Contributions to Statistics

V. Fedorov · W. G. Müller
I. N. Vuchkov (Eds.)

Model Oriented Data-Analysis

A Survey of Recent Methods

Physica-Verlag
A Springer-Verlag Company

V. Fedorov · W. G. Müller
I. N. Vuchkov (Eds.)

Model Oriented Data-Analysis

A Survey of Recent Methods

Proceedings of the 2nd IIASA-workshop in
St. Kyrik, Bulgaria, May 28 - June 1, 1990

With 37 Figures

Physica-Verlag

A Springer-Verlag Company

Series Editors
Werner A. Müller
Peter Schuster

Editors
Prof. Dr. Valery Fedorov
Department of Applied Statistics
University of Minnesota
1994 Buford Avenue, St. Paul
Minnesota, USA

Dr. Werner G. Müller
Department of Economical Statistics
University of Economics
Augasse 2-6
A-1060 Vienna

Prof. Dr. Ivan N. Vuchkov
Head of the Laboratory of Organization
and Automation of Experimental Research
Higher Institute of Chemical Technology
1156 Sofia, Bulgaria

ISBN 3-7908-0624-2 Physica-Verlag Heidelberg
ISBN 0-387-91422-6 Springer-Verlag New York

CIP-Titelaufnahme der Deutschen Bibliothek
Model oriented data-analysis : a survey of recent methods /
Valery Fedorov ... - Heidelberg : Physica-Verl., 1992
(Contributions to statistics)
ISBN 3-7908-0624-2
NE: Fedorov, Valery [Hrsd.]

7120/7130-543210 - Printed on acid-free paper

PREFACE

In July 1987 the International Institute for Applied System Analysis (IIASA) has, together with some national Academies of Sciences, started a series of international workshops on 'Model-Oriented Data Analysis'. The first meeting, that took place at Wartburg Castle, was co-sponsered by the Karl-Weierstraß Institute for Mathematics of the Academy of Sciences of the GDR. The proceedings were published by Springer Verlag in 1988.

As a continuation IIASA and the Academy of Sciences of Bulgaria organized a second workshop in St. Kyrik, Bulgaria from 28.5 to 1.6. 1990, the proceedings of which constitute this volume. The main topics of this meeting were:

I Optimal Design, II Regression Analysis, III Quality Engineering and Applications

Part I contains various generalizations of experimental design theory for nonstandard regression models.

The survey paper by A.Atkinson comprises results related to the models with prior information. It reveals that a number of regression problems, for instance estimation of parameters for nonlinear response and model discrimination can be considered from general positions thus clarifying the ideas of convex experimental design theory. Numerous examples help to evaluate the efficiency of this theory and to understand the main difficulties a practitioner can face while constructing optimal designs.

The paper by A.Donev complements these results addressing mainly to the model discrimination problem for several competing polynomial models.

In practice an experimental design frequently has to satisfy some natural constraints. For instance not to exceed a prescribed level by the cost of measurements, weights of supporting points or density of supporting points being finite, and so on. In the paper by V.Fedorov the corresponding modifications of the equivalence theorem are formulated and discussed.

There are many experimental situations where the underlying response has to be approximated by a simpler and more treatable model. For this case R.Schwabe describes the characteristics of a randomized design which meets both tasks of approximation and estimation.

A.Pazman and L.Pronzato propose a method for optimal design construction, when one applies to the constrained least squares estimators. Their approach is essentially based on the geometrical structure of response functions and on introduction of a penalty function.

The question of how batch sequential design performs in a nonlinear estimation problem is discussed by W.G.Müller and B.M.Pötscher. They propose a quasi-batch sequential method, derive its asymptotic properties and give simulation results for small samples.

L.Pronzato and E.Walter in this section survey the up-to-date methodology in non-sequential Bayesian design, providing some illustrative examples.

H.Yonchev proposes the use of optimal composite designs for linear regression models, when controlled variables belong to multidimensional simplexes (so-called experiments with mixture). He illuminates his results with a numerical example.

The pattern recognition problem is reduced to the method of estimation and the design of regression experiments in N.Manolov's article.

An algorithm for constructing optimizing distribution, solving problems like maximum likelihood estimation, is presented by B.Torsney and A.Alahmadi. The performance of the algorithm is investigated in the optimal regression design context.

Part II deals with general regression methods, reporting various modern approaches to the problem.

J.Višek presents two methods of adaptive estimation of linear regression models, which are essentially based on the assumption of symmetricity of the distribution of observation errors. He suggests a measure of symmetry, which can be used as a characteristic of model stability and gives the corresponding theoretical results as well as two examples with a classical data-set and simulated data.

B.Kovachev uses the concept of almost linear regression models to handle non-linear regression problems with normally distributed errors. He finds, that for some of them there exist finite dimensional sufficient statistics and he proposes some modifications of leasts squares estimation.

Using a bootstrap technique in nonlinear regression analysis H.Läuter manages to increase its efficiency, explicitely using information about the structure of the model. The results can be used as a good pattern for the use of resampling techniques in statistical analysis.

S.Hadživukovic and E.Nikolic-Djoric survey the approaches on L_1-regression and computational procedures. A corresponding empirical study is given.

The problem of selection of variables and models in regression analysis is challenged by B.Droge. Together with a short theoretical survey he describes the implementation of the discussed algorithm on a PC.

Part III presents some contributions based on statistical methods of experimental design quality improvement techniques.

Probably most explicitely these facts are expressed in the article by I.Vuchkov and L.Boyadjieva, where they discuss optimal designs under Taguchi-type optimality criteria (minimizing a process variance, conditioned on keeping a target value).

In the same framework C.Hirotsu presents various data processing techniques that to some extent go beyond the traditional analysis of variance approach (which he consequently calls BANOVA).

The problem of inadequate description of a nonlinear dynamic process by linearization and constant parameter models is investigated in the contribution by K.Velev, I.Vuchkov and V.Tsochev. They compare two main types of models: parametric ones in the form of difference equations and nonparametric ones in the form of convolution integrals.

The final contribution by A.Zhigljavsky describes asymptotic properties of the likelihood ratio test for detecting rectangular change in mean for normally distributed random variables.

Both above given techniques can be used for on-line quality control.

August, 1991 V.V.Fedorov, W.G.Müller, I.V.Vuchkov

TABLE OF CONTENTS

Part I:

OPTIMAL DESIGN

OPTIMUM EXPERIMENTAL DESIGNS FOR PARAMETER ESTIMATION AND FOR DISCRIMINATION BETWEEN MODELS IN THE PRESENCE OF PRIOR INFORMATION.

A.C.Atkinson,
Department of Statistical and Mathematical Sciences, London School of Economics, London, WC2A 2AE, UK

1. INTRODUCTION.

The theory of the optimum design of experiments, together with the associated General Equivalence Theorem (Kiefer,1959; Kiefer and Wolfowitz, 1960), leads to designs for many situations, both standard and non-standard. In standard applications, such as D-optimum designs for polynomial response surface models, the design depends upon the terms in the model, but not on the values of the associated parameters. However, D-optimum designs for nonlinear models, found by local linearization of the model about prior point estimates of the parameters (Box and Lucas, 1959), do depend on the unknown parameter values. If the prior estimates are poor, the design will be inefficient. Conversely, if the prior estimate is good, the designed experiment will be unnecessary. Similarly, the T-optimum designs of Atkinson and Fedorov (1975a, 1975b) for discriminating between models depend upon which model is true and on the parameter values of the true model. Such designs, optimum at a single point in parameter space, are said to be locally optimum (Chernoff, 1953).

The inefficiency of locally optimum designs arises because the point prior information used in the construction of the designs does not adequately reflect the lack of knowledge of the parameter values. In this paper examples are given of the use of an extension of the General Equivalence Theorem which incorporates information about the prior distribution of the parameters. By using the expectation of the design criterion over this prior distribution a new design criterion is obtained, for which an equivalence theorem holds. Thus the checks for optimality of a proposed design and the algorithms for construction of designs are available for these extended criteria, just as they are for the original criteria of D- and T-optimality. The chief distinguishing feature of the new designs is that they frequently have more points of support than the locally optimum designs.

The paper starts in Section 2 with four examples which will be used throughout to illustrate the designs and their properties. Sections 3 and 4 are concerned respectively with locally optimum designs for parameter estimation and for discrimination between models. In both sections the standard form of the General Equivalence Theorem is

used to demonstrate the optimality of the designs. The extended General Equivalence Theorem is introduced in Section 5 and, in Section 6, applied to designs for parameter estimation. The section also includes a discussion of general properties of designs incorporating prior information and the effect on the design of changes in the prior distribution. Section 7 describes designs for discrimination between models when there is a prior probability for the truth of each model and, within each model, a prior distribution of the parameters. The paper concludes in Section 8 with a discussion of related problems and literature.

2. EXAMPLES.

In all examples it is assumed that second-order error assumptions hold and that estimation is by least squares.

Example 1. Truncated Quadratic Model.

The expected value of the response Y is related to the single explanatory variable x by the truncated quadratic relationship

$$E(Y) = \eta(x, \beta, \theta) = \beta\, x\theta(1 - x\theta) = \beta\, f(x, \theta)\,, (0 \leq x \leq 1/\theta)$$
$$= 0, \text{ otherwise.} \qquad (1)$$

For known θ this is a standard linear model with a single parameter β, except that the expected value of the response is constrained to be non-negative. The model is related to those used in pharmacokinetic studies to describe the flow of a drug through a subject, although such models usually involve linear combinations of exponential terms. In this interpretation $1/\theta$, which would vary between subjects, is the time to complete elimination of the drug. The maximum of the curve, corresponding to the maximum concentration of the drug, is $\beta/4$: interest is in estimation of β. Observations for which $x\theta > 1$ are not informative about the value of β, although they may be about θ.

This simple model demonstrates clearly the properties of designs in the presence of prior information. For a given value of θ the variance of $\hat{\beta}$, the least squares estimate of β, is minimised by putting all trials at the point where the response is a maximum, that is at $x = 1/(2\theta)$. If the value of θ is not known a priori, but is described by a prior distribution, this locally optimum design could be used with θ replaced by its expected value. But there may be values of θ within the prior distribution for which concentration of the design on one value of x will give estimates of β with large, or even infinite, variance. The designs derived in this paper are intended to provide, for example, a small value of the expected variance of $\hat{\beta}$ taken over the distribution of θ. As

we shall see, such designs can be very different from those which maximize the expected information about β. ∎

Example 2. First Order Decay.

A simple model arising from chemical kinetics is that for first order decay in which

$$E(Y) = \eta(x, \theta) = e^{-\theta x}, \ (x, \ \theta \geq 0). \tag{2}$$

Linearization of the model about the prior value θ_o gives

$$\begin{aligned} E(Y) &= \eta(x, \theta_o) + (\theta - \theta_o) \left. \frac{\partial \eta(x, \theta)}{\partial \theta} \right|_{\theta = \theta_o} + \cdots \\ &= \eta(x, \theta_o) + (\theta - \theta_o) f(x), \end{aligned} \tag{3}$$

where $f(x) = -x \ \exp(-\theta_o x)$.

The relationship between (3) and (1) is expressed more forcefully by writing

$$\begin{aligned} E(Y) - \eta(x, \theta_o) &= (\theta - \theta_o) f(x) \\ &= \beta \ f(x). \end{aligned} \tag{4}$$

The variance of $\hat{\beta}$ is again minimized by performing all trials where $f(x)$ is a maximum, that is at $x = 1/\theta_o$ when $\eta = e^{-1}$. As in Example 1, if the true value of θ is far from θ_o, the variance of $\hat{\beta}$ will be large, because experiments will be performed where $f(x)$ is small. In such regions the value of the response is near zero or one, providing little information about θ. ∎

Example 3. Two Models for Decay.

An alternative to the exponential decay model (2) is the inverse polynomial

$$\eta_2(x, \phi) = 1 \ /(1 + \phi x), \ (x, \phi \geq 0). \tag{5}$$

It may be hard to discriminate between these two models. If one of the models is known to be true, although it is not known which one, the most efficient designs are those of Section 4. These locally T-optimum designs lead to experiments at two values of x in order to maximize the expected value of the residual sum of squares for the false model. ∎

Example 4. Two Linear Models.

The two models of Example 3 are both nonlinear in the parameters. Some additional insight into the structure of the designs comes from considering linear models. As an example let

$$\eta_1(x, \beta_1) = \beta_{10} + \beta_{11} e^{x} + \beta_{22} e^{-x} \tag{6}$$

and

$$\eta_2(x, \beta_2) = \beta_{20} + \beta_{21}x + \beta_{22}x^2. \tag{7}$$

Both models are linear in three parameters and so will exactly fit any three point design. Designs for discriminating between the two models will therefore need at least four points of support. ∎

In Examples 3 and 4 only one model can be true. If however the two competing models are not separate but nested, so that one is a special case of the other, either one or both may be true. The design implications are mentioned briefly in Section 4.

Whether the designs are the locally optimum designs of Sections 3 and 4 or those incorporating prior information of later sections, only non-sequential designs will be discussed in this paper. Sequential experimentation, where possible, provides a more efficient way of learning about parameters and models. But, at each stage of a sequential procedure, design considerations similar to those of this paper will be of importance.

3. LOCALLY *D*-OPTIMUM DESIGNS FOR PARAMETER ESTIMATION.

3.1. The General Equivalence Theorem.

In this section the General Equivalence Theorem of optimum design theory is stated in a form suitable for extension to include prior information. Silvey (1980, Chapter 3) gives a careful discussion of the theorem with a notation similar to that used here.

For the linear model $E(Y) = F\beta$, where F is an $n \times p$ matrix with ith row $f^t(x_i)$, a function of m known explanatory variables, the information matrix for the least squares estimates of the parameters β is

$$F^tF = \sum f(x_i)f^t(x_i).$$

In the continuous, or approximate, theory the exact n-trial design is replaced by the design measure ξ over the design region $\mathcal{X}$. This measure puts weight w_i at the point x_i. The information matrix is then written as

$$M(\xi) = \int_{\mathcal{X}} f(x)f^t(x)\xi(dx) = \int_{\mathcal{X}} m(x)\xi(dx).$$

Optimum design theory is concerned with designs which minimize the convex function $\Psi\{M(\xi)\}$. Let this design be given by the measure ξ^* and let the measure $\bar{\xi}$ put unit mass at the point x. The derivative of $\Psi\{M(\xi)\}$ at ξ in the direction $\bar{\xi}$ is

$$\phi(x, \xi) = \lim_{\alpha \to 0+} \frac{1}{\alpha} \left[\Psi\{(1-\alpha)M(\xi) + \alpha\, M(\bar{\xi})\} - \Psi\{M(\xi)\}\right].$$

The General Equivalence Theorem then states the equivalence of the three conditions:
(i). ξ^* minimizes $\Psi\{M(\xi)\}$.
(ii). min $\phi(x, \xi^*) \geq 0$.
(iii). $\phi(x, \xi^*)$ achieves its minimum at the points of support of the design.

The best known example is the equivalence of D- and G-optimality for linear models in which

$$\Psi\{M(\xi)\} = -\log |M(\xi)|, \tag{8}$$

so that the determinant of the information matrix is maximized or, equivalently, the determinant of $M^{-1}(\xi)$ is minimized. Also, if the standardized variance of the estimated response at x is

$$d(x, \xi) = f^t(x) M^{-1}(\xi) f(x), \tag{9}$$

$$\phi(x, \xi) = p - d(x, \xi). \tag{10}$$

It is customary to write

$$\max_{x \in \mathcal{X}} d(x, \xi) = d(\bar{\xi})$$

when the second condition of the theorem becomes $\bar{d}(\xi^*) = p$, the condition for G-optimality.

The theorem suggest algorithms for the construction of designs. In the approximate or continuous theory for D-optimality, designs are built by adding points where $d(x, \xi)$ is a maximum. The process can be speeded by the removal of design points for which the variance is low (Wu and Wynn, 1978). Similarly, algorithms for the construction of exact designs (Fedorov, 1972, *p.*164; Mitchell, 1974; Atkinson and Donev, 1989) add points with high variance or exchange them for design points with low variance.

Of particular importance in the construction of designs with prior information is the number of points of support of the design. For linear models the number of points of support of the optimum design is bounded by $p(p+1)/2$, a result which follows from the additivity of $M(\xi)$ and Carathéodory's Theorem (Silvey, 1980, Appendix 2). Optimum designs with a greater number of points will have an information matrix identical to that of a design satisfying this bound. For locally optimum designs found by linearisation of nonlinear models, the number of design points is often p. However there is in general no bound on the number of support points for the designs of Sections 6 and 7 in which the expectation of the design criterion is minimized. A second property of these Bayesian designs is that the derivative function $\phi(x, \xi)$ is often appreciably flatter than that for the locally optimum designs. The implications of this property for the construction of optimum designs is discussed in Section 6.4.

3.2 Locally D-Optimum Designs.

The locally D-optimum design found from the linearised model for first-order decay maximizes $M(\xi)$ with $f(x)$ given by (3). To extend the equivalence theorem to designs for nonlinear models with a vector parameter requires the extension of the Taylor series expansion leading to (3) .If θ in the model $E(Y) = \eta(x, \theta)$ is of dimension p, then the $p \times 1$ vector $f^t(x)$ is given by the p partial derivatives

$$f^t(x_i) = \{\partial\eta(x_i, \theta)/\ \partial\theta_j\}|_{\theta=\theta_o}, (j = 1, ..., p). \tag{11}$$

The extended design matrix F has ith row $f^t(x_i)$ and the locally D-optimum design maximizes $|F^tF|$, where the derivatives are evaluated at θ_o. The General Equivalence Theorem of Section 3.1 then applies to this linearized model.

Example 2. First Order Decay.

For this one parameter example we have already seen that $f(x_i) = -x_i \exp(-\theta_o x_i)$. The locally D-optimum design for θ which maximizes

$$|M(\xi)| = \int_{\mathcal{X}} f^2(x)\xi(dx)$$

concentrates all experimental effort at the value of x for which $f(x)$ is a maximum. This confirms the result of Section 2 that all trials should be performed at $x = 1/\theta_o$.

This design illustrates two aspects of optimum design theory. One is that for $p = 1$ the bound on the maximum number of support points $p(p + 1)/2$ is one, so that the design satisfies this condition. The second is that the design satisfies points ii and iii of the General Equivalence Theorem. Figure 1 shows a plot of $d(x, \xi^*)$ for $\theta_o = 1$: the function has a maximum value of 1, that is p, and this maximum occurs at the point of support of the design, namely $x = 1$.

4. LOCALLY T-OPTIMUM DESIGNS FOR DISCRIMINATION BETWEEN TWO MODELS.

A description is given in this section of designs for discriminating between two models. References to work on the more complicated problem of discrimination between three or more models are given in Section 8.

The optimum design for discriminating between two models depends upon which model is true. Without loss of generality let this be the first model and write

$$\eta_t(x) = \eta_1(x, \theta_1). \tag{12}$$

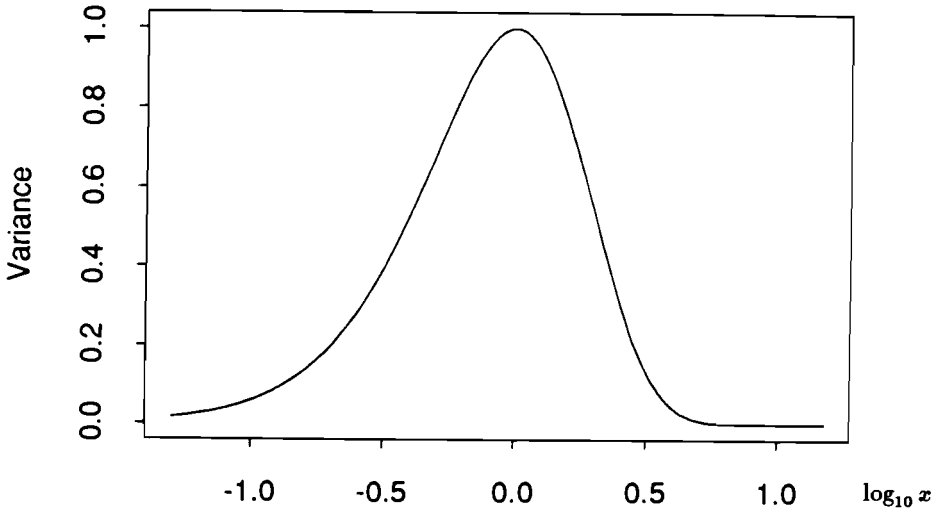


FIGURE 1. Example 2 (First Order Decay): the variance function $d(x, \xi^*)$ for the locally D-optimum design when $\theta_o = 1$.

A good design for discriminating between the models will then provide a large lack of fit sum of squares for the second model. When the second model is fitted to the data, the least squares parameter estimates will depend on the experimental design as well as on both the value of θ_1 and on the errors. In the absence of errors the parameter estimates are

$$\hat{\theta}_2(\xi) = \min_{\theta_2} \int_{\mathcal{X}} \{\eta_t(x) - \eta_2(x, \theta_2)\}^2 \xi(dx), \tag{13}$$

yielding a residual sum of squares

$$\Delta_2(\xi) = \int [\eta_t(x) - \eta_2\{x, \hat{\theta}_2(\xi)\}]^2 \xi(dx). \tag{14}$$

For linear models $n\Delta_2(\xi)/\sigma^2$ is the non-centrality parameter of the χ^2 distribution of the residual sum of squares for the second model. Designs which maximize $\Delta_2(\xi)$ are called T-optimum to emphasize the connection with testing models. The T-optimum design maximizing (14) provides the most powerful F test for lack of fit of the second model when the first is true. When the models are nonlinear in the parameters, the exact F test is replaced by asymptotic results, but we still design to maximize (14).

For linear models with extended design matrices F_1 and F_2 and parameter vectors β_1 and β_2 the least squares estimates $\hat{\beta}_2$ minimizing (13) are

$$\hat{\beta}_2 = (F_2^t F_2)^{-1} F_2^t F_1 \beta_1 \tag{15}$$

when only model 2 is fitted to the data. Further understanding of the designs for linear models comes from consideration of a combined model. If the two models are separate, that is F_1 and F_2 have no terms in common, they can be combined to yield the model

$$E(Y) = F\beta = F_1\beta_1 + F_2\beta_2.$$

In this combined model $\beta_2 = 0$ corresponds to model 1 being correct. However the models will frequently have terms in common, sometimes, as in Example 4, only a constant, but often other terms as well. The combined model is then

$$E(Y) = F\beta = F_1\beta_1 + \tilde{F}_2\tilde{\beta}_2 = \tilde{F}_1\tilde{\beta}_1 + F_2\beta_2 \tag{16}$$

where $\tilde{F}_2\tilde{\beta}_2$ is the complement of $F_1\beta_1$ in the combined model $F\beta$, and similarly for $\tilde{F}_1\tilde{\beta}_1$. The non-centrality parameter (14) for models with some terms in common is

$$n\Delta_2(\xi_n)/\sigma^2 = \tilde{\beta}_1^t\{\tilde{F}_1^t\tilde{F}_1 - \tilde{F}_1^tF_2(F_2^tF_2)^{-1}F_2^t\tilde{F}_1\}\tilde{\beta}_1, \tag{17}$$

which makes explicit the dependence of $\Delta_2(\xi_n)$ on the elements of $F_1\beta_1$ not included in the second model. If $\tilde{\beta}_1$ is a scalar, designs maximizing (17) minimize the variance of the estimate of $\tilde{\beta}_1$ in the combined model (16) and so do not depend on the value of $\tilde{\beta}_1$. However if $\tilde{\beta}_1$ is a vector, the T-optimum design will depend on the parameter values.

If model 2 is true, rather than model 1, the T-optimum design will maximize the non-centrality parameter when model 1 is fitted to the data. The design criterion to be maximized is then $\Delta_1(\xi_n)$, the analogue of (17) with 1's and 2's interchanged. If model 1 is a special case of model 2, model 2 must be true, since it is assumed that one of the models is true. Then the complement $\tilde{\beta}_1$ will be empty and the only non-centrality parameter to be maximized is $\Delta_1(\xi_n)$, which gives information as to whether the larger model is justified. If it is not and model 1 is all that is required, $\tilde{\beta}_2 = 0$ and the non-centrality parameter $\Delta_1(\xi_n)$ will be identically zero for all designs.

The quantity $-\Delta_2(\xi_n)$ is another example of a convex function to which the General Equivalence Theorem applies. To establish notation for the derivative function let the T-optimum design yield the parameter estimate $\theta_2^* = \hat{\theta}_2(\xi^*)$. Then

$$\Delta_2(\xi^*) = \int_{\mathcal{X}} \{\eta_t(x) - \eta_2(x, \theta_2^*)\}^2 \xi(dx). \tag{18}$$

The squared difference between the true and predicted responses at x, for this design, is

$$\phi_2(x, \xi^*) = \{\eta_t(x) - \eta_2(x, \theta_2^*)\}^2, \tag{19}$$

with $\phi_2(x,\xi)$ being the difference for any other design. The following conditions on the design are then equivalent:

(i). The T-optimum design ξ^* maximizes $\Delta_2(\xi)$.

(ii). $\phi_2(\xi^*) \leq \Delta_2(\xi^*)$, for all $x \in \mathcal{X}$.

(iii). At the points of the optimum design $\phi_2(\xi^*) = \Delta_2(\xi^*)$.

(iv). For any non-optimum design, that is one for which $\Delta_2(\xi) < \Delta_2(\xi^*)$,

$$\sup_{x \in \mathcal{X}} \phi_2(x,\xi) > \Delta_2(\xi^*).$$

These results are, in all important respects, the same as those for D-optimality in Section 3.1 and lead to similar methods of design construction and verification.

Example 4. Two Linear Models (continued).

Without loss of generality we take the first model as true, just as was done in the theoretical development. Then the T-optimum design depends on the values of the parameters β_{11} and β_{12}, but not on the value of β_{10}, since both models contain a constant. We consider only one pair of parameter values, taking as the true model

$$\eta_t(x) = 4.5 - 1.5\ e^{x} - 2\ e^{-2x}. \tag{20}$$

This function, which has a value of -1.448 at $x = -1$, rises to a maximum of 1.036 at $x = 0.144$, before declining to -0.131 at $x = -1$. It can be well approximated by the quadratic polynomial (7). The T-optimum design for discriminating between the two models is found by numerical maximization of $\Delta_2(\xi)$ to be

$$\xi^* = \begin{Bmatrix} -1 & -0.669 & 0.144 & 0.957 \\ 0.253 & 0.428 & 0.247 & 0.072 \end{Bmatrix} \tag{21}$$

for which $\Delta_2(\xi^*) = 1.087 \times 10^{-3}$. A strange feature of this design is that half the weight is on the first and third design points and half on the other two.

For the particular parameter values of (20) the design is not symmetrical and does not span the experimental region. It contains only four design points, the minimum number, in general, for discrimination between two three parameter models. As an illustration of the equivalence theorem, $\phi_2(x,\xi^*)$ is plotted in Fig. 2. The maximum value of $\phi_2(x,\xi^*)$ is indeed equal to $\Delta_2(\xi^*)$, the maximum occuring at the points of the optimum design. The minimum values of zero occur where the two fitted models coincide. Incremental experiments at these points would be non-informative for discrimunation between the models. ∎

Example 3. Two Models for Decay (continued).

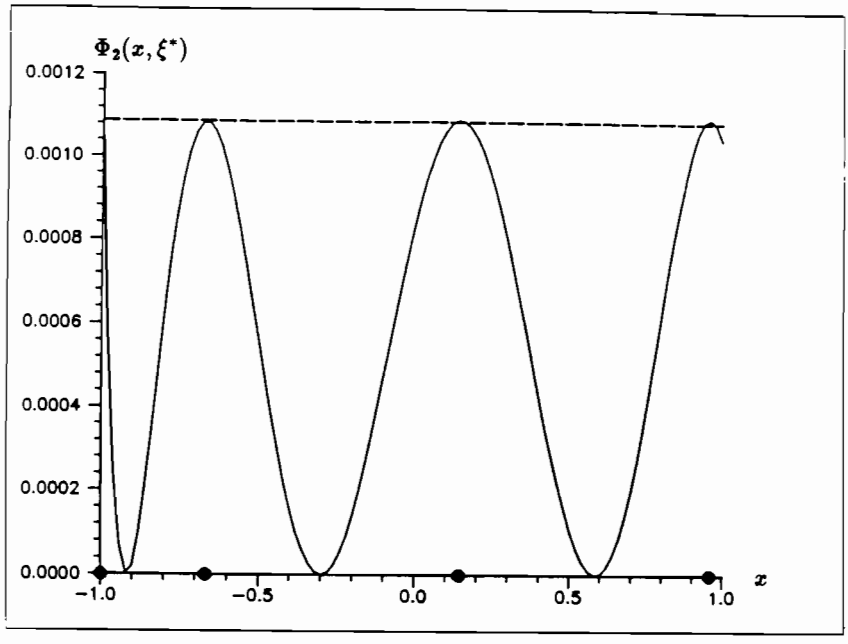


FIGURE 2. Example 4 (Two Linear Models): the derivative function $\phi_2(x, \xi^*)$ for the locally T-optimum design for discriminating between the two models.

Both models in Example 4 are linear in the parameters. We now find the T-optimum design for discriminating between two nonlinear models, using as an example the two models for decay (2) and (5).

Let the first model be true with $\theta_1 = 1$ so that

$$\eta_t(x) = e^{-x}, \ (x \geq 0). \tag{22}$$

The T-optimum design again maximizes the non-centrality parameter $\Delta_2(\xi)$ (14), the only small complication introduced by the nonlinearity of $\eta_2(x, \theta_2)$ being the iterative calculation of the nonlinear least squares estimates $\hat{\theta}_2(\xi)$. The iterative numerical maximization of $\Delta_2(\xi)$ thus contains an iterative fit at each function evaluation.

The T-optimum design when $\theta_1 = 1$ is

$$\xi^* = \left\{ \begin{array}{cc} 0.327 & 3.34 \\ 0.3345 & 0.6655 \end{array} \right\}, \tag{23}$$

a two-point design allowing discrimination between these one-parameter models. In Section 3.2 the locally D-optimum design for θ_1 when $\theta_1^o = 1$ put all trials at $x = 1$. The design given by (23) divides the design weight between points either side of this

value. Confirmation that this is the optimum design comes again from the Equivalence Theorem. The plot of $\phi_2(x,\xi^*)$ in Fig. 3 has two maxima with the value of $\Delta_2(\xi^*)$, which is 1.038×10^{-2}. Since both models are one at $x = 0$, experiments at this point are not informative and $\phi(x,\xi^*) = 0$. It is also zero at the point of intersection of the true model and model 2 with parameters estimated from the optimum design. A third non-informative point is at $x = \infty$, when both models predict zero for the response. ∎

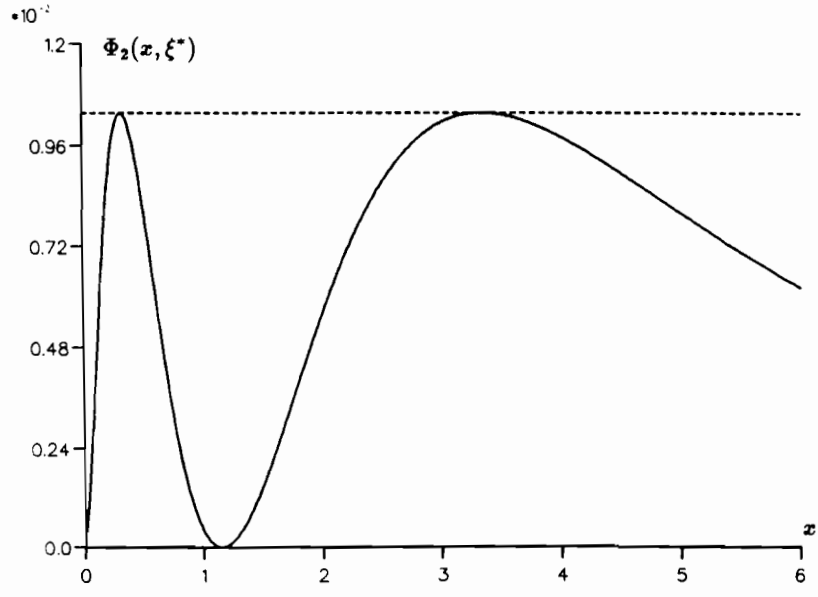


FIGURE. 3. Example 3 (Two Models for Decay): derivative function $\phi_2(x,\xi^*)$ for the locally T-optimum design for discriminating between two nonlinear models.

5. A GENERAL EQUIVALENCE THEOREM INCORPORATING PRIOR INFORMATION.

In this section the General Equivalence Theorem of Section 3.1 is extended to include dependence of the information matrix on a vector parameter θ. We write the information matrix as

$$M(\xi,\theta) = \int_{\mathcal{X}} f(x,\theta) f^t(x,\theta) \xi(dx) = \int_{\mathcal{X}} m(x,\theta) \xi(dx).$$

The generalization is to consider design criteria of the form

$$\Psi\{M(\xi)\} = E_\theta \Psi\{M(\xi,\theta)\}.$$

For the one parameter examples of Section 2 reasonable extensions of D-optimality would be to find designs to maximize the expected information about the parameter, or to minimize the expected variance of the parameter estimate. The results of Section 6.2 show that these designs are not the same.

There are similarly several generalizations of D-optimality when θ is a vector. The obvious generalization of (8) is to take

$$\Psi_I\{M(\xi)\} = -E_\theta \log |M(\xi,\theta)| = E_\theta \log |M^{-1}(\xi,\theta)|. \tag{24}$$

Another possibility is

$$\Psi_{II}\{M(\xi)\} = \log\ E_\theta |M^{-1}(\xi,\theta)| \tag{25}$$

which, when $p = 1$, reduces to minimizing the expected variance of the parameter estimate. Five possible generalizations of D-optimality are listed in Table 1, together with their derivative functions, for each of which an equivalence theorem holds (Dubov, 1977; Fedorov, 1981). These criteria are compared in Section 6.2. For the present we notice that, from a Bayesian viewpoint, not all criteria correspond to preposterior expected loss, although Criterion I does.

TABLE 1. Equivalence Theorem for Bayesian Versions of D-Optimality: Design Criteria and Derivative Functions.

	Criterion $\Psi\{\mathbf{M}(\xi)\}$	Derivative Function $\phi(x,\xi)$
I	$E \log\lvert\mathbf{M}^{-1}\rvert$	$p - E\ \mathrm{tr}\ \mathbf{M}^{-1}\mathbf{m}(x,\theta)$
II	$\log E\lvert\mathbf{M}^{-1}\rvert$	$p - E\{\lvert\mathbf{M}^{-1}\rvert\ \mathrm{tr}\ \mathbf{M}^{-1}\ \mathbf{m}(x,\theta)\}/\ E\lvert\mathbf{M}^{-1}\rvert$
III	$\log\lvert E\mathbf{M}^{-1}\rvert$	$p - E\{\ \mathrm{tr}\ \mathbf{M}^{-1}\ (E\mathbf{M}^{-1})\ \mathbf{M}^{-1}\ \mathbf{m}(x,\theta)$
IV	$\log\ \{E\lvert\mathbf{M}\rvert\}^{-1}$	$p - E\{\lvert\mathbf{M}\rvert\ \mathrm{tr}\ \mathbf{M}^{-1}\ \mathbf{m}(x,\theta)\}/\ E\lvert\mathbf{M}\rvert$
V	$\log\ \lvert E\mathbf{M}\rvert^{-1}$	$p - \mathrm{tr}\ (E\mathbf{M})^{-1}\ \mathbf{m}(x,\theta)$

In this table $E\mathbf{M}$ is short for $E_\theta\ \mathbf{M}(\xi,\theta)$, etc.

For T-optimum designs the extension is to take the expectation over parameters and models of the non-centrality parameters $\Delta_2(\xi)$ (14) and $\Delta_1(\xi)$, the latter being obtained when model 1 is fitted with model 2 true. As with the extensions of D-optimality this yields a convex design function to which the General Equivalence theorem applies. In the

case of T-optimality the derivative function is the expectation of the derivative functions for each parameter value. However, for some extensions of D-optimality, $\phi(x,\xi)$ is more complicated.

These results provide a means whereby the uncertainty in the prior estimates of the parameters is translated into a spread of design points. In the standard theory the criteria are defined by matrices $M(\xi)$ which are linear combinations, with positive coefficients, of elementary information matrices $m(x)$ corresponding to designs with one support point. But in, for example, the extensions of D-optimality, dependence is on such functions of matrices as $E_\theta M^{-1}(\xi,\theta)$ or $E_\theta|M(\xi,\theta)|$, the non-additive nature of which precludes the use of Carathéodory's theorem. As a result the number of support points is no longer bounded by $p(p+1)/2$. The examples of the next two sections show how the non-additive nature of the criterion leads to designs with appreciable spread of the points of support.

6. DESIGNS FOR PARAMETER ESTIMATION WITH PRIOR INFORMATION.

6.1. The Truncated Quadratic Model, Example 1 (continued).

As a first example of design criteria incorporating prior information we calculate some designs for the truncated quadratic model (1), concentrating in particular on Criterion II, given by (25). In this one parameter example this reduces to minimizing the expected variance of the parameter estimate. We contrast this design with that maximizing the expected information about β.

The derivative function for Criterion II is given in Table 1. It is convenient when referring to these derivatives to follow (10) and call $d(x,\xi) = p - \phi(x,\xi)$ the expected variance. Then for Criterion II

$$d(x,\xi) = \frac{E_\theta|M^{-1}(\xi,\theta)|d(x,\xi,\theta)}{E_\theta|M^{-1}(\xi,\theta)|}\ , \tag{26}$$

where $d(x,\xi,\theta) = f^t(x,\theta)M^{-1}(\xi,\theta)f(x,\theta)$. The expected variance is thus a weighted combination of the variance of the predicted response for the various parameter values. In the one parameter case the weights are the variances of the parameter estimates. From the equivalence theorem it follows that the points of support of the optimum design are at the maxima of (26), where $d(x,\xi^*) = p$.

Suppose that the prior for θ is discrete with mass p_m on the value θ_m. The design criterion (25) to be minimized is

$$E_\theta M^{-1}(\xi,\theta) = \sum_m p_m/\ f^2(x,\theta_m), \tag{27}$$

with $f(x, \theta)$ given in (1). To illustrate the properties of the design let the prior for θ put weight 0.2 on the five values 0.3, 0.6, 1, 1.5 and 2. Trials at values of $x > 1/\theta$ yield a zero response. Thus for $\theta = 2$ a reading at any value of x above 0.5 will be non-informative. Unless the design contains some mass at values less than this, the criterion (27) will be infinite. Yet the locally optimum designs, at $x = 1/2\theta$, for the three smallest parameter values all concentrate mass on a single x value at or above 0.5.

The expected values required for the criterion (27) are found by summing over the five parameter values. Table 2 gives three optimum continuous designs for Criterion II. The first was found by searching over the convex design space [0, 1], the second and third designs by grid search over respectively 20 and 10 x values. The designs have either two or three points, more than the single point indicated by Carathéodory's Theorem for the locally optimum designs.The design for the coarser grid has three points, the others two. That the three point design is optimum can be checked from the plot of $d(x, \xi^*)$ in Fig.4.

TABLE 2. Example 1 (Truncated Quadratic Model): Continuous optimum designs ξ^* minimizing the expected variance of the parameter estimate (Criterion II).

	Region			Criterion Value
(a)	Convex [0, 1]			32.34
	x 0.3430	1		
	w^* 0.6951	0.3049		
(b)	20 point grid			32.37
	x 0.35	1		
	w^* 0.7034	0.2966		
(c)	10 point grid			32.95
	x 0.3	0.4	1	
	w^* 0.4528	0.2406	0.3066	

The design ξ^* puts weight w^* at the point x.

The expected variance is 1, *i.e.* p, at the the three design points and less than 1 at the

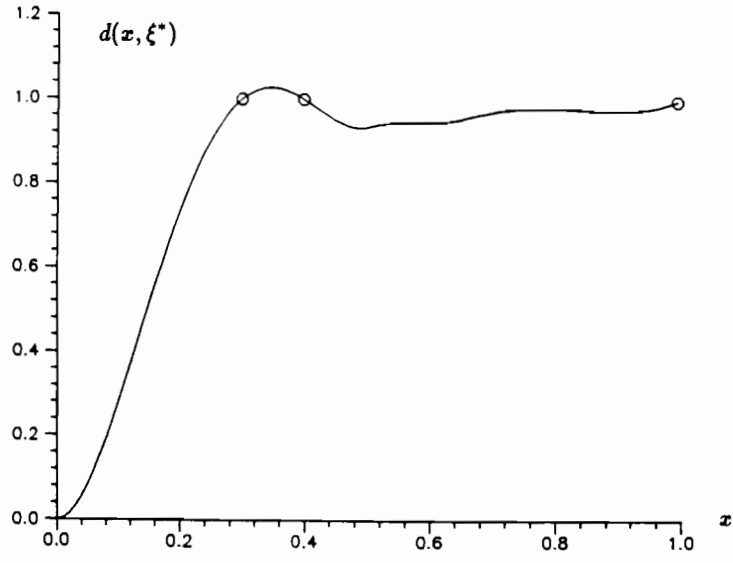


FIGURE 4. Example 1 (Truncated Quadratic): the expected variance function $d(x, \xi^*)$ for the three-point design minimizing the expected variance of $\hat{\beta}(27)$ when θ has a five-point prior.

other 7 points of the discrete design region. However it is 1.027 at $x = 0.35$, which is not part of the coarse grid. Searching over a finer grid leads to the optimum design in which the weights at 0.3 and 0.4 are almost combined, yielding a two-point design. It is clear why the number of design points has changed. But such behaviour is infrequent for the standard design criteria when the additivity property holds. Of course, for such criteria for a single parameter model, all optimum designs would require only one design point.

The effect of the spread of design points is to ensure that there is no value of θ for which the design is very poor. The appearance of Figure 4 indicates that it is the sum of several rather different curves arising from the various values of θ. However not all design criteria lead to a spread of design points. If we use instead a criterion like V in which the expected information about β is maximized, (27) is replaced by maximization of

$$E_\theta M(\xi, \theta) = \sum_m p_m f^2(x, \theta_m). \tag{28}$$

For the coarse grid the optimum design is at the single point $x = 0.3$. The effect of little, or no, information about β for a specific θ value may well be outweighed by the information obtained for other θ values. This is not the case for designs using (27) when

variances can be infinite for some parameter values, whereas the information is bounded at zero.

6.2. A Comparison of Design Criteria.

The results of Section 6.1 illustrate the striking difference between designs which minimize expected variance and those which maximize expected information. In this section we use the first-order decay model, Example 2, to compare the five generalizations of D-optimality listed in Table 1.

When $p = 1$ the five criteria reduce to the three listed in Table 3, in which the expectation of integer powers of the infomation matrix, in this case a scalar, are maximized or minimized as appropriate. The values of the power parameter are also given in Table 3. The equivalence theorem for these criteria involves an expected variance of the weighted form

$$d(x,\xi) = E_\theta\{a(\theta)d(x,\xi,\theta)\}/\ E_\theta\{a(\theta)\},$$

where the weights $a(\theta)$ are given in Table 3. For Criterion I, $a(\theta) = 1$, so that the combination of variances is unweighted.

TABLE 3. Equivalence Theorem for Bayesian Versions of D-Optimality: Reduction of criteria of Table 1 for single parameter models.

	Criterion min $\Phi\{\mathbf{M}(\xi,\theta)\}$	Power Parameter	Expected Variance Weight $a(\theta)$
I	$-\mathrm{E}_\theta \log \mathbf{M}(\xi,\theta)$	0	1
II, III	$\mathrm{E}_\theta\, \mathbf{M}^{-1}(\xi,\theta)$	-1	$\mathbf{M}^{-1}(\xi,\theta)$
IV, V	$-\mathrm{E}_\theta\, \mathbf{M}(\xi,\theta)$	1	$\mathbf{M}(\xi,\theta)$

For a numerical comparison of these criteria we use Example 2 with, again, five equally probable values of θ, now $1/7$, $1/\sqrt{7}$, 1, $\sqrt{7}$ and 7. For each parameter value the locally D-optimum design is at $x = 1/\theta$, so that the design times are uniformly spaced in log time.

The designs for the three one-parameter criteria are given in Table 4. The most satisfactory design arises from Criterion I in which $E_\theta \log |M(\xi,\theta)|$ is maximized. This design puts weights in the approximate ratio of 2:1:1 within the range of the optimum designs for the individual parameter vaues. By comparison, the design for Criterion II,

in which the expected variance is minimized, puts 96.69% of the weight on $x = 0.1754$. This difference arises because, in the locally D-optimum design for the linearised model, $var(\hat{\theta}) \propto \theta^2 e^2$. Large parameter values, which result in rapid reactions and experiments at small values of x, are therefore estimated with large variances, relative to small parameter values. Designs with Criterion II accordingly tend to choose experimental conditions in order to reduce these large variances. The reverse is true for the design with Criterion V, in which the maximization of expected information leads to a one-point design dominated by the smallest parameter value, for which the optimum design is at $x = 7$.

TABLE 4. Example 2 (First Order Decay): comparison of optimum designs satisfying criteria of Table 4.

Criterion	Power	x	w^*
I	0	0.2405	0.4781
		1.4863	0.2707
		3.9907	0.2512
II, III	-1	0.1754	0.9669
		2.5529	0.0331
IV, V	1	6.5217	1

The numerical results of this section indicate that Criterion I is most satisfactory. We have already mentioned the Bayesian justification for this criterion. A third argument comes from the equivalence theorem. For each value of θ the locally optimum design will have the same maximum value for the variance, in general p. The results of Table 3 show that the weight $a(\theta)$ for Criterion I is unity. The criterion therefore provides an expected variance which precisely reflects the importance of the different θ values as specified by the prior distribution. In other criteria the weights $a(\theta)$ can be considered as distorting the combination of the already correctly scaled variances.

Despite these arguments, there may be occasions when the variance of the parameter estimates is of prime importance and Criterion II is appropriate. For Example 1 this criterion produced an appealing design in Section 6.1, because the variance of $\hat{\beta}$ for the locally optimum design does not depend on θ. But the results of the present section support the use of the Bayesian criterion in which $E_\theta \log |M^{-1}(\xi, \theta)|$ is minimized. In Example 2 a further advantage of the design using Criterion I is that a close approximation to the continuous design is found by replacing the weights in Table 4 by 2, 1

and 1 trials.

6.3. The Effect of the Prior Distribution.

The comparisons of criteria in Section 6.2 used a single 5-point prior for θ. In this section the effect of the spread of this prior on the design is investigated together with the effect of more plausible forms of prior. Criterion I is used throughout with Example 2.

The more general five point prior for θ puts mass of 0.2 at the points $1/\nu$, $1/\sqrt{\nu}$, 1, $\sqrt{\nu}$ and ν. In Section 6.2 taking $\nu = 7$ yielded a 3-point design. When $\nu = 1$ the design problem collapses to the locally optimum design with all weight at $x = 1$. Table 5 gives optimum designs for these and three other values of ν giving 1, 2, 3, 4 and 5-point designs as ν increases. The design for $\nu = 100$ almost consists of weight 0.2 on each of the separate locally optimum designs for the very widely spaced parameter values. A prior with this range but more parameter values might be expected to give a design with more design points. As one example, a 9-point uniform prior wih support ν^{-1}, $\nu^{-3/4}$, $\nu^{-1/2}$, ..., $\nu^{3/4}$, ν with ν again equal to 100 produces an 8-point design. Rather than explore this path any further we let Table 5 demonstrate one way in which increasing prior uncertainty leads to an increase in the number of design points. In assessing such results, although it may be interesting to observe the change in the designs, it is the efficiencies of the designs for a variety of prior assumptions that is of greater practical importance.

An alternative to these discrete uniform priors in log θ is a normal prior in log θ. This corresponds to a prior assessment of θ values in which $k\theta$ is as likely as θ/k and θ has a lognormal distribution. An effect of continuous priors such as these on the design criteria is to replace the summations in the expectations by integrations. However, numerical routines for the evaluation of integrals reduce to the calculation once more of weighted sums.

The normal distribution used as a prior was chosen to have the same variance τ on the log θ scale as the 5-point discrete prior with $\nu = 7$, which gave rise to a 3-point design. The normal prior was truncated to have range -2.5τ to 2.5τ and this range was then divided into 7 equal intervals on the log θ scale to give weights for the values of θ. To assess the effect of this discretization the calculation was repeated with the prior divided into 15 intervals. The two optimum designs are given in Table 6. There are slight differences between these 5-point designs. However the important results are the efficiencies of Table 7, calculated on the assumption that the 15 point normal prior holds.

TABLE 5. Example 2 (First Order Decay): dependence of design on range of prior distribution: optimum designs for Criterion I with five-point prior distribution over $1/\nu$, $1/\sqrt{\nu}$, 1, $\sqrt{\nu}$ and ν.

ν	x	w^*
1	1	1
3	0.6505	0.7690
	1.5750	0.2310
7	0.2405	0.4781
	1.4863	0.2707
	3.9907	0.2512
13	0.1109	0.3371
	0.4013	0.1396
	1.2840	0.1955
	6.1466	0.3279
100	0.0106	0.2137
	0.1061	0.1992
	1.0610	0.2000
	10.6490	0.2009
	99.9987	0.1862

TABLE 6. Example 2 (First Order Decay): optimum designs for discretized lognormal priors.

Prior	x	w^*
7 point	0.1012	0.0873
	0.2299	0.1459
	0.6208	0.3653
	1.6588	0.2671
	4.2274	0.1344
15 point	0.1079	0.1083
	0.3329	0.2489
	0.7415	0.2189
	1.4051	0.2496
	3.7389	0.1743

The optimum design for the 7-point prior has an efficiency of 99.95%, indicating the irrelevance of the kind of differences shown in Table 6. More importantly, the 3-point design for the 5-point uniform prior has an efficiency of 92.58%. The 4-trial exact design derived from this by replacing the weights in Table 4 with 2, 1 and 1 trials is scarcely

TABLE 7. Example 2 (First Order Decay): Efficiencies of optimum designs for various priors using criterion I when the true prior is the 15 point lognormal.

Prior Used In Design	Efficiency %
One point	23.45
5 point uniform, $\nu = 7$	92.58
Exact design for $\nu = 7$	92.18
7 point lognormal	99.95
15 point lognormal	100

less efficient. The only poor design is the one-point locally optimum design.

6.4. Algorithms and the Equivalence Theorem.

Results such as those of Table 6 suggest that there is appreciable robustness of the designs to mis-specification of the prior distribution. A related intepretation is that the optima of the design criteria are flat for Bayesian designs. This interpretation is supported by plots of the expected variance for some of the designs of Table 6.

The plot of $d(x, \xi^*)$ for the locally optimum design putting all weight at $x = 1$ was given in Fig. 1. The curve is sharply peaked, indicating that designs with trials far from $x = 1$ will be markedly inefficient. However the curve for the design for the five-point uniform prior with $\nu = 7$, Fig. 5, is appreciable flatter, with three shallow peaks at the three design points. The curve for the 5-point design for the 15-point normal prior , Fig. 6, is sensibly constant over a 100-fold range of x, indicating a very flat optimum.

The flatness of the optima for designs with prior information has positive and negative aspects. The positive aspect, illustrated in Table 7, is the near optimum behaviour of designs quite different from the optimum design: the negative aspect is the numerical problem of finding the precisely optimum design, if such is required.

The standard algorithms of optimum design theory were mentioned briefly in Section 3.1. They consist of adding mass at the point at which $d(x, \xi)$ is a maximum. For the design of Fig. 1, with a sharp maximum, the algorithms converge, albeit relatively slowly, since convergence is first-order. For flat derivative functions, such as that of Fig. 6, our limited experience is that these algorithms are useless, an opinion supported by the comments of Chaloner and Larntz (1989, Section 4). One difficulty is that small

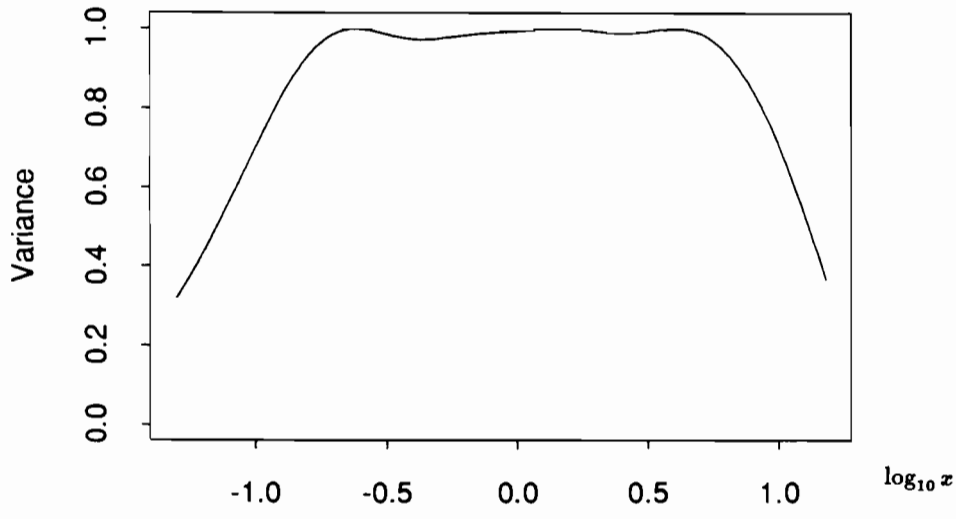


FIGURE 5. Example 2 (First Order Decay): variance function $d(x, \xi^*)$ for the three point design, optimum for the five-point uniform prior with $\nu = 7$.

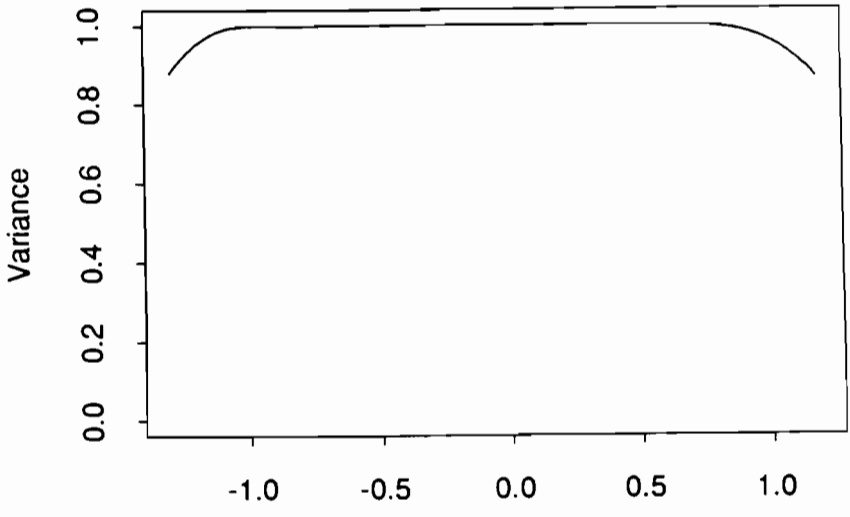


FIGURE. 6. Example 2 (First Order Decay): variance function $d(x, \xi^*)$ for the five point design, optimum for the 15-point normal prior.

amounts of mass are added to the design at numerous distinct points; the pattern to which the design is converging does not emerge.

The designs described in this paper were found using numerical optimization applied to the design criterion, alternating with inspection of the derivative function to

indicate regions in which the search for the optimum should be concentrated. In all examples three iterations of optimization and inspection led to designs in which the maximum expected variance equaled 1 ± 0.0001, so that the equivalence theorem was sensibly satisfied. The optimization routines used were quasi-Newton algorithms with numerical derivatives: NAG routines on the Cyber at Imperial College and the Vax at LSE, CMLIB on the Vax at the University of Minnesota. To apply these algorithms for unconstrained optimization, transformations were used to ensure that the design constraints were satisfied. Examples are given by Atkinson (1969).

7. DISCRIMINATION BETWEEN MODELS WITH PRIOR INFORMATION.

7.1. True Model Known.

In this section the extension of the General Equivalence Theorem in Section 5 is used to incorporate prior information into the T-optimum designs of Section 4. We continue to work with only two competing models. First it will be assumed that it is known which model is true, expectations being taken only over the parameters of the true model. Then, in Section 7.2, a prior probability is assigned to the truth of each model and the expectation of the design criterion is taken over this distribution. In both cases the resulting equivalence theorem is a straightforward generalization of that of Section 4.

To begin we generalize the earlier notation, to make explicit the dependence of the design criterion on model and parameters. If, as before, model 1 is true, the non-centrality parameter (18) becomes $\Delta_2(\xi, \theta_1)$ with the squared difference in the true and predicted responses (19) written as $\phi_2(x, \xi, \theta_1)$. Although we shall not explicitly need the notation, for every design and parameter value θ_1, the least squares estimates of the parameters of the second model (13) are $\hat{\theta}_2(\xi, \theta_1)$.

Let E_1 denote expectation with respect to θ_1. Then if we write

$$\Delta_2(\xi) = E_1 \Delta_2(\xi, \theta_1) \text{ and}$$

$$\phi_2(x, \xi) = E_1 \phi_2(x, \xi, \theta_1), \tag{29}$$

the equivalence theorem of Section 4 applies to this composite criterion.

Example 3. Two Models for Decay (continued).

The two models (1) and (5) are respectively exponential decay and an inverse polynomial. In Section 4 it was shown that if the exponential model is true with $\theta_1 = 1$, the T-optimum design (23) puts unequal design weight at the two points 0.327 and

3.34. Table 8 lists some designs obtained by putting a prior distribution on θ_1. If two equiprobable values of θ_1 are taken at 1/3 and 3, a 3-point design results. A very similar design results from taking the three values 1/3, 1 and 3. However for the four more dispersed θ_1 values 1/8, 1/2, 2 and 8 the resulting design has 5 unequally weighted points of support from $x = 0.0514$ to $x = 22.52$. To show that this is indeed the Bayesian T-optimum design, we can again use the equivalence theorem, this time in the form (29). Fig. 7 is a plot of $\phi_2(x, \xi^*)$ against log x. There are five maxima at the design points which are equal to the value of $\Delta_2(\xi^*)$, that is 4.225×10^{-3}. As in other applications of the theorem, we see that the design is optimum. ∎

TABLE 8. Example 3 (Two Models for Decay): dependence of design on prior for θ.

θ	x	w^*
1	0.327	0.3345
	3.34	0.6655
1/3, 3	0.1160	0.1608
	1.073	0.4014
	9.345	0.4378
1/3, 1, 3	0.1443	0.1749
	1.0726	0.3616
	7.9817	0.4635
1/8, 1/2, 2, 8	0.05149	0.0966
	0.3450	0.1899
	1.3932	0.2343
	4.8266	0.2001
	22.521	0.2791

7.2. True Model Unknown.

Let the prior probability that model j is true be π_j, with, of course, $\pi_1 + \pi_2 = 1$. Then the expected value of the non-centrality parameter, taken over models and over parameters within models is, by extension of (29)

$$\Delta(\xi) = \pi_1 E_1 \Delta_2(\xi, \theta_1) + \pi_2 E_2 \Delta_1(\xi, \theta_2)$$

with the expected squared difference in responses given by

$$\phi(x, \xi) = \pi_1 E_1 \phi_2(x, \xi, \theta_1) + \pi_2 E_2 \phi_1(x, \xi, \theta_2). \qquad (30)$$

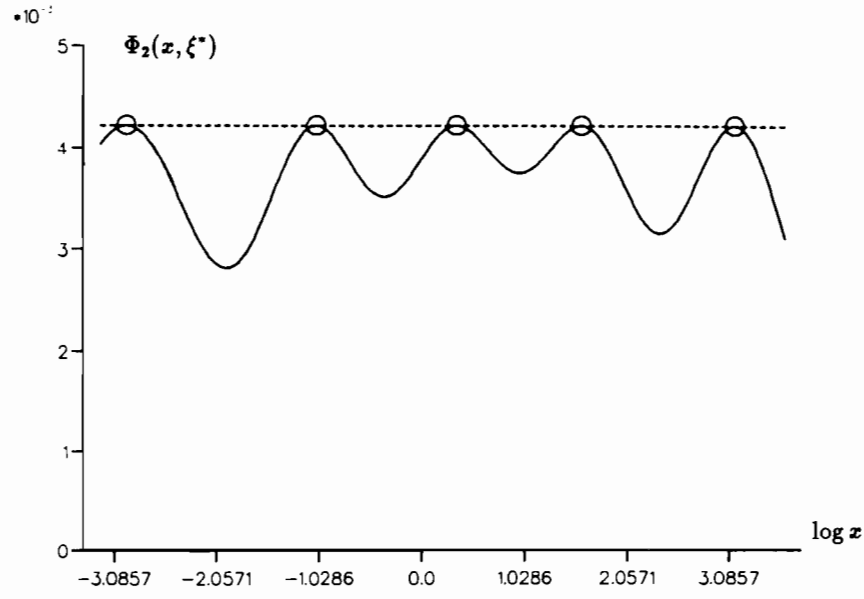


FIGURE. 7. Example 3 (Two Models for Decay): the derivative function $\phi_2(x, \xi^*)$ for the five-point T-optimum design when θ_1 has a four-point prior.

That is, for each model assumed true, the expected value is calculated of the quantity disproving the other model. These values are then combined according to the prior probabilities π_j. The equivalence theorem applies to this more general design criterion as it did to its special case (29).

Example 4. Two Linear Models (continued).

The locally T-optimum design for discriminating between these two 3-parameter models given in (21) puts trials at four points. We now consider a prior specification which gives rise to a five-point design.

Table 9 details one prior yielding a five-point design. The prior probability that model 1 is true is 0.6 and, conditional on this, there are ten prior values of the parameters whereas, for model 2, there are only 5. The optimum design

$$\xi^* = \begin{Bmatrix} -1 & -0.6634 & 0.1624 & 0.8466 & 1 \\ 0.2438 & 0.4265 & 0.2535 & 0.0206 & 0.0556 \end{Bmatrix} \tag{31}$$

differs from the non-Bayesian design (21) in spanning the range of x. However, like that design, it places relatively little experimental effort at the higher values of x.

TABLE 9. Example 4 (Two Linear Models): prior distribution of parameters yielding the 5 point design (31) and the derivative function of Fig. 8

Model 1 $\pi_1 = 0.6$				Model 2 $\pi_2 = 0.4$			
β_{10}	β_{11}	β_{12}	$p_1(\beta)$	β_{20}	β_{21}	β_{22}	$p_2(\beta)$
4.5	−1.5	−2.0	0.25	1.0	0.5	−2.0	0.23
4.0	−1.0	−2.0	0.14	0.8	0.4	−2.0	0.33
4.5	−2.0	−1.5	0.11	1.0	0.6	−1.5	0.17
5.0	−1.5	−1.5	0.06	1.2	0.5	−1.5	0.15
4.0	−2.0	−1.0	0.05	0.8	0.6	−1.0	0.12
4.5	−1.5	−1.5	0.08				
4.0	−1.5	−2.0	0.05				
4.0	−2.0	−2.0	0.12				
4.5	−2.0	−2.0	0.07				
5.0	−1.5	−2.0	0.07				

The prior probabilities of the parameters $p_j(\beta)$ are conditional on the models

The plot of the derivative function $\phi(x,\xi)$ in Fig. 8 shows that (31) is the optimum design. Comparison of this figure with that for the non-Bayesian design, Fig. 3, is informative. In Fig. 3 $\phi(x,\xi)$ goes to zero at the three points where the two models intersect. However the corresponding plot for the Bayesian design does not go to zero, as, for each x, there will always be some combination of parameter values for which the experiment is informative. ∎

These examples illustrate the way in which prior information can be incorporated into designs for discriminating between models. In the second example we assumed independence of the prior distributions of the parameters within models. It might sometimes be more realistic to consider priors which give equal weight to parameter values yielding similarly shaped response curves under the two models. We have also assumed discrete joint prior distributions within models. The case of continuous joint prior distributions would involve no new ideas, but would require the use of numerical integration. For these Bayesian designs the extension to three or models would seem to be straightforward: expectations can be taken over all non-centrality parameters yielding a smooth, well behaved design criterion.

8. DISCUSSION.

The main result used in this paper is the extension of the standard equivalence the-

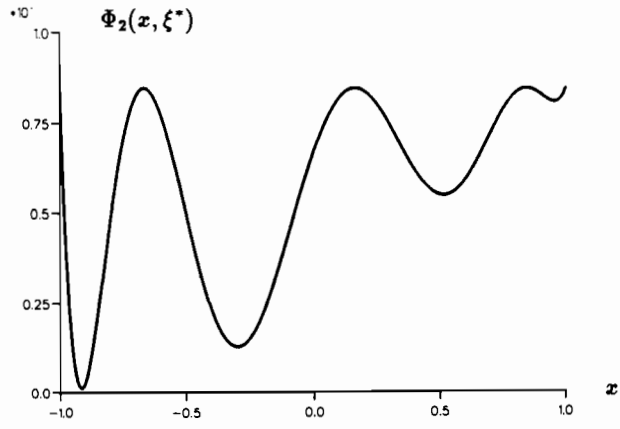


FIGURE. 8. Example 4 (Two Linear Models): the derivative function $\phi(x, \xi)$ for the Bayesian T-optimum design with two model prior given by Table 9.

orem of Section 3.1 to incorporate prior information, yielding the General Equivalence Theorem of Section 5. This theorem has then been exemplified by extensions to the familiar criteria of D- and T-optimality. The equivalence theorem for these expectation criteria has a long, implicit history. The earliest proof seems to have been due to Whittle (1973), but the implications, particularly for the number of design points, are not clearly stated. The first complete discussion, including examples of designs, is due to Chaloner and Larntz (1989) who consider logistic regression. Chaloner (1988) briefly treats the more general case of design for genralized linear models. Earlier work does not consider either the number of design points, nor the properties of the derivative function, which are of importance in the construction of designs. Läuter (1974, 1976) proves the theorem in the generality required, but only gives examples of designs for composite criteria for linear models. Atkinson and Cox (1974) use the theorem for Criterion I of Table 1 with linear models. Cook and Nachtsheim (1982) are likewise concerned with designs for linear models. Pronzato and Walter (1985) calculate numerical optimum designs for some nonlinear problems, but do not mention the equivalence theorem. Fedorov and Atkinson (1988) give a more algebraic discussion of the properties of the designs for the criteria of Table 1. The examples of Section 6 are discussed in fuller detail by Atkinson and Fedorov (1992).

T-optimum designs for two models were introduced by Atkinson and Fedorov (1975a). A full discussion of designs for three or more models is given by Atkinson and Fedorov (1975b). The Bayesian extension of T-optimality was introduced by de

Leon and Atkinson (1991), who give details of the proof of the equivalence theorem using (30). Atkinson and Donev (1992) in a book length treatment of optimum experimental designs give much related material in Chapter 19 for designs in the presence of prior information and in Chapter 20 for designs for discriminating between models. Similar methods can be extended to other design criteria. For example, Atkinson et al (1992) provide c-optimum designs for properties of compartmental models, such as the conditions of maximum yield, or the area under the curve. Again, increasing variablity in the prior distribution of the parameters results in an increasing spread of design points. In all applications, if the prior information used in calculating the designs is also to be used in the analysis of the experiments, the information matrices used in this work require augmentation by prior information. Pilz (1983) provides a survey.

REFERENCES

Atkinson, A.C. (1969). Constrained maximisation and the design of experiments. *Technometrics* 11: 616-618.

Atkinson, A.C., Chaloner, K., Herzberg, A.M. and Juritz, J. (1992). Optimum experimental designs for properties of a compartmental model. Submitted for publication.

Atkinson, A.C. and Cox, D.R. (1974). Planning experiments for discriminating between models (with discussion). *J. R. Statist. Soc. B* 36 : 321 – 348.

Atkinson, A.C. and Donev, A.N. (1989). The construction of exact D-optimum experimental designs with application to blocking response surface designs. *Biometrika* 76: 515-526.

Atkinson, A.C. and Donev, A.N. (1992). *Optimum Experimental Designs.* Oxford: Clarendon Press.

Atkinson, A.C. and Fedorov, V.V. (1975a). The design of experiments for discriminating between two rival models. *Biometrika* 62: 57-70.

Atkinson, A.C. and Fedorov, V.V. (1975b).Optimal design: experiments for discriminating between several models. *Biometrika* 62: 289-303.

Atkinson, A.C. and Fedorov, V.V. (1992). Examples of the optimum design of experiments for linear and nonlinear models in the presence of prior information. Submitted for publication.

Box, G.E.P. and Lucas, H.L. (1959). Design of experiments in nonlinear situations. *Biometrika* 46: 77-90.

Chaloner, K. (1988). An approach to experimental design for generalized linear models. In V. Fedorov and H. Läuter (Eds), *Model-Oriented Data Analysis.* Berlin: Springer

Chaloner, K. and Larntz, K. (1989). Optimal Bayesian design applied to logistic regression experiments. *J. Statist. Planning Inf.* 21: 191-208.

Chernoff, H. (1953). Locally optimal designs for estimating parameters. *Ann. Math. Statist.* 24: 586-602.

Cook, R.D. and Nachtsheim, C.J. (1982). Model robust, linear-optimal designs. *Technometrics* 24: 49-54.

de Leon, A.P. and Atkinson, A.C. (1991). Optimum experimental design for discriminating between two rival models in the presence of prior information. *Biometrika* 78 (in press).

Dubov, E.L. (1977). *D*-optimal designs for nonlinear models under the Bayesian approach. In V.V. Nalimov (Ed.), *Regression Experiments.* Moscow University Press (in Russian).

Fedorov, V.V. (1972). *Theory of Optimal Experiments.* New York: Academic Press.

Fedorov, V.V. (1981). Active regression experiments. In V.B. Penenko (Ed.), *Mathematical Methods of Experimental Design.* Novosibirsk: Nauka (in Russian).

Fedorov, V.V. and Atkinson, A.C. (1988). The optimum design of experiments in the presence of uncontrolled variability and prior information. In Y. Dodge, V.V. Fedorov and H.P. Wynn (Eds), *Optimal Design and Analysis of Experiments.* Amsterdam: North Holland.

Kiefer, J. (1959). Optimum experimental designs (with discussion). *J. R. Statist. Soc. B* 21 : 272 – 319.

Kiefer, J. and Wolfowitz, J. (1960). The equivalence of two extrema problems. *Can. J. Math.* 12: 363-366.

Läuter, E. (1974). Experimental design in a class of models. *Math. Oper. Statist.* 5, 379-396.

Läuter, E. (1976). Optimal multipurpose designs for regression models. *Math. Oper. Statist.* 7: 51-68.

Mitchell, T.J. (1974). An algorithm for the construction of '*D*-optimal' experimental designs. *Technometrics* 16: 203-210.

Pilz, J. (1983). *Bayesian Estimation and Design in Linear Models.* Leipzig: Teubner.

Pronzato, L. and Walter,E. (1985). Robust experiment design via stochastic approximation. *Math. Biosci.* 75: 103-120.

Silvey, S.D. (1980). *Optimal Design.* London: Chapman and Hall.

Whittle, P. (1973). Some general points in the theory of optimal experimental design. *J. R. Statist. Soc. B* 35 : 123 – 130.

Wu, C.F.J. and Wynn, H.P. (1978). The convergence of general step length algorithms for regular optimum design criteria. *Ann. Statist.* 6: 1286-1301.

DESIGNS WITH IMPROVED DETECTABILITY OF LACK OF FIT

Alexander. N. Donev
Dept. of Automation, Higher Institute of Chemical Technology
1156 Sofia, Bulgaria

1. INTRODUCTION.

This paper is concerned with the choice of additional trials for the detection of lack of fit of a model. It is well known that the choice of a design is very much dependent on the choice of a model for the experiment. The right choice however depends on the intervals in which the factors vary during the experiment and therefore we cannot be sure that the choice is correct. For example, it is possible for the relationship to be of different orders in the different factors while we customary expect the orders all to be the same. It is important to be able to check such assumptions. Many designs widely used in practice do not allow for such a check. In this paper we restrict our attention to the factorials and composite designs which have very good properties if the model is correctly selected. They however do not always allow to discover if the model is inadequate because of the presence of terms of a higher order polynomial.

In the following section the effect of the inadequacy of the model is discussed along with some related work. Considerations in the choice of additional trials, examples and discussion are given in Section 3.

2. EFFECT OF INADEQUACY.

We assume some functional relationship

$$E(Y) = \Psi(x_1, x_2, \ldots, x_m) \qquad (1)$$

connecting the expected value of the response Y with the factors x in the design region. We shall be concerned with situations where this relationship is linear in the parameters:

$$Y(x) = \Phi(x,\beta) + \varepsilon = \sum_{i=1}^{P} \beta_i w_i + \varepsilon,$$

where x is a mx1 vector of the coded factors, β is a Px1 vector of the parameters of the model which are to be estimated from the data obtained in the experiment, w is a Px1 vector formed

by the values of the approximating functions and ε is the experimental error assumed to be normally distributed with zero mean and variance σ^2_ε. The design region is assumed to be cuboidal. The most popular approximating functions are the polynomials. We shall restrict our discusion to those of first and second order. It is desirable for the prediction $\hat{Y}(x)$ to be as close as possible to the true value of the response E(Y). The design is usually chosen in order to satisfy some criterion of optimality for the model parameters. For example, the D-optimum N trial exact design minimizes the content of the confidence ellipsoid for the parameters for a given confidence level. The LSE (least square estimates) of the model parameters ensure that the quantity

$$s^2_R = \sum_{i=1}^{N} (Y_i - \hat{Y}_i)^2/(N-p) \qquad (2)$$

is a minimum. In (2) Y_i is the value of the response measured in the ith trial.

As the true approximating function is usually not known another source of error, apart from the experimental one ε included in the model, is the systematic error, or bias, arising from the inability of the approximating function $\Phi(x,\beta)$ exactly to match the expectation function (1). It is always necessary to check for lack of fit, that is the inadequacy of the model. The usual way of doing this is to test the hypothesis that the variance σ^2_L caused by both the possible inadequacy and the experimental error and the variance of the experimental error σ^2_ε are equal, leading to a formal F test. This problem has been studied by many authors, for example by Atkinson (1972, 1973) and Box & Draper (1987). An independent estimate of σ^2_ε is usually obtained either from a separate sample or from replicated measurements of the design trials. In the numerator of the F test there should be an estimate of the variance σ^2_L giving evidence of lack of fit. Often as an estimate the quantity s^2_R calculated from (2) is used. Many designs however do not allow for obtaining a value of s^2_R which shows the effect of the inadequacy if it exists. Moreover, several widely used designs suffer from the disadvantage that s^2_R remains unchanged when the true model includes terms of higher order.

Let us first consider the case when factorial designs are used and the assumed model is of 1 order, i.e.

$$E(Y) = \beta_o + \sum_{i=1}^{m} \beta_i x_i. \qquad (3)$$

If our assumption about the true model is wrong and the correct model includes second order terms it can be seen that the

estimates b_i of the parameters β_i, i = 1, 2, ..., m, obtained from such a design will be unbiased, but the effect of the second order terms will be confounded with the estimate of β_o. It is not difficult also to see that the variance s_R^2 for the inadequate model is the same as if it were calculated from the correct model. Therefore it should not be used in the goodness of fit test.

Similar confounding of the effects appears if fractions of the factorials are used. The quantity s_R^2 gives no evidence of lack of fit.

If composite designs are used the assumed model is usually of second order in the factors:

$$E(Y) = \beta_o + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m-1} \sum_{i=j+1}^{m} \beta_{ij} x_i x_j + \sum_{i=1}^{m} \beta_{ii} x_i^2.$$

If the correct model however has terms of higher order, for example $\beta_{ijj} x_i x_j^2$ and $\beta_{iii} x_i^3$, they will cause bias in the estimates of β_i. All other parameters will be unbiased. Therefore it is also easy to see that the variance s_R^2 will be the same if the true model has all interactions of the factors equal to zero and its value will be underestimated in the more general case of a third order true model.

These designs are good according to criteria of optimality for the model parameters but bad according to the possibility to test the model for lack of fit. The reason for confounding of the factors is that $x_i^2 = 1$ for $x_i = \pm 1$ and $x_i^3 = x_i$ for $x_i = 1$, 0 or -1. Therefore the list of designs which are insensible to the test of lack of fit caused by omitted higher order terms in the model can be essentially extended. The value of s_R^2 will not give enough evidence of lack of fit if the design points have coordinates (-1, 1) for the first order model and (-1, 0, 1) for second order model because the estimates will be confounded although in a more complicated way.

Customarily this problem is solved by design of experiments simultaneously providing information about both the original regression model and one which includes additional terms of a higher order (for example, Atkinson, 1972, Box & Draper, Ch.13, 1987). The efficiency of the design for estimating both kinds of parameters is investigated. However such designs, which provide a good check of the adequacy of the model, may provide poor estimates of the original parameters if the model is in fact adequate (Atkinson, 1972). In the next section an alternative way to solve the problem is illustrated. Additional trials are used to obtain an estimate of σ_L^2 which will show if there are omitted terms in the model.

3. EXAMPLES AND DISCUSSION.

In this section several examples will be given to illustrate the effect of using additional trials to detect possible inadequacy of the model due to higher order terms in one of the factors. All examples are simulated. As the exact effect obviously depends on the unknown values of the omitted parameters we shall always state the true model.

An estimate of σ_L^2 will be obtained from the results in the additional design of size L . It is

$$s_L^2 = L^{-1} \sum_{i=1}^{L} (Y_{ai} - \hat{Y}_{ai})^2. \qquad (5)$$

In (5) Y_{ai} is the ith additional measurement while $\hat{Y}_{ai}$ is the prediction of the model which is to be checked for adequacy at the point x_{ai}. In order to obtain a relevant estimate of s_L^2 which provides information about the lack of fit when it exists, Donev (1990) suggests choosing the L trials to maximize $|Y_{ai} - \hat{Y}_{ai}|$ for some i under a variety assumptions about possible departures from the true model.

For each of the examples 2 different additional designs are compared. The designs are listed with the values of s_{R*}^2 and s_{L*}^2 if the model is adequate and s_R^2 and s_L^2 if it is not. The degrees of freedom in all cases were chosen to be equal: N - p. In the tables H denotes 0.5 and $T = \sqrt{1/3}$.

Example 1 (Table 1). The true model is

$$E(Y) = 12.5 + 2.05x_1 - 4.33x_2 + 5.16x_3 + 6.6x_1^2,$$

while we expect a first order model.

Example 2 (Table 2). The true model is

$$E(Y) = 12.5 + 2.05x_1 - 4.33x_2 + 5.16x_3 + 6.6x_1^2 - 3x_2^2 - 3.6x_3^2,$$

while we expect a first order model.

Example 3 (Table 3). The true model is

$$E(Y) = 12.5 + 2.05x_1 - 4.33x_2 + 5.16x_3 + 0.98x_1^2x_2^2 - 2.05x_1x_3 + 4.96x_2x_3 + 3.78x_1^2 + 6.2x_2^2 - 4.9x_3^2 + 6.6x_1^3,$$

while we expect a second order model.

Example 4 (Table 4). The true model is

$$E(Y) = 12.5 + 2.05x_1 - 4.33x_2 + 5.16x_3 + 0.98x_1^2x_2^2 - 2.05x_1x_3$$
$$+ 4.96x_2x_3 + 3.78x_1^2 + 6.2x_2^2 - 4.9x_3^2$$
$$+ 6.6x_1x_2^2 - 4.8x_1x_3^2 + 3.8x_1^3,$$

while we expect a second order model.

For Examples 1 and 2 the parameters of the models were obtained from a factorial design. For these designs Donev (1990) suggests that the L additional trials x_i should be set to zero while the other factors can vary in their whole intervals. In Examples 3 and 4 composite designs were used for the estimation of the parameters. The additional trials in this case should be constructed following the more complicated rules: $x_i = \pm 1$; if $\sum_{i=2}^{m} \beta_{iii} > 0$ and $\beta_{iii} > 0$ then $x_i = 0$, and if $\beta_{iii} < 0$ then $x_i = \pm 1$, for i = 2, ..., m, but if $\sum_{i=2}^{m} \beta_{iii} < 0$ the optimality conditions for x_i, i = 2, ..., m, are reversed.

The results in the tables show large values of s_L^2 when the model is inadequate due to omitted higher order terms and the conditions derived in the previous chapter are achieved. Even in the designs which do not exactly follow the rule s_L^2 is bigger if compared to s_{R*}^2. It is interesting to note that the exception, the first design in Table 2, is ineffective because the absolute values of the factors in the trials are the same. Therefore such an arrangement of trials should be avoided. This results can be extended for the case when the inadequacy is caused by more than one factor.

This approach is suggested as an alternative to the one which proposes the construction of a design satisfying both the requirements of the criteria of optimality for parameter estimation and those for high detecability of lack of fit. The additional trials, even when their number is small, are shown to be effective. At a reasonable extra experimental effort we are able learn more about the investigated system. Therefore they should complement every response surface design.

TABLE 1. Additional trials for check of lack of fit of 1 order model obtained from a factorial design when the term $6.6x_1^2$ is omitted.

x_1	x_2	x_3		
H	1	-1	s^2_{R*}	1.052
-H	1	-1	s^2_{L*}	2.255
-H	-1	1	s^2_R	1.052
H	-1	1	s^2_L	27.748

x_1	x_2	x_3		
0	-1	-1	s^2_{R*}	1.052
0	1	-1	s^2_{L*}	2.702
0	-1	1	s^2_R	1.052
0	1	1	s^2_L	47.584

TABLE 2. Additional trials for check of lack of fit of 1 order model obtained from a factorial design when the terms $6.6x_1^2 - 3x_2^2 - 3.6x_3^2$ are omitted.

x_1	x_2	x_3		
H	-H	-H	s^2_{R*}	1.052
-H	H	-H	s^2_{L*}	2.075
-H	-H	H	s^2_R	1.052
H	H	H	s^2_L	2.075

x_1	x_2	x_3		
0	1	1	s^2_{R*}	1.052
1	0	1	s^2_{L*}	1.632
-1	-1	0	s^2_R	1.052
1	1	0	s^2_L	30.012

TABLE 3. Additional trials for check of lack of fit of 2 order model obtained from a composite design when the term $6.6x_1^3$ is omitted.

x_1	x_2	x_3		
-T	T	-T	s^2_{R*}	2.675
-T	-T	T	s^2_{L*}	3.793
T	T	T	s^2_R	2.675
T	-T	-T	s^2_L	10.440

x_1	x_2	x_3		
-T	1	-1	s^2_{R*}	2.675
-T	-1	1	s^2_{L*}	4.495
T	1	1	s^2_R	2.675
T	-1	-1	s^2_L	12.280

TABLE 4. Additional trials for check of lack of fit of 2 order model obtained from a composite design when the terms $6.6x_1x_2^2$ - $4.8x_1x_2^2$ + $3.8x_1^3$ are omitted.

x_1	x_2	x_3		
H	1	-1	s^2_{R*}	1.052
-H	1	-1	s^2_{L*}	2.255
-H	-1	1	s^2_R	1.052
H	-1	1	s^2_L	27.748

x_1	x_2	x_3		
0	-1	-1	s^2_{R*}	1.052
0	1	-1	s^2_{L*}	2.702
0	-1	1	s^2_R	1.052
0	1	1	s^2_L	47.584

4. REFERENCES.

Atkinson, A.C. (1972). Planning Experiments to Detect Inadequate Regression Models. Biometrika, 59(2), 275 - 293.

Atkinson, A.C. (1973). Multifactor Second Order Designs for Cuboidal Regions. Biometrika, 60(1), 15 - 19.

Box, G.E.P. & Draper, N.R. (1987). Empirical Model-Building and Response Surfaces. John Wiley & Sons, Inc.

Donev, A.N. (1990). Designs for Checking Lack of Fit. Submitted for publication.

Lucas, J.M. (1976). Which Response Surface Design is Best. Technometrics, 18, 411 - 417.

VARIOUS CONSTRAINTS IN EXPERIMENTAL DESIGN

Fedorov V. V.
CLSEM, Academy of Sciences, USSR

I. Introduction

Experimental design problems considered in this paper are basically related to the standard linear regression model:

$$y_{ij} = \theta^T f(x_i) + \varepsilon_{ij}, \qquad (1)$$

$$i=1,\dots,n, \quad j=1,\dots,r_i, \quad \sum r_i = N,$$

where $\theta \in R^m$ are unknown parameters, $f^T(x) = (f_1(x),\dots,f_m(x))$ are given functions, supporting points x_i can be chosen from some set X, ε_{ij} are uncorrelated random errors with zero means and variances equal 1.

For the best linear unbiased estimator of unknown parameters the accumulated "accuracy" is described by the information matrix:

$$M(\xi) = N^{-1} \sum p_i f(x_i) f^T(x_i), \quad p_i = r_i/N,$$

which is completely defined by design $\xi = \{x_i, p_i\}_1^N$. In the context of the convex design theory:

$$M(\xi) = \int f(x) f^T(x) \xi(dx),$$

where $\xi(dx)$ is a probability measure or (continuous) design with the supporting set belonging to X : $\operatorname{supp} \xi \subset X$. The subscript corresponding to the area of integration will be used only when it will be essential for understanding. A design

$$\xi^* = \underset{\xi}{\text{Arg min}}\ \Psi[\mathbf{M}(\xi)] \qquad (2)$$

is called (Ψ-)optimal.

In the traditional case minimization has to be over the set of all possible probability measures Ξ with supporting sets belonging to X. For a practitioner it means that one has to find an optimal design with a given number of observations. Of course, the reality can be worse and more constraints can be imposed. For instance, the cost of observations may depend upon x with the total cost of the experiment not exceeding some level. Sometimes together with the parameters of model (1) one may wish to estimate the parameters of some competing model. Then additionally to (2) it is reasonable to demand that the corresponding information matrix is not very "small". In the observation network optimization problem it is usually not sensible to locate several sensors at the same site nor with very small distances between them. This leads to the restriction of the number of sensors per square unit. In terms of continuous designs it means that the density of the design measure has to be restricted.

Thus additionally to (2) one has to consider design problems when the structure of Ξ is more complicated than in the traditional experimental design theory, which is very briefly surveyed in Section II. In Sections III-V the various types of constraints are considered: and the main focusing on the similarities among thecorresponding results rather than on the discrepancies between them.

II. Standard Equivalence Theorem

The optimization problem (2) has been intensively studied since Kiefer's pioneering paper (1959). In this section we shall summarize the major properties of the traditional optimal designs.

Assume that:

(a) X is compact;

(b) $f(x)$ are continuous functions in X, $f \in R^m$;

(c) $\Psi(\mathbf{M})$ is a convex function;

(d) there exists q such that

$$\{\xi : \Psi[\mathbf{M}(\xi)] \le q < \infty\} = \Xi(q) \neq \varnothing;$$

(e) for any $\xi \in \Xi(q)$ and $\overline{\xi} \in \Xi$:

$$\Psi[(1-\alpha)\mathbf{M}(\xi)+\alpha\mathbf{M}(\overline{\xi})] = \Psi[\mathbf{M}(\xi)] + \alpha\int\psi(x,\xi)\overline{\xi}(dx) + \tau(\alpha,\xi,\overline{\xi}),$$

where $\tau(\alpha,\xi,\overline{\xi})=o(\alpha)$.

Assumptions (c) and (e) are most essential and restrictive for the theory. Fortunately the majority of the popular optimality criteria satisfy them, such as D- and linear criteria. But there exist some natural and widely used criteria which do not satisfy (e)(for instance, the minimax ones). One can face similar troubles even for "good" criteria when an optimal design happens to be singular: see Silvey (1980).

Theoreml. If (a)-(e) hold, then:

1. For any optimal design there exists a design with the same information matrix and containing no more than $n_0 = m(m+1)/2$ supporting points.

2. A necessary and sufficient condition for a design ξ^* to be optimal is fulfillment of the inequality

$$\min_{x \in X} \psi(x,\xi^*) \ge 0. \qquad (3)$$

3. The set of optimal designs is convex.

4. $\psi(x,\xi^*)$ achieves zero almost everywhere in $\operatorname{supp} \xi^*$.

Proof. The proof of this theorem is well known and is only sketched here to clarify the main ideas which are used in the subsequent sections.

The proof of the first part of the theorem is based on Caratheodory's theorem and on the fact that any information matrix can be considered as an element of the convex hull of the elementary information matrices:

$$m(x) = f(x)f^{T}(x) \in R^{m(m+1)/2}, \quad x \in X.$$

Necessity and sufficiency of (3) follows from the fact that the following inequality:

$$\min_{\xi \in \Xi} \lim_{\alpha \to 0} \Psi[(1-\alpha)\mathbf{M}(\xi^{*}) + \alpha \mathbf{M}(\xi)] \geq 0 \quad (4)$$

is a necessary and sufficient condition of optimality of ξ^{*}. If (e) holds, then (4) can be easy transformed to:

$$\min_{\xi \in \Xi} \int \psi(x,\xi^{*})\xi(dx) = \min_{x} \psi(x,\xi) \geq 0.$$

The third part of the theorem follows directly from the convexity of the objective function.

Integration of both parts of the expression from (e) with respect to $\xi^{*}(dx)$ confirms the final section of the theorem.

Theorem 1 is the basic one in convex design theory and its various modifications has been extensively discussed in the statistical literature: see Fedorov (1972), Fedorov and Malyutov (1972), Whittle (1973), Silvey (1980).

Example 1. For D-criterion, when $\Psi(\mathbf{M}) = -\ln|\mathbf{M}|$ and

$$\psi(x,\xi) = m - d(x,\xi), \quad d(x,\xi) = f(x)^{T}\mathbf{M}^{-1}(\xi)f(x) \ ,$$

the theorem can be reformulated in the more traditional form (its point 1 is omitted):

The following problems:

$$\xi^{*} = \operatorname*{Arg\,max}_{\xi} \ln |\mathbf{M}(\xi)| ;$$

$$\xi^* = \operatorname{Arg}\min_{\xi}\max_{x\in X} d(x,\xi);$$

$$\max_{x\in X} d(x,\xi) = m;$$

are equivalent.

This is Kiefer's celebrated equivalence theorem.

III. Linear constraints

Constraints linear with the respect to the design measure mainly arise in experiments when the cost of observations depends upon controlled variables. The optimization problem can be stated now in the following way:

$$\xi^* = \operatorname{Arg}\min_{\xi} \Psi[M(\xi)] \tag{5}$$

$$\text{s.t.} \int \xi(dx) = 1, \qquad C(\xi) = \int \phi(x)\xi(dx) \le 0, \tag{6}$$

where $\phi(x) = (\phi_1(x),\ldots,\phi_l(x))^T$.

Example 2. Let the functions $\zeta_\alpha(x)$, $\alpha=1,\ldots,l$, describe the losses when observation is taken at point x. Assume that the total loss for a particular α can not exceed C_α. Then

$$\sum r_i \zeta_\alpha(x_i) \le C_\alpha, \qquad \alpha = 1,\ldots,l,$$

where r_i is the number of observations at point x_i.

For continuous designs the latter inequality takes the form:

$$\int \phi(x)\xi(dx) \le 0,$$

where $\phi_\alpha(x) = \zeta_\alpha(x) - c_\alpha$, $c_\alpha = C_\alpha/N$.

We consider the optimization problem (6) under assumptions (a)-(e) adding to them

(b') $\phi(x)$ are continuous in X.

Theorem 2. If (a)-(e),(b') hold, then

1. For any optimal design there exists a design with the same information matrix and containing no more than $n_0 = m(m+1)/2 + 1$ supporting points.

2. A necessary and sufficient condition for a design ξ^* to be optimal is fulfillment of the inequality

$$\min_{x \in X} q(x,u^*,\xi^*) \geq 0,$$

where

$$q(x,u,\xi) = \psi(x,\xi) + u^T\phi(x),$$

$$u^* = \operatorname{Arg}\max_{u \in U'} \min_{x \in X} q(x,u,\xi^*),$$

$$U' = \{u: u \in R^1,\ u_\alpha \geq 0\}.$$

3. The set of optimal designs is convex.

4. $q(x,u^*,\xi^*)$ achieves zero almost everywhere in $\operatorname{supp} \xi^*$.

Proof. To prove now the first part of the theorem it is necessary to notice that any couple $\{\mathbf{M}(\xi),C(\xi)\}$ belongs to the convex hull of

$\{m(x),\ \phi(x)\} \in R^{m(m+1)/2+1},\ x \in X.$

To prove the second part of the theorem one has to add to (4) the constraints (6):

$$\min_{\xi \in \Xi} \int \psi(x,\xi^*)\xi(dx) \geq 0, \quad (7)$$

$$\text{s.t.} \quad \int \phi(x)\xi(dx) \leq 0. \quad (8)$$

The fulfillment of (7) and (8) are necessary and sufficient condition for the optimality of ξ^*. But unlike the standard case there is generally no single point design (see comments to (4)) simultaneously satisfying (7) and (8).

The Lagrangian technique (see, for instance, Laurent (1972), Ch. 7) leads to the duality of optimization problem (7), (8) with the following maximin problem:

$$\max_{u\in U'} \min_{\xi} \int q(x,u,\xi^*)\xi(dx),$$

or equivalently

$$\max_{u\in U'} \min_{x\in X} q(x,u,\xi^*)$$

(see, for instance, Fedorov and Gaivoronski (1984)) confirming the assertion of the theorem.

The proof of two last parts of the theorem is identical to the standard case.

Note 1. The existence of a solution of (7), (8) with no more than $(l+1)$ supporting points follows from Caratheodory's theorem .

Example 3. Let us consider the design problem for one dimension polynomial response and D-criterion:

$f_\alpha(x) = x^{\alpha-1}$, $|x| \le 1$, $\Psi(\mathbf{M}) = -\ln|\mathbf{M}|$,
with linear constraints:

$$\int_{-1}^{1} \phi(x)\xi(dx) \le 0,$$

and let $\{f,\phi\}$ constitute a Chebyshev system on $|x|\le 1$.

From example 1 it follows that

$$q(x,u,\xi) = m - \sum \mathbf{M}^{-1}_{\alpha\beta} x^{\alpha-1} x^{\beta-1} + u^T\phi(x),$$

i. e. $q(x,u,\xi)$ is a linear combination of $2m+1$ Chebyshev's functions with some nonzero coefficients. Therefore (see, for instance, Karlin and Studden (1966)) this function has no more than $2m+1$ roots and subsequently has no more than $m+1/2$ (if l is even) or $m+(l+1)/2$ (if l is odd) minima on the interval $|x|\le 1$. But in accordance with Theorem 2 they have to coincide

with the support points. So for this case the number of support points is essentially less than n_0.

IV.Nonlinear Convex Constraints

The approach considered in the previous section can be usedfor the more general design problem:

$$\xi^* = \underset{\xi}{\text{Arg min}}\ \Psi[\mathbf{M}(\xi)], \quad (9)$$

$$\text{s. t.} \quad \Phi(\xi) \le 0, \quad \Phi \in R^l. \quad (10)$$

Assume additionally to (a)-(e),(b') that:

(c') $\Phi(\xi)$ are convex;

(e') $\Phi[(1-\alpha)\xi + \alpha\bar{\xi}] = \Phi(\xi) + \alpha\int\phi(x,\xi)\bar{\xi}(dx) + \tau(\alpha,\xi,\bar{\xi})$, where $\tau_k(\alpha,\xi,\bar{\xi}) = o(\alpha)$, $k = 1,\ldots,l$, ξ and $\bar{\xi}$ are defined in (e) with $\Xi(q)$ and Ξ satisfying (10).

The analysis of (9),(10) are mainly based on ideas of Theorem 2 and on the possibility of linearization of $\Phi(\xi)$ near an optimal design (compare with Gaivoronski (1984) and Lee (1988)).

All the final results can described by Theorem 2 with functions $\phi(x,\xi)$ defined in (e') $\Phi(\xi) = 0$. We shall refer to Theorem 2' in the case of nonlinear constraints, but one has to remember about assumptions (c'),(e').

Example 4. Let $\Psi = -\ln|\mathbf{M}|$ and $\Phi_k = -\ln|\mathbf{M}_k| - c_k$, where

$$\mathbf{M}_k(\xi) = \int f_k(x) f_k^T(x)\xi(dx).$$

Then the design problem corresponds to the case when one wishes to find a D-optimal design for the response $\theta^T f(x)$ and to be sure that this design is efficient for some competing responses $\theta_k^T f_k(x)$. Taking into account that:

$$\psi(x,\xi) = m - d(x,\xi),$$

$$\phi_k(x,\xi) = m_k - d_k(x,\xi),$$

$$d_k(x,\xi) = f_k^T(x)\mathbf{M}_k^{-1}(\xi)f_k(x),$$

and assuming that $f(x)$ and $f_k(x)$, $k=1,\ldots,l$ are continuous in X and c_k are not very small (to provide fulfillment of (d) together with (10)) it is not difficult to check the validity of Theorem 2'. From this theorem it follows that:

a necessary and sufficient condition for optimality of ξ^* is existence of $u^* \in U'$ such that

$$d(x,\xi^*) + \sum u_k^* d_k(x,\xi^*) \le m + \sum u_k^* m_k$$

while $\Phi(\xi) = 0$;

almost everywhere in $\operatorname{supp} \xi^*$

$$d(x,\xi^*) + \sum u_k^* d_k(x,\xi^*)] = m + \sum u_k^* m_k.$$

A number of similar examples for various optimality criteria can be found in Lee (1988).

Theorems 1 - 2' can be considered as specific cases of the Kuhn-Tucker Theorem, and, of course, its versions and generalizations of this theorem can help to extend the previous results.

For instance, theKuhn-Tucker Theorem for the case with a continuum of constraints (see Pshenichny (1969), Ch. 5.2) allows analysis of the following design problems:

$$\xi^* = \operatorname*{Arg\,min}_{\xi} \Psi[\mathbf{M}(\xi)], \quad (11)$$

$$\text{s. t.} \quad \Phi(\xi,\lambda) \le 0, \quad \Phi \in R^1, \quad \lambda \in \Lambda \subset R^l. \quad (12)$$

Let there be in addition to the previous assumptions:

(c'') $\Phi(\xi,\lambda)$ is convex for all $\lambda \in \Lambda$ and Λ is compact;

(e'') $\Phi[(1-\alpha)\xi + \alpha\bar{\xi}, \lambda] = \Phi(\xi,\lambda) + \alpha\int \phi(x,\xi,\lambda)\bar{\xi}(dx) + \tau(\alpha,\xi,\bar{\xi},\lambda)$,

where $\tau(\alpha,\xi,\bar{\xi},\lambda) = o(\alpha)$.

Then the above mentioned theorem leads to

Theorem 3. A necessary and sufficient condition for a design ξ^* to be optimal is the existence of such u^* and $\lambda_k^* \in \Lambda$ that :

$$\min_{x \in X} q(x,u^*,\xi^*) \geq 0, \quad (13)$$

where $q(x,u,\xi) = \psi(x,\xi) + u^T \phi(x,\xi)$, $\Phi(\xi^*,\lambda^*) = 0$, $\phi_k(x,\xi) = \phi(x,\xi,\lambda_k^*)$, $U' = \{u: u \in R^{l+1}, u_k \geq 0\}$, $k = 1,\ldots,l+1$.

Assume that all λ_k^* are known. Then Theorem 3 states that (11), (12) are equivalent to (9),(10) with $\Phi(\xi)=(\Phi(\xi,\lambda_1^*),\ldots,\Phi(\xi,\lambda_{l+1}^*))^T$. This makes it evident how to use the results ofthe previous theorems.

Example 5. As in example 4 suppose one wishes to find a D-optimal design for the response $\theta^T f(x)$ and to be sure that this design is efficient for some competing nonlinear response $\eta(x,\lambda)$, i. e.

$$-\ln|M(\xi,\lambda)| \leq G,$$

$$M(\xi,\lambda) = \int f(x,\lambda) f^T(x,\lambda) \xi(dx), \quad f(x,\lambda) = \partial\eta(x,\lambda)/\partial\lambda, \quad \lambda \in \Lambda \subset R^l.$$

The combination of the results of example 4 and Theorem 3 transforms (13) to:

$$d(x,\xi^*) + \sum u_k^* d_k(x,\xi^*) \leq m + l \sum u_k^* ,$$

$$d_k(x,\xi) = f(x,\lambda_k^*) M^{-1}(\xi,\lambda_k^*) f(x,\lambda_k^*), \quad k = 1,\ldots,l+1.$$

If $f(x)=f(x,\lambda')$, where λ' is a prior value of the parameters λ, this example can be considered as a particular case of the design problem for the nonlinear response.

V. Directly Constrained Design Measures

A number of experimental design problems can be formulated as optimization problems with explicitly bounded measures (see Fedorov (1986), (1989), Wynn (1982)):

$$\xi^* = \underset{\xi}{\text{Arg min}}\ \Psi[\mathbf{M}(\xi)], \quad (14)$$

$$\text{s. t.} \qquad \xi(dx) \le \Phi(dx), \ \int_X \Phi(dx) = C \ge 1. \quad (15)$$

As in to the moment space theory (see Fedorov (1989), Karlin and Studden (1966), Krein and Nudelman (1973)) ξ^* can be called a Ψ,Φ-optimal design.

Assume additionally to (a)-(e) that:

(f) $\Phi(dx)$ is atomless, i. e.

$$\lim_{\Delta X \to 0} \int_{\Delta X} \Phi(dx) = 0.$$

Sets Ξ and $\Xi(q)$ in (e) have to satisfy (15).

Let $\overline{\Xi}$ be a set of design measures such that $\xi(\Delta x) = \Phi(\Delta x)$ for any $\Delta X \subset X$. A function $\phi(x,\xi)$ is said to separate sets X_1 and X_2 with respect to the measure $\Phi(dx)$ if for two sets $\Delta X_1 \in X_1$ and $\Delta X_2 \in X_2$ with equal nonzero measures:

$$\int_{\Delta X_1} \phi(x,\xi)\Phi(dx) \le \int_{\Delta X_2} \phi(x,\xi)\Phi(dx). \quad (16)$$

Theorem 4. If assumptions (a)-(f) hold, then:

1. $\xi^* \in \overline{\Xi}$ exists.

2. A necessary and sufficient condition of Ψ,Φ-optimality of $\xi^* \in \overline{\Xi}$ is that $\phi(x,\xi^*)$ separates $X^* = \text{supp}\ \xi^*$ and $X \setminus X^*$.

Proof. The results of the theorem are strongly related to the moment spaces theory, and the proof is based on the corresponding ideas.

The existence of an optimal design follows from the compactness of the set of information matrices. The compactness of the latter is provided by (a), (b) and (f). The fact that at least one optimal design belong to $\overline{\Xi}$ is the corollary of Liapunov's Theorem on the range of a vector measure (see Karlin and Studden, 1966, Ch. VIII).

Necessity follows from the fact that if there exist $\Delta X_1 \subset \operatorname{supp} X^*$ and $\Delta X_2 \subset X \setminus X^*$ with equal nonzero measures such that:

$$\int_{\Delta X} \psi(x,\xi^*)\Phi(dx) > \int_{\Delta X_2} \psi(x,\xi^*)\Phi(dx),$$

then deletion of the first set from the supporting set with the subsequent inclusion of the second one causes the decrease of Ψ. This contradicts the optimality of ξ^*.

Now assume that $\xi^* \in \overline{\Xi}$ is nonoptimal and $\xi \in \overline{\Xi}$ is optimal, i.e.:

$$\Psi[M(\xi^*)] > \Psi[M(\xi)] + \delta, \qquad \delta > 0.$$

Let $\overline{\xi} = (1-\alpha)\xi^* + \alpha\xi$, then:

$$\Psi[M(\overline{\xi})] \le (1-\alpha)\Psi[M(\xi^*)] + \alpha\Psi[M(\xi)]$$

$$< (1-\alpha)\Psi[M(\xi^*)] + \alpha\{\Psi[M(\xi^*)] - \delta\} = \Psi[M(\xi)^*] - \alpha\delta. \quad (17)$$

Simultaneously:

$$\Psi[M(\overline{\xi})] = \Psi[M(\xi^*)] + \alpha \int_X \psi(x,\xi^*)\xi(dx) + o(\alpha)$$

$$= \Psi[M(\xi)] + \alpha\{\int_E \psi(x,\xi^*)\Phi(dx) - \int_D \psi(x,\xi^*)\Phi(dx)\} + o(\alpha)$$

$$\ge \Psi[M(\xi)] + o(\alpha), \quad (18)$$

where E and D describe the difference between the supporting sets for ξ^* and ξ.

The comparison of (17) and (18) gives a contradiction, and this completes the proof.

Note 2. The comparison of Theorems 1 and 4 gives a hint how the latter one can be generalized when to constraints (15) one adds (6), or (10), or (12). For this purpose thefunction $\psi(x,\xi)$ has to be replaced by a corresponding function $q(x,u,\xi) = \psi(x,\xi) + u^T\phi(x,\xi)$.

REFERENCES

Fedorov, V. V. (1972). Theory of Optimal Experiments. Academic Press, New York.

Fedorov, V. V. (1989). Optimal Design with Bounded Density: Optimization Algorithms of the Exchange Type. J.S.P.I., 22, 1-13.

Fedorov, V. V. and M. B. Malyutov (1972). Design of Experiments in Regression Problems. Math. Oper. Forschung und Stat. 2, 281 - 320.

Fedorov, V. V. and A. Gaivoronski (1984). Design of Experiments under Constraints. WP-84-8. International Institute for Applied System Analysis, Austria, Laxenburg.

Gaivoronski, A. (1986) Linearization Methods for Optimization of Functionals which Depend on Probability Measures. Mathematical Programming Study. 28, 157-181.

Karlin, S. and W. J. Studden (1966). Tchebycheff Systems: with Applications in Analysis and Statistics. Wiley and Sons, New York.

Kiefer, J. (1959). Optimal Experimental Design. J. R. Statist. Soc., B, 21, 272-319.

Krein, M. and A. Nudelman (1977). The Markov Moment Problem and Extremal Problems. Translation Mathem. Monographs 50 (American Mathematical Society, Providence, EI).

Laurent, P. J. (1972). Approximation et Optimization. Hermann, Paris.

Lee, C. M.-S., (1988). Constrained Optimal Designs. J.S.P.I., 18, 377-389.

Pshenichniy, B. N., (1969). Necessary Conditions of Extremum. Nauka, Moscow (in Russian).

Silvey, S. D., (1980). Optimal Design. Chapman and Hall, London.

Whittle, P., (1973). Some general Points in the Theory of Optimal Experimental Design. J. Roy. Statist. Soc. Ser. B..35, 123-130.

On randomized designs for regression

Rainer Schwabe

Freie Universität Berlin, 1. Mathematisches Institut, Arnimallee 2-6, D-W-1000 Berlin 33, Germany

Abstract: In situations where little is known about the underlying model fitting a response function results in uncertainty in prediction caused by the necessary approximation and by observational noise. For such a situation Ermakov (1975) has proposed a randomized design for selecting the sites at which observations are to be taken. We present that the expected values of the order statistics connected with Ermakov's randomization measure are close to both the optimum locations known from approximation theory resp. the statistical theory of optimal designs as desired.

AMS Subject Classification: Primary 62K05; Secondary 62J05; 41A10.

Key Words: experimental design; polynomial regression; interpolation; Vandermonde determinant; order statistics; Legendre polynomials.

1 Introduction and general considerations

We consider the problem of fitting a response surface in situations when very little is known about the underlying shape of this surface. Thus we are faced with the task to approximate the surface by a combination of some simple functions and we have to take into account that evaluations of the response surface may be corrupted by noise.

To be more specific let $\mu : T \to \mathbb{R}$ be a (unknown) response function over a region T of interest and let us assume that for any setting $t \in T$ it is possible to obtain an observation

$$X(t) = \mu(t) + Z(t) \tag{1.1}$$

where $Z(t)$ may be some random error with zero expectation: $E(Z(t)) = 0$. Our aim is

to find a linear combination $\sum_{j=1}^{n} \beta_j a_j$ of previously chosen regression funtions $a_j : T \to \mathbb{R}, j = 1, \ldots, n$, which is *close* to μ on the region T. Equivalently we are interested in the parameter vector $\beta = (\beta_1, \ldots, \beta_n)'$ if the set $\{a_1, \ldots, a_n\}$ of regression functions is linearly independent on T.

For this purpose we want to perform n experiments at n (different) sites $t_1, \ldots, t_n \in T$. According to (1.1) we are going to observe

$$X_i(t_i) = \mu(t_i) + Z_i(t_i), \tag{1.2}$$

$i = 1, \ldots, n$. Now in the absence of random noise i.e. $Z(t) \equiv 0$, the most reasonable fit is the interpolation of the observations $X_i(t_i) = \mu(t_i)$, because then μ is perfectly fitted in case $\mu = \sum_{j=1}^{n} \beta_j a_j$ is a linear combination itself. Thus β has to be chosen to solve the n linear equations

$$X_i(t_i) = \sum_{j=1}^{n} \beta_j a_j(t_i), \tag{1.3}$$

$j = 1, \ldots, n$, which have the unique solution

$$\beta = A^{-1} X \tag{1.4}$$

if the matrix $A := (a_j(t_i))_{i=1,\ldots,n}^{j=1,\ldots,n}$ is regular, $X := (X_1(t_1), \ldots, X_n(t_n))'$. The regularity of A means that the set of regression functions $\{a_1, \ldots, a_n\}$ restricted to the set $\{t_1, \ldots, t_n\}$ is still linearly independent.

On the other hand, if the random errors are uncorrelated and have equal variance $\mathrm{Var}(Z(t)) = \sigma^2$ (which will be assumed throughout the rest of the paper) and if the linear model $\mu = \sum_{j=1}^{n} \beta_j a_j$ holds true, β can be estimated by the least squares estimator $\widehat{\beta}$ in case A is regular. Then $\widehat{\beta} = \widehat{\beta}(X)$ can be a calculated by solving the normal equations

$$\sum_{i=1}^{n} a_k(t_i) X_i(t_i) = \sum_{j=1}^{n} \sum_{i=1}^{n} a_k(t_i) a_j(t_i) \widehat{\beta}_j, \tag{1.5}$$

$k = 1, \ldots, n$, which turn out to have the unique solution

$$\widehat{\beta} = A^{-1} X \tag{1.6}$$

for regular A. This, of course, means again that the fitted function $\widehat{\mu} = \sum_{j=1}^{n} \widehat{\beta}_j a_j$ meets the observations.

In the general setting of unknown structure of the response function μ and in the presence of random noise we deduce from (1.4) and (1.6) that for regular A

$$\widehat{\beta} = A^{-1} X \tag{1.7}$$

is the natural choice for the estimator of the parameter β in the approximating linear combination $\sum_{j=1}^{n} \beta_j a_j$ for μ. To cover more general situations where A is not regular

e. g. if there are more observations than approximating regression functions, we can see from (1.3) and (1.5) that $\widehat{\beta}$ should be chosen to solve the normal equations (cf. (1.5)).

The performance of the estimator $\widehat{\beta}$ which will be measured by the quality of the fit in the L_2-sense depends on the location of the sites $t_1, \ldots, t_n$ where the observations are taken. Thus a good choice of $t_1, \ldots, t_n$ should result in a small value for the mean squared L_2-distance between the estimated and the true response function

$$E\left(\int_T \left(\sum_{j=1}^n \widehat{\beta}_j a_j(t) - \mu(t)\right)^2 dt\right) = \int_T E\left(\left(\sum_{j=1}^n \widehat{\beta}_j a_j(t) - \mu(t)\right)^2\right) dt. \tag{1.8}$$

By (1.8) this criterion is equivalent to the minimization of the average mean squares error of the prediction $\widehat{\mu} = \sum_{j=1}^n \widehat{\beta}_j a_j$ at t where the average is taken over the region T.

The problem of a good choice of the sites $t_1, \ldots, t_n$ has been investigated in the field of approximation theory in the absence of random noise and in the theory of optimal experimental design if the approximating model is assumed to be true. In general the two designs, i. e. the choices of $t_1, \ldots, t_n$, motivated by considerations of approximation theory resp. of optimal design theory differ from each other. (For the approximation theory we refer e. g. to Cheney (1966) and for the theory of optimal experimental design to Fedorov (1972), Bandemer et al. (1977), and Bandemer and Näther (1980).) As a compromise Ermakov (1975) suggested to use a randomized design where the sites are chosen according to a common probability distribution the density of which is proportional to the squared determinant of the corresponding design matrix, i. e. for the density ρ of the randomized design holds

$$\begin{aligned} \rho(t_1, \ldots, t_n) &= c \cdot \left(\det\left((a_j(t_i))_{i=1,\ldots,n}^{j=1,\ldots,n}\right)\right)^2 \\ &= c \cdot \det\left(\left(\sum_{i=1}^n a_k(t_i) a_j(t_i)\right)_{k=1,\ldots,n}^{j=1,\ldots,n}\right) \end{aligned} \tag{1.9}$$

for some positive constant c (see also Ermakov et al. (1983), Ermakov and Zhigljavskij (1987), and Ermakov (1989)). It was also shown by him that the resulting estimator $\widehat{\beta}$ is unbiased for the parameter β of the best approximating linear combination $\sum_{j=1}^n \beta_j a_j$ to μ in L_2. In particular, if $\{a_1, \ldots, a_n\}$ is orthonormal on T with respect to the scalar product in L_2, i. e. $\int_T a_j(t) a_k(t) dt = 1$ or 0 according to $j = k$ or $j \neq k$, then $\widehat{\beta}_j$ is unbiased for the j-th Fourier coefficient associated with a_j:

$$E(\widehat{\beta}_j) = \int_T \mu(t) a_j(t) dt. \tag{1.10}$$

Here the expectation is taken over both random noise $Z_1, \ldots, Z_n$ and randomization measure according to ρ and, as before, μ and $a_1, \ldots, a_n$ are assumed to be in L_2. Note also that the density ρ is proportional to the determinant of Fisher's information matrix in case of Gaussian noise.

In what follows we deal with the special situation of polynomial approximation on a real interval. We mention some specific results from optimal design and approximation theory in section 2, present a simulation on the shape of the distribution of the randomization procedure in section 3, give some exact results concerning this distribution in section 4, and end up with some remarks on further investigations.

2 Fitting polynomials

As mentioned above we are going to consider the problem of fitting a polynomial $\sum_{j=1}^{n} \beta_j t^{j-1}$ on the real interval $T = [0,1]$. For more general intervals $[a,b] \subseteq \mathbb{R}$ results can immediately be obtained by means of linear transformations since the quality of the fit is not affected by them.

For convenience we have written down the polynomial as a linear combination of the monomials $1, t, t^2, \ldots, t^{n-1}$. Instead of using the monomials $a_j(t) = t^{j-1}$ for the regression function we can also employ the normalized Legendre polynomials $a_j = P_{j-1}$ on $[0,1]$ with $P_0(t) = 1, P_1(t) = \sqrt{12}(t - \frac{1}{2}), P_2(t) = \sqrt{180}(t^2 - t + \frac{1}{6})$ etc. which constitute an orthonormal set of regression functions $\{P_0, \ldots, P_{n-1}\}$ for any n on $[0,1]$. However, this change is again a linear transformation and yields the same fit.

In case of the absence of random noise a reasonable choice for the sites $t_1, \ldots, t_n$ are the n distinct roots of the Legendre polynomial P_n of degree n on $[0,1]$. For this choice the resulting interpolating polynomials converge in L_2 to the response function μ with increasing n according to a theorem of Erdös and Turán (1937) (cf. Szegö (1959), p.331, Cheney (1966), p.137). Moreover for fixed n with observations taken at these nodes we can determine the value of $\int_0^1 \mu(t)dt$ exactly by means of the Gauss-Jacobi mechanical quadratare if μ is a polynomial of degree less than $2n$ (see Szegö (1959), p. 47, Cheney (1966), p. 110). Additionally, as has been pointed out by Ermakov and Sedunov (1979), this choice of the sites results in an *optimal (in number of points) unbiased (in the L_2-metric) design of an experiment for polynomial regression* of degree n.

For a true polynomial model of degree $n-1$, i.e. $\mu(t) = \sum_{j=1}^{n} \beta_j t^{j-1}$, with random noise Smith (1918), Guest (1958), and Hoel (1958) have shown that the $n-2$ roots of the first derivative of the Legendre polynomial P_{n-1} of degree $n-1$ on $[0,1]$ plus the two end points 0 and 1 of this interval, i.e. the roots of $t(1-t)P'_{n-1}(t)$, are a good allocation for $t_1, \ldots, t_n$. This choice minimizes the maximal variance

$$\max_{0 \le t \le 1} E\left((\widehat{\mu}(t) - \mu(t))^2\right) = \max_{0 \le t \le 1} E\left(\left(\sum_{j=1}^{n} (\widehat{\beta}_j - \beta_j) t^{j-1}\right)^2\right) \qquad (2.1)$$

of the prediction for the response function on $T = [0,1]$ (G-optimality) and minimizes simultaneously the generalized variance $\det(\mathrm{cov}(\widehat{\beta})) = \det(E((\widehat{\beta} - \beta)(\widehat{\beta} - \beta)'))$ of the

estimator for the whole parameter vector (D-optimality). The criterion (1.8) under consideration reduces for a true model to the linear criterion

$$E\left(\int_T \left(\sum_{j=1}^n (\hat{\beta}_j - \beta_j)a_j(t)\right)^2 dt\right) = \text{Trace}(E((\hat{\beta} - \beta)(\hat{\beta} - \beta)') \cdot U) \qquad (2.2)$$

with $U = \left(\int_T a_j(t)a_k(t)dt\right)_{j=1,\ldots,n}^{k=1,\ldots,n}$. We mention that in the present case we obtain for the members u_{jk} of U :

$$u_{jk} = \int_0^1 t^{j+k-2}dt = \frac{1}{j+k-1} \qquad (2.3)$$

if the a_j are the monomials resp. U equal to the identity matrix in case of an orthonormal set $\{a_1, \ldots, a_n\}$. In the literature the linear criterion (2.2) has been coined Q-optimality (cf. Fedorov (1972), p. 142) resp. I-optimality (cf. Bandemer et al. (1977), p. 185). Studden (1977) has shown that for the problem of polynomial regression an approximate design with the same supporting points as the D-(G-)optimal one but with different weights is close to minimize (2.2). However, choosing $t_1, \ldots, t_n$ as roots of $t(1-t)P'_{n-1}(t)$ is a good approximation to this design.

For the present situation the density ρ of Ermakovs's randomized design (1.9) equals the squared Vandermonde determinant multiplied by some constant c independent of $t_1, \ldots, t_n$:

$$\rho(t_1, \ldots, t_n) = c \cdot \Pi_{i<j}(t_i - t_j)^2. \qquad (2.4)$$

Furthermore, since ρ is proportional to the inverse of the generalized variance the maximum value of $\rho(t_1, \ldots, t_n)$ is achieved for $t_1, \ldots, t_n$ being the n distinct roots of $t(1-t)P'_{n-1}(t)$, i.e. the support points of the D-optimal design. On the other hand side the randomized design should also be close to the roots of P_n, i.e. the nodes for polynomial interpolation. In a private communication Ermakov has conjectured that the expectation of the order statistics $(T_{(1)}, \ldots, T_{(n)})$ of a randomized design $(T_1, \ldots, T_n)$ generated according to the density ρ are *very close* to those roots of P_n.

3 Simulations

In order to get an impression of the shape of the randomization measure associated with ρ for fitting polynomials we have generated random numbers according to (2.4). We have used the von Neumann rejection method to generate 10 000 n-dimensional random numbers $(t_1, \ldots, t_n)$ for fitting polynomials of degree $n-1 = 1, 1\,000$ for $n-1 = 2, \ldots 8$, and 200 for $n-1 = 9, \ldots, 11$ respectively. Each sample $(t_1, \ldots, t_n)$ has been transformed to the ordered sample $(t_{(1)}, \ldots, t_{(n)})$, i.e. $\{t_1, \ldots, t_n\} = \{t_{(1)}, \ldots, t_{(n)}\}$ and $t_{(1)} < t_{(2)} < \ldots < t_{(n)}$. Then the means $\overline{t_{(1)}}, \ldots, \overline{t_{(n)}}$ have been calculated from the ordered samples to

obtain an estimate for the expectation terms $E(T_{(1)}), \ldots, E(T_{(n)})$ of the order statistics $(T_{(1)}, \ldots, T_{(n)})$ of a random allocation $(T_1, \ldots, T_n)$ according to the density ρ.

The results of this simulation study suggest that the means $\overline{t_{(1)}}, \ldots, \overline{t_{(n)}}$ and consequently $E(T_{(1)}), \ldots, E(T_{(n)})$ are close to the ordered roots of the Legendre polynomial P_n. Numerical values of the means and the roots are listed in TABLE I.

TABLE I: Simulated and exact values of $E(T_{(k)})$, roots of P_n and $t(1-t)P'_{n-1}(t)$

$n=2$				$n=3$				$n=4$			
P_n	$\overline{t_{(k)}}$	$ET_{(k)}$	P'_{n-1}	P_n	$\overline{t_{(k)}}$	$ET_{(k)}$	P'_{n-1}	P_n	$\overline{t_{(k)}}$	$ET_{(k)}$	P'_{n-1}
0.2113	0.2005	0.2000	0.0000	0.1127	0.0988	0.1000	0.0000	0.0694	0.0605	0.0588	0.0000
0.7887	0.7980	0.8000	1.0000	0.5000	0.4986	0.5000	0.5000	0.3300	0.3195	0.3200	0.2764
				0.8873	0.9008	0.9000	1.0000	0.6700	0.6852	0.6800	0.7236
								0.9306	0.9426	0.9412	1.0000

$n=5$				$n=6$			$n=7$			$n=8$		
P_n	$\overline{t_{(k)}}$	$ET_{(k)}$	P'_{n-1}	P_n	$\overline{t_{(k)}}$	P'_{n-1}	P_n	$\overline{t_{(k)}}$	P'_{n-1}	P_n	$\overline{t_{(k)}}$	P'_{n-1}
0.0469	0.0376	0.0385	0.0000	0.0338	0.0275	0.0000	0.0254	0.0193	0.0000	0.0199	0.0154	0.0000
0.2308	0.2116	0.2178	0.1727	0.1694	0.1572	0.1175	0.1292	0.1165	0.0849	0.1017	0.0903	0.0641
0.5000	0.4965	0.5000	0.5000	0.3807	0.3728	0.3574	0.2971	0.2865	0.2656	0.2372	0.2256	0.2041
0.7692	0.7816	0.7822	0.8273	0.6193	0.6234	0.6426	0.5000	0.4975	0.5000	0.4083	0.4027	0.3954
0.9531	0.9615	0.9615	1.0000	0.8306	0.8472	0.8825	0.7029	0.7130	0.7344	0.5917	0.5923	0.6046
				0.9662	0.9736	1.0000	0.8708	0.8793	0.9151	0.7628	0.7745	0.7959
							0.9746	0.9792	1.0000	0.8983	0.9101	0.9359
										0.9801	0.9840	1.0000

$n=9$			$n=10$			$n=11$			$n=12$		
P_n	$\overline{t_{(k)}}$	P'_{n-1}	P_n	$\overline{t_{(k)}}$	P'_{n-1}	P_n	$\overline{t_{(k)}}$	P'_{n-1}	P_n	$\overline{t_{(k)}}$	P'_{n-1}
0.0159	0.0122	0.0000	0.0130	0.0107	0.0000	0.0109	0.0074	0.0000	0.0092	0.0071	0.0000
0.0820	0.0726	0.0501	0.0675	0.0621	0.0402	0.0565	0.0478	0.0330	0.0479	0.0431	0.0276
0.1933	0.1825	0.1614	0.1603	0.1536	0.1306	0.1349	0.1259	0.1078	0.1150	0.1072	0.0904
0.3379	0.3306	0.3184	0.2833	0.2828	0.2610	0.2405	0.2357	0.2174	0.2063	0.2017	0.1836
0.5000	0.4966	0.5000	0.4256	0.4231	0.4174	0.3652	0.3631	0.3521	0.3161	0.3134	0.3002
0.6621	0.6656	0.6816	0.5744	0.5838	0.5826	0.5000	0.5004	0.5000	0.4374	0.4354	0.4317
0.8067	0.8171	0.8386	0.7167	0.7274	0.7390	0.6348	0.6356	0.6479	0.5626	0.5623	0.5683
0.9180	0.9267	0.9499	0.8397	0.8512	0.8694	0.7595	0.7611	0.7826	0.6839	0.6876	0.6998
0.9841	0.9873	1.0000	0.9325	0.9431	0.9598	0.8651	0.8736	0.8922	0.7937	0.8057	0.8164
			0.9870	0.9896	1.0000	0.9435	0.9481	0.9670	0.8850	0.8957	0.9096
						0.9891	0.9916	1.0000	0.9521	0.9600	0.9724
									0.9908	0.9919	1.0000

For illustrative purposes we present the histograms for the lower half sample of the

ordered random numbers $t_{(1)}, \ldots, t_{(n/2)}$ in case $n = 8$ in FIG. 1. The sequence of pictures in this figure is supplemented by the histogram of the collected random numbers $t_1, \ldots, t_n$

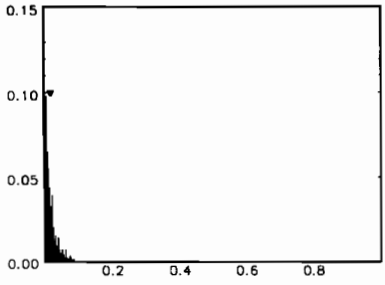


FIG. 1.a: $n = 8$, Frequencies of $t_{(1)}$

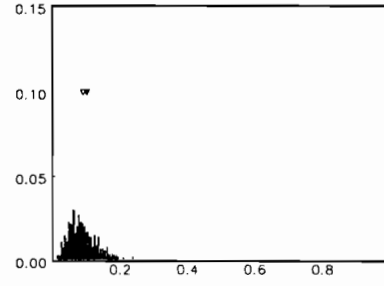


FIG. 1.b: $n = 8$, Frequencies of $t_{(2)}$

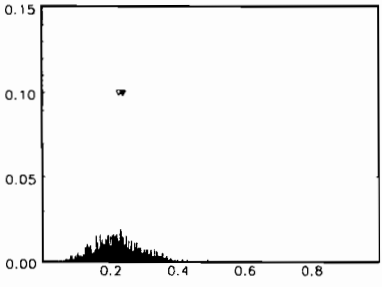


FIG. 1.c: $n = 8$, Frequencies of $t_{(3)}$

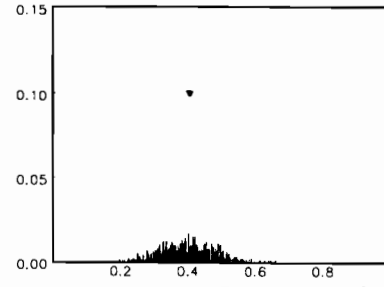


FIG. 1.d: $n = 8$, Frequencies of $t_{(4)}$

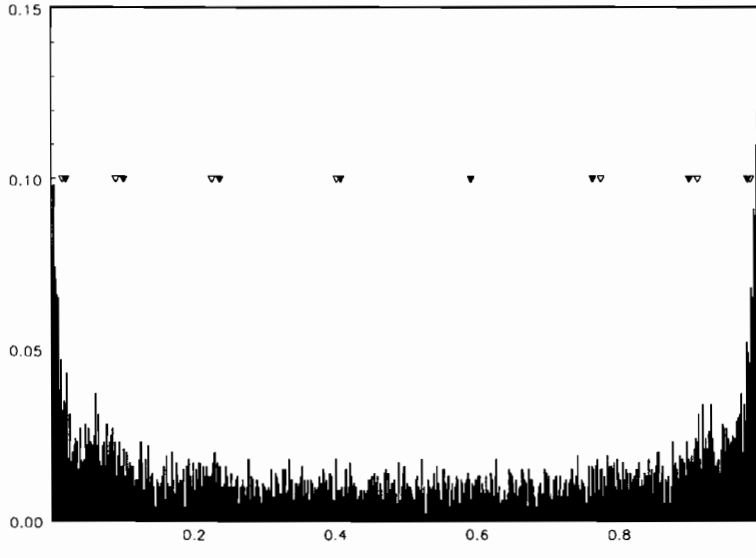


FIG. 1.e: $n = 8$, Frequencies of $t_1, \ldots, t_8$

showing an approximation to the one-dimensional marginal density of $T = (T_1, \ldots, T_n)$. (We recall that for the present density ρ the components $T_1, \ldots, T_n$ of T are identically distributed). The location of the means $\overline{t_{(1)}}, \ldots, \overline{t_{(n)}}$ and the corresponding roots of the Legendre polynomial P_n are indicated by simple and solid triangles respectively.

4 Some exact results

Despite the apparent closeness in the simulation we can notice that the means are a little bit more scattered than the roots of P_n. This suggests that the means are shifted towards the corresponding roots of $t(1-t)P'_{n-1}(t)$ which are also listed in TABLE I. This observation led us to compute the expectation $E(T_{(k)}), 1 \leq k \leq n$, exactly in some situations where it is possible.

Lemma 1.

Let T be distributed according to the density ρ defined in (2.4). Then for the distribution function $F_{T_{(n)}}$ of the largest member $T_{(n)}$ of the order statistics it holds

$$F_{T_{(n)}}(s) = s^{n^2} \tag{4.1}$$

for $0 \leq s \leq 1$.

Proof.

Let α denote a multi-index, i.e. $\alpha = (\alpha_1, \ldots \alpha_n)$ and $\alpha_i \in \{0, 1, 2, \ldots\}$, $i = 1, \ldots, n$, and let the magnitude of α be defined by the L_1-norm: $|\alpha| = \sum_{i=1}^n \alpha_i$.

Since $\rho(t_1, \ldots, t_n)$ is essentially a product of $\frac{1}{2}n(n-1)$ factors of the type $(t_i - t_j)^2$ we can conclude that ρ is a polynomial of degree $n(n-1)$. Moreover all components of the polynomial are exactly of degree $n(n-1)$:

$$\begin{aligned} \rho(t_1, \ldots, t_n) &= c \cdot \textstyle\prod_{i<j}(t_i - t_j)^2 \\ &= c \cdot \textstyle\sum_{|\alpha|=n(n-1)} (w_\alpha \prod_{i=1}^n t_i^{\alpha_i}) \end{aligned} \tag{4.2}$$

where w_α are some (integer valued) weights. Thus we obtain

$$\begin{aligned} F_{T_{(n)}}(s) &= P(T_1 \leq s, T_2 \leq s, \ldots, T_n \leq s) \\ &= \int_0^s \cdots \int_0^s \rho(t_1, \ldots, t_n) dt_n \ldots dt_1 \\ &= c \cdot \textstyle\sum_{|\alpha|=n(n-1)} w_\alpha \prod_{i=1}^n \int_0^s t_i^{\alpha_i} dt_i \\ &= c \cdot \textstyle\sum_{|\alpha|=n(n-1)} w_\alpha \prod_{i=1}^n \frac{1}{\alpha_i+1} s^{\alpha_i+1} \\ &= c \cdot \textstyle\sum_{|\alpha|=n(n-1)} w_\alpha \left(\prod_{i=1}^n \frac{1}{\alpha_i+1}\right) s^{\sum_{i=1}^n (\alpha_i+1)} \\ &= \tilde{c} \cdot s^{n^2}. \end{aligned}$$

Since $F_{T_{(n)}}(1) = 1$ we get $\check{c} = 1$ which completes the proof. □

From the distribution function we can compute the expected value of the largest member $T_{(n)}$ of the order statistics:

$$\begin{aligned} E(T_{(n)}) &= \int_0^1 (1 - F_{T_{(n)}}(s))ds \\ &= 1 - \int_0^1 s^{n^2} ds \\ &= 1 - \frac{1}{n^2+1}. \end{aligned} \tag{4.3}$$

This result also could have been obtained using the density $f_{T_{(n)}}(s) = n^2 s^{n^2-1}$ of $T_{(n)}$. By considerations of symmetry we get $E(T_{(1)}) = \frac{1}{n^2+1}$ for the smallest member $T_{(1)}$ of the order statistics $(T_{(1)}, \ldots, T_{(n)})$. The quantities $E(T_{(1)})$ listed in TABLE II are smaller than the corresponding smallest roots $z_1^{(n)}$ of the Legendre polynomials P_n.

TABLE II: Expectation of the smallest order statistics vs. smallest root of P_n

n	2	3	4	5	6	7	8	9	10	11	12
$z_1^{(n)}$	0.2113	0.1127	0.0694	0.0469	0.0338	0.0254	0.0199	0.0159	0.0130	0.0109	0.0092
$E(T_{(1)})$	0.2000	0.1000	0.0588	0.0385	0.0270	0.0200	0.0154	0.0122	0.0099	0.0082	0.0069

In particular this result holds true for large n since $z_1^{(n)} \sim \frac{1}{4} j_1^2 n^{-2} \approx 1.4458 n^{-2}$ where j_1 is the first positive zero of the Bessel function of the first kind of order zero (see Szegö (1959),p. 190f and p. 119) and $E(T_{(1)}) \sim n^{-2}$. Hence $E(T_{(1)}) \sim 0.69 z_1^{(n)}$ and $E(T_{(1)})$ is close to $z_1^{(n)}$ but not substantially closer than to zero, which is the corresponding smallest root of $t(1-t)P'_{n-1}(t)$.

Additionally we have computed the one- and two-dimensional marginal distributions of the order statistics $(T_{(1)}, \ldots, T_{(n)})$ for n up to 5. For this purpose we have used the representation (4.2) for the density ρ. The sum occuring in (4.2) already consists of 201 different terms for $n = 4$ and 3081 for $n = 5$ respectively. As in the proof of Lemma 1 we get

$$\begin{aligned} P(T_1 \le s, \ldots, T_k \le s) &= \int_0^s \cdots \int_0^s \int_0^1 \cdots \int_0^1 \rho(t_1, \ldots, t_n) dt_n \ldots dt_{k+1} dt_k \ldots dt_1 \\ &= c \cdot \sum_{|\alpha|=n(n-1)} w_\alpha \left(\prod_{i=1}^n \frac{1}{\alpha_i + 1} \right) s^{k + \sum_{i=1}^k \alpha_i} \\ &= \sum_{\ell=0}^{n^2} \tilde{w}_{k,\ell} s^\ell \end{aligned} \tag{4.4}$$

where $\tilde{w}_{k,\ell} = c \cdot \sum_{\alpha : |\alpha| = n(n-1), \alpha_1 + \ldots + \alpha_k = \ell - k} w_\alpha \prod_{i=1}^n \frac{1}{\alpha_i + 1}$ if $\ell \ge k$ and $\tilde{w}_{k,\ell} = 0$ if $\ell < k$.

Since the components of $(T_1, \ldots, T_n)$ are exchangeable we obtain for the distribution function of the k-th order statistics, $k = 1, \ldots, n$:

$$\begin{aligned} F_{T_{(k)}}(s) &= \sum_{m=k}^{n} (-1)^{m-k} \binom{m-1}{k-1} \binom{n}{m} P(T_1 \le s, \ldots, T_m \le s) \\ &= \sum_{\ell=k}^{n^2} \left(\sum_{m=k}^{n} (-1)^{m-k} \binom{m-1}{k-1} \binom{n}{m} \tilde{w}_{m,\ell} \right) s^{\ell} \end{aligned} \tag{4.5}$$

(see David (1981), p. 105). The coefficients of these polynomials have been determined by means of formal computation for $k = 1, \ldots, n$ and $n \le 5$ (see TABLE III for $k > n/2$; we recall that $F_{T_{(k)}}(s) = 1 - F_{T_{(n-k+1)}}(1-s)$ by the properties of symmetry of ρ).

TABLE III: Distribution functions of $\max_{i=1,\ldots,k} T_i$ and the order statistics

n	k	$P(T_1 \le s, \ldots, T_k \le s)$	$F_{T_{(k)}}(s)$
2	2	s^4	s^4
3	2	$3s^8 - 12s^7 + 28s^6 - 30s^5 + 12s^4$	$-2s^9 + 9s^8 - 36s^7 + 84s^6 - 90s^5 + 36s^4$
	3	s^9	s^9
4	3	$4s^{15} - 30s^{14} + 140s^{13} - 355s^{12} + 492s^{11} - 350s^{10} + 100s^9$	$-3s^{16} + 16s^{15} - 120s^{14} + 560s^{13} - 1420s^{12} + 1968s^{11} - 1400s^{10} + 400s^9$
	4	s^{16}	s^{16}
5	3	$250s^{21} - 2625s^{20} + 13370s^{19} - 43890s^{18} + 105952\frac{1}{2}s^{17} - 200745s^{16} + 302376s^{15} - 355320s^{14} + 315840s^{13} - 204190s^{12} + 90420s^{11} - 24500s^{10} + 3062\frac{1}{2}s^9$	$6s^{25} - 75s^{24} + 900s^{23} - 6900s^{22} + 32950s^{21} - 106890s^{20} + 263900s^{19} - 564300s^{18} + 1125675s^{17} - 2022150s^{16} + 3023760s^{15} - 3553200s^{14} + 3158400s^{13} - 2041900s^{12} + 904200s^{11} - 245000s^{10} + 30625s^9$
	4	$5s^{24} - 60s^{23} + 460s^{22} - 2030s^{21} + 5376s^{20} - 8680s^{19} + 8360s^{18} - 4410s^{17} + 980s^{16}$	$-4s^{25} + 25s^{24} - 300s^{23} + 2300s^{22} - 10150s^{21} + 26880s^{20} - 43400s^{19} + 41800s^{18} - 22050s^{17} + 4900s^{16}$
	5	s^{25}	s^{25}

The expected values of the order statistics can again be calculated via $E(T_{(k)}) = \int_0^1 (1 - F_{T_{(k)}}(s))ds$. These values are given in TABLE I together with the simulation results and the corresponding roots of P_n and $t(1-t)P'_{n-1}(t)$ respectively. It can be seen

that the expected values are located between the corresponding roots. The associated densities $f_{T_{(k)}}$ of the order statistics are plotted in FIG. 2.

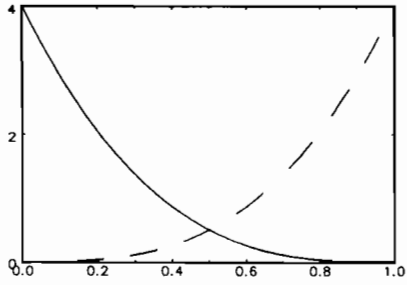


FIG. 2.a: $f_{T_{(k)}}$, $n = 2$

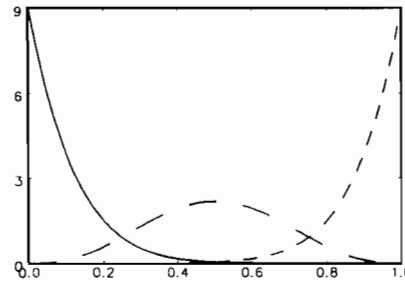


FIG. 2.b: $f_{T_{(k)}}$, $n = 3$

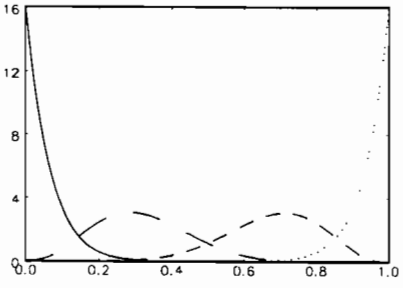


FIG. 2.c: $f_{T_{(k)}}$, $n = 4$

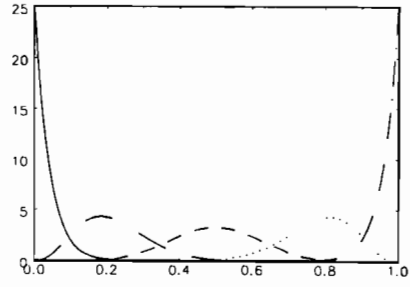


FIG. 2.d: $f_{T_{(k)}}$, $n = 5$

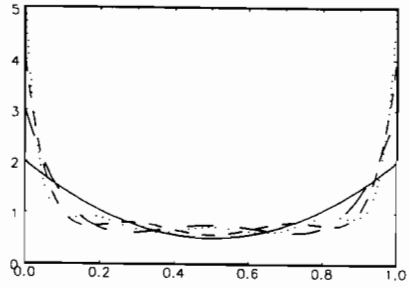


FIG. 3: f_{T_i}, $n = 2, \ldots, 5$

Letting $k = 1$ in (4.4) we get the one-dimensional marginal distributions F_{T_i} and hence the marginal densities

$$f_{T_i}(s) = \sum_{\ell=0}^{n^2-1} (\ell+1)\tilde{w}_{1,\ell+1} s^\ell \qquad (4.6)$$

which are given in FIG. 3. Obviously $f_{T_i} = \frac{1}{n}\sum_{k=1}^{n} f_{T_{(k)}}$ and f_{T_i} is symmetric, i.e. $f_{T_i}(s) = f_{T_i}(1-s)$.

As in (4.4) we can calculate the two-dimensional marginal distributions

$$\begin{aligned} F_{T_i,T_j}(s,t) &= P(T_1 \le s, T_2 \le t) \\ &= \sum_{\ell=1}^{2n-1} \sum_{m=1}^{2n-1} \tilde{\tilde{w}}_{\ell,m}\, s^\ell t^m \end{aligned} \qquad (4.7)$$

where $\tilde{\tilde{w}}_{\ell,m} = c \cdot \sum_{\alpha:|\alpha|=n(n-1),\alpha_1=\ell-1,\alpha_2=m-1} w_\alpha \prod_{i=1}^{n} \frac{1}{\alpha_i+1}$ and hence the densities $f_{T_i,T_j}(s,t) = \sum_{\ell=0}^{2n-2}\sum_{m=0}^{2n-2}\left((\ell+1)(m+1)\,\tilde{\tilde{w}}_{\ell+1,m+1}\right) s^\ell t^m$ which are displayed in FIG. 4.

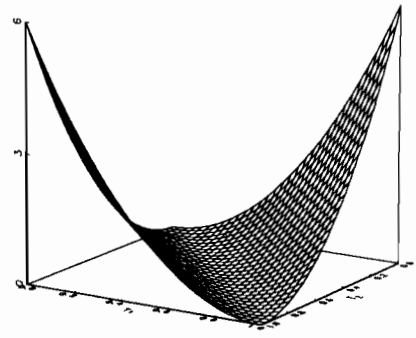


FIG. 4.a: f_{T_i,T_j}, $n = 2$

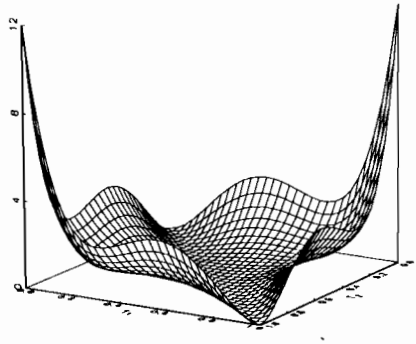


FIG. 4.b: f_{T_i,T_j}, $n = 3$

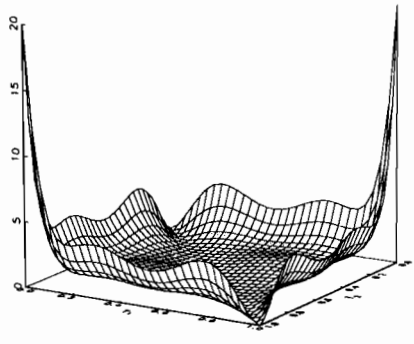


FIG. 4.c: f_{T_i,T_j}, $n = 4$

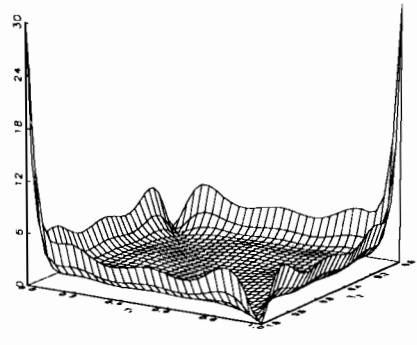


FIG. 4.d: f_{T_i,T_j}, $n = 5$

5 Concluding remarks

The results obtained in the previous sections give rise to the impression that the shape of the randomized design associated with the density ρ proposed by Ermakov (1975) is close to both the allocations known to be of great use in experimental design and approximation theory respectively. Further investigations are to be made in higher dimensions.

For the present situation of fitting polynomials on a real interval we suppose that the one-dimensional marginal of the randomization measures is converging to the arc sine law or some appropriate modification of it with increasing degree n (cf. Kiefer and Studden (1976)). In particular, we expect a local limit theorem to hold, that means that the marginal density f_{T_1} tends to the density of the limiting distribution which in case of the arc sine law equals to $f(t) = \left(\pi\sqrt{t(1-t)}\right)^{-1}$, the density of a beta distribution with parameters $\frac{1}{2}$ and $\frac{1}{2}$ .This behaviour seems to be due to the fact that the distributions of

the roots of P_n resp. $t(1-t)P_n'(t)$ converge to the arc sine law (see Szegö (1959), p. 121). This assumption is also indicated by FIG. 3.

All formal computations, simulations, and graphics were done on a 386 personal computer (33MHz) by means of the GAUSS386 programming language. The bounds on the degree of the polynomials under consideration and on the number of generated random number for the various degrees are due to the limitations of runtime, workspace, and accuracy of the calculations.

Acknowledgement

The author wishes to express his thanks to Professor S. M. Ermakov for his encouraging interest in the problem and to Professor V. V. Fedorov for his helpful comments. A substantial part of this work has been done during a visit at Leningrad State University.

References

Bandemer, H. (Ed.) (1977): *Theorie and Anwendung der optimalen Versuchsplanung I. Handbuch zur Theorie.* Akademie-Verlag, Berlin.

Bandemer, H. and W. Näther (1980): *Theorie und Anwendung der optimalen Versuchsplanung II. Handbuch zur Anwendung.* Akademie-Verlag, Berlin.

Cheney, E.W. (1966). *Introduction to Approximation Theory.* McGraw-Hill, New York.

David, H.A. (1981). *Order Statistics. 2nd ed.* Wiley, New York.

Erdös, P. and P. Turán (1937). On interpolation I. Quadrature- and mean-convergence in the Lagrange-interpolation. *Ann. Math.* **38**, 142-155.

Ermakov, S.M. (1975). *Die Monte-Carlo Methode und verwandte Fragen.* Deutscher Verlag der Wissenschaften, Berlin and Oldenbourg, München.

Ermakov, S.M. (1989). Random interpolation in the theory of experimental design. *Comput. Statist. Data Anal.* **8**, 75-80.

Ermakov, S.M. et al. (1983). *Mathematical Theory of Experimental Design.* Nauka, Moscow (in Russian).

Ermakov, S.M. and E.V. Sedunov (1979). On unbiased designs for regression experiments in a finite-dimensional function space. *Vestnik Leningrad Univ. Math.* **7**, 11-21.

Ermakov, S.M. and A.A. Zhigljavskij (1987). *Mathematical Theory of Optimal Experiments.* Nauka, Moscow (in Russian).

Fedorov, V.V. (1972). *Theory of Optimal Experiments.* Academic Press, New York.

Guest, P.G. (1958). The spacing of observations in polynomial regression. *Ann. Math. Statist.* **29**, 294-299.

Hoel, P.G. (1958). Efficiency problems in polynomial estimation. *Ann. Math. Statist.* **29**, 1134-1145.

Kiefer, J. and W.J. Studden (1976). Optimal designs for large degree polynomial regression. *Ann. Statist.* **4**, 1113-1123.

Smith, K. (1918). On the standard deviation of adjusted and interpolated values of an observed *polynomial function* and its constants and the guidance towards a proper choice of the distribution of observations. *Biometrika* **12**, 1-85.

Studden, W.J. (1977). Optimal designs for integrated variance in polynomial regression. In: S.S. Gupta, D.S. Moore, Eds., *Statistical Decision Theory and Related Topics II,* Academic Press, New York, 411-420.

Szegö, G. (1959). *Orthogonal Polynomials, revised ed.* Am. Math. Soc. Coll. Pub. **23**.

NONLINEAR EXPERIMENTAL DESIGN FOR CONSTRAINED LS ESTIMATION*

Andrej PÁZMAN[1] and Luc PRONZATO[2]

[1]Mathematical Institute of the Slovak Academy of Sciences, Štefánikova 49, CS-81473 Bratislava, Czechoslovakia
[2]Laboratoire des Signaux et Systèmes, CNRS/ESE, Plateau de Moulon, 91192 Gif-sur-Yvette cedex, France

1. INTRODUCTION

This paper is devoted to the problem of optimal experimental design for nonlinear regression models defined by

$$y(x) = \eta(\underline{\theta}, x) + \varepsilon(x), \ (x \in \mathcal{X}, \underline{\theta} \in \Theta), \tag{1}$$

with normal errors

$$\varepsilon(x) \sim \mathcal{N}(0, \sigma^2).$$

The function $\eta(\underline{\theta}, x)$ is the response (or model) function, $\underline{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)^T$ denotes the vector of parameters to be estimated, with $\underline{\theta} \in \Theta$, $\mathcal{R}^p \supset \Theta$. The design variable x (which can be vector valued) belongs to some design space $\mathcal{X}$. In what follows, $\eta(\underline{\theta}, x)$ will be assumed to admit continuous second order derivatives $\dfrac{\partial^2 \eta(\underline{\theta}, x)}{\partial\theta_i \partial\theta_j}$ in every interior point $\underline{\theta}$ of Θ ($\underline{\theta} \in \text{int}\,\Theta$) for any x in $\mathcal{X}$. The boundary $\partial\Theta$ of Θ will be further assumed to be attainable as a limit of points from int Θ. A classical situation corresponds to a parameter space defined by

$$\Theta = [\theta_{m_1}, \theta_{M_1}] \times [\theta_{m_2}, \theta_{M_2}] \times \ldots \times [\theta_{m_p}, \theta_{M_p}], \tag{2}$$

but such an assumption is not required by the presented method. Fixed-size designs (with size N) will be considered,

$$X := \{x_1, x_2, \ldots, x_N\},$$

with possible replications ($x_i = x_j$ for some $i \neq j$). The observations $y(x_i)$ will be assumed to be independent. The experimental design problem consists in choosing the design variables X in an optimal way according to some optimality criterion.

This is a classical set-up in experimental design, as described for instance in the recent surveys by Ford *et al.* (1989) and Walter and Pronzato (1990). We are interested in parameter estimation, so that the design criterion must be related to some measure of uncertainty on the

* This paper was initiated while the first author was visiting the Laboratoire des Signaux et Systèmes

parameter estimates. A standard approach is then based on the asymptotic normality of the least-squares (LS) estimator $\hat{\underline{\theta}}$ (which here coincides with the maximum likelihood estimator),

$$\hat{\underline{\theta}} := \arg \min_{\underline{\theta} \in \Theta} \sum_{i=1}^{N} (y(x_i) - \eta(\underline{\theta}, x_i))^2. \tag{3}$$

One has asymptotically,

$$\hat{\underline{\theta}} \sim \mathcal{N}(\overline{\underline{\theta}}, M_X^{-1}(\overline{\underline{\theta}})), \tag{4}$$

where $\overline{\underline{\theta}}$ is the true value of $\underline{\theta}$ and where

$$\{M_X(\underline{\theta})\}_{ij} := \frac{1}{\sigma^2} \sum_{k=1}^{N} \frac{\partial \eta(\underline{\theta}, x_k)}{\partial \theta_i} \frac{\partial \eta(\underline{\theta}, x_k)}{\partial \theta_j}$$

is the (Fisher) information matrix for the parameter vector $\underline{\theta}$ and the design X. Equation (4) is then the rationale for the use of design criteria given by $\Phi(M_X(\overline{\underline{\theta}}))$, where Φ is any criterion function (to be minimized) used in experimental design for linear models. Since the true parameter value $\overline{\underline{\theta}}$ in (4) is unknown, modified criteria such as

$$\Phi(M_X(\underline{\theta}^\circ)), \text{ where } \underline{\theta}^\circ \text{ is some prior nominal value for } \underline{\theta}, \tag{5a}$$

$$\int_{\Theta} \Phi(M_X(\underline{\theta}))\, \pi(\underline{\theta})\, d\underline{\theta}, \text{ where } \pi(\underline{\theta}) \text{ is some prior distribution for } \underline{\theta}, \tag{5b}$$

$$\max_{\underline{\theta} \in \Theta} \Phi(M_X(\underline{\theta})), \tag{5c}$$

have been considered in literature (see e.g. the survey (Walter and Pronzato, 1990)).

If σ is "very small" compared to the nonlinearity of the model (1), or if a sequential design can be used, the asymptotic approximation (4) for the distribution of $\hat{\underline{\theta}}$ is reasonable, and the previous approaches are justified. However, in other situations, the true density of $\hat{\underline{\theta}}$ can be quite different from the normal distribution (4), so that a "classical" optimal design obtained from (5a, b, c) can reveal to be far from optimal in practice. For instance, Pázman (1989) shows that two designs giving the same information matrix (not depending on $\underline{\theta}$)) can contain a different information about $\underline{\theta}$. An approximation $q_X(\hat{\underline{\theta}} \,|\, \overline{\underline{\theta}})$ of the true density of $\hat{\underline{\theta}}$, more precise than (4) and almost exact in some nonlinear models (see Section 2), has been derived by Pázman (1984).

The new approach to be presented considers the distribution of $\hat{\underline{\theta}}$ on int Θ and on $\partial\Theta$ in a unified way (which is important from a computational point of view). While the distribution $q_X(\hat{\underline{\theta}} \,|\, \overline{\underline{\theta}})$ was obtained for the ordinary LS estimator, we slightly modify this estimator near $\partial\Theta$ by adding a penalty function to the LS criterion (3),

$$\tilde{\underline{\theta}} := \arg \min_{\underline{\theta} \in \Theta} \{\frac{1}{\sigma^2} \sum_{i=1}^{N} (y(x_i) - \eta(\underline{\theta}, x_i))^2 + 2\, w(\underline{\theta})\}. \tag{6}$$

The new expression $\tilde{q}_X(\tilde{\underline{\theta}} \,|\, \overline{\underline{\theta}})$ for the density of the constrained LS estimates $\tilde{\underline{\theta}}$, derived in (Pázman and Pronzato, 1990), is presented in Section 3. The penalty function $w(\underline{\theta})$ is chosen such that $w(\underline{\theta}) \geq 0$ ($\underline{\theta} \in \Theta$), and $w(\underline{\theta})$ is non-constant just near the boundary of Θ, so that $\tilde{\underline{\theta}} \neq$

$\hat{\underline{\theta}}$ only near $\partial\Theta$ (Section 4). The design optimality criterion to be considered corresponds to the mean-square error for $\underline{\theta}$, and is a generalization of the A-optimality criterion used in linear models,

$$\Psi_{\overline{\underline{\theta}}}(X) = \int_{\Theta} \| \tilde{\underline{\theta}} - \overline{\underline{\theta}} \|^2 \, \tilde{q}_X(\tilde{\underline{\theta}} \mid \overline{\underline{\theta}}) \, d\tilde{\underline{\theta}}. \tag{7}$$

Other criteria could be considered in a similar way. Note, however, that a criterion based on the entropy of the density $\tilde{q}_X(\tilde{\underline{\theta}} \mid \overline{\underline{\theta}})$ would not take the bias of the estimate $\tilde{\underline{\theta}}$ into account, and could therefore lead to a density concentrated on $\partial\Theta$ whatever the location of $\overline{\underline{\theta}}$ in Θ. The criterion (7) depends on the unknown value $\overline{\underline{\theta}}$, so that a modification similar to (5b) could also be considered,

$$\Psi(X) = \int_{\Theta} \left(\int_{\Theta} \| \tilde{\underline{\theta}} - \underline{\theta} \|^2 \, \tilde{q}_X(\tilde{\underline{\theta}} \mid \underline{\theta}) \, d\tilde{\underline{\theta}} \right) \pi(\underline{\theta}) \, d\underline{\theta}, \tag{8}$$

where $\pi(\underline{\theta})$ is some prior distribution for $\underline{\theta}$. A stochastic approximation algorithm which permits to minimize criteria such as (7-8) without any evaluation of mathematical expectation is described in Section 5. Various examples are treated in Section 6.

2. THE PROBABILITY DENSITY OF THE (UNCONSTRAINED) LS ESTIMATES $\hat{\underline{\theta}}$

The expression of $q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$ and its main properties presented in earlier papers are recapitulated. Let $\underline{\eta}_X(\underline{\theta})$ denote the vector of response functions

$$\underline{\eta}_X(\underline{\theta}) := (\eta(\underline{\theta}, x_1), \eta(\underline{\theta}, x_2), \ldots, \eta(\underline{\theta}, x_N))^T.$$

We consider designs X such that

(i) $\underline{\theta} \in \Theta \rightarrow \underline{\eta}_X(\underline{\theta}) \in \mathcal{R}^N$ is one-to-one,

(ii) the matrix $\dfrac{\partial \underline{\eta}_X(\underline{\theta})}{\partial \underline{\theta}^T}$ has full rank (equal to p), i.e. $M_X(\underline{\theta})$ is non singular for any $\underline{\theta} \in \Theta$.

Let us introduce the following matrices

$$P_X^{\underline{\theta}} := \frac{1}{\sigma^2} \frac{\partial \underline{\eta}_X(\underline{\theta})}{\partial \underline{\theta}^T} M_X^{-1}(\underline{\theta}) \frac{\partial \underline{\eta}_X^T(\underline{\theta})}{\partial \underline{\theta}}, \tag{9}$$

$$\{Q_X(\hat{\underline{\theta}}, \underline{\theta})\}_{ij} := \{M_X(\hat{\underline{\theta}})\}_{ij} + \frac{1}{\sigma^2} \left(\underline{\eta}_X(\hat{\underline{\theta}}) - \underline{\eta}_X(\underline{\theta}) \right)^T (I - P_X^{\hat{\underline{\theta}}}) \frac{\partial^2 \underline{\eta}_X(\underline{\theta})}{\partial \theta_i \partial \theta_j}, \tag{10}$$

a good approximation of the probability density of $\hat{\underline{\theta}}$ is then given by

$$q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}}) := \frac{\det Q_X(\hat{\underline{\theta}}, \overline{\underline{\theta}})}{(2\pi)^{p/2} \det^{1/2} M_X(\hat{\underline{\theta}})} \exp\left(- \frac{1}{2\sigma^2} \| P_X^{\hat{\underline{\theta}}} (\underline{\eta}_X(\hat{\underline{\theta}}) - \underline{\eta}_X(\overline{\underline{\theta}})) \|^2 \right), \tag{11}$$

where $\|.\|$ denotes the euclidian norm. This expression was derived in (Pázman, 1984) in the non-asymptotic case, and, by independent investigations, in (Skovgaard, 1985; Hougaard, 1985) as an asymptotic approximation of the true density. The properties of $q_X(\hat{\underline{\theta}} \,|\, \overline{\underline{\theta}})$ for a fixed-size design have been investigated in (Pázman, 1987a, 1987b, 1990). Two important notions are there

(i) the expectation surface

$$\mathcal{E}_X := \{\eta_X(\underline{\theta});\ \underline{\theta} \in \Theta\}, \tag{12}$$

(ii) the curvature $k_X(\underline{\theta})$ of this surface $\mathcal{E}_X$ at any point $\underline{\theta} \in \Theta$,

$$k_X(\underline{\theta}) := \sup_{\underline{v} \in \mathcal{R}^p} \frac{\| (I - P_X^{\underline{\theta}}) \sum_{i,j=1}^{p} v_i \frac{\partial^2 \eta_X(\underline{\theta})}{\partial\theta_i \partial\theta_j} v_j \|}{\sigma^2\, \underline{v}^T M_X(\underline{\theta})\, \underline{v}}, \tag{13}$$

which is also known as the intrinsic measure of nonlinearity (Bates and Watts, 1980). (Note that the expression (13) does not depend on σ.) Consider the number α defined by

$$\Pr\{\chi_N^2 > \alpha^2\} = \beta, \tag{14}$$

where β is nearly zero (0.05 for instance), and where χ_N^2 is the χ^2 random variable with N degrees of freedom. The expression (11) for $q_X(\hat{\underline{\theta}} \,|\, \overline{\underline{\theta}})$ is then correct for every $\hat{\underline{\theta}} \in \Theta$ such that

$$(\sigma\, k_X(\hat{\underline{\theta}}))^{-1} > \alpha, \tag{15}$$

and

$$\frac{1}{\sigma^2} \| P_X^{\hat{\underline{\theta}}} (\eta_X(\hat{\underline{\theta}}) - \eta_X(\overline{\underline{\theta}})) \|^2 \le \alpha^2. \tag{16}$$

The true density is nearly zero when (16) is not satisfied, and we will take $q_X(\hat{\underline{\theta}} \,|\, \overline{\underline{\theta}}) = 0$ by definition in such a case. Equation (14) ensures that 100(1-β) % of the samples are in the sphere

$$\mathcal{G}(\alpha) := \{\underline{y} \in \mathcal{R}^N;\ \frac{1}{\sigma} \| \underline{y} - \eta_X(\overline{\underline{\theta}}) \| < \alpha\}.$$

Equation (15) ensures that for every $\underline{y}$ in $\mathcal{G}(\alpha)$ the function

$$\underline{\theta} \to \| \underline{y} - \eta_X(\underline{\theta}) \|^2$$

admits only one stationary point which satisfies (16), and this point is equal to $\hat{\underline{\theta}}(\underline{y})$. For univariate models (dim $\underline{\theta}$ = 1) and for so-called "flat models" (see (Pázman, 1990)), the density $q_X(\hat{\underline{\theta}} \,|\, \overline{\underline{\theta}})$ is "almost exact", in the sense that

$$\Pr\{S\} = \int_S q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})\, d\hat{\underline{\theta}}$$

has an error not exceeding 2β for any measurable set S. Even if the model is non-flat, it follows from asymptotic considerations (Skovgaard, 1985; Hougaard, 1985) that $q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$ is more exact that the classical normal density (4). This density $q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$ can be quite different from (4), as illustrated on Figure 1. Note that (14, 15) prescribe a maximum on the admissible value of σ.

3. THE PROBABILITY DENSITY OF THE CONSTRAINED LS ESTIMATES $\tilde{\underline{\theta}}$

The expression (11) is valid only for $\hat{\underline{\theta}} \in$ int Θ, and the distribution on $\partial\Theta$ is unknown (it corresponds to all the estimates that would lie outside Θ if the constraints where not taken into account). There are several reasons why $\Pr\{\hat{\underline{\theta}} \in \text{int } \Theta\}$ can be much smaller than one, leading to situations where the distribution on $\partial\Theta$ cannot be neglected ($\overline{\underline{\theta}}$ is close to $\partial\Theta$, σ is large, and/or the design contains little information —it is almost degenerated— so that $q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$ widely spreads outside Θ). In order to take into account the estimates that are on $\partial\Theta$ we proceed as mentioned in the introduction, i.e. we consider the estimate $\tilde{\underline{\theta}} = \tilde{\underline{\theta}}(\underline{y})$ defined by (6).

The penalty function $w(\underline{\theta}) \geq 0$ will be chosen so as to satisfy the following requirements.

(i) It is continuous on Θ with continuous second order derivatives on int Θ, and is constant on some inner part Θ_0 of Θ. As a consequence, $\tilde{\underline{\theta}}(\underline{y}) = \hat{\underline{\theta}}(\underline{y})$ if $\hat{\underline{\theta}}(\underline{y}) \in \Theta_0$.

(ii) Its value on $\partial\Theta$ is infinite, $w(\underline{\theta}) = \infty$ iff $\underline{\theta} \in \partial\Theta$, so that there is no estimate left on $\partial\Theta$, and all the least-squares estimates $\hat{\underline{\theta}}(\underline{y})$ which are on $\partial\Theta$ are shifted by (6) onto the set [int Θ - Θ_0].

(iii) The second order derivative $\dfrac{\partial^2 w(\underline{\theta})}{\partial\underline{\theta}\partial\underline{\theta}^T}$ is positive definite on [int Θ - Θ_0].

The probability density of $\tilde{\underline{\theta}}$, of the same accuracy as $q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$, is derived in (Pázman and Pronzato, 1990).

$$\tilde{q}_X(\tilde{\underline{\theta}} \mid \overline{\underline{\theta}}) := \frac{\det\left(Q_X(\tilde{\underline{\theta}},\ \overline{\underline{\theta}}) - \dfrac{1}{\sigma^2} \underline{u}_X^T(\tilde{\underline{\theta}}) \dfrac{\partial^2 \underline{\eta}_X(\tilde{\underline{\theta}})}{\partial\underline{\theta}\partial\underline{\theta}^T} + \dfrac{\partial^2 w(\tilde{\underline{\theta}})}{\partial\underline{\theta}\partial\underline{\theta}^T} \right)}{(2\pi)^{p/2} \det{}^{1/2} M_X(\tilde{\underline{\theta}})}$$

$$\times \exp\left(- \frac{1}{2\sigma^2} \| P_X^{\tilde{\underline{\theta}}} (\underline{\eta}_X(\tilde{\underline{\theta}}) - \underline{\eta}_X(\overline{\underline{\theta}})) + \underline{u}_X(\tilde{\underline{\theta}}) \|^2 \right), \qquad (17)$$

where

$$\underline{u}_X(\underline{\theta}) := \frac{\partial \underline{\eta}_X(\underline{\theta})}{\partial\underline{\theta}^T} M_X^{-1}(\underline{\theta}) \frac{\partial w(\underline{\theta})}{\partial\underline{\theta}}, \qquad (18)$$

and where $P_X^{\underline{\theta}}$ and Q_X are still given by (9-10).

One can readily verify that $\tilde{q}_X(\tilde{\underline{\theta}} \mid \overline{\underline{\theta}}) = q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$ when $\tilde{\underline{\theta}} \in \Theta_o$. The geometrical notions used to derive $\tilde{q}_X(\tilde{\underline{\theta}} \mid \overline{\underline{\theta}})$ are the same as for $q_X(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$, and the validity of $\tilde{q}_X(\tilde{\underline{\theta}} \mid \overline{\underline{\theta}})$ still relies on equations (14-16).

4. THE CHOICE OF $w(\underline{\theta})$ WHEN Θ IS A p-DIMENSIONAL INTERVAL

When Θ is given by (2), it seems reasonable to take $w(\underline{\theta})$ as

$$w(\underline{\theta}) = \sum_{i=1}^{p} w_i(\theta_i), \tag{19}$$

where, $\forall\ i = 1, \ldots, p$,

(i) $w_i(\theta_i) = 0$ if $\theta_i \in [\theta_{m_i} + \Delta_i, \theta_{M_i} - \Delta_i]$,

(ii) $\dfrac{\partial^2 w_i(\theta_i)}{\partial \theta_i^2} > 0$ if $\theta_i \notin [\theta_{m_i} + \Delta_i, \theta_{M_i} - \Delta_i]$,

(iii) $\lim\limits_{\theta_i \to \theta_{m_i}} w_i(\theta_i) = \lim\limits_{\theta_i \to \theta_{M_i}} w_i(\theta_i) = \infty$,

with $\Delta_i \in \mathcal{R}$ small compared to $\theta_{M_i} - \theta_{m_i}$.

Consider a real function f continuous on [0, 1[with continuous first and second order derivatives f' f'' on this interval. Assume that $f(0) = 0$, $\lim\limits_{x \to 1} f(x) = \infty$ and that f, f', f'' are strictly positive on]0, 1[. Possible choices for f are for instance

$$f(x) = \operatorname{tg}\left(\frac{\pi}{2} x\right), \tag{20}$$

or

$$f(x) = \frac{1}{1-x} - 1. \tag{21}$$

The functions w_i can then be chosen in the following way,

$$\begin{cases} w_i(\theta_i) = K\, f\left(\left(\dfrac{\theta_i - \theta_{M_i} + \Delta_i}{\Delta_i}\right)^{\beta}\right) \text{ if } \theta_i \in [\theta_{M_i} - \Delta_i, \theta_{M_i}] \\ w_i(\theta_i) = 0 \text{ if } \theta_i \in [\theta_{m_i} + \Delta_i, \theta_{M_i} - \Delta_i] \\ w_i(\theta_i) = K\, f\left(\left(\dfrac{\theta_{m_i} + \Delta_i - \theta_i}{\Delta_i}\right)^{\beta}\right) \text{ if } \theta_i \in [\theta_{m_i}, \theta_{m_i} + \Delta_i], \end{cases} \tag{22}$$

with $K \in \mathcal{R}_+$

5. ALGORITHMIC PROCEDURE FOR THE COMPUTATION OF THE OPTIMAL EXPERIMENTAL DESIGN

The computation of the optimal design involves the following steps.

(i) Compute the classical A-optimal design,

$$X_A = \arg \min_X \text{trace } M_X^{-1}(\overline{\underline{\theta}}). \tag{23}$$

This design will be taken as the initial one for the optimization procedure (iii).

(ii) Check the curvature condition (15) for X_A and any $\hat{\underline{\theta}}$ in Θ satisfying (16)

(note that it can be computationally easier to check (15) for any $\hat{\underline{\theta}}$ in Θ).

If this condition is not satisfied, the noise level is too large with respect to the curvature of the expectation surface. A first solution (not always feasible) is then to reduce σ. A second solution is to restrict the design space in order to reduce the curvature. Note that a design of size N which consists of replications of only p different design points gives a curvature equal to zero, so that it is advisable to begin the whole procedure with a design of size p.

(iii) Optimize the design criterion (7) or (8).

Under some classical assumptions (Dvoretzky, 1956; Saridis, 1974), stochastic approximation techniques permit to optimize a criterion such as (7) or (8) without any evaluation of the criterion, thereby avoiding repetitive evaluations of mathematical expectations. The stochastic gradient algorithm, applied to the minimization of (7), corresponds to the following iterative procedure

$$X^{(k+1)} = X^{(k)} - \lambda^{(k)} \| \tilde{\underline{\theta}}^{(k)} - \overline{\underline{\theta}} \|^2 \frac{\partial \tilde{q}_X(\tilde{\underline{\theta}}^{(k)}, \overline{\underline{\theta}})}{\partial X}, \tag{24}$$

where, at each iteration k, $\tilde{\underline{\theta}}^{(k)}$ is randomly selected in Θ with a uniform distribution. The minimization of (8) could be performed with the same procedure, with $\overline{\underline{\theta}}$ generated according to the prior distribution $\pi(.)$ (independently of $\tilde{\underline{\theta}}$) at each iteration. When $X^{(k)}$ does not belong to the admissible domain, it is projected on its boundary. The step-size $\lambda^{(k)}$ must satisfy the conditions

$$\lambda^{(k)} \geq 0, \sum_{k=0}^{\infty} \lambda^{(k)} = \infty, \sum_{k=0}^{\infty} {\lambda^{(k)}}^2 < \infty.$$

The most common practice is to use the harmonic sequence

$$\lambda^{(k)} = \frac{a}{k}, \; a > 0. \tag{25}$$

The convergence can be accelerated by changing the value of $\lambda^{(k)}$ only when the angle between the gradients at iterations k-1 and k is greater than 90°. Stochastic gradient algorithms have

already been used in the context of experimental design for the optimization of criteria such as (5b) (see e.g. (Pronzato and Walter, 1985; Walter and Pronzato, 1987)) for a description of stochastic gradient algorithms with step-size normalization).

(iv) Repeat (ii) for the final design.

This procedure will be applied in Appendix B to different examples.

6. EXAMPLES

Example 1:

The response function is given by

$\eta(\theta, x) = \exp(-\theta x)$, ($x \in \mathcal{X} = [0, 2]$, $\theta \in \Theta = [0, 10]$).

Figure 1 presents the distribution $q_X(\hat{\theta} \mid \overline{\theta})$ (11) and the asymptotic normal distribution (4) as a function of $\hat{\theta}$ ($\hat{\theta} \in$ int Θ) for $\overline{\theta} = 5$ and $\sigma^2 = 0.25$. Note that the two distributions coincide when $\hat{\theta} = \overline{\theta}$, as can be seen from equations (10-11). The bounds on the parameters are not taken into account for both distributions.

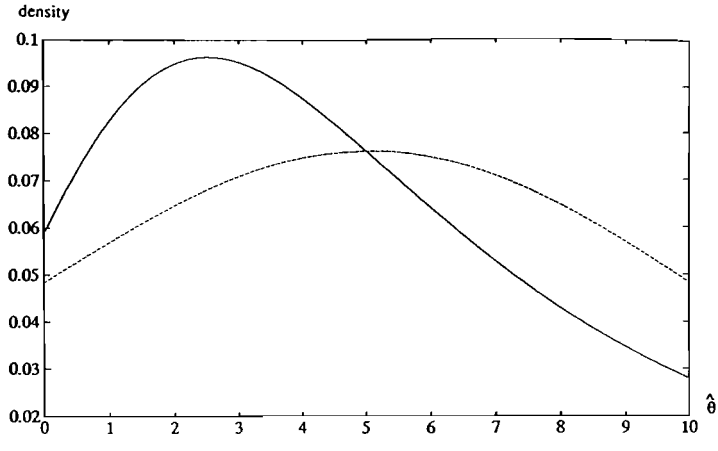


FIGURE 1 asymptotic normal density (---) and density $q_X(\hat{\theta} \mid \overline{\theta})$ (—).

We now consider the distribution of the constrained LS estimates ($0 \le \hat{\theta} \le 10$), for $\overline{\theta} = 1$, $\sigma^2 = 0.25$ and $X = \{0.1, 0.2\}$, with the rational penalty function $w(\theta)$ given by (21, 22). The value of Δ which defines the inner part Θ_0 of Θ where $\tilde{q}_X(\tilde{\theta} \mid \overline{\theta})$ coincides with $q_X(\hat{\theta} \mid \overline{\theta})$ is taken equal to 0.5 ($\Theta_0 = [0.5, 9.5]$). The influence of the scalar K (22) on the distribution $\tilde{q}_X(\tilde{\theta} \mid \overline{\theta})$ in int Θ - Θ_0 has been considered in (Pázman and Pronzato, 1990). When K is small (so that the influence of $w(\theta)$ on $\tilde{\theta}$ is negligible when θ is close to Θ_0) the distribution is concentrated near the outer boarder of int Θ - Θ_0, while it is concentrated near the inner boarder

of int Θ - Θ_0 when K is large. Values of K between 0.01 and 1 where found to give a distribution reasonably spread on int Θ - Θ_0 (which is important from a computational point of view), and we use K = 0.1. The corresponding optimal experimental design (of size 2) obtained according to the procedure of Section 5 is approximately given by $X^* = \{0.32, 0.32\}$. An evaluation of the criterion $\Psi_{\overline{\underline{\theta}}}$ by numerical integration gives $\Psi_{\overline{\underline{\theta}}}(X^*) = 5.70$ and $\Psi_{\overline{\underline{\theta}}}(X_A) = 86.4$. The initial A-optimal design ($X_A = \{1, 1\}$) is therefore far from being optimal according to the new criterion $\Psi_{\overline{\underline{\theta}}}$. Note that the curvature condition (15) does not need to be checked for X^* since X^* consists of replications.

Finally, we consider the criterion Ψ (8), where a normal prior distribution $\pi(\theta)$ is given for θ, $\theta \sim \mathcal{N}(5.5, 1.5^2)$. The optimal design of size 2 obtained with the stochastic gradient algorithm (24) (harmonic sequence (25), a = 0.05) is approximately equal to $\{0.18, 0.18\}$. It can be compared to the optimal design of size 2 for the criterion (5b), with $\Phi(M) = \text{trace}\,(M^{-1})$, which is given by $\{1.61, 1.61\}$ (Walter and Pronzato, 1987).

Example 2:

We consider the Michaelis-Menten model function

$$\eta(\underline{\theta}, x) = \frac{\theta_1 x}{\theta_2 + x}, \quad (x \in \mathcal{X} = [0, 2]).$$

The true value $\overline{\underline{\theta}}$ is fixed to $\overline{\underline{\theta}} = (0.1, 1.7)^T$, and the noise variance to $\sigma^2 = 25 \times 10^{-6}$. We use the tangent penalty function $w(\underline{\theta})$ given by (19, 20, 22), with $\Delta_i = 0.1(\theta_{M_i} - \theta_{m_i})$ and K = 0.01. Figure 2 presents a 3-dimensional plot of $\tilde{q}_X(\tilde{\underline{\theta}} \,|\, \overline{\underline{\theta}})$ for the design $X = \{0.5, 1.5\}$ and the admissible parameter domain $\Theta = [0, 0.25] \times [0, 4]$ (note that $\mathcal{E}_X$ (12) has a curvature $\mathcal{K}_X$ (13) equal to zero since the size of X is equal to dim $\underline{\theta}$).

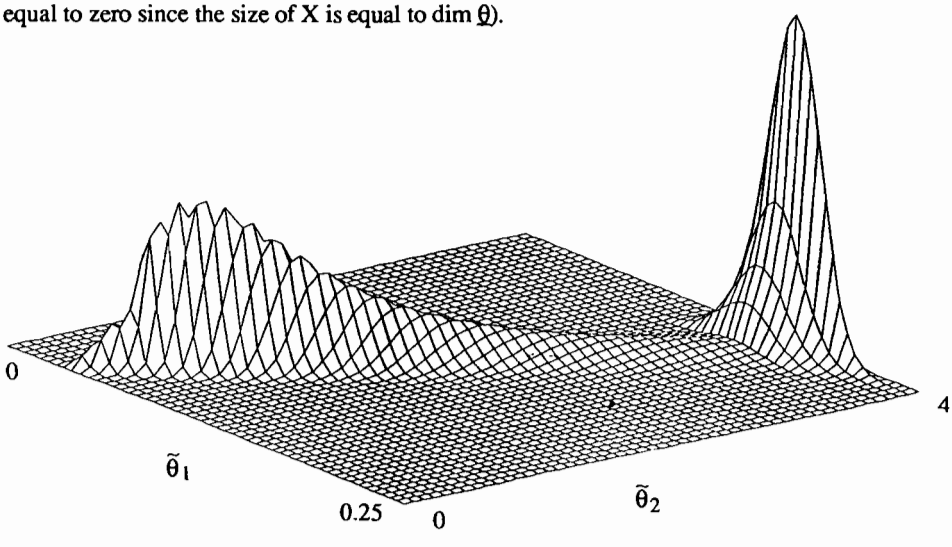


FIGURE 2 density $\tilde{q}_X(\tilde{\underline{\theta}} \,|\, \overline{\underline{\theta}})$.

The A-optimal design of size 2 is given by $X_A = \{0.5187, 2\}$. When $\Theta = [0, 0.25] \times [0, 10]$, the optimal design for the criterion $\Psi_{\overline{Q}}$ (7), obtained via the stochastic approximation algorithm described in Section 5, is approximately given by $X^* = \{0.7, 2\}$. The evaluation of the criterion by numerical integration then gives $\Psi_{\overline{Q}}(X_A) = 4.51$ and $\Psi_{\overline{Q}}(X^*) = 4.26$.

REFERENCES

Bates, D.M. and Watts, D.G. (1980). Relative curvature measures of nonlinearity. *J. R. S. S.*, **B42**: 1-25.

Dvoretzky, A. (1956). On stochastic approximation. In *Proceedings of the Berkeley Symposium on Mathematical Statistics and Probability*, Vol. 1: 39-45.

Ford, I., Kitsos, C.P. and Titterington, D.M. (1989). Recent advances in nonlinear experimental design. *Technometrics*, **31**,

Hamilton, D.C. and Watts, D.G. (1985). A quadratic design criterion for precise estimation in nonlinear regression models. *Technometrics*, **27**: 241-250.

Hougaard, P. (1985). Saddlepoint approximations for curved exponential families. *Stat. and Prob. Letters*, **3**: 161-166.

Pázman, A. (1984). Probability distribution of the multivariate nonlinear least squares estimates. *Kybernetika*, **20**: 209-230.

Pázman, A. (1987a). On formulas for the distribution of nonlinear LS estimates. *Statistics*, **18**: 3-15.

Pázman, A. (1987b). Flat nonlinear regression models. In V.V. Fedorov and H. Läuter (Eds.), *Model-Oriented Data Analysis*, Lecture Notes in Economics and Math. Systems, n°297, Springer-Verlag, Berlin, 120-124.

Pázman, A. (1989). On information matrices in nonlinear experimental design. *J. Stat. Planning and Inference*, **21**: 253-263.

Pázman, A. (1990). Almost exact distributions of estimators II - Flat nonlinear regression models. *Statistics*, **21**(1): 21-33.

Pázman, A. and Pronzato, L. (1990). Nonlinear experimental design with bounded parameter space. Rapport interne LSS-SUPELEC, Gif-sur-Yvette, France.

Pronzato, L. and Walter, E. (1985). Robust experiment design via stochastic approximation. *Mathematical Biosciences*, **75**: 103-120.

Saridis, G.N. (1974). Stochastic approximation methods for identification and control - a survey. *IEEE Trans. Automatic Control*, **AC-19**(6): 798-809.

Skovgaard, I.M. (1985). Large deviation approximations from maximum likelihood estimators. *Prob. Math. Statist.*, **6**: 89-107.

Walter, E. and Pronzato, L. (1987). Robust experiment design: between qualitative and quantitative identifiabilities. In E. Walter (Ed.), *Identifiability of Parametric Models*, Pergamon, Oxford, 104-113.

Walter, E. and Pronzato, L. (1990). Qualitative and quantitative experiment design for phenomenological models: a survey. *Automatica*, **26**(2): 195-213.

Batch Sequential Design for a Nonlinear Estimation Problem

Werner G. Müller, Benedikt M. Pötscher *

Abstract

A method for constructing batch sequential designs for a nonlinear problem is presented. The limiting behaviour is investigated for a particular model and simulation results are provided.

1 Introduction

As is well known (e.g. Fedorov (1972) or Ford et al. (1989)) the optimal design measure in a nonlinear setup depends upon the the unknown parameter, which is to be estimated. This creates a circular problem, for which two solutions have been proposed in the literature. First, construction of the optimal design based on a prior guess θ_0 of the parameter vector θ, or second, sequential methods, where the parameter estimators are updated during the experiment and the design is then based upon the current estimators. Procedures of the second type can be performed either as a batch sequential or as a fully sequential method (i.e. batches of size one), where after each batch of observations the estimation and the design are updated. Although the fully sequential method is expected to be theoretically superior to a batch sequential procedure (with batchsize > 1), in a number of applications practical reasons can lead to a preference for the latter procedure, as taking observations in batches may for instance be cheaper than taking them individually.

2 A Nonlinear Design Problem

The model of interest is the regression equation:

$$y_i = \theta_1 x_i + \theta_2 x_i^2 + \epsilon_i \tag{2.1}$$

where y_i is the response variable, x_i is the design variable , θ_1 and $\theta_2 \neq 0$ are parameters and the errors ϵ_i are independently identically distributed with zero mean and unit variance. The design variable x_i is assumed to take its values in the interval $[-1, 1]$ only.

*Department of Statistics, University of Economics Vienna, Augasse 2-6, A-1060 Vienna and Department of Statistics, University of Vienna, Universitätsstraße 5, A-1030 Vienna

The goal is to estimate the value x, which optimizes the response, i.e. to estimate the nonlinear function $g(\theta) = \frac{-\theta_1}{2\theta_2}$, leading to a nonlinear design problem.

This example has been frequently used in the literature (e.g. Ford & Silvey (1980), Ford et al. (1985), Wu (1985) and Chaloner (1988)) to illustrate the performance of optimal design methods in a nonlinear setup, since it is simple enough to allow an analytical treatment.

A reasonable and widely used design criterion is the asymptotic variance of the (pseudo) maximum likelihood estimator $\hat{g}_N$ of $g(\theta)$, derived under the assumption of normal errors and fixed design. Since this asymptotic variance suggests the approximation

$$N \operatorname{Var}(\hat{g}_N) = \frac{1}{4\theta_2^2} c_g^T J_N^{-1} c_g \tag{2.2}$$

the design criterion becomes [1]

$$\Phi(J_N, \theta) = c_g^T J_N^{-1} c_g$$

where $c_g = (-2\theta_2)\frac{\partial g(\theta)}{\partial \theta} = \begin{pmatrix} 1 \\ 2g(\theta) \end{pmatrix}$, and $J_N = \begin{pmatrix} \sum_{i=1}^N x_i^2 & \sum_{i=1}^N x_i^3 \\ \sum_{i=1}^N x_i^3 & \sum_{i=1}^N x_i^4 \end{pmatrix}$ is the information matrix for N observations. It is well known, that the non-sequential optimal design for this situation takes values only at $x = -1$ and $x = 1$ with the design measure given by:

$$p(1) = \begin{cases} 1/2 + g(\theta) & \text{if } |g(\theta)| \leq 1/2 \\ 1/2 + g(\theta)^{-1}/4 & \text{if } |g(\theta)| > 1/2 \end{cases}$$

and

$$p(-1) = \begin{cases} 1/2 - g(\theta) & \text{if } |g(\theta)| \leq 1/2 \\ 1/2 - g(\theta)^{-1}/4 & \text{if } |g(\theta)| > 1/2 \end{cases}$$

The fully sequential design is found by minimizing $\Phi(J_i, \hat{\theta})$ with respect to the design variable x_i, where $\hat{\theta}$ is the estimator from sample size $i-1$, see Silvey (1980). The k-th batch of the batch sequential design is obtained as follows:

$$\text{Choose the spectrum}(x_{k1}, \ldots, x_{kn_k}) \text{ which minimizes } \Phi(J_{N_k}, \hat{\theta}_{k-1}),$$

where $N_k = \sum_{j=1}^k n_j$, n_j is the batch length of the j-th batch, $n_j \geq 1$, and $\hat{\theta}_{k-1}$ is the ML-estimator for θ after the $k-1$-th batch. [2] Of course, if $n_j = 1$ for all j, this reduces to the fully sequential design. Since optimization of $\Phi(J_{N_k}, \hat{\theta}_{k-1})$ is computationally burdensome or requires algorithms from approximative design theory, we consider in the following an alternative method, which can be viewed as an approximation to the batch sequential design. We call this method quasi-batch sequential design, which is given by the rule:

$$\text{Sequentially choose } x_{ki} \text{ which minimizes } \Phi(J_{N_{k-1}+i}, \hat{\theta}_{k-1}) \tag{2.3}$$

[1] Ford et al. (1985) criticise the choice of (2.2) as a design criterion, since it is based on a fixed non-sequential design, Wu (1985), however, provides asymptotic justification for this choice.

[2] For ease of notation the j-th element of the k-th batch is here denoted by x_{kj}, i.e. $x_{kj} = x_{N_{k-1}+j}$ in the original notation. For convenience, we keep both notations, as no confusion seems possible. We also use the convention $N_0 = 0$.

Since minimization of Φ in (2.3) may be computationally awkward, we shall instead, following the literature, choose the next design point by maximizing the Gateaux-derivative of $\log \Phi$ in the direction $(x_{ki}, x_{ki}^2)'(x_{ki}, x_{ki}^2)$, rather than by (2.3).

Chaloner (1989) suggests an alternative approach, namely to augment the design at N_{k-1} observations in such a way that the resulting design is closest to the non-sequential design for N_k observations according to some closeness criterion. For batch sequential design in a different framework see also Abdelbasit & Placket (1983).

3 The Quasi Batch Sequential Design

It is easy to see, that maximizing the Gateaux-derivative mentioned above with respect to $x_{ki} \in [-1, 1]$ is equivalent to maximizing the scalar function

$$d_{(N_{k-1}+i-1)}(x_{ki}) = \left((x_{ki}, x_{ki}^2) J_{N_{k-1}+i-1}^{-1} c_{\hat{\vartheta}(k-1)}\right)^2, \tag{3.1}$$

where $c_{\hat{\vartheta}(k-1)} = (1, 2g(\hat{\theta}_{(k-1)}))'$. It has been shown by Ford & Silvey, 1980, that this function can have its maximum only at $x = -1$ or $x = 1$, which therefore are the only candidates for design points.

An explicit solution for the optimization problem (3.1) can now be given quite analogously as in Ford & Silvey (1980) for the fully sequential case. From the first N_{k-1} observations of the experiment N_{k-1}^- of these will be taken at $x = -1$ and $N_{k-1}^+ = N_{k-1} - N_{k-1}^-$ at $x = 1$. Let $\bar{y}_{k-1}^-$ denote the mean of the N_{k-1}^- observations on y at $x = -1$; $\bar{y}_{k-1}^+$ is defined analogously. Then $\bar{y}_{k-1}^- = -\hat{\theta}_{1(k-1)} + \hat{\theta}_{2(k-1)}$, $\bar{y}_{k-1}^+ = \hat{\theta}_{1(k-1)} + \hat{\theta}_{2(k-1)}$, and hence $2\hat{g}_{(k-1)} = (\bar{y}_{k-1}^- - \bar{y}_{k-1}^+)/(\bar{y}_{k-1}^- + \bar{y}_{k-1}^+)$. After $N_{k-1} + i - 1$ observations the information matrix is given by the 2×2 matrix with diagonal elements equal to $N_{k-1} + i - 1$ and off-diagonal elements equal to $(N_{k-1} + i - 1)^+ - (N_{k-1} + i - 1)^-$. Simple algebra then yields, the positive proportionality factor being the same,

$$d_{(N_{k-1}+i-1)}(-1) \propto ((N_{k-1} + i - 1)^+)^2 (\bar{y}_{k-1}^+)^2,$$

$$d_{(N_{k-1}+i-1)}(+1) \propto ((N_{k-1} + i - 1)^-)^2 (\bar{y}_{k-1}^-)^2.$$

Hence, similarly as in Ford & Silvey, 1980 for the fully sequential case, the design rule for the quasi batch sequential design can be described as follows: The i-th observation of the k-th batch, i.e. the $(N_{k-1} + i)$-th observation, is taken at $+1$ or -1 according to whether

$$(N_{k-1} + i - 1)^+ |\bar{y}_{k-1}^+| \quad < \text{ or } \geq \quad (N_{k-1} + i - 1)^- |\bar{y}_{k-1}^-|. \tag{3.2}$$

Of course the design rule (3.2) needs to be initialized. If we define $\bar{y}_0^+ = \bar{y}_0^- = 0$, it suffices in principle to fix the first two design points at $+1$ and -1, respectively (in case this allocation is chosen randomly it must not depend upon (ϵ_i)). However, if $n_1 > 2$ the remaining design points in the first batch will then be all set equal to -1 by the rule (3.2). Hence, if $n_1 > 1$, we may, as an alternative initialization of (3.2), want to fix the design points in the first batch a priori and invoke (3.2) only for $k \geq 2$.

Note that the design rule (3.2) allows one to calculate the design of the k-th batch $(x \quad, \ldots, x \quad)$ using only the first $N \quad$ observations. It may then be advantageous to

rearrange $(x_{k1}, \ldots, x_{kn_k})$ prior to taking observations of the dependent variable, such that only one change from 1 to -1 occurs in the batch. This avoids frequent setup changes, which may be costly. [3]

4 Asymptotics of Quasi Batch Sequential Design

The limiting behaviour of quasi batch sequential design is studied in this section. A proof of convergence of fully sequential designs in the particular example given above is provided in Ford & Silvey (1980). The argument given in that paper seems to be incomplete, however, as those authors assume the validity of a law of large numbers for a certain optionally sampled sequence of i.i.d. variables without providing a proof. This lacuna in the proof is closed in Lemmas 2 in the Appendix by utilizing a result of Doob (1936). Given this amendement, Ford & Silvey's (1980) proof can be generalized to provide a convergence proof for the more general case of quasi batch sequential designs. As a corollary consistency and asymptotic normality of the parameter estimators are obtained. The proofs of the Theorem and Corollary can be found in the Appendix. There we also outline how the results of this section continue to hold if the errors ϵ_i are only assumed to be a martingale difference sequence. For related results see Maljutov (1988) and Wu (1985).

Theorem: Under the maintained assumptions the quasi batch sequential design converges to the non-sequential optimal design based on the true parameter value (given by (4)), if the batch lenghts are bounded. I.e., if $n_i \leq \nu < \infty$ for all $i \geq 1$ (in particular if $n_i = \nu$), then

$$N^-/N \to p(-1) = |\theta_1 + \theta_2|/(|\theta_1 + \theta_2| + |\theta_2 - \theta_1|).$$

$$N^+/N \to p(+1) = |\theta_2 - \theta_1|/(|\theta_1 + \theta_2| + |\theta_2 - \theta_1|).$$

almost surely as $N \to \infty$.

The Theorem allows one to derive the asymptotic properties of the estimators $\hat{\theta}$ and $\hat{g}$ based on the quasi batch sequential design. Here $\hat{\theta}$ and $\hat{g}$ denote the estimators for a sample of size N and $\bar{y}^+ = \frac{1}{N^+}\sum_{i \in I_n^+} y_i$, $\bar{y}^- = \frac{1}{N^-}\sum_{i \in I_n^-} y_i$, where I_N^+ denotes the set of indices $i \leq N$ with $x_i = 1$ and I_N^- is defined analogously. The symbol $\to^d$ denotes convergence in distribution.

Corollary: Under the maintained assumptions the estimators $\hat{\theta}$ and $\hat{g}$ are strongly consistent. Furthermore, $\sqrt{N}(\hat{g} - g) \to^d N(0, (2\theta_2)^{-2} c_g' M^- c_g)$, where $M_{11} = M_{22} = 1$ and $M_{12} = M_{21} = p(1) - p(-1)$, from $M = limN^{-1}J_N$ and M^- is any g-inverse. If the optimal design is not degenerate then also $\sqrt{N}(\hat{\theta} - \theta) \to^d N(0, M^{-1})$.

5 Simulation Results

The small sample behaviour of quasi batch sequential designs was studied by means of a simulation experiment. In order to make results comparable with those reported in Ford &

[3] The asymptotic properties of the procedure are not affected by this rearrangement as long as the errors are assumed to be i.i.d., as may be shwon by arguments similar to those given in the Appendix.

design method	mean($\hat{g}_{25}$)	m.s.e.($\hat{g}_{25}$).10^4	mean(N_{25}^-)	Var(N_{25}^-)
fully sequential	-0.1257	6.090	15.524	0.470
batch sequential	-0.1248	6.186	15.620	0.572
quasi batch sequential	-0.1247	6.237	15.471	0.531
non-sequential (a)	-0.1248	6.569	15.645	0.229
non-sequential (b)	-0.1265	7.315	12.510	0.250
random (c)	-0.1263	14.165	12.180	48.579

Table 1: Performance characteristics for different design techniques.

Silvey (1980) for fully sequential designs the same simulation setup was used. Model(2.1) with $\theta = (1, 4)$ and $\theta = (1, 1)$, respectively, was used to generate samples of size 100, where the x_i were chosen by various design rules described below. The experiment was repeated 1000 times. At sample sizes 25,50,75 and 100 the same characteristics of the inference process as in Ford & Silvey (1980), i.e., the mean squared error of $\hat{g}$, were calculated. We found no significant differences between the performance of quasi batch sequential and fully sequential design for sample size 50 and larger. (In fact an experiment with purely random design was not significantly inferior.) For this reason we report only the results of the simulation for samples of size 25. As the results for $\theta = (1, 1)$ are quite similar to the corresponding results for $\theta = (1, 4)$ we report only the latter. In this case the response function has its maximum at $x = 0.125$.

The following design methods were studied: fully sequential design, batch sequential and quasi batch sequential design (5 batches of lenght 5) [4] and several non sequential designs, namely (a) non-sequential optimal design under perfect information, i.e. $N_{25}^- = 15.625$, (b) non-informative non-sequential design, i.e. $N_{25}^- = 12.5$ and (c) pure random design. [5]

Table 1 presents the performance characteristics of the design methods given above ordered by the empirical mean squared error of the estimator $\hat{g}$. Unexpectedly the non-sequential optimal design did not perform. An explanation can be found in the work of Schwabe (1989), who proved the superiority of sequential over nonsequential methods, when the optimal designs can not be realized exactly (as in this case). The difference in performance between fully, batch and quasi batch sequential design is not substantial, while informative (a), non-informative (b) and random (c) design are clearly dominated. These results seem to justify the use of quasi batch sequential procedures in expensive experiments.

Figures 1 and 2 show the empirical distributions of the estimator $\hat{g}$ for N=5,10,15 observations (solid, dashed, dotted line), based on fully sequential and quasi batch sequential designs, respectively. It can be seen that even for small samples the empirical distributions are not dramatically different, although the distributions in Figure 1 are slightly more concentrated.

[4] In the first batch two design points were chosen as $+1$, two as -1 and the remaining point was chosen randomly as ± 1 with probability 1/2.

[5] Since the non sequential design (a) is not exactly realizable for $N = 25$ we proceed as follows: 15 of the design points were chosen equal -1 and 9 points equal $+1$. The remaining point was randomly chosen with $P(-1) = 5/8$. The non sequential design (b) was constructed analogously. For the pure random design each x_i was chosen randomly from $\{-1, +1\}$ with $P(-1) = P(1) = 1/2$ in each simulation run.

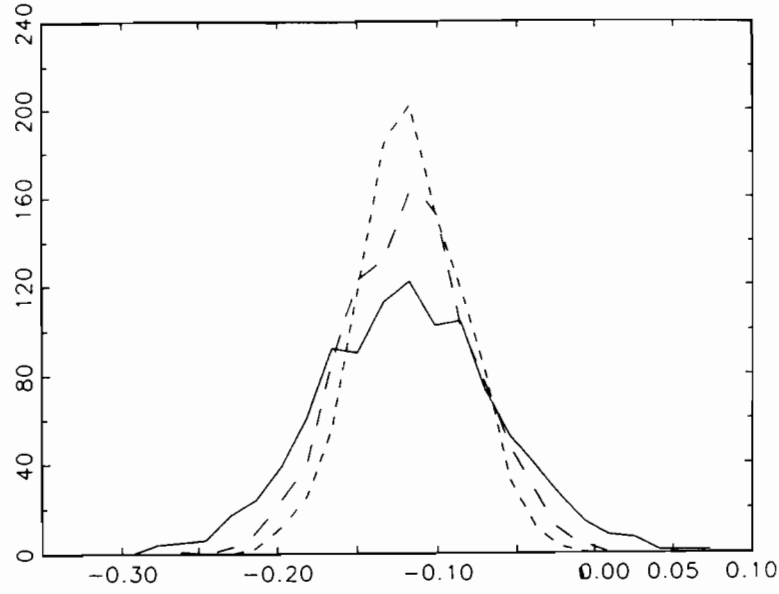


Figure 1: Empirical distribution of $\hat{g}_5, \hat{g}_{10}, \hat{g}_{15}$ for fully sequential design.

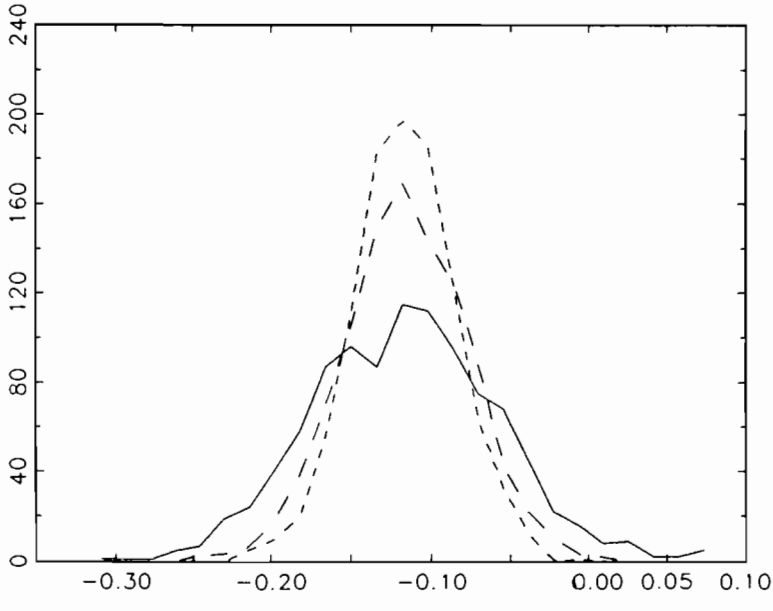


Figure 2: Empirical distribution of $\hat{g}_5, \hat{g}_{10}, \hat{g}_{15}$ for quasi batch sequential design.

vector n	mean($\hat{g}_{25}$)	m.s.e.($\hat{g}_{25}$).10^4	mean(N_{25}^-)	Var(N_{25}^-)
(5,5,5,5,5)	-0.1257	6.237	15.52	0.548
(2,2,17,2,2)	-0.1245	6.377	15.40	0.612
(5,5,5,5,5)*	-0.1247	6.398	15.47	0.531
(17,2,2,2,2)*	-0.1253	6.432	15.51	0.484
(2,2,2,2,17)	-0.1238	6.435	15.48	1.246
(17,2,2,2,2)	-0.1236	6.502	15.41	0.371
(2,17,2,2,2)	-0.1257	6.551	15.49	0.620
(2,2,2,17,2)	-0.1244	6.786	15.42	0.944

Table 2: Performance characteristics for different quasi batch sequential designs.

Table 2 provides information about performance characteristics of quasi batch sequential procedures for different batch lengths. For samples of size $N = 25$ and $k = 5$ batches different choices for the vector $n = (n_1, \ldots, n_5)$ have been investigated.

The first batch was initialized as described above, except the cases marked by an asterisk, for which perfect information was used. The simulation showed no clear indication for the preference of any choice of vector n in this example. All the results for the empirical mean squared error remained within the information gain of one additional information.

References

K.M. Abdelbasit and R.L. Plackett. Experimental design for binary data. *Journal of the American Statistical Association*, 78(381):90–98, 1983.

K. Chaloner. Optimal bayesian experimental design for estimating the turning point of a quadratic regression. *Communication in Statistics, Theory & Methods*, 18:1385–1400, 1988.

J.L. Doob. Note on probability. *Annals of Mathematics*, 37:363–367, 1936.

V.V. Fedorov. *Theory of Optimal Experiments*. Academic Press, New York, 1972.

I. Ford and S.D. Silvey. A sequentially constructed design for estimating a nonlinear parametric function. *Biometrika*, 67:381–388, 1980.

I. Ford, D.M. Titterington, and C.F.J. Wu. Inference and sequential design. *Biometrika*, 72:545–551, 1985.

I. Ford, D.M. Titterington, and C.P. Kitsos. Recent advances in nonlinear experimental design. *Technometrics*, 31(1):49–60, 1989.

P. Gänssler and W. Stute. *Wahrscheinlichkeitstheorie*. Springer Verlag, Berlin, Heidelberg, New York, 1977.

C.C. Heyde and D.J. Scott. Invariance principles for the law of the iterated logarithm for the martingales and processes with stationary increments. *Annals of Probability*, 1:428–436, 1973.

M.B. Maljutov. Design and analysis in generalized regression model f. In V.V. Fedorov and H. Läuter, editors, *Lecture Notes in Economical and Mathematical Systems*, pages 72–76, Springer Verlag, Berlin, 1988.

B.M. Pötscher. *Optional Skipping of Martingale Differences and Related Sequences.* Technical Report, Department of Economics, Working Paper, University of Maryland, 1990.

R. Schwabe. *Adaptive Designs for Linear Problems.* Technical Report A-89-26, Fachbereich Mathematik, Forschungsbericht, Freie Universit t Berlin, 1989.

S.D. Silvey. *Optimal Design.* Chapman and Hall, London, 1980.

C.F.J. Wu. Asymptotic inference from sequential design in a nonlinear situtation. *Biometrika*, 72:553–558, 1985.

6 Appendix

Let $(\Omega, \mathcal{A}, \mathcal{P})$ denote the probability space on which all random variables are defined.

Lemma 1: Under the assumptions of Section II, the quasi batch sequential design given by (3.2) satisfies: $N^+ \to \infty$ and $N^- \to \infty$ a.s. as $N \to \infty$.

Proof: It is sufficient to prove the Lemma for $N = N_k$. Suppose for some $\omega \in \Omega$ we have

$$N_k^-(\omega) = n \quad \text{for all } k \geq k^*(\omega). \tag{6.1}$$

Then condition (3.2) implies

$$|\sum_{i \in I^+_{N_k}} y_i(\omega)| < |\sum_{i \in I^-_{N_k}} y_i(\omega)| = const(\omega) < \infty \quad \text{for all } k \geq k^*(\omega).$$

It follows that

$$\limsup_{k \to \infty} |\sum_{i \in I^+_{N_k}} y_i(\omega)| = |\sum_{i \in I^+_{N_{k^*(\omega)}}} y_i(\omega) + \sum_{i=N_{k^*(\omega)}+1}^{N_k} y_i(\omega)| \leq const(\omega),$$

Hence we have

$$\limsup_{k \to \infty} |\sum_{i=N_{k^*(\omega)}+1}^{N_k} y_i(\omega)| < \infty \tag{6.2}$$

on the event defined by (7.1). On this event the expression $|\sum_{i=N_{k^*(\omega)}+1}^{N_k} y_i|$ coincides with $|\sum_{i=N_{k^*(\omega)}+1}^{N_k}(\epsilon_i + \theta_1 + \theta_2)|$. Since ϵ_i is i.i.d. (with finite variance) it follows, that $\limsup_{s \to \infty} |\sum_{i=1}^{s}(\epsilon_i + \theta_1 + \theta_2)| = \infty$ a.s.. Hence in view of (7.2) the event defined by (7.1) has probability zero. Since the event $\{N_k^- < \infty\}$ is a countabular union of the above events we arrive at a contradiction. Thus $N_k^- \to \infty$ a.s.. The result for N_k^+ is proved analogously. **qed**

Lemma 2: Suppose the assumptions of section 2 hold and let the design be generated by (3.2). Then

$$\lim_{N\to\infty} \frac{1}{N^+} \sum_{i\in I_N^+} y_i = \theta_1 + \theta_2 \text{ and } \lim_{N\to\infty} \frac{1}{N^-} \sum_{i\in I_N^-} y_i = \theta_2 - \theta_1 \quad a.s..$$

Proof: Almust surely both values 1 and -1 occur infinitely often in the design (x_i) in view of Lemma 1. Ignoring a subset of probability zero in the following, the stopping times

$$\mu_j = \min\{i \geq 1 : \text{card}(I_i^+) = j\},$$

where $\text{card}(A)$ denotes the cardinality of a set A, are well-defined and finite. Furthermore the event $\{\mu_j = k\}$ depends only on $(x_1, \ldots, x_k)$ and hence is measurable with respect to $(\epsilon_1, \ldots, \epsilon_{k-1})$ (and the initializing design points) in view of the design rule (3.2). Define $z_j = y_{\mu_j}$ and $B_s = \frac{1}{s}\sum_{j=1}^{s} z_j$. Then the sequence $\frac{1}{N^+}\sum_{i\in I_N^+} y_i$ is a subsequence of the sequence $(B_s(\omega))$ (possibly repeating values of $B_s(\omega)$). Hence it suffices to prove $B_s \to \theta_1 + \theta_2$ a.s. as $s \to \infty$. Observe that $x_{\mu_j} = 1$ by construction of μ_j. Therefore $z_j = \theta_1 + \theta_2 + \epsilon_{\mu_j}$ and it remains to show that $\frac{1}{s}\sum_{j=1}^{s} v_j \to 0$ a.s., where $v_j = \epsilon_{\mu_j}$. Now, since (ϵ_i) is i.i.d., since the initializing design points are independent of (ϵ_i), since the stopping times μ_j are predetermined (i.e. $\{\mu_j = k\}$ belongs to $\mathcal{G}_{k-1}$, the σ-field generated by $\{\epsilon_1, \ldots \epsilon_{k-1}\}$ and the initializing design points) and are strictly increasing, it follows from a result by Doob (1936) that (v_j) is also i.i.d. with the same distribution as (ϵ_i), cf. also Pötscher (1990). Kolmogorov's law of large numbers now completes the proof. The second half of the lemma is now proved analogously. **qed**

Note that Lemma 2 does not holds only for quasi batch sequential designs but for any design (x_i) satisfying (a) the design contains an infinite number each of 1 and -1 a.s. and (b) x_i is measurable w.r.t. $\mathcal{G}_{i-1}$.

Proof of the Theorem: Since the batch length is assumed to be bounded it is sufficient to prove the result for $N = N_k$ with $k \geq 1$. For r a natural number let ${}_rN$ denote the index at which the r-th change from 1 to -1 occurs in the design, i.e. ${}_rN$ is the r-th smallest index such that $x_{{}_rN} = 1$ and $x_{{}_rN+1} = -1$ holds. Let ${}_rN^-$ (${}_rN^+$) denote the number of observations taken at $x = -1$ ($x = +1$) within the first ${}_rN$ observations. Since $N_k^+ \to \infty$ and $N_k^- \to \infty$ a.s. as $k \to \infty$ by Lemma 1, the random variable ${}_rN$ is a.s. finite and ${}_rN^+, {}_rN^-$ are a.s. well defined. Of course ${}_rN^+$ and ${}_rN^-$ are a.s. positive for $r > 1$, and ${}_rN^+ \to \infty$, ${}_rN^- \to \infty$ and ${}_rN \to \infty$ a.s. as $r \to \infty$. Let $k(r)$ denote the number of batches preceeding the r-th change from $+1$ to -1, i.e. $k(r)$ is determined such that $N_{k(r)} \leq {}_rN < N_{k(r)+1}$ holds. As the batch length is assumed to be bounded we clearly have $k(r) \to \infty$ as $r \to \infty$. Furthermore, note that $N_{k(r)}^+ > 0$ and $N_{k(r)}^- > 0$ a.s. hold for $r > \nu/2$. Applying now (3.2) to the $({}_rN + 1)$-th observation we obtain

$$\frac{{}_rN^-}{N_{k(r)}^-} \Big| \sum_{i\in I_{N_{k(r)}}^-} y_i \Big| \leq \frac{{}_rN^+}{N_{k(r)}^+} \Big| \sum_{i\in I_{N_{k(r)}}^+} y_i \Big| \quad a.s., \tag{6.3}$$

where $I_{N_{k(r)}}^-$ is the index set corresponding to the observations in the first $k(r)$ batches taken at $x = -1$ and $I_{N_{k(r)}}^+$ its complement relative to $\{i : 1 \leq i \leq N_{k(r)}\}$. Since Lemma

1 shows that $N^+_{k(r)} \to \infty$ and $N^-_{k(r)} \to \infty$ a.s. as $r \to \infty$ we obtain from Lemma 2

$$\lim_{r\to\infty} \frac{1}{N^-_{k(r)}} \Big| \sum_{i\in I^-_{N_{k(r)}}} y_i \Big| = |\theta_1 - \theta_2| \quad a.s., \tag{6.4}$$

and

$$\lim_{r\to\infty} \frac{1}{N^+_{k(r)}} \Big| \sum_{i\in I^+_{N_{k(r)}}} y_i \Big| = |\theta_1 + \theta_2| \quad a.s.. \tag{6.5}$$

Dividing (7.3) by ${}_rN$ we obtain using (7.4) and (7.5)

$$|\theta_1 - \theta_2| \liminf_{r\to\infty} {}_rN^-/{}_rN \le |\theta_1 + \theta_2| \liminf_{r\to\infty} {}_rN^+/{}_rN \quad a.s.$$

Applying the design rule (3.2) to the $({}_rN)$-th observation we get

$$\frac{{}_rN^-}{N^-_{k(r)-1}} \Big| \sum_{i\in I^-_{N_{k(r)-1}}} y_i \Big| > \frac{{}_rN^+ - 1}{N^+_{k(r)-1}} \Big| \sum_{i\in I^+_{N_{k(r)-1}}} y_i \Big| \quad a.s.,$$

on the event $\{{}_rN = N_{k(r)}\}$ and

$$\frac{{}_rN^-}{N^-_{k(r)}} \Big| \sum_{i\in I^-_{N_{k(r)}}} y_i \Big| > \frac{{}_rN^+ - 1}{N^+_{k(r)}} \Big| \sum_{i\in I^+_{N_{k(r)}}} y_i \Big| \quad a.s., \tag{6.6}$$

on the event $\{{}_rN > N_{k(r)}\}$. Again dividing by ${}_rN$ we obtain in any case

$$|\theta_1 - \theta_2| \liminf_{r\to\infty} {}_rN^-/{}_rN \ge |\theta_1 + \theta_2| \liminf_{r\to\infty} {}_rN^+/{}_rN \quad a.s.$$

This gives

$$|\theta_1 - \theta_2| \liminf_{r\to\infty} {}_rN^-/{}_rN = |\theta_1 + \theta_2| \liminf_{r\to\infty} {}_rN^+/{}_rN \quad a.s. \tag{6.7}$$

Similarly we get

$$|\theta_1 - \theta_2| \limsup_{r\to\infty} {}_rN^-/{}_rN = |\theta_1 + \theta_2| \limsup_{r\to\infty} {}_rN^+/{}_rN \quad a.s. \tag{6.8}$$

Observing that ${}_rN = {}_rN^- + {}_rN^+$, it follows from (7.7) and (7.8) for $\theta_1 \neq 0$ (note that $\theta_2 \neq 0$)

$$\lim_{r\to\infty} {}_rN^-/{}_rN = |\theta_1 + \theta_2|/(|\theta_1 + \theta_2| + |\theta_2 - \theta_1|) \quad a.s.$$

If $\theta_1 = 0$, dividing (7.3) as well as (7.6),(33) by ${}_rN^-$ gives

$$1 \le \liminf_{r\to\infty} {}_rN^+/{}_rN^- \le \limsup_{r\to\infty} {}_rN^+/{}_rN^- \le 1 \quad a.s.$$

observing that $\theta_2 \neq 0$. Hence

$$\lim_{r\to\infty} {}_rN^-/{}_rN = 1/2 = |\theta_1 + \theta_2|/(|\theta_1 + \theta_2| + |\theta_2 - \theta_1|) \quad a.s.$$

If furthermore ${}^rN^-$ and ${}^rN^+$ denote the r-th change from -1 to 1 in the design, we obtain analogously as above

$$\lim {}^rN^-/{}^rN = |\theta_1 + \theta_2|/(|\theta_1 + \theta_2| + |\theta_2 - \theta_1|) \quad a.s.$$

Observing that N_k^-/N_k is monotonic between changes completes the proof. **qed**

Proof of the Corollary: Since $\hat{\theta} = \frac{1}{2}(\bar{y}^+ - \bar{y}^-, \bar{y}^+ + \bar{y}^-)$ consistency follows from Lemma 2. Next observe that $\sqrt{N}(\hat{\theta} - \theta) = (N^{-1}J_N)^{-1}\frac{1}{\sqrt{N}}\sum_{i=1}^N (x_i, x_i^2)'\epsilon_i$ and that $N^{-1}J_N$ converges to M in view of theTheorem. From a standard martingale central limit theorem applied to $(x_i, x_i^2)'\epsilon_i$, cf. e.g. Gänssler & Stute (1977), Th.9.3.2., and the Cramér-Wold device we obtain $\frac{1}{\sqrt{N}}\sum_{i=1}^N (x_i, x_i^2)'\epsilon_i \to^d N(0, M)$. Observe that the conditional Lindeberg condition is satisfied for a linear combination $(\alpha x_i + \beta x_i^2)\epsilon_i$, since ϵ_i is i.i.d. with finite second moment and

$$E((\alpha x_i + \beta x_i^2)\epsilon_i^2 I_{(|\alpha x_i + \beta x_i^2||\epsilon_i| > \delta\sqrt{N})}/\mathcal{G}_{i-1}) \leq (|\alpha| + |\beta|)^2 E(\epsilon^2 I_{(|\epsilon_i| > \frac{\delta\sqrt{N}}{|\alpha|+|\beta|})}).$$

Consequently the last claim in the Corollary follows, since the optimal non sequential design is nondegenerate iff M is nonsingular. As an immediate consequence we obtain the asymptotic distribution for $\sqrt{N}(\hat{g} - g)$ in the nondegenerate case. Finally observe that M is singular iff $p(1) = 1$ or $p(-1) = 1$, i.e. $g = 1/2$ or $g = -1/2$. As the proofs for both cases are similar we give only the proof for the case $g = 1/2$. Rewrite $\sqrt{N}(\hat{g} - g)$ as $-\sqrt{N}\bar{y}^+/(\bar{y}^+ + \bar{y}^-)$. By Lemma 2 the denominator converges to $2\theta_2$ and $N^+/N \to p(1) = 1$ by the Theorem. It hence suffices to establish $\frac{N^+}{\sqrt{N}}\bar{y}^+ \to^d N(0,1)$ as $c_g' M^- c_g = 1$ holds. Now $\frac{N^+}{\sqrt{N}}\bar{y}^+ = N^{-1/2}\sum_{i=1}^N \delta_i\epsilon_i$ where $\delta_i = 1$ on the event $\{\mu_k = i \text{ for some } k \geq 1\}$. and $\delta_i = 0$ else. Clearly, δ_i is $\mathcal{G}_{i-1}$-measurable and hence $(\delta_i\epsilon_i)$ is a martingale difference sequence. Observing once more that $N^+/N \to 1$ a.s., it follows that the norming condition in the martingale central limit theorem is satisfied. Furthermore, since $|\delta_i\epsilon_i| \leq |\epsilon_i|$ also the Lindeberg condition is seen to hold. Consequently, $N^{-1/2}\sum_{i=1}^N \delta_i\epsilon_i \to^d N(0,1)$, which completes the proof. **qed**

Inspection of the above given proofs show that the Theorem and Corollary from Section 4 still hold if the errors (ϵ_i) are more generally assumed to be a martingale difference sequence w.r.t. $(\mathcal{G}_i)$ satisfying $E(\epsilon_i^2/\mathcal{G}_{i-1} = 1$, the conditional Lindeberg condition, and the law of the iterated logarithm (sufficient conditions on (ϵ_i) such that the law of the iterated logarithm holds can be found in Heyde & Scott (1973)). The following modifications have then to be made in the proofs above: first, in the proof of Lemma 1 we now deduce $\limsup_{s\to\infty} |\sum_{i=1}^s(\epsilon_i + \theta_1 + \theta_2)| = \infty$ a.s. from the law of the iterated logarithm. Second, to establish $\frac{1}{s}\sum_{j=1}^s v_j \to 0$ a.s. in the proof of Lemma 2 we now make use of the fact that (v_j) is again a martingale difference sequence with $E(v_j^2) = 1$ as shown in Pötscher (1990) (see also the working paper version of the present paper for more details), and hence satisfies a strong law of large numbers, cf. Gänssler & Stute (1977), Korollar 6.7.2. The rest of the proofs remain essentially unchanged.

NONSEQUENTIAL BAYESIAN EXPERIMENTAL DESIGN FOR RESPONSE OPTIMIZATION

Luc Pronzato and Eric Walter,

Laboratoire des Signaux et Systèmes, CNRS / Ecole Supérieure d'Electricité
Plateau de Moulon, 91192 Gif-sur-Yvette Cedex, France

1. INTRODUCTION

Response optimization corresponds to the maximization of a dependent response variable y with respect to some independent input variables $\underline{x}$ (operating conditions). In many practical situations, including optimal quality control, the exact dependence of y on $\underline{x}$ is unknown, and, moreover, y is subject to random variability. A possible policy is then to maximize the expectation of y. Inference regarding the system can be drawn from measuring y at various values of $\underline{x}$. While replications of measurements at the same $\underline{x}$ inform us on the random part of y, measurements at different $\underline{x}$ also inform us on its deterministic part, denoted in what follows by η. The number of possible measurements at different $\underline{x}$ is often very limited for economical, technical or ethical reasons so that an optimal choice of these values $\underline{x}^i$ has to be performed.

The classical response surface methodology (see e.g. (Montgomery, 1976)) involves a sequential determination of the appropriate region for the optimal inputs $\underline{x}^*$. A small region $\mathcal{X}^{(k)}$ of the admissible experimental domain $\mathcal{X}$ is considered at the kth step. If the region $\mathcal{X}^{(k)}$ is far from $\underline{x}^*$, η is approximated over $\mathcal{X}^{(k)}$ by a linear function of $\underline{x}$, while a quadratic function of $\underline{x}$ is used when $\mathcal{X}^{(k)}$ moves closer to $\underline{x}^*$. Classically, prespecified experimental conditions (e.g. central composite designs) are applied at each step to obtain the parameter estimates to be used to determine the optimal inputs $\underline{x}^*$.

We consider here a situation where the response optimization problem has to be solved for a series of similar processes, so that prior knowledge on the possible values of the model parameters is available. A sequential determination of the appropriate region for the operating conditions for each process may then not be reasonable, and prior knowledge must be used to design a single-shot experiment on the whole feasible experimental domain $\mathcal{X}$.

Classical prespecified designs used in response surface methodology have five major drawbacks in this context.

(i) They imply a large number of measurements.

(ii) All parameters receive equal attention, regardless of their influence on the intended use of the model.

(iii) Prior information resulting from previous experiments on the same type of process is not taken into account.

(iv) The approach is inherently local and cannot take the constraints defining $\mathcal{X}$ into account.

(v) The model response is assumed to be a linear or a quadratic function of $\underline{x}$, which may not be valid on the whole domain $\mathcal{X}$.

This paper suggests an alternative approach, based on a Bayesian optimality criterion that avoids these drawbacks. It does not require a large number of measurements (i) and aims at explicitly taking into account the intended application to response optimization (ii), prior information on the model parameters (iii) and possible constraints on the input variables (iv). It also permits to use other model structures than polynomial functions of $\underline{x}$ (v).

Section 2 introduces the response optimization problem and defines the conditional loss to be used for the estimation and experimental design procedures. The Bayesian estimator and experimental design criterion are presented in Section 3. The design policy corresponds to L_B-optimality. Classical design policies for parameter estimation such as D-optimality could also be used in the nonsequential context considered here. A numerical example is used in Section 4 to compare an approach based on D-optimality and maximum likelihood estimation with the one of Section 3, and to illustrate the robustness of the Bayesian approach to misspecifications in the priors.

2. RESPONSE OPTIMIZATION

The quality index to be maximized will be described as

$$y(\underline{x}) = \eta(\overline{\underline{\theta}}, \underline{x}) + \varepsilon(\underline{x}), \quad (\underline{x} \in \mathcal{X}, \overline{\underline{\theta}} \in \Theta), \tag{1}$$

with i.i.d. normal errors $\varepsilon(\underline{x}) \sim \mathcal{N}(0, \sigma^2)$. The function $\eta(\underline{\theta}, \underline{x}) = \underset{y|\underline{\theta}}{E}\{y(\underline{x})\}$ is the model response, $\underline{\theta} = (\theta_1, \ldots, \theta_p)^T$ denotes the vector of parameters, with $\underline{\theta} \in \Theta$, $\mathcal{R}^p \supset \Theta$, and $\overline{\underline{\theta}}$ is the unknown true value of these parameters. In what follows $\eta(\underline{\theta}, \underline{x})$ is assumed to admit second order derivatives $\dfrac{\partial^2 \eta(\underline{\theta}, \underline{x})}{\partial \underline{\theta}\, \partial \underline{\theta}^T}$ in every interior point $\underline{\theta}$ of Θ ($\underline{\theta} \in \text{int}\,\Theta$). The input variable $\underline{x}$ (a m-dimensional vector) belongs to an admissible design space $\mathcal{X}$, $\mathcal{R}^m \supset \mathcal{X}$.

Usually, $\eta(\underline{\theta}, \underline{x})$ is approximated by a low-order polynomial in some region of interest of the independent variables. When the initial estimate of the optimum operating conditions are remote from the optimum, the curvature of the response surface

$$\mathcal{S}_{\underline{\theta}} = \{\eta(\underline{\theta}, \underline{x}); \underline{x} \in \mathcal{X}\}$$

can be neglected, and a first-order polynomial approximation can be used. The method of steepest ascent (Box and Wilson, 1951; Brooks and Mickey, 1961; Montgomery, 1976) then allows sequential movements along the direction of maximum increase of the response. When $\underline{x}$ is closer to the optimum, the curvature of $\mathcal{S}_{\underline{\theta}}$ can no longer be neglected. The model response $\eta(\underline{\theta}, \underline{x})$ is then described by a quadratic function of $\underline{x}$

$$\eta(\underline{\theta}, \underline{x}) = \theta_0 + \underline{q}^T\underline{x} + \frac{1}{2}\underline{x}^T Q \underline{x},$$

or equivalently by

$$\eta(\underline{\theta}, \underline{x}) = \underline{z}^T(\underline{x})\,\underline{\theta}, \tag{2}$$

with

$$\underline{z}^T(\underline{x}) = (1, x_1, x_2, \ldots, x_m, \tfrac{1}{2}x_1^2, \tfrac{1}{2}x_2^2, \ldots, \tfrac{1}{2}x_m^2, x_1x_2, x_1x_3, \ldots, x_1x_m, x_2x_3, \ldots, x_2x_m, \ldots, x_{m-1}x_m), \tag{3a}$$

and

$$\underline{\theta} = (\theta_0, q_1, q_2, \ldots, q_m, Q_{11}, Q_{22}, \ldots, Q_{mm}, Q_{12}, Q_{13}, \ldots, Q_{1m}, Q_{23}, \ldots, Q_{2m}, \ldots, Q_{(m-1)m})^T. \tag{3b}$$

Such a quadratic model response will be used in the example of Section 4, however, this hypothesis is not essential, and we shall simply assume that $\eta(\underline{\theta}, \underline{x})$ is linear in $\underline{\theta}$, so that it can be written as (2). Vectors $\underline{z}(\underline{x})$ different from (3a) can then be used, thereby allowing more general model structures than quadratic functions. Although it raises important and interesting problems, deterministic deviations of $y(\underline{x})$ from the model $\eta(\underline{\theta}, \underline{x})$ will be neglected. For situations where such an approximation is unacceptable one can refer for instance to (Blight and Ott, 1975) for the estimation and prediction problems and to (Pesotchinsky, 1982; Sacks and Ylvisaker, 1985; Sacks and Schiller, 1988; Sacks *et al.*, 1989) for the experimental design problem.

For any $\underline{\theta}$ in Θ, let $\underline{x}^*(\underline{\theta})$ denote the optimal value of $\underline{x}$

$$\underline{x}^*(\underline{\theta}) = \arg \max_{\underline{x} \in \mathcal{X}} \eta(\underline{\theta}, \underline{x}). \tag{4}$$

Approaching $\underline{x}^*(\overline{\underline{\theta}})$ first requires estimating $\underline{\theta}$. Classically, the final purpose of the experiment is not taken into account during the experimental design. However, as shown in Section 3, the definition of a conditional loss function can be used to derive an optimality criterion for the experiment which is closely connected to the response optimization problem. This loss function $\mathcal{L}(\hat{\underline{\theta}} \,|\, \overline{\underline{\theta}})$ is defined as the cost of estimating the parameters by $\hat{\underline{\theta}}$ when their true value is $\overline{\underline{\theta}}$. We wish to minimize $y(\underline{x}^*(\overline{\underline{\theta}})) - y(\underline{x}^*(\hat{\underline{\theta}}))$. The observations are not available at the design step and

we take $\mathcal{L}(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$ as the average difference $\underset{\underline{y} \mid \overline{\underline{\theta}}}{E}\{y(\underline{x}^*(\overline{\underline{\theta}})) - y(\underline{x}^*(\hat{\underline{\theta}}))\}$. From (1) this loss function (to be minimized) can be written as

$$\mathcal{L}(\hat{\underline{\theta}} \mid \overline{\underline{\theta}}) = \eta(\overline{\underline{\theta}}, \underline{x}^*(\overline{\underline{\theta}})) - \eta(\overline{\underline{\theta}}, \underline{x}^*(\hat{\underline{\theta}})). \tag{5}$$

It will now be used to derive a Bayesian estimator of $\underline{\theta}$ and to define an optimality criterion for the experiment.

Remark: An alternative parametrization of a response function quadratic in $\underline{x}$ could also be considered (Chatterjee and Mandal, 1981; Mandal, 1989), given by

$$\eta(\underline{\theta}, \underline{x}) = x_0 + \frac{1}{2}(\underline{x} - \underline{x}^*)^T Q(\underline{x} - \underline{x}^*),$$

where $\underline{x}^*$ is included in the parameters to be estimated, so that

$\underline{\theta} = (x_0, x_1^*, \ldots, x_m^*, Q_{11}, Q_{22}, \ldots, Q_{mm}, Q_{12}, Q_{13}, \ldots, Q_{1m}, Q_{23}, \ldots, Q_{2m}, \ldots, Q_{(m-1)m})^T$.

With this approach, the computation of $\underline{x}^*$ is explicitly taken into account when designing an experiment for estimating $\underline{\theta}$. However, the model response is nonlinear with respect to the parameters $\underline{x}^*$, so that classical design optimality criteria depend on the unknown value of $\underline{x}^*$. A Bayesian approach is suggested to get round this difficulty, but the cost (in terms of the expected response) of assuming that the parameters are $\hat{\underline{\theta}}$ when their true value is $\overline{\underline{\theta}}$ is not taken into account. Moreover, the approach seems to be restricted to ellipsoidal (Chatterjee and Mandal, 1981) or rectangular (Mandal, 1989) experimental regions. ◊

3. BAYESIAN ESTIMATION AND DESIGN

Let $\underline{y}_X$ be the N-dimensional vector of all observations performed on the process using the design X (of fixed size N), $X = \{\underline{x}^1, \underline{x}^2, \ldots, \underline{x}^N\}$, with possible replications ($\underline{x}^i = \underline{x}^j$ for some $i \neq j$). $\mathcal{L}(\hat{\underline{\theta}} \mid \overline{\underline{\theta}})$ depends on $\underline{y}_X$ through the estimate $\hat{\underline{\theta}}(\underline{y}_X)$, and a Bayesian risk $r(X)$ can be introduced,

$$r(X) = \underset{\underline{\theta}, \underline{y}_X}{E}\{\mathcal{L}(\hat{\underline{\theta}}(\underline{y}_X) \mid \underline{\theta})\} = \int p(\underline{y}_X) \left(\int \mathcal{L}(\hat{\underline{\theta}}(\underline{y}_X) \mid \underline{\theta})\, p(\underline{\theta} \mid \underline{y}_X)\, d\underline{\theta} \right) d\underline{y}_X. \tag{6}$$

The minimum risk estimator is then defined as

$$\hat{\underline{\theta}}_B(\underline{y}_X) \in \arg\min_{\hat{\underline{\theta}} \in \Theta} \int \mathcal{L}(\hat{\underline{\theta}} \mid \underline{\theta})\, p(\underline{\theta} \mid \underline{y}_X)\, d\underline{\theta} = \arg\min_{\hat{\underline{\theta}} \in \Theta} \underset{\underline{\theta} \mid \underline{y}_X}{E}\{\mathcal{L}(\hat{\underline{\theta}} \mid \underline{\theta})\},$$

or equivalently, from (5) and the linearity of $\eta(\underline{\theta}, \underline{x})$ with respect to $\underline{\theta}$ (2),

$$\hat{\underline{\theta}}_B(\underline{y}_X) \in \arg\min_{\hat{\underline{\theta}} \in \Theta} \mathcal{L}(\hat{\underline{\theta}} \mid \underset{\underline{\theta} \mid \underline{y}_X}{E}\{\underline{\theta}\}), \tag{7}$$

(the prior distribution $p(\underline{\theta})$ and the feasible parameter set Θ are assumed to be such that $E_{\underline{\theta}|\underline{y}_X}\{\underline{\theta}\} \in \Theta$). From (5), (7) can also be written

$$\hat{\underline{\theta}}_B(\underline{y}_X) \in \{\hat{\underline{\theta}} \in \Theta;\ \underline{x}^*(\hat{\underline{\theta}}) = \arg\max_{\underline{x}\in\mathcal{X}} \eta(E_{\underline{\theta}|\underline{y}_X}\{\underline{\theta}\}, \underline{x})\},$$

or equivalently

$$\hat{\underline{\theta}}_B(\underline{y}_X) \in \{\hat{\underline{\theta}} \in \Theta;\ \underline{x}^*(\hat{\underline{\theta}}) = \underline{x}^*(E_{\underline{\theta}|\underline{y}_X}\{\underline{\theta}\})\}.$$

$\hat{\underline{\theta}}_B(\underline{y}_X)$ can therefore be taken as the posterior mean,

$$\hat{\underline{\theta}}_B(\underline{y}_X) = E_{\underline{\theta}|\underline{y}_X}\{\underline{\theta}\}.$$

Note that this result is similar to the one obtained for loss functions $L(\hat{\underline{\theta}}|\underline{\theta})$ quadratic in $\hat{\underline{\theta}}$.

Replacing $\hat{\underline{\theta}}$ by $\hat{\underline{\theta}}_B$ in the expression (6) of the Bayesian risk $r(X)$, and taking (5) into account, one can write $r(X)$ as

$$r(X) = \int \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))\, p(\underline{\theta})\, d\underline{\theta} - \int p(\underline{y}_X) \left(\int \eta(\underline{\theta}, \underline{x}^*(\hat{\underline{\theta}}_B(\underline{y}_X)))\, p(\underline{\theta}|\underline{y}_X)\, d\underline{\theta} \right) d\underline{y}_X,$$

or equivalently, with the linearity of $\eta(\underline{\theta}, \underline{x})$ with respect to $\underline{\theta}$,

$$r(X) = \int \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))\, p(\underline{\theta})\, d\underline{\theta} - \int \eta(\hat{\underline{\theta}}_B(\underline{y}_X), \underline{x}^*(\hat{\underline{\theta}}_B(\underline{y}_X)))\, p(\underline{y}_X)\, d\underline{y}_X. \tag{8}$$

Given a prior distribution $p(\underline{\theta})$, the risk $r(X)$ can then be evaluated, at least in principle, for any design X and used as an optimality criterion for experimental design. However, the optimization of $r(.)$ with respect to X will require many such evaluations, so that we need some simplifying hypotheses and approximations.

Firstly, we shall assume that $\underline{\theta} \sim \mathcal{N}(\bar{\underline{\theta}}, \Omega)$. The marginal distribution $p(\underline{y}_X)$ is then $\mathcal{N}(Z_X\bar{\underline{\theta}}, \sigma^2 I_N + Z_X \Omega Z_X^T)$, where I_N is the N-dimensional identity matrix and Z_X is the N x p dimensional matrix the ith row of which is equal to $\underline{z}^T(\underline{x}^i)$. The posterior mean is then equal to

$$\hat{\underline{\theta}}_B(\underline{y}_X) = \left(\frac{1}{\sigma^2} Z_X^T Z_X + \Omega^{-1}\right)^{-1} \left(\frac{1}{\sigma^2} Z_X^T \underline{y}_X + \Omega^{-1}\bar{\underline{\theta}}\right), \tag{9}$$

and elementary algebraic calculations show that its predictive distribution is $\mathcal{N}(\bar{\underline{\theta}},\ \Omega - \left(\frac{1}{\sigma^2} Z_X^T Z_X + \Omega^{-1}\right)^{-1})$. The Bayesian estimate $\hat{\underline{\theta}}_B(\underline{y}_X)$ given by (9) will be used to obtain the estimated optimal inputs $\underline{x}^*(\hat{\underline{\theta}}_B(\underline{y}_X))$ via (4).

Secondly, we shall use a second-order power expansion of $\eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))$ around $\bar{\underline{\theta}}$,

$$\eta(\underline{\theta}, \underline{x}^*(\underline{\theta})) = \eta(\bar{\underline{\theta}}, \underline{x}^*(\bar{\underline{\theta}})) + (\underline{\theta} - \bar{\underline{\theta}})^T \frac{\partial \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta}}\Big|_{\bar{\underline{\theta}}} + \frac{1}{2}(\underline{\theta} - \bar{\underline{\theta}})^T \frac{\partial^2 \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta} \partial \underline{\theta}^T}\Big|_{\bar{\underline{\theta}}} (\underline{\theta} - \bar{\underline{\theta}}) + \ldots$$

Assuming that $\tilde{\underline{\theta}} \in \text{int}\,\Theta$, that $\underline{x}^*(\tilde{\underline{\theta}}) \in \text{int}\,\mathcal{X}$ is a stationary point of $\eta(\tilde{\underline{\theta}}, \underline{x})$ and that $\dfrac{\partial \underline{x}^{*T}(\underline{\theta})}{\partial \underline{\theta}}\Big|_{\tilde{\underline{\theta}}}$ exists, we compute the gradient vector and the Hessian matrix involved in this expansion. One has

$$\frac{\partial \eta(\tilde{\underline{\theta}}, \underline{x})}{\partial \underline{x}}\Big|_{\underline{x}^*(\tilde{\underline{\theta}})} = \underline{0}, \tag{10}$$

which gives

$$\frac{\partial \eta(\tilde{\underline{\theta}}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta}}\Big|_{\tilde{\underline{\theta}}} = \frac{\partial \underline{x}^{*T}(\underline{\theta})}{\partial \underline{\theta}}\Big|_{\tilde{\underline{\theta}}} \frac{\partial \eta(\tilde{\underline{\theta}}, \underline{x})}{\partial \underline{x}}\Big|_{\underline{x}^*(\tilde{\underline{\theta}})} = \underline{0},$$

which in turn implies

$$\frac{\partial \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta}}\Big|_{\tilde{\underline{\theta}}} = \frac{\partial \eta(\underline{\theta}, \underline{x}^*(\tilde{\underline{\theta}}))}{\partial \underline{\theta}}\Big|_{\tilde{\underline{\theta}}}.$$

From (2) the gradient vector thus satisfies

$$\frac{\partial \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta}}\Big|_{\tilde{\underline{\theta}}} = \underline{z}(\underline{x}^*(\tilde{\underline{\theta}})).$$

The Hessian matrix is then given by

$$\frac{\partial^2 \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta} \partial \underline{\theta}^T}\Big|_{\tilde{\underline{\theta}}} = \frac{\partial \underline{z}(\underline{x})}{\partial \underline{x}^T}\Big|_{\underline{x}^*(\tilde{\underline{\theta}})} \frac{\partial \underline{x}^*(\underline{\theta})}{\partial \underline{\theta}^T}\Big|_{\tilde{\underline{\theta}}}. \tag{11}$$

As a particular case, consider the quadratic model response (2), (3a) and (3b). Equation (10) gives $\underline{x}^*(\tilde{\underline{\theta}}) = -\,\tilde{Q}^{-1}\,\tilde{\underline{q}}$. Taking (3a) and (3b) into account, after elementary but lengthy algebraic calculations, one obtains

$$\frac{\partial \underline{z}(\underline{x})}{\partial \underline{x}^T}\Big|_{\underline{x}^*(\tilde{\underline{\theta}})} = -\,\frac{\partial \underline{x}^{*T}(\underline{\theta})}{\partial \underline{\theta}}\Big|_{\tilde{\underline{\theta}}} \tilde{Q},$$

which together with (11) gives

$$\frac{\partial^2 \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta} \partial \underline{\theta}^T}\Big|_{\tilde{\underline{\theta}}} = -\,A(\tilde{\underline{\theta}})\,\tilde{Q}\,A^T(\tilde{\underline{\theta}}), \tag{12}$$

with

$$A(\tilde{\underline{\theta}}) = \frac{\partial \underline{x}^{*T}(\underline{\theta})}{\partial \underline{\theta}}\Big|_{\tilde{\underline{\theta}}}. \tag{13}$$

Replacing $\eta(., \underline{x}^*(.))$ in (8) by its second-order expansion, one obtains

$$r(X) \simeq \frac{1}{2N} \Psi_{LB}(X),$$

with

$$\Psi_{LB}(X) = \text{trace}\left(\frac{\partial^2 \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta} \partial \underline{\theta}^T} \Big|_{\tilde{\underline{\theta}}} M_B^{-1}(X) \right), \tag{14}$$

where $M_B(X)$ is the Bayesian information matrix (per sample) (Pilz, 1983) given by

$$M_B(X) = \frac{1}{N} \left(\frac{1}{\sigma^2} Z_x^T Z_x + \Omega^{-1} \right). \tag{15}$$

To show that $\Psi_{LB}(X)$ is an L_B-optimality criterion (to be minimized), we must prove that the Hessian matrix $\frac{\partial^2 \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta} \partial \underline{\theta}^T} \Big|_{\tilde{\underline{\theta}}}$ is semi-definite positive. When this matrix is given by (12), it is non-negative definite when $\tilde{Q}$ is negative definite, i.e. when $\eta(\tilde{\underline{\theta}}, \underline{x})$ is maximum in $\underline{x} = \underline{x}^*(\tilde{\underline{\theta}})$. More generally, let $f(\underline{\theta})$ denote the function $\eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))$, where $\underline{x}^*(\underline{\theta})$ is given by (4). Assume that a convex neighborhood $\mathcal{U}$ of $\tilde{\underline{\theta}}$ exists, $\Theta \supset \mathcal{U}$. $\forall\, \underline{\theta}^1, \underline{\theta}^2 \in \mathcal{U}$, $\forall\, \alpha \in [0, 1]$, one has

$$f((1-\alpha)\underline{\theta}^1 + \alpha\underline{\theta}^2) = \eta((1-\alpha)\underline{\theta}^1 + \alpha\underline{\theta}^2, \underline{x}^*((1-\alpha)\underline{\theta}^1 + \alpha\underline{\theta}^2)),$$

$$= (1-\alpha)\, \eta(\underline{\theta}^1, \underline{x}^*((1-\alpha)\underline{\theta}^1 + \alpha\underline{\theta}^2)) + \alpha\, \eta(\underline{\theta}^2, \underline{x}^*((1-\alpha)\underline{\theta}^1 + \alpha\underline{\theta}^2)),$$

$$\leq (1-\alpha)\, \eta(\underline{\theta}^1, \underline{x}^*(\underline{\theta}^1)) + \alpha\, \eta(\underline{\theta}^2, \underline{x}^*(\underline{\theta}^2)) = (1-\alpha)\, f(\underline{\theta}^1) + \alpha\, f(\underline{\theta}^2).$$

The function f is thus convex, which implies that the Hessian matrix (11) is semi-definite positive and that Ψ_{LB} is an L_B-optimality criterion.

A general equivalence theorem for L_B-optimal continuous design measures can be proved (Pilz, 1983; Chaloner, 1984). It is used to define an algorithmic procedure guaranteed to converge to an L_B-optimal design measure (Pilz, 1983). Using a result from Chaloner (1984) we know that there exists an L_B-optimal design measure with at most $r(2p-r+1)/2$ different support points, with $r = \text{rank}\left(\frac{\partial^2 \eta(\underline{\theta}, \underline{x}^*(\underline{\theta}))}{\partial \underline{\theta} \partial \underline{\theta}^T} \Big|_{\tilde{\underline{\theta}}} \right)$.

Since we are interested here in fixed-size designs, we suggest to use the exchange algorithm presented by Pilz (1983). As it is generally the case for algorithms for exact designs, the convergence is not proved. For each problem we therefore perform several optimizations choosing various initial designs (the determination of an optimal design measure can be of help for this choice), and perform local optimizations (using standard nonlinear programming techniques) when the algorithm is no longer able to progress. This exchange algorithm could probably be improved following the ideas used in recent algorithms for D-optimality (see e.g. (Yonchev, 1988; Atkinson and Donev, 1989) and the references therein).

The optimal experiment for the criterion (14) depends on the values of N, $\tilde{\underline{\theta}}$, Ω and σ^2. The value of N can be fixed *a priori*, and it is always possible to determine the optimal experiment for $N' > N$ in order to evaluate how much could be gained if $N' - N$ additional

measurements were performed. The robustness of the design with respect to misspecifications in the values of $\tilde{\underline{\theta}}$, Ω and σ^2 is now illustrated by an example.

4. EXAMPLE

Consider a response variable y, with two input variables x_1 and x_2. These input variables must satisfy the following constraints, which define $\mathcal{X}$,

$$\sum_{i=1}^{2} x_i \leq 1,\ x_i \geq 0,\ i = 1, 2. \tag{16}$$

A quadratic model response is assumed to describe y correctly on the admissible domain for the inputs. We define $\eta(\underline{\theta}, \underline{x})$ as

$$\eta(\underline{\theta}, \underline{x}) = q_1 x_1 + q_2 x_2 + \frac{1}{2}(Q_{11} x_1^2 + 2 Q_{12} x_1 x_2 + Q_{22} x_2^2), \tag{17}$$

with

$$\underline{\theta} = (q_1, q_2, Q_{11}, Q_{22}, Q_{12})^T,\ \underline{x} = (x_1, x_2)^T. \tag{18}$$

4.1. Dependence of ξ^* on Ω and σ^2

Due to the expression of the Bayesian information matrix (15), the L_B-optimal experiment only depends on Ω and σ^2 through their ratio. Assuming that $\Omega/\sigma^2 = \alpha\, I_5$, $\alpha \in \mathcal{R}^+$, one can compute the L_B-optimal design measure $\xi^*(\alpha^o)$ associated with a given value α^o, and evaluate the efficiency of $\xi^*(\alpha^o)$ when $\alpha \neq \alpha^o$,

$$\varepsilon_{LB}(\xi^*(\alpha^o)|\alpha) = \frac{\Psi_{LB}(\xi^*(\alpha|\alpha))}{\Psi_{LB}(\xi^*(\alpha^o|\alpha))}. \tag{19}$$

Figure 1 presents the evolution of $\varepsilon_{LB}(\xi^*(\alpha^o|\alpha))$ as a function of α, $\alpha \in [1, 100]$, when $\alpha^o = 10$ and $\tilde{\underline{\theta}} = (3, 3, -10, -10, 0)^T$. A prior over-estimation of α (i.e. choosing $\alpha^o > \alpha$) is clearly of little consequence (the efficiency remains close to 1), while a prior under-estimation of α can lead to a design with small efficiency. This study is of course insufficient to assess the generality of this result; however, such tests of robustness can always be performed on any practical problem.

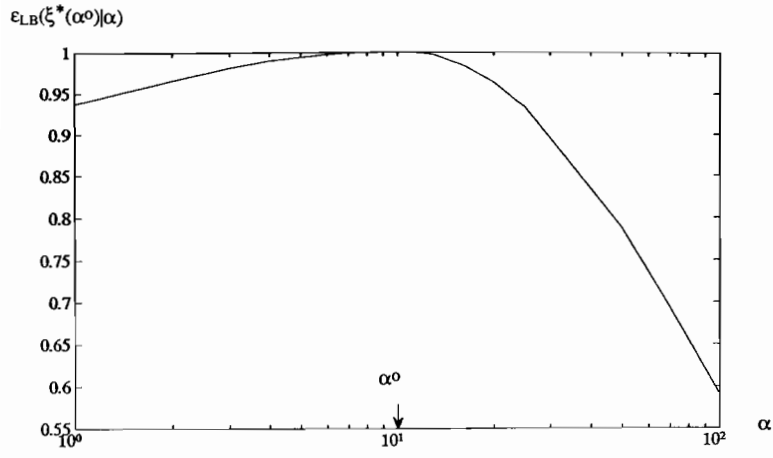


FIGURE 1 Efficiency $\varepsilon_{LB}(\xi^*(\alpha^o)|\alpha)$ (19) of the optimal design for $\alpha^o = 10$ as a function of α.

4.2. Dependence of ξ^* on $\underline{\theta}$, comparison with a non-Bayesian approach

Designs. Experimental design for parameter estimation has received considerable attention from statisticians (see e.g. the books (Fedorov, 1972; Silvey, 1980; Pazman, 1986) and the survey paper (Walter and Pronzato, 1990)). Any criterion from the general class given by Kiefer (1974) could be considered for estimating the parameters in the linear regression model (2). For the sake of brevity, only D-optimality (which is the most widely used) will be considered here. D-optimal design is defined by the criterion (to be maximized)

$$\Psi_D(X) = \det (Z_x^T Z_x). \tag{20}$$

The final purpose of the experiment is not taken into account. The parameters are estimated via maximum likelihood as

$$\hat{\underline{\theta}}_{ML}(\underline{y}_x) = (Z_x^T Z_x)^{-1} Z_x^T \underline{y}_x. \tag{21}$$

They are then used to obtain the estimated optimal inputs $\underline{x}^*(\hat{\underline{\theta}}_{ML}(\underline{y}_x))$ via (4).

D- and L_B-optimal discrete designs of size 5, respectively denoted by X_D and X_{LB}, have been computed for the example defined by (16)-(18). The D-optimal design was found to be

$$X_D = \{(0, 1), (1, 0), (0, 0.5), (0.5, 0), (0.5, 0.5)\}. \tag{22}$$

We assumed that $\Omega/\sigma^2 = 10 \times I_5$ and considered two values of $\underline{\theta}$, namely

$$\underline{\theta}_1 = (5, 10, -10, -10, -5)^T, \tag{23}$$

and

$$\tilde{\underline{\theta}}_2 = (3, 3, -10, -10, 0)^T. \tag{24}$$

Using the exchange algorithm described in (Pilz, 1983), we obtained

$$X_{LB}(\tilde{\underline{\theta}}_1) = \{(0, 1), (1, 0), (0.481, 0.519), (0.481, 0.519), (0.481, 0.519)\}, \tag{25}$$

and

$$X_{LB}(\tilde{\underline{\theta}}_2) = \{(0, 1), (1, 0), (0, 0.897), (0.533, 0.467), (0.533, 0.467)\}. \tag{26}$$

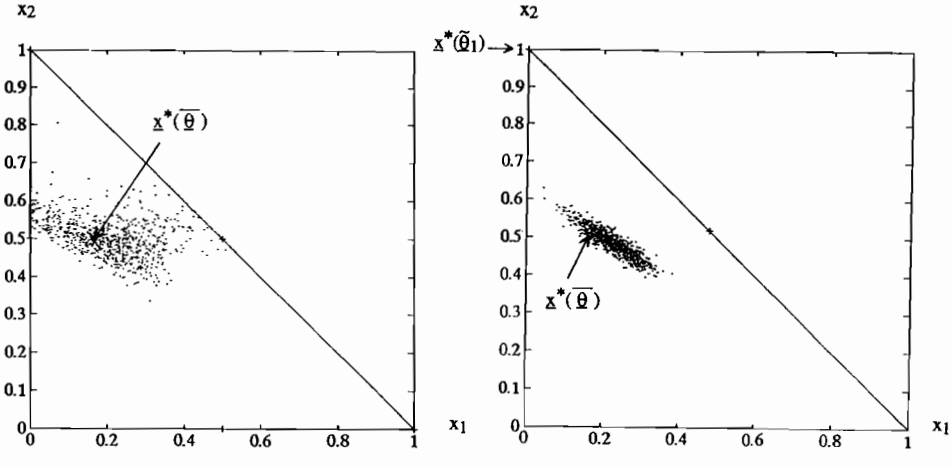
Simulations. Assume first that the prior is $\tilde{\underline{\theta}}_1$ (23). For both X_D and $X_{LB}(\tilde{\underline{\theta}}_1)$ we generated 1000 vectors of observations $\underline{y}_x^{(i)}$ according to

$$\underline{y}_x^{(i)} = Z_x \overline{\underline{\theta}} + \underline{\varepsilon}^{(i)}, \; i = 1,\ldots, 1000,$$

with $\underline{\varepsilon}^{(i)}$ normally distributed $\mathcal{N}(\underline{0}, 0.1 \times I_5)$. In order to test the robustness of the L_B-optimal policy with respect to errors in the prior mean $\tilde{\underline{\theta}}$, we chose $\overline{\underline{\theta}}$ different from $\tilde{\underline{\theta}}_1$,

$$\overline{\underline{\theta}} = (3.75, 7.5, -7.5, -13.33, -5)^T.$$

Estimated optimal inputs $\hat{\underline{x}}^{*(i)}$ were obtained for each $\underline{y}_x^{(i)}$, i = 1,..., 1000, and their locations are given on Figure 2a for X_D and Figure 2b for X_{LB}.



2a: D-optimal design (22) and maximum likelihood estimation (21)

2b: L_B-optimal design (25) and Bayesian estimation (9)

FIGURE 2 Location of the estimated optimal inputs.

The highest concentration of the $\hat{\underline{x}}^{*(i)}$, i = 1,..., 1000, around the true optimal input $\underline{x}^*(\overline{\underline{\theta}})$ is obtained for the Bayesian approach of Section 3 (Figure 2b). Although the prior information on the location of $\underline{x}^*$ is quite inexact, the bias in the location of $\underline{x}^*$ remains reasonable.

Assume now that the prior is $\tilde{\underline{\theta}}_2$ (24). For both X_D and $X_{LB}(\tilde{\underline{\theta}}_2)$ we generate 1000 vectors of observations $\underline{y}_x^{(i)}$ according to

$$\underline{y}_x^{(i)} = Z_x\, \overline{\underline{\theta}}^{(i)} + \underline{\varepsilon}^{(i)},\ i = 1,\ldots,\ 1000, \tag{27}$$

with $\underline{\varepsilon}^{(i)}$ and $\overline{\underline{\theta}}^{(i)}$ independently distributed $\mathcal{N}(\underline{0},\ 0.1 \times I_5)$ and $\mathcal{N}(\underline{\theta}^o,\ I_5)$ respectively. In order to test the robustness of the L_B-optimal policy with respect to errors in the prior mean $\tilde{\underline{\theta}}$, we assume that $\underline{\theta}^o$ can differ from $\tilde{\underline{\theta}}_2$, and parametrize $\underline{\theta}^o$ as a function of a scalar β,

$$\underline{\theta}^o(\beta) = (3+2\beta,\ 3+2\beta,\ -10,\ -10,\ 0)^T. \tag{28}$$

When $\beta = 0$, $\underline{\theta}^o(\beta) = \tilde{\underline{\theta}}_2$, and β is a measure of the error in the prior mean. Figure 3 presents the locus of the optimal inputs $\underline{x}^*(\underline{\theta}^o(\beta))$ when β varies from -1 to 1. Rather large errors in the prior location of the optimal input $\underline{x}^*(\tilde{\underline{\theta}}_2)$ are therefore considered.

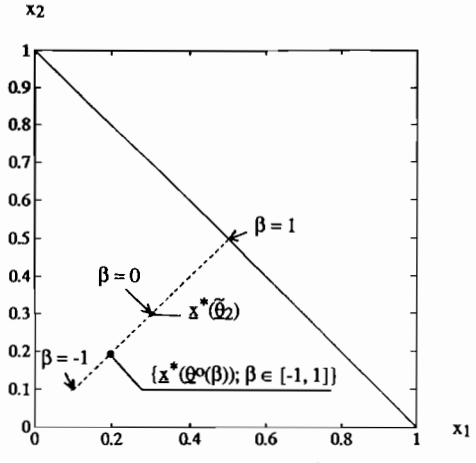


FIGURE 3 Optimal inputs $\underline{x}^*(\underline{\theta}^o(\beta))$ ($\underline{\theta}^o(\beta)$ given by (28), $\beta \in [-1, 1]$) and prior optimal input $\underline{x}^*(\tilde{\underline{\theta}}_2)$ ($\tilde{\underline{\theta}}_2$ given by (24)).

We then evaluate the following relative risk

$$\rho(X, \beta) = \frac{\sum_{i=1}^{1000} \eta(\overline{\underline{\theta}}^{(i)}, \underline{x}^*(\overline{\underline{\theta}}^{(i)})) - \eta(\overline{\underline{\theta}}^{(i)}, \hat{\underline{x}}^{*(i)})}{\sum_{i=1}^{1000} \eta(\overline{\underline{\theta}}^{(i)}, \underline{x}^*(\overline{\underline{\theta}}^{(i)}))}, \beta \in [-1,1], X = X_D, X_{LB}(\tilde{\theta}_2), \quad (29)$$

where the estimated optimal inputs, $\hat{\underline{x}}^{*(i)}$, i = 1,..., 1000, are determined from the simulated observations obtained according to (27). Figure 4 presents the evolution of $\rho(X, \beta)$ as a function of β for the D-optimal design (22) combined with maximum likelihood estimation (21) and for the L_B-optimal design (26) combined with posterior mean estimation (9). The second policy gives better results whatever the value of β between -1 and 1, and the relative risk is more than halved for almost all values of β.

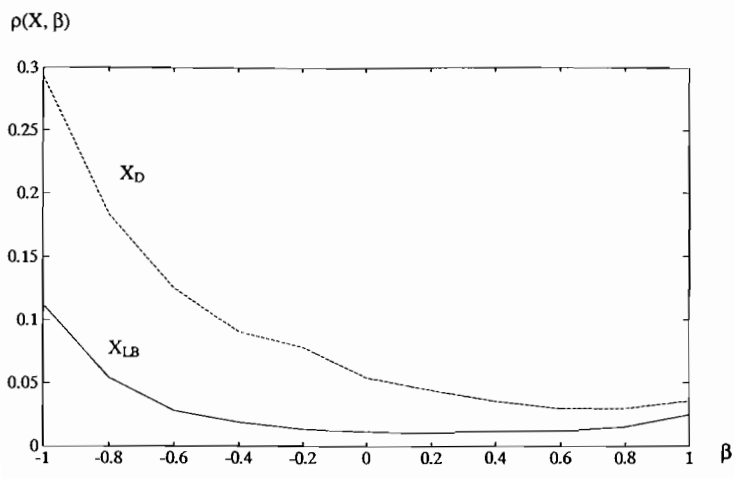


FIGURE 4 Relative risk $\rho(X, \beta)$ (29) as a function of β for the two policies X_D (22) -----, and X_{LB} (26) ——.

5. CONCLUSIONS

A Bayesian experimental design procedure has been suggested to be used when one is interested in response optimization rather than in a precise estimation of all the model parameters. After some simplifications, it has been formulated as the minimization of an L_B-optimality criterion. The resulting approach is computationally almost as simple as traditional D-optimal design, but gives better results regarding the intended model application. It could be

used in situations where a series of similar processes have to be studied, with a small number of measurements on each of them. First simulation results exhibit some insensitivity of the performances of the approach with respect to errors in the prior distribution. Further studies are required to assess such qualitative results, but in any practical situation simulated data can be used to test these robustness properties. Designs of size $N \leq \dim(\underline{\theta})$ are allowed, and all the examples that we considered with $N = \dim(\underline{\theta})$ yielded experiments involving replications, thereby requiring a small number of measurements on each process.

The model robustness issue has not been considered here. The model response was assumed to be properly described by the function $\eta(\underline{\theta}, \underline{x})$. Robustness with respect to errors in the model structure is considered for instance in (Blight and Ott, 1975; Sacks and Ylvisaker, 1985; Sacks and Schiller, 1988, Sacks *et al.* 1989), where some deterministic error components are superimposed to the response, with prior knowledge on their possible values. Another approach would consist in considering bounded disturbances from the function $\eta(\underline{\theta}, \underline{x})$. The results presented in (Pronzato and Walter, 1988, 1989) concerning experiment design for bounded error models could then be of help.

REFERENCES

Atkinson, A.C., and Donev, A.N. (1989). The construction of exact D-optimum experimental designs with application to blocking response surface designs. *Biometrika*, **76**(3) : 515-526.

Blight, B.J.N., and Ott, L. (1975). A Bayesian approach to model inadequacy for polynomial regression. *Biometrika*, **62** (1) : 79-88.

Box, G.E.P., and Wilson, K.B. (1951). On the experimental attainment of optimum conditions (with discussion). *J. Royal Stat. Soc.*, **B13**(1) : 1-45.

Brooks, S.H., and Mickey, R.M. (1961). Optimum estimation of gradient direction in steepest ascent experiments. *Biometrics*, **17** : 48-56.

Chaloner, K. (1984). Optimal Bayesian experimental design for linear models. *The Annals of Stat.*, **12**(1) : 283-300.

Chatterjee, S.K., and Mandal, N.K. (1981). Response surface designs for estimating the optimal point. *Calcutta Statist. Assoc. Bull.*, **30** : 145-169.

Fedorov, V.V. (1972). *Theory of Optimal Experiments*. Academic Press, New York.

Kiefer, J. (1974). General equivalence theory for optimum designs (approximate theory). *The Annals of Stat.*, **2**(5) : 849-879.

Mandal, N.K. (1989). D-optimal designs for estimating the optimum point in a quadratic response surface - rectangular region. *J. of Statistical Planning and Inference*, **23** : 243-252.

Montgomery, D.C. (1976). *Design and Analysis of Experiments*.Wiley, New York.

Pazman, A. (1986). *Foundations of Optimum Experimental Design*. Veda, Bratislava.

Pesotchinsky, L. (1982). Optimal robust designs: Linear regression in R^k. *Annals of Stat.*, **10**(2) : 511-525.

Pilz, J. (1983). *Bayesian Estimation and Experimental Design in Linear Regression Models*. Teubner Texte zur Mathematik, Leipzig.

Pronzato, L., and Walter, E. (1988). Experiment design for membership-set estimation: linear models with homogeneous and heterogeneous measurement errors. In Y. Dodge, V.V. Fedorov and H.P. Wynn (Eds.), *Optimal design and Analysis of Experiments*. North-Holland, Amsterdam, pp. 195-205.

Pronzato, L., and Walter, E. (1989). Experiment design in a bounded error context: comparison with D-optimality. *Automatica*, **25**(3) : 383-391.

Sacks, J., and Ylvisaker, D. (1985). Model robust design in regression: Bayes theory. *Proc. of the Berkeley Conf. in Honor of J. Neyman and J. Kiefer*, **2** : 667-679.

Sacks, J., and Schiller, S. (1988). Spatial designs. In S.S. Gupta and J.O. Berger (Eds.), *Statistical Decision Theory and Related Topics IV*. Springer, Berlin, pp. 385-399.

Sacks, J., Welch, W.J., Mitchell, T.J., and Wynn, H.P. (1989). Design and analysis of computer experiments (with discussion). *Statistical Science*, **4**(4) : 409-435.

Silvey, S.D. (1980). *Optimal Design*. Chapman and Hall, London.

Walter, E., and Pronzato, L., (1990). Qualitative and quantitative experiment design for phenomenological models: a survey. *Automatica*, **26**(2) : 195-213.

Yonchev, H. (1988). New computer procedures for constructing D-optimal designs. In Y. Dodge, V.V. Fedorov and H.P. Wynn (Eds.), *Optimal design and Analysis of Experiments*. North-Holland, Amsterdam, pp. 71-80.

OPTIMAL COMPOSITE SEQUENTIAL DESIGNS FOR EXPERIMENTS WITH MIXTURE AND PROCESS VARIABLES

H. Yonchev
Higher Institute of Chemical Technology - Sofia,
Dept. of Automation, Sofia 1156, Bulgaria

1. INTRODUCTION

The majority of investigations for developing new products of high quality are based on experiments with different kinds of mixtures. The special nature of these experiments, known as mixture experiments, is due to the fact that in a q-component mixture the sum of the proportions of the components is unity. If the proportion of the i-th component is denoted by x_i then

$$\sum_{i=1}^{q} x_i = 1, \qquad \text{and} \tag{1}$$

$$0 \le x_i \le 1, \quad i = 1,2,\ldots,q\ . \tag{2}$$

The experimental region formed by the constraints (1) and (2) is (q-1)-dimensional regular simplex. In many cases the experiment is performed in a subarea of the simplex formed by the additional constraints A_i and B_i imposed by economic or technological considerations on the mixture components

$$0 \le A_i \le x_i \le B_i \le 1, \quad i=1,2, \ldots, q \tag{3}$$

The proportions x_i are called "related" or mixture variables.

The temperature, the pressure or the reaction time of the technological process of manufacturing the product are called "process variables". They are varied in coded form in a hypercube defined by the constraints

$$-1 \le x_i \le 1, \quad i=q+1, q+2, \ldots, m \tag{4}$$

The number of the "process variables" is r=m-q, where by m is denoted the total number of variables

The success of statistical modeling of the mixture properties using both kinds of variables depends on the information obtained by the experimental designs. Specific problems arise while designing optimal experimental plans in that case due to the necessity of working with mixture variables in a simplex or its subarea while the process variables are varied in a hypercube in Euclidean factor space.

The designs can be judged by various criteria. In the majority of problems arising in the practice the following six requirements mentioned by

Box and Draper (1975) are to be taken into account. The design should:

1. Generate a satisfactory distribution of information throughout the region of interest;
2. Ensure that the fitted value at $\vec{x}$, $\hat{Y}(x)$ be as close as possible to the true value $\eta(\vec{x})$ at $\vec{x}$;
3. Allows designs of increasing order to be built up sequentially;
4. Require a minimum number of experimental points;
5. Not require an impractical large number of levels of the predictor variables;
6. Give good detectability of lack of fit.

In this paper a method and algorithm for constructing by computer a new kind of designs for experiments with mixture and process variables are proposed. They are based on the six important requirements mentioned above.

To satisfy the first and the second ones of them the design points are distributed in the factor space according to D- an G-optimality criteria.

To satisfy the third criterion the design matrix is made as a composition of designs for models of increasing order. Then a sequence of points is added to ensure the requirements of the fourth criterion. This gives the experimenter the possibility of choosing a design with the minimum number of experimental trials needed.

The fifth criterion is accounted by searching the design points on the set of "candidates" with a limited number of levels for each coordinate. For example the possible set of "candidates" are the points of support of the continuous D-optimum designs.

The detectability of lack of fit is facilitated by the possibility of choosing the number of design points i.e. the degrees of freedom for determining the residual variance.

The new kind of designs is called "Optimal composite sequential designs", (OCSD). The general idea of OCSD was presented by Yonchev (1990) where it was developed for experiment with "process variables" only.

2. OPTIMAL COMPOSITE SEQUENTIAL DESIGNS

2.1. Some basic definitions and assumptions

It is assumed that the response surface can be described by the equation

$$Y_i = \vec{f}^T(\vec{x}_i)\vec{\beta} + \varepsilon_i, \quad i=1,2, \ldots, N , \tag{5}$$

where Y_i is the experimental value of the response obtained in the i-th run, $\vec{x}$ is a m×1 vector of predictor variables for the i-th run; $\vec{f}$ is a vector of k functions modeling the dependence of the response at $\vec{x}_i$. $\vec{\beta}$ is a k×1 vector of model coefficients; ε_i is the experimental error for the i-th run. The errors are uncorrelated, with mean zero and constant variance $\sigma_\varepsilon^2 = 1$. The covariance matrix of the least squares estimated parameters $\vec{\beta}$ is $(F^TF)^{-1}\sigma_\varepsilon^2$, where $F=(\vec{f}_i^T(\vec{x}_i))$, i=1,2, ..., N. The variance of prediction at a point $\vec{x}$ is given by

$$d(\vec{x}) = \vec{f}^T(\vec{x})(F^TF)^{-1}\vec{f}(\vec{x})\sigma_\varepsilon^2 . \tag{6}$$

A design with $F=F^*$ is said to be D-optimal with respect to the model (5) if it minimizes the determinant of the covariance matrix $(F^TF)^{-1}$ over the factor space χ, i.e.

$$\det (F^{*T}F^{*})^{-1} = \min_{\chi} (F^{T}F)^{-1} . \qquad (7)$$

The D-optimality criterion is essentially a parameter estimation criterion giving the smallest possible confidence region for the parameter estimates.

A design is said to be G-optimal one if it minimizes max $d(\vec{x})$, where the maximum is taken over the all possible vectors $\vec{x}$ of predictor variables. G-optimality is a response estimation criterion which minimizes the maximum value of the variance of prediction at the points of the factor space χ. A good introduction to D- and G- optimality is provided by the review of St. John and Draper (1975).

2.2. The general idea of developing optimal composite sequential designs

The general equation (5) is reduced to the following form

$$Y_i = \vec{f}_1^{T}(\vec{x}_i)\vec{\beta}_1 + \vec{f}_2^{T}(\vec{x}_i)\vec{\beta}_2 + \varepsilon_i, \; i=1,2, \ldots, N , \qquad (8)$$

where $\vec{f}_1^{T}(\vec{x}_i)$ and $\vec{f}_2^{T}(\vec{x}_i)$ are vectors of k_1 and k_2 functions correspondingly; $\vec{\beta}_1$ and $\vec{\beta}_2$ are $k_1 \times 1$ and $k_2 \times 1$ vectors of the model coefficients ($k_1 + k_2 = k$);

The following notations are also used

$$P_1 = \vec{f}_1^{T}(\vec{x}_i)\vec{\beta}_1 , \qquad (9)$$

$$P_2 = \vec{f}_1^{T}(\vec{x}_i)\vec{\beta}_1 + \vec{f}_2^{T}(\vec{x}_i)\vec{\beta}_2 , \qquad (10)$$

and

$$P_2^{*} = \vec{f}_2^{T}(\vec{x}_i)\vec{\beta}_2, i=1,2, \ldots, N , \qquad (11)$$

$$Y_i = P_2 + \varepsilon_i , \text{ or} \qquad (12)$$

$$Y_i = P_2 + P_2^{*} + \varepsilon_i , \quad i=1,2, \ldots, N . \qquad (13)$$

It is assumed that the polynomial P_1 of order n_1 is good for beginning the experimental investigation but it is possibly underestimating the shape of the response surface and a model P_2 of order n_2, ($n_2 > n_1$) will give a better fit. Taking into account this fundamental assumption the process of constructing the experimental plan is developed into the following four stages.

Stage 1. A design with a minimal number of observations and possibly best informative properties is constructed for the model P_1. Usually it is a saturated D-optimal design with $N_1 = k_1$ points and will be denoted by ξ_1. The points of the design ξ_1 are situated in the block A shown in table 1.

Stage 2. The design ξ_1 is augmented with a block of k_2 additional points (block B) to obtain the saturated near D-optimum design ξ_2 for the model P_2. These points can be used for checking the goodness of fit of P_1 and to improve its predictive properties. If the model P_1 does not fit, the design ξ_2 can be

used for evaluating k coefficients of the model of order P_2.

Stage 3. The points in the block B are arranged in decreasing order of the maximum value of the variance of prediction, calculated for model of order n_1 and designs with k_1+1, k_1+2, ..., k_1+k_2 points. This ordering allows the experimenter to choose a design with a desirable number of points for checking the lack of fit of the model of order n_1 or to improve its predictive properties.

Stage 4. To check the goodness of fit of the model of order n_2 and to obtain better estimates of its coefficients additional observations are needed. Their number depends on many different conditions but in rare cases it exceeds k_2. To give the experimenter the possibility of choosing the number of desired additional observations a group of k points (block C) are sequentially added to the design ξ_2. To improve the predictive properties of model P_2 the points of block C are found using the criterion of G-optimality. So the (k+1)-th point $\vec{x}^*_{k+1}$ is searched in the whole factor space as a point with maximum value of the variance of prediction

$$\sigma^2\{\hat{Y}(\vec{x}^*_{k+1})\} = \max_{\chi} \vec{f}^T(\vec{x})(F_k^T F_k)^{-1}\vec{f}(\vec{x})\sigma_\varepsilon^2 , \qquad (14)$$

where F_k is the augmented matrix of the design with k points and model P_2. The next point $\vec{x}^*_{k+2}$ is searched in the same way for the design with k+1 points and model P_2. So the points of block C together with block A and block B constitute a sequence of G-optimal designs for model P_2.

TABLE 1

No	x_1 x_2 ... x_q x_{q+1} x_{q+2} ... x_m
1 2 ⋮ k_1	BLOCK A
k_1+1 k_1+2 ⋮ $k=k_1+k_2$	BLOCK B
k+1 k+2 ⋮ 2k	BLOCK C

The approach of combining two criteria using D-optimality to obtain saturated designs and to augment it with additional points was used earlier by Vuchkov, Yonchev, Damgaliev, Tsochev and Dikova (1978). Here this approach is used to construct optimal composite sequential designs.

3. THE ALGORITHM FDOPCMP FOR CONSTRUCTING OPTIMAL COMPOSITE SEQUENTIAL DESIGNS FOR EXPERIMENTS WITH MIXTURE AND PROCESS VARIABLES

Different versions of the general algorithm for generating OCSD are worked out depending on the factor space being used. They take into account the peculiarities of searching the design points in a hypercube, in a simplex or in a subarea of the simplex defined by (3). But all of them are divided into two big groups: 1. Algorithms for searching the designs in the whole continuous factor space and 2. Algorithms for searching the design points on a given preliminary finite set of "candidate points". The algorithm FDOPCMP from the second group will be used to illustrate the main peculiarities of the algorithms developed for constructing OCSD for experiments with mixture and process variables.

The stages of FDOPCMP follow the four stages of constructing OCSD described in section 2.

Stage 1. Constructing a saturated D-optimum design for model of order n_1

1.1. The structure of the models P_1 and P_2 is specified

1.2. A set S_1 of L_1 "candidate points" for searching D-optimal designs for models of order P_1 is generated. For example the set S_1 can be formed by the support points of the continuous D-optimal design for models of order n_1.

1.3. Using the procedure FDOP of Yonchev (1988) a saturated D-optimal design $\xi_1(k_1)$ with $N_1=k_1$ points is found on the set S_1. The design is included in block A.

1.4. The values of $M^{-1}\left(\xi_1(k_1)\right)$, det $M\left(\xi_1(k_1)\right)$, $d(\vec{x}_i)$, i=1,...,L_1 are calculated and saved.

Stage 2. Constructing an optimal design for a model P_2 of order n_2.

2.1. A set S_2 of L_2 "candidate points" for constructing D-optimal design for model P_2 is generated.

2.2. The points of S_2 are randomly distributed into R groups with p points each.

2.3. An initial design $\xi_0(k)$ with k-points is constructed. Its first k_1 points are formed by the design $\xi_1(k_1)$. The next k_2 points are taken at random from S_2. The values of M $\left(\xi_0(k)\right)$, det $M\left(\xi_0(k)\right)$ are calculated an saved.

2.4. The first group of S_2 is added to the initial design forming a "candidate list" with H=k+p points. The values of M_H^{-1}, det M_H and $d_H(\vec{x}_i)$, i=k_1+1, k_1+2, ..., H are determined.

2.5. The point $\vec{x}_{min}$ with a minimum value of d(H) is found on the "candidate list" with $H_1=H-k_1$ points (The points of the design $\xi_1(k_1)$ are excluded).

2.6. The point $\vec{x}_{min}$ is deleted from the "candidate list" in which H-1

points are left. The values of M^{-1}, det M and $d(\vec{x}_i)$, i=k_1+1, k_1+2, ..., H are updated for H_1-1 points using the formulae

$$M^{-1}_{H-1}=M^{-1}_H+\left(M^{-1}_H\vec{f}(\vec{x}_{min})\right)\left(M^{-1}_H\vec{f}(\vec{x}_{min})\right)^T/\left(1-\vec{f}^T(\vec{x}_{min})\ M^{-1}_H\vec{f}(\vec{x}_{min})\right) \quad (15)$$

$$d_{H-1}(\vec{x}_i)=d_H(\vec{x}_i)+\left(\vec{f}^T(\vec{x}_i)M^{-1}_H\vec{f}(\vec{x}_{min})\right)^2/\left(1-\vec{f}^T(\vec{x}_{min})M^{-1}_H\vec{f}(\vec{x}_{min})\right) \quad (16)$$

$$\det M_{H-1}=\det M_H\left(1-\vec{f}^T(\vec{x}_{min})M^{-1}_H\vec{f}(\vec{x}_{min})\right) \quad (17)$$

2.7. The procedure is repeated from point 2.5. and a second point with minimum value of d_H is deleted from the "candidate list". In this way points with minimum value of d_H are sequentially deleted until k points are left in the "candidate list". A design $\xi_1(k)$ is obtained and one "little excursion" is counted out.

2.8.The design $\xi_1(k)$ is taken as a new initial design if the following condition is fulfilled

$$\det M(\xi_1(k))/\det M(\xi_0(k)) > 1+\epsilon \quad (18)$$

where ϵ is a sufficiently small numeral.

2.9. Another group of p points from S is added to the new initial design (or to the old one depending on the condition (18)) and a new "candidate list" is formed. The points are added one by one, updating at each step M^{-1}, det M and $d(\vec{x}_i)$, i=k_1+1, k_1+2, ..., H by the formulae (15), (16) and (17) transformed for addition of points.

2.10. A "little excursion" is made on the new "candidate list" and the procedure is repeated R times until the set set S_2 is exhausted. The sequence of R "little excursions" form an "excursion" over the set S_2. At the end of the "excursion" a design $\xi_R(k)$ is found.

An excursion is successful if the following condition is fulfilled

$$\det M(\xi_R(k))/\det M(\xi_0(k)) > 1+\epsilon \quad (19)$$

2.11. If the excursion is successful a new one is performed including in the "candidate list" the design $\xi_R(k)$. In the case of unsuccessful excursion the old design $\xi_0(k)$ is included.

2.12. The Stage 2 is finished after a given number t of unsuccessful excursions is performed. The best design obtained is denoted by $\xi_k(k)$ and includes block A and block B shown in table 1.

Stage 3. Rearranging the points in block B

3.1. The values of the variance of prediction $d_i=\sigma^2_i\{\hat{Y}_i\}$, i=$k_1$+1, k_1+2, ...,K for a model P_1 are calculated in the points of block B using the formula

$$d_i = \vec{f}_1^T(\vec{x}_i)(F_1^T F_1)^{-1}\vec{f}_1(\vec{x}_i), \quad i=k_1+1,\ k_1+2,\ \ldots,\ K \qquad (20)$$

where F_1 is the augmented matrix of the design $\xi_1(k_1)$ for model P_1 obtained at the end of the first stage of the algorithm.

3.2. The points of block B are rearranged in decreasing order of maximum values of the variance of prediction, calculated for model P_1 and designs with $k_1+1,\ k_1+2,\ \ldots,\ K$ points.

Stage 4. Augmenting the design for model P_2

4.1. The variance of prediction $d_i=\sigma^2\{\hat{Y}(\vec{x}_i)\}$ is calculated in each point of the set $S=S_1+S_2$ by the formula

$$d_i=\sigma^2\{\hat{Y}(\vec{x}_i)\}=\vec{f}^T(\vec{x}_i)(F_k^T F_k)^{-1}\vec{f}(\vec{x}_i), \quad i=1,2,\ldots,L\ , \qquad (21)$$

where F_k is the augmented matrix of the design $\xi_k(k)$. The values of d_i are saved.

4.2. The point $\vec{x}_{max}$ with maximum value of d_i is found.

4.3. The point $\vec{x}_{max}$ is added to the design $\xi_k(k)$ with k+1 points

4.4. For the design $\xi_{k+1}(k)$ are updated the values of d_i in L+1 points of S, $M_{k+1}^{-1}=(F_{k+1}^T F_{k+1})^1$ and d_{k+1} using the transformed formulae (15),(16) and (17).

4.5. The procedure is repeated from point 4.2. and a new point with maximum value of d_i, found on the set of L-1 points of S is added to the design $\xi_{k+1}(k)$. A design with k+2 points is obtained.

4.6. The procedure of sequentially adding new points terminates whenever a given number of points is added. Normally k points are added.

4. SOME COMMENTS AND EXAMPLES

Three kinds of optimal composite sequential designs can be generated for experiments with mixture and process variables:

1. The design is composite with respect to the mixture variables
2. The design is composite with respect to the process variables
3. The design is composite with respect to both mixture and process variables

The following example illustrate the constructing of OCSD by the algorithm FDOPCMP.

Example 1. In the table 2 is shown an optimal composite sequential design in three mixture variables x_1, x_2, x_3 and three process variables x_4, x_5, x_6. The first 21 points form a saturated D-optimal design ξ_1 for a second order model P_1 with respect to both kinds of variables ($n_1=2$, $n_3=2$). The model P_1 is given by the polynomial:

$$\hat{y} = \sum_{i=1}^{3} b_i x_i + \sum_{i=1}^{5} \sum_{i<j}^{6} b_{ij} x_i x_j + \sum_{i=4}^{6} b_{ii} x_i^2 \qquad (22)$$

The design is found at the first stage of the search by the procedure FDOP over the set S_1. To obtain the set S_1 the coordinates of its points are found as a full combination of the levels [0; 0.5; 1] and [-1; 0; 1] which correspond to the support of the continuous D-optimal designs in mixture and process variables. The coordinate 0.333 is also added.

The next four points (22, 23, 24 and 25) are forming a block B which augments the design ξ_1 to a saturated near D- optimal one ξ_2 for a model of third order (n_2=3) with respect to the mixture variables and second order (n_3=2) with respect to the process variables P_2:

$$\hat{y} = \sum_{i=1}^{3} b_i x_i + \sum_{i=1}^{5} \sum_{i<j}^{6} b_{ij} x_i x_j + \sum_{i=1}^{2} \sum_{i<j}^{3} c_{ij} x_i x_j (x_i - x_j) + b_{123} x_1 x_2 x_3 + \sum_{i=4}^{6} b_{ii} x_i^2 \qquad (23)$$

TABLE 2

No	x_1	x_2	x_3	x_4	x_5	x_6	No	x_1	x_2	x_3	x_4	x_5	x_6
1	0.000	0.500	0.500	1	1	1	26	0.788	0.212	0.000	1	1	1
2	0.000	0.000	1.000	-1	-1	-1	27	0.788	0.000	0.212	-1	0	1
3	0.000	0.500	0.500	0	0	-1	28	0.212	0.788	0.000	1	1	1
4	0.500	0.500	0.000	-1	1	-1	29	0.333	0.333	0.333	1	0	1
5	0.000	0.000	1.000	1	1	-1	30	0.000	0.000	1.000	0	-1	1
6	0.000	0.000	1.000	-1	0	1	31	0.000	0.788	0.212	-1	1	-1
7	0.333	0.333	0.333	-1	-1	1	32	0.788	0.000	0.212	1	-1	-1
8	1.000	0.000	0.000	1	-1	1	33	0.212	0.000	0.788	1	-1	-1
9	0.000	1.000	0.000	1	1	-1	34	0.788	0.212	0.000	-1	-1	0
10	0.000	0.000	1.000	1	-1	0	35	0.000	0.212	0.788	-1	1	-1
11	0.500	0.500	0.000	1	-1	-1	36	0.333	0.333	0.333	0	1	0
12	1.000	0.000	0.000	1	1	-1	37	0.000	0.788	0.212	1	-1	-1
13	0.000	0.000	1.000	-1	1	0	38	0.788	0.000	0.212	-1	1	-1
14	0.500	0.000	0.500	1	0	0	39	0.000	0.000	1.000	1	1	1
15	0.000	1.000	0.000	1	-1	1	40	0.788	0.212	0.000	0	0	-1
16	1.000	0.000	0.000	-1	1	1	41	0.212	0.788	0.000	0	-1	1
17	1.000	0.000	0.000	-1	-1	-1	42	0.000	0.212	0.788	1	-1	1
18	0.000	1.000	0.000	-1	-1	-1	43	0.212	0.000	0.788	-1	1	-1
19	0.500	0.500	0.000	0	0	0	44	1.000	0.000	0.000	1	1	0
20	0.000	1.000	0.000	-1	1	1	45	1.000	0.000	0.000	0	-1	1
21	0.500	0.000	0.500	0	1	1	46	0.000	1.000	0.000	1	1	-1
22	0.000	0.788	0.212	-1	-1	1	47	0.000	1.000	0.000	-1	-1	-1
23	0.212	0.788	0.000	-1	0	0	48	0.000	1.000	0.000	-1	1	1
24	0.212	0.000	0.788	-1	0	1	49	0.000	0.212	0.788	1	0	-1
25	0.000	0.212	0.788	-1	-1	1	50	1.000	0.000	0.000	-1	0	-1

The points of the block B are searched on the set S_2, obtained as a full combination of the levels [0.000; 0.500; 1.000; 0.788; 0.212 0.333] of the

mixture variables and [-1; 0; 1] of the process-variables. At the third stage of the algorithm they are rearranged in decreasing order of the values of the maximum variance of prediction $d(n_1, n_3)$ calculated sequentially for a designs with 22, 23, 24 and 25 points and a model P_1. The points 26÷50 constitute a sequence of designs found by the G-optimality criterion over the set $S=S_1+S_2$ and a model P_2.

In the table 3 are given the values of variance of prediction and $\det(F^TF)$ for the different models and designs which can be obtained on the base of the optimal composite sequential design.

TABLE 3

No	$\det(F^TF)_{n_1,n_3}$	$\det(F^TF)_{n_2,n_3}$	$d(n_1,n_3)$	$d(n_2,n_3)$
21	2.706E -19		2.887	
22	2.486E -19		2.861	
23	1.991E -19		2.546	
24	1.548E -19		2.545	
25	1.233E -19	5.946E -35	2.312	5.334
26	1.722E -19	1.413E -34	2.188	5.192
27	1.409E -19	3.405E -34	2.073	3.039
28	1.262E -19	5.540E -34	2.073	2.760
29	1.010E -19	8.663E -34	2.054	2.335
30	1.513E -19	1.238E -33	1.623	2.024
31	1.709E -19	1.650E -33	1.477	1.981
32	1.956E -19	2.224E -33	1.426	1.837
33	1.877E -19	2.923E -33	1.409	1.767
34	1.881E -19	3.834E -33	1.408	1.743
35	1.842E -19	5.094E -33	1.379	1.664
36	1.772E -19	6.711E -33	1.343	1.395
37	2.046E -19	8.104E -33	1.333	1.360
38	2.403E -19	9.818E -33	1.317	1.351
39	3.226E -19	1.206E -32	0.957	1.128
40	3.184E -19	1.362E -32	0.922	1.105
41	3.231E -19	1.546E -32	0.837	0.990
42	3.184E -19	1.685E -32	0.834	0.911
43	2.963E -19	1.788E -32	0.823	0.882
44	3.328E -19	1.894E -32	0.823	0.853
45	3.785E -19	2.001E -32	0.786	0.812
46	4.262E -19	2.093E -32	0.729	0.808
47	4.689E -19	2.211E -32	0.721	0.804
48	5.186E -19	2.356E -32	0.708	0.787
49	5.175E -19	2.514E -32	0.677	0.739
50	5.559E -19	2.638E -32	0.662	0.712

Optimal sequential designs composite with respect to both kinds of variables are constructed in the same way. The basic difference arises while generating the sets of "candidate points".

On the base of the algorithm FDOPCMP a FORTRAN-77 program is developed. The computer experiments are conducted on VAX 11/750 VMS computer. A catalogue of optimal composite sequential designs is generated for polynomial models of order $n_1=2$ and $n_2=3$ for up to ten variables. The designs are composite with

respect to mixture variables, process variables and both kind of variables.

5. REFERENCES

Box, G.E.P. and Draper, N.R. (1975). Robust Designs. Biometrika 62:347-352.

St. John, R.C. and Draper, N.R.(1975). D-optimality for regression designs: a review, Technometrics, 17:15-24.

Vuchkov, I., Yonchev, H.A., Damgaliev, D.L., Tsochev, V.K. and Dikova, T.D. (1978). Catalogue of Sequentially Generated Designs. Department of Automation, Higher Institute of Chemical Technology, Sofia, Bulgaria.

Yonchev, H.A. (1988). New Computer Procedures for Constructing D-optimal Designs. Optimal Design and Analysis of Experiments, Proceedings of the International Conference - Workshop, Neuchatel, Switzerland, Elsevier Science Publishers, 71-80.

Yonchev H.A. (1990) Optimal Composite Sequential Designs. Submitted for publication to REBRAPE, Brazil.

DESIGN OF EXPERIMENT SUPPLYING TRAINING SAMPLE FOR PATTERN RECOGNITION

N. E. Manolov,
Higher Institute of Chemical Technology,
Department of Automation, Sofia, Bulgaria

1. INTRODUCTION

There are many kinds of objects that can be investigated by means of experimental designs. One of them is case when input variables are continuous and one or several outputs are discreet (with two levels). In this case decision function between 2 areas in the space of input variables x, corresponding to 2 qualitative values of output may be polynomial and its coefficients may be estimated using pattern recognition methods. Of importance is how many experiments will be necessary to obtain a decision function, possessing a satisfactory predictive ability. This paper proposes design of experiments, solving some specific aspects of the above mentioned problem.

2. PROBLEM STATEMENT

Let us assume, that we have to investigate an object with 2 conditions of output: y=1 or y=-1, corresponding to 2 uncrossing areas of $\underline{x}$ values ω_1 and ω_2 in the multivariate space of inputs. The problem of describing such an object by polynomial decision function $d(\underline{x})=0$ such that

$$d(\underline{x}_i) < 0 \qquad \text{if } \underline{x}_i \in \omega_1 \quad \text{and}$$

$$d(\underline{x}_i) > 0 \qquad \text{if } \underline{x}_i \in \omega_2 \qquad (1)$$

can be resolved by an iterative version of the least squares method, known as Ho-Kashyap algorithm (1965).

Let $\underline{x}^T=(1,x_1,x_2,..,x_m,x_1x_2,..,x_{m-1}x_m,x_1^2,..,x_m^2)$ and $d(\underline{x})=\underline{w}^T\underline{x}$ and let suppose $\underline{x} = -\underline{x}$, if $\underline{x} \in \omega_2$. Then we can replace (1) by condition $\underline{w}^T\underline{x} > 0$, or by equation

$$\underline{w}^T\underline{x}_i = y_i \qquad i=1,2,\ldots,Np \qquad (2)$$

where $y_i>0$, $\underline{w}$ is a vector of classifier, $\underline{x}_i$ are pattern vectors

and Np the is number of patterns.

Let matrix

$$X = (\underline{x}_1 | \underline{x}_2 | \ldots | \underline{x}_{Np})^T$$

then equalities (2) may be written as follows

$$X\underline{w} = \underline{y}, \qquad (3)$$

where $\underline{y} = (y_1 | y_2 | \ldots | y_{Np})^T$. Now the unknown w can be estimated by the following iterative procedure:

$$\begin{aligned} \underline{w}(1) &= (X^T X)^{-1} X^T \underline{y}(1) \\ \underline{e}(k) &= X\,\underline{w}(k) - \underline{y}(k) \\ \underline{w}(k+1) &= \underline{w}(k) + c\,(X^T X)^{-1} X^T [\underline{e}(k) + |\underline{e}(k)|] \\ \underline{y}(k+1) &= \underline{y}(k) + c\,[\underline{e}(k) + |\underline{e}(k)|] \end{aligned} \qquad (4)$$

where $0<c\leq 1$; $|\underline{e}|$ is a vector, composed from the absolute values of the components of $\underline{e}$; k is number of iteration.

Proof of its convergence is given by Ho and Kashyap (1966) in the case of separability of the patterns.

Solving the problem of design the experiment supplying patterns for a learning procedure, we must take into account the following peculiarities:

1.Experimental points (patterns) must be located as near as possible to the decision boundary between 2 areas in the space of input $\underline{x}$ (Fukunaga 1972).

2.We need an approximately equal number of patterns corresponding to ω_1 and ω_2.

It is evident,that we can't take into consideration the above conditions before we know the true location of the decision boundary. Therefore we come to the idea of sequential design of the training experiments.

3. SIMPLE EXAMPLE FOR SEQUENTIAL DESIGN

Consider the situation where we have 2 independent input variables x_i limited by conditions:

$$x_{i,min} \leq x_i \leq x_{i,max} \qquad i=1,2 \qquad (5)$$

Let us assume that 2 patterns $\underline{x}(1) \in \omega_1$ and $\underline{x}(2) \in \omega_2$ are known and their belonging are established by an experiment.Then we can calculate the components of $\underline{x}(3)$ so that $\underline{x}(1)$, $\underline{x}(2)$ and $\underline{x}(3)$ form a regular simplex. Now we establish belonging of the new pattern $\underline{x}(3)$ to one of the two classes by a new experiment. Let $\underline{x}(3) \in \omega_1$.Disposing of two patterns from ω_1 and one from ω_2 we can reflect point $\underline{x}(1)$ replacing it by a new point $\underline{x}(4)$ and establishing its belonging.So we can formulate the following rules:

1.A point from the current simplex must be reflected, if it is not unique in its own class.

2.We must reflect the older of the two points having the same belonging. in this way we always ensure two apex of the simplex from class ω_i and one from ω_j, $i\neq j$, $i,j=1,2$.

(Reflection, can be done using the same formulae as in the classical simplex method.)

The motion of the simplex continues until some of the limits (5) are broken.

At the end of this procedure, we dispose of the training sample, satisfying necessary conditions formulated above - patterns are located near the true boundary and the number of observations from each of 2 classes is approximately equal as is obvious from following example.

Example 1

Let $-1 \le x_i \le 1, i=1,2$ and belonging of 2 patterns is known after an experiment respectively $\underline{x}(1)=\langle 0.1 \quad 1\rangle^T \in \omega 1$, $\underline{x}(2)=\langle 0.3 \quad 1\rangle^T \in \omega 2$. The results of a simulated experiment are given in a table 1. Second order polynomial is used as decision function; w estimated by (4) after 100 steps is:

$\underline{w}^T = \langle -.179805 \quad .305571 \quad .363424 \quad -.143261 \quad -.130971 \quad -.208544 \rangle$

Table 1 Training sample and experimental belonging of patterns

No	x_1	x_2	class	No	x_1	x_2	class
1	0.1	1.0	1	10	0.5	0.30718	2
2	0.3	1.0	2	11	0.4	0.13398	1
3	0.2	0.82679	2	12	0.6	0.13398	1
4	0.0	0.82679	1	13	0.7	0.30718	2
5	0.1	0.65359	1	14	0.8	0.13398	2
6	0.3	0.65359	2	15	0.7	-0.03923	1
7	0.2	0.48038	1	16	0.9	-0.03923	1
8	0.4	0.48038	2	17	1.0	0.13398	2
9	0.3	0.30718	1				

The plot of training patterns and estimated decision function is shown in Figure 1.

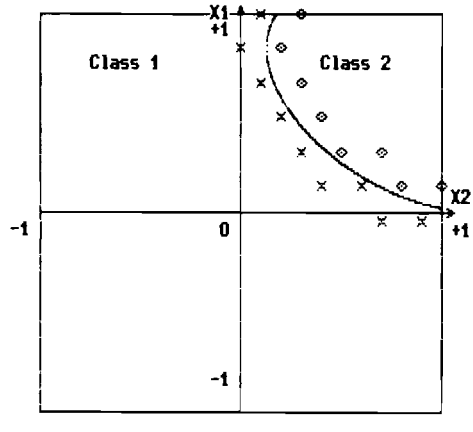


FIGURE 1. Plot of training patterns and estimated decision function

4. GENERALIZED ALGORITHM FOR SEQUENTIAL DESIGN

Despite its simplicity this method is only applicable to 2-dimensional tasks. In general, we propose the following approach: An initial experimental design can be chosen after the same considerations as with regression problems.It is convenient to use a D-optimal symmetrical design. After application of Ho-Kashyap's procedure we have first approximations of decision function $d(\underline{x})=\underline{w}^T(1)\underline{x}=0$. Having this first approximation of $\underline{w}$ it is clear, that we can better predict the response of the points, located far away from the decision boundary,and there is the biggest uncertainty in points, satisfying the equality $\underline{w}^T(1)\underline{x}=0$. Consequently we shall get richest information about the object making in next experiment so as to satisfy equality $\underline{w}^T(1)\underline{x}=0$. There are many options for the choice of points $\underline{x}$, satisfying $\underline{w}^T(1)\underline{x}=0$. One of them is the D-optimal strategy the advantages of which are well known.

By increasing the number of points we collect a training sample, in which the new points are situated closer and closer to the needed decision function $d(\underline{x})$. They carry much more information than the old patterns, situated in a distance. It is most convenient to use the value of $|d(\underline{x})|$ as closeness measure. The patterns for which this measure is highest could be rejected from the training sample and be replaced with new ones, bearing much more information. Thus the volume of the training sample remains constant, independent by the number of experiments. This improves the convergence of procedure (4). Thus we come to approximate equality of patterns number, representing two classes.

The above mentioned considerations could be summarized in the following algorithm:

1. Chose the initial design and order of decision function;
2. Carry out an experiment in the points of initial design;
3. Estimation of $\underline{w}(1)$ by Ho-Kashyap algorithm
4. If $e_i<0$ for $i=1,2,...,Np$ order of decision function is inconvenient, then go to 1;
5. If $k=K_{max}$ then stop;
6. Generate a new point $\underline{x}(N+1)$ satisfying condition $\underline{w}^T(k)\underline{x}(N+k)=0$, and such that $|\det[X^T(N+k)X(N+k)]|$ to have maximal value;
7. Reject x such that $|\underline{w}^T(k)\underline{x}|$ to have maximal value;
8. Carry out an experiment in the new point; then go to 3.

(N is number of points in the initial design; K_{max} is total number of iterations)

Example 2

The algorithm considered above was tested by a simulated experiment. Following decision function was used:

$$d(\underline{x}) = 0.2+0.1x_1-0.3x_2+0.4x_1x_2-0.5x_1^2-0.2x_2^2=0 \qquad (6)$$

The design of experiment,the belonging of points and predictive ability of classifier are given in table 2. Plots of training patterns, real and estimated decision functions are

shown in Fig. 2. Estimated classifier is:

$\underline{w}=($ .779338 .353493 -1.16874 1.32043 -1.97171 -.543722$)^T$

Table 2 Training sample, experimental belonging of patterns and predictive ability of estimated classifier

No	x_1	x_2	Class	predictive ability,(%)	No	x_1	x_2	Class	predictive ability,(%)
1	1	1	1		18	-1	-0.79	2	95.6
2	1	-1	1		19	0.7	-1	1	95.2
3	-1	1	1		20	0.69	0	2	96.5
4	-1	-1	2		21	0.5	0.75	1	96.9
5	1	0	1		22	0.67	-1	1	97.3
6	0	1	1		23	0.64	-1	1	97.4
7	-1	0	1		24	-0.45	0	2	97.7
8	0	-1	2		25	-0.2	0.31	2	98.0
9	0	0	2		26	0.48	0.6	1	98.6
10	0.78	-1	1	91.2	27	-0.52	0	2	98.9
11	-1	-0.35	1	91.5	28	0.79	-0.1	1	98.8
12	-0.2	0.41	1	92.0	29	0.78	-0.1	1	99.1
13	0	0.29	2	92.1	30	0.3	0.59	2	98.7
14	-1	-0.61	1	88.2	31	-1.0	-0.75	2	98.9
15	0.72	-1	1	90.3	32	0.64	-1	1	99.1
16	-1	-0.72	1	92.0	33	0.4	0.6	2	99.2
17	0.64	0	2	93.5	34	-0.54	0	2	99.1

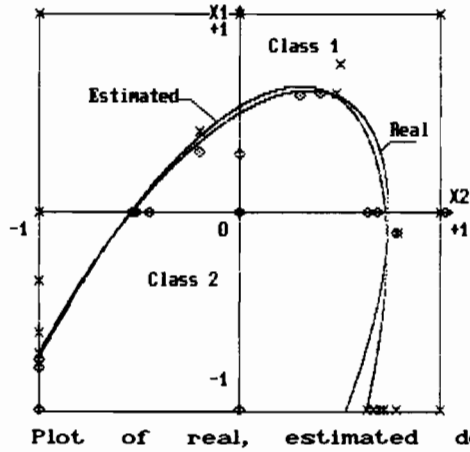


FIGURE 2 Plot of real, estimated decision functions and training sample

The above considered case is applicable for such objects for which the belonging of their points depends only on $\underline{x}$ coordinates and has not any probabilistic character. If $d(\underline{x})=0$ is true then $P(\underline{x}\in\omega_1)=1$ for each $\underline{x}$ such that $d(\underline{x})>0$. In the tasks existing in practice there are many cases when $P(\underline{x}\in\omega_1)<1$ although $d(\underline{x})>0$ and P is continuous function of $\underline{x}$. Usually, as the Euclidean distance between $\underline{x}$ and decision function increases as the probability $P(\underline{x}\in\omega_1)$ is near to 1. Statistical methods in the pattern recognition are based on presentation of classes by their conditional probability densities $P(\underline{x}/\omega_i)$, so

not only the belonging of the patterns but the possibility of apparition of each point x has stochastic nature. That is why the methods of design of experiments can not be used in statistical classification tasks in their classical formulation. Known are only a few investigations of influence of sample size to classifier design (Fukunaga and Hayes 1989).

Let us suppose that the probability of belonging of $\underline{x}$ to the class $\omega 1$ changes following a normal distribution function in the direction of the perpendicular to the surface of the decision function

$$P(\underline{x} \in \omega_1) = \Phi\left((\underline{x}-\underline{x}_o)^T(\underline{x}-\underline{x}_o)\,\mathrm{sign}[d(\underline{x})]/\sigma\right) \qquad (7)$$

where $\Phi(.)$ is function of normal distribution, σ is standard deviation, and $\underline{x}_o$ is the nearest point to $\underline{x}$, such that $d(\underline{x})=0$. This point can be found by minimization of distance $\|\underline{x}-\underline{x}_o\|$ provided that $d(\underline{x})=0$. Lagrange multipliers can be used.

Lets minimize function

$$J(\underline{x},\underline{x}_o) = \sum_{i=1}^{m} (x_{oi} - x_i)^2 \qquad (8)$$

where m is the number of independent input variables x_i

Consider the case when the order of decision function is 2.Then the partial derivatives $J(\underline{x},\underline{x}_o)$ and $d(\underline{x})$ are as follows

$$\partial J(\underline{x},\underline{x}_o)/\partial x_i = 2(x_i - x_{oi}) \qquad (9)$$

$$\partial d(\underline{x})/\partial x_i = w_o + \sum_{k=1}^{i-1} w_{ki}x_k + \sum_{k=i+1}^{m} w_{ik}x_k + 2w_{ii}x_i \qquad (10)$$

$$i=1,2,\ldots,m$$

Applying Lagrange multipliers one can obtain the following system of equations:

$$\begin{cases} 2(x_i - x_{oi}) + \lambda\left(w_o + \sum_{k=1}^{i-1} w_{ki}x_k + \sum_{k=i+1}^{m} w_{ik}x_k + 2w_{ii}x_i\right) = 0 \\ \qquad\qquad (i=1,2,\ldots,m) \\ d(\underline{x}) = 0 \end{cases} \qquad (11)$$

where λ is a Lagrange multiplier. After some transformations of (11),we get a system of m+1 equations. First m of them are linear with respect to $\underline{x}$.

$$A(\lambda)\underline{x} = \underline{b}(\lambda) \qquad (12)$$

where $A(\lambda)$ is a m×m matrix

$$A(\lambda) = \begin{Vmatrix} 2(1+\lambda w_{11}) & w_{12} & \cdots & w_{1m} \\ w_{12} & 2(1+\lambda w_{22}) & \cdots & w_{2m} \\ \vdots & & & \vdots \\ w_{1m} & \cdots & \cdots & 2(1+\lambda w_{mm}) \end{Vmatrix} = 2I + \lambda W \qquad (13)$$

$$\underline{b}(\lambda) = 2\underline{x}_o - \lambda\underline{w}_m \qquad (14)$$

$\underline{x}_o = (x_{o1} \ldots x_{om})^T$, $\underline{w}_m = (w_1 \ldots w_m)^T$ and W is m×m matrix,

$$W = \| w_{ij} \| \qquad i,j = 1,2,\ldots,m \qquad (15)$$

Now system (11) can be written as follows:

$$\begin{cases} (2I + \lambda W)\underline{x} = \underline{b}(\lambda) \\ d(\underline{x}) = 0 \end{cases} \qquad (16)$$

One can find the solution x of (16) by minimizing the absolute value $|d(\underline{x})|$ with respect to λ and solving first linear part of a system on each step of an iterative procedure.

It is interesting to test above proposed sequential D-optimal procedure to an object such that probability of belonging of its output to 2 classes changes in the way considered above. It is evident that if this probability changes according to (7) and $d(\underline{x})=0$, then $P(\underline{x} \in \omega_1)=P(\underline{x} \in \omega_2)=0.5$, so there is the largest possibility of error at the decision function surface. The fact that $P(\underline{x} \in \omega_1) > 0.5$ for each $\underline{x}$ located near decision boundary if $d(\underline{x}) > 0$ and $P(\underline{x} \in \omega_2) > 0.5$ if $d(\underline{x}) < 0$ allows to collect a true information about the pattern's belonging when the sequential procedure is run. The separability conditions can be violated if a point has a wrong belonging (for example, if an experiment shows that $\underline{x}(k) \in \omega_i$ and $d[\underline{x}(k)] < 0$, where k is the number of iterations of sequential design procedure). Such a pattern will be rejected from the training sample and replaced by a new experimental point. When this procedure is finished after N steps, we have an estimate of classifier $\underline{w}(N)$.Then among the patterns, that had been present in the training sample, we can find some points $\underline{x}_{er}$, that are classified incorrectly by $\underline{w}(N)$.If $\underline{w}(N)$ is an unbiased estimate of true value $\underline{w}$ then estimate

$$s^2 = \frac{1}{Np-1} \sum_{i=1}^{Ne} \| \underline{x}_{er} - \underline{x}_o \|^2 \qquad (17)$$

will be an estimate of σ in (7); Ne is number of patterns classified incorrectly.

One can use s for determination of a confidence bound round estimate of decision function $d(\underline{x}) = \underline{w}(N)^T\underline{x}$. Thus the belonging of the points, located in a distance less than 2s will not be predicted reliably. Out of this area the probability of errors is practically equal to 0.

The numerical simulation of such an object of investigation is possible using a random vector $\varepsilon \sim N[0,\sum]$, $\sum=\sigma^2 I$, where I is an identify matrix. The belonging of x can be obtained proving the sign of the function $d(\underline{x}+\varepsilon)$, and then x is used in learning procedure without any changes.

Example 3

A numerical experiment has been simulated by using a second order decision function $d(\underline{x}+\varepsilon)$ of 2 variables and a random vector ε with a covariance matrix $\Sigma = \sigma^2 I$, where σ=0.05. Initial experimental design is the same as in *Example* 2. The main results are shown in the table 3. Plots of wrong-predicted patterns, mathematical expectation of real decision function (the same as in *Example* 2) and estimated decision function are shown in Figure 3. Estimated classifier $\underline{w}$ after 120 experiments is:

$\underline{w} = (\ 1.28382 \quad .582984 \quad -1.77598 \quad 2.04184 \quad -3.26945 \quad -.927592)^T$

Table 3 Predictive ability of estimated and real decision functions

Number of patterns N	predictive ability of $\underline{w}(N)$, (%)	predictive ability of $d(\underline{x})=0$ (6)	Number of wrong predicted patterns Ne	s
18	91.0	96.1	-	-
30	93.2	96.1	-	-
60	94.2	96.1	-	-
90	95.0	96.1	18	0.0183
108	95.1	96.1	15	0.0242
120	95.2	96.1	20	0.0207

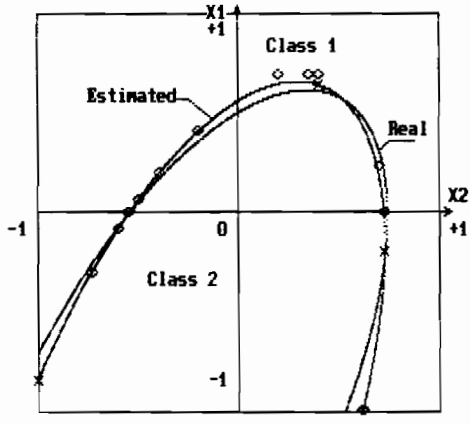


FIGURE 3 Plot of real, estimated decision functions and wrong classified points

REFERENCES

Ho Y. C., Kashyap R. L. (1965). An Algorithm for Linear Inequalities and Its Applications, IEEE Trans. Electronic Computers EC-14, 5.

Ho Y. C., Kashyap R. L. (1966). A Class of Iterative procedures for Linear Inequalities, J.STAM Contr., 4, 112-115.

Fukunaga, K. (1972). Introduction to Statistical Pattern Recognitions, Academic Press, New York.

Fukunaga, K., Hayes R. R.,(1989).Effects of Sample Size in Classifier Design, IEEE Trans. on Pattern Analysis & Machine Intelligence, v.11, 873-885

FURTHER DEVELOPMENT OF ALGORITHMS FOR CONSTRUCTING OPTIMIZING DISTRIBUTIONS

BEN TORSNEY and ABDULHADI M. ALAHMADI
Department of Statistics,
University of Glasgow
Scotland, U.K.

ABSTRACT

A class of multiplicative algorithms, indexed by functions which depend on derivatives and a free parameter is proposed for constrained maximization problems which require the calculation of an optimizing probability distribution. The performance of the algorithm is investigated in constructing D-optimal designs under optimal choices of the parameter and in constructing c-optimal designs starting from difficult initial designs.

KEYWORDS: OPTIMIZATION, OPTIMIZING DISTRIBUTIONS, DIRECTIONAL DERIVATIVES, OPTIMAL DESIGN, MULTIPLICATIVE ALGORITHMS.

1. INTRODUCTION

There are a variety of problems in the statistical arena which demand the calculation of an optimizing probability distribution or measure and hence are examples of the general problems we consider. These include maximum likelihood estimation problems and optimal regression design problems. Also some results in probability theory can be established from the solution to such problems (see Torsney (1986)) and some approaches to image processing or image reconstruction tasks generate examples in which several optimizing distributions are sought (see Torsney (1988)). Our interest in this contribution is to explore a class of algorithms for the solution of such problems which often cannot be obtained in closed form. The problem of interest is formally defined in section 2 and optimality conditions are given in section 3. In section 4 the class of algorithms is proposed and properties of these are outlined in section 5. Results of using them in optimal design problems are reported in sections 6 and 7.

2. A HIERARCHY OF PROBLEMS

We consider the following general problems.

Problem (P1)

"Maximise $\varphi(p)$ over $\mathcal{P} = \{p = (p_1, p_2, \ldots, p_J): p_j \geq 0, \sum p_j = 1\}$".

Problem (P2)

"Maximise $\psi(X)$ over the convex hull of the points $G(v_1)$, $G(v_2)$, ..., $G(v_J)$, where $G(\cdot)$ is a given one to one function and $\mathcal{V} = \{v_1, v_2, \ldots, v_J\}$ is a known set of vector (or matrix) vertices of fixed dimension. That is, solve (P1) for

$$\varphi(p) = \psi\{E_p[G(v)]\}, \quad X = E_p[G(v)] = \sum p_j G(v_j)."$$

3. OPTIMALITY CONDITIONS

We focus attention on Problem (P2) and define optimality conditions in terms of what might be called point to point directional derivatives.

3.1. Directional Derivatives

Let

$$f(X,Y,\varepsilon) = \psi\{(1-\varepsilon)X + \varepsilon Y\}$$

$$F_\psi\{X,Y\} = \lim_{\varepsilon \downarrow 0} \frac{f(X,Y,\varepsilon) - \psi(X)}{\varepsilon} = \left.\frac{df(X,Y,\varepsilon)}{d\varepsilon}\right|_{\varepsilon=0^+}$$

$$F_\psi^{(2)}\{X,Y\} = \left.\frac{d^2 f(X,Y,\varepsilon)}{d\varepsilon^2}\right|_{\varepsilon=0^+}$$

Whittle (1973) called $F_\psi\{X,Y\}$ the directional derivative of $\psi(\cdot)$ at X in the direction of Y. It is a derivative which can exist even if $\psi(\cdot)$ is not differentiable but we will in general wish to assume differentiability of $\psi(\cdot)$ and then $F_\psi(X,Y) = (Y-X)^T \partial\psi/\partial X$.

Let $F_j = F_\psi\{X, G(v_j)\}$. We call F_j a vertex directional derivative of $\psi(\cdot)$ at X. If $\psi(\cdot)$ is differentiable, then so is the function $\varphi(p) = \psi\{E_p(G(v))\}$, and

$$F_j = d_j - \sum_{i=1}^{J} p_i d_i, \quad d_j = \partial\varphi/\partial p_j.$$

3.2. Conditions for Local Optimality

(a) If $\psi(\cdot)$ is differentiable at $X^* = E_{p^*}\{G(v)\}$, then $\psi(X^*)$ is a local maximum of $\psi(\cdot)$ in the feasible region of problem (P2) if,

$$F_j^* = F_\psi\{X^*, G(v_j)\} \begin{cases} = 0, & \text{if } p_j^* > 0 \\ \leq 0, & \text{if } p_j = 0 \end{cases} \qquad \text{(i)},$$

$$F_j^{*(2)} = F_\psi^{(2)}\{X^*, G(v_j)\} \leq 0, \text{ if } p_j > 0 \qquad \text{(ii)}.$$

See Whittle (1973) for a proof. If $\psi(\cdot)$ is concave on its feasible region then the first order stationarity condition (i) is both necessary and sufficient for a solution to (P2), a result known as the General Equivalence Theorem in Optimal Design.

4. A CLASS OF ALGORITHM

Problems (P1) and (P2) have a distinctive set of constraints, namely the variables $p_1, p_2, \ldots, p_J$ must be nonegative and sum to 1. An iteration which neatly submits to these and has some respectable properties is

$$p_j^{(r+1)} = p_j^{(r)} f(d_j,\delta) / \sum_{i=1}^{J} p_i^{(r)} f(d_i,\delta) , \qquad (4.1)$$

where now $d_j = \partial\varphi/\partial p_j | p = p^{(r)}$, while $f(d,\delta)$ satisfies the following conditions:

(a) $f(d,\delta) > 0$;
(b) $f(d,\delta)$ is strictly increasing in d for some set of δ-values, say $\delta>0$;
(c) $f(d,0) =$ constant $\neq 0$;
(d) the variable δ is a free parameter.

This type of iteration was first proposed by Torsney (1977), taking $f(d,\delta) = d^{\delta}$, with $\delta > 0$. Subsequent empirical studies include Silvey et al (1978), which is a study of the choice of δ when $f(d,\delta) = d^{\delta}$, and Torsney (1988), which mainly considers $f(d,\delta) = e^{\delta d}$ in a variety of applications, including estimation and image processing problems. We continue these investigations exploring other choices of $f(d,\delta)$ for which an approximate optimal finite δ can be determined.

Of course other iterations for problems like (P2) have been proposed. Vertex direction algorithms which perturb one p_j and change the others proportionately were first proposed by Fedorov (1972) and Wynn (1972). These are useful when many of the p_j are zero at the optimum as happens in design problems. At the other extreme, when all p_j are positive at the optimum or when it has been established which are positive, constrained steepest ascent or Newton type iterations may be appropriate. See Wu (1978) and Atwood (1976,1980) on these respectively. It is in a context intermediate to these, when only a few optimal weights might be zero that iteration (4.1) is to be recommended in its raw form. See Torsney (1983) for further discussion of this.

5. PROPERTIES OF PROPOSED ALGORITHM

5.1. General properties

Under the conditions imposed on $f(d,\delta)$, iterations under (4.1) possess the following properties.

(i) $p^{(r)}$ is always feasible.

(ii) $F_{\varphi}\{p^{(r)}, p^{(r+1)}\} \geq 0$ with equality when the d_j corresponding to nonzero p_j are equal (in which case $p^{(r+1)} = p^{(r)}$). This can be seen by letting a positive random variable Z take the value $\partial\varphi/\partial p_j$ with probability p_j $(p_j = p_j^{(r)})$. Then

$$F_{\varphi}(p^{(r)}, p^{(r+1)}) = \mathrm{Cov}(Z, f(Z,\delta))/E\{f(Z,\delta)\}.$$

If $f(Z,\delta)$ is increasing in Z it must have nonnegative covariance with Z. This result implies that an increase in the criterion can be obtained by stepping from $p^{(r)}$ to $p^{(r+1)}$ though it does not guarantee that $\varphi(p^{(r+1)}) \geq$

$\varphi(p^{(r)})$.

(iii) In relation to Problem (P2) let $\text{supp}(p) = \{v_j \in \mathcal{V} : p_j > 0\}$ denote the support of the distribution p. Under the above iteration $\text{supp}(p^{(r+1)}) \subseteq \text{supp}(p^{(r)})$.

(iv) An iterate $p^{(r)}$ is a fixed point of the iteration if the derivatives $\partial\varphi/\partial p_j^{(r)}$ corresponding to nonzero $p_j^{(r)}$ share a common value. This is a necessary but not a sufficient condition for $p^{(r)}$ to solve (P1) or (P2). Thus in view of the conditions for (local) optimality, a solution to (P2) is a fixed point of the iteration but so also are the solutions to (P2) for any subset of $\mathcal{V}$.

(v) Let $g(\delta) = F(p^{(r)}, p^{(r+1)})$. Then

$$g'(\delta) = \text{Cov}(D,G),$$

where

$$G = \{\partial f(D,\delta)/\partial\delta\}/f(D,\delta) = \partial \ell n\{f(D,\delta)\}/\partial\delta,$$

and D is a random variable taking the value d_j with probability q_j, $q_j = p_j f(d_j,\delta)/\Sigma p_i f(d_i,\delta)$.

5.2. Properties of Specific Cases

5.2.1. To begin with we consider the two choices $f(d,\delta) = d^\delta$ and $f(d,\delta) = e^{\delta d}$ together. These share two properties, namely:

(a) if there is a unique maximum derivative at $p^{(r)}$, say $d_t = \partial\varphi/\partial p_t|_{p = p^{(r)}}$, then $p^{(r+1)} \to e_t$ as $\delta \to \infty$, where e_t is the t^{th} unit vector;

(b) $g(\delta) = F(p^{(r)},p^{(r+1)})$ is nondecreasing in δ. The first property is trivial. In respect of the second we note that the function G(D) of 5.1 (v) is given by $G(D,\delta) = \ell nD$ and $G(D,\delta) = D$ in the two cases respectively. Both are increasing functions and therefore $g'(\delta) = \text{Cov}(D,G(D,\delta)) \geq 0$.

Note care must be taken in interpreting the latter. In the optimal design context the vector e_t corresponds to a single point design. For a number of optimal design criteria $\varphi(e_t) = -\infty$. The implication is that for such criteria iteration (4.1) is unlikely to be monotonic and possibly not convergent if δ is large. In fact non-convergence occurs under the following combinations:

$$\varphi(p) = \pi_{j=1}^{J} p_j,\ f(d,\delta) = d^\delta,\ \delta = 2;$$

$$\varphi(p) = -\sum_{j=1}^{J} p_j^{-t},\ f(d,\delta) = d^\delta,\ \delta = 2/(t+1);$$

$$\varphi(p) = -\sum_{j=1}^{J} p_j \ell n p_j,\ f(d,\delta) = e^{\delta d},\ \delta = 2\ .$$

In each case iterations oscillate between two values unless the initial value is the optimizing p^*, which is $p_j^* = 1/J$ for each $\varphi(p)$.

In contrast this optimum is attained in one step from any initial $p^{(o)}$ if $\delta = 1, 1/(t+1), 1$ respectively in the three examples. An implication would seem to be that iteration (4.1) would be convergent if not monotonic at least for $\delta < 1$, $\delta < 1/(t+1)$, $\delta < 1$ in the three examples respectively. For larger δ we recall that properly 5.1(ii) only guarantees an increase in

the criterion if we take a small enough step from $p^{(r)}$ to what we have defined to be $p^{(r+1)}$. This would mean a different formula from (4.1) for the next iterate. If we adopt such a method property (b) suggests taking $\delta = \infty$. The revised iterative rule would then be a vertex direction one but not a steepest ascent method since $F_\psi(X,Y)$ depends on the distance between X and Y. Constrained steepest ascent techniques choose directions which maximise normalised directional derivatives.

5.2.2. We again consider two cases of $f(d,\delta)$, namely $f(d,\delta) = \ell n(e+\delta d)$ and $f(d,\delta) = F(\delta d)$ where $F(x)$ is increasing in x and bounded above so that it must have an asymptote as $x \to \infty$. Examples include cumulative distribution functions. In these examples the following is true:

(a) $p^{(r+1)} \to p^{(r)}$ as $\delta \to \infty$;
(b) $g(\delta)$ is maximised by some finite δ, say δ^*.

The first is again trivial. It implies that $g(\infty) = g(0) = 0$ since $F(p,p) = 0$. Given that $g(\delta) \geq 0$ from 5.1(ii), property (b) follows.

It is a possibility then that convergence, if not monotonicity are obtained for any δ. An optimal choice might be the δ^* of (b). In general there is no explicit formula for δ^* in terms of $p^{(r)}$ and $d = \partial\varphi/\partial p|_{p=p^{(r)}}$, (terms on which it must depend), but we can suggest an approximation to it in the case $f(d,\delta) = F(\delta d)$. Recall that $g'(\delta)$ is a covariance between a random variable D and $G(D,\delta)$ where $G(D,\delta) = \partial\ell n\{f(D,\delta)\}/\partial D$. Thus $g'(\delta)$ is likely to be zero if δ is such that $G(D,\delta)$ has a turning point in the range of $d_1, \ldots, d_J$.

Now
$\partial G(d,\delta)/\partial d = \partial^2 \ell n\{f(d,\delta)\}/\delta d \partial\delta$,
and for $f(d,\delta) = F(\delta d)$ this derivative has value $H(x)$ where $x = \delta d$ and

$$H(x) = \frac{F'(x)}{F(x)} + \frac{xF''(x)}{F(x)} - \frac{x[F'(x)]^2}{[F(x)]^2}$$

Let $H(x^*) = 0$. A possibly simplistic suggestion is to approximate δ^* by $\delta^* = x^*/\sum p_i d_i$ or by corresponding terms based on other moments of the d_i's. We focus attention on this choice of δ in the next section.

6. CONSTRUCTION OF OPTIMAL DESIGNS: EMPIRICAL RESULTS ON CONVERGENCE

6.1. We report the performance of iteration (4.1) in calculating D-optimal designs when $f(d,\delta)$ satisfies the conditions of section 5.2.2. and $\delta = \delta^* = x^*/\sum p_i d_i$.

Optimal regression design problems are examples of (P2) in which

(i) $V \subset R^k$ and is called the (induced) design space.
(ii) $G(v) = \underline{v}\,\underline{v}^T$.
(iii) X is a symmetric k×k matrix.
(iv) a variety of criteria $\psi(\cdot)$ have been considered including $\psi(X) = \ell n\det(X)$ which is the D-optimal criterion.

We calculate D-optimal designs for five examples considered by Silvey et al (1978) and Wu (1978). The examples are defined by their design spaces.

Example 1. $V = V_1 = \{(1,-1,-1)^T, (1,-1,1)^T, (1,1,-1)^T, (1,2,2)^T\}$

Example 2. $U = U_2 = \{(1,-1,-1)^T, (1,-1,1)^T, (1,1,-1)^T, (1,2,3)^T\}$

Example 3. $U = U_3 = \{(1,-1,-2)^T, (1,-1,1)^T, (1,1,-1)^T, (1,2,2)^T\}$

Example 4. $U = U_4 = \{(1,1,-1,-1)^T, (1,-1,1,-1)^T, (1,-1,-1,-1)^T$
$(1,2,2,-1)^T, (1,1,-1,1)^T, (1,-1.5,1,1)^T$
$(1,-1,-1,2)^T\}$

Example 5. $U = U_5 = U_4 \cup \{1,1,1.5,1)^T\}$

In Tables 1-3 of section 7 we report the number of iterations needed to achieve max $F_j \leq 10^{-n}$, n=1,2,3,4 under three choices of $f(d,\delta)$. It is clear that on the whole convergence is slow in terms of numbers of iterations. However arguably it is fast to begin with. It must be remembered too that at each iteration only first derivatives are required. One marginally positive result is that convergence is faster under the case $f(d,\delta) = c - \exp(-\delta d)$ with c=1.0001.
Convergence was slower for larger values of c. Interestingly if $c \doteq 1$ and δ is small then $f(d,\delta) \doteq \delta d$. Iterations are then approximately those under $f(d,\delta) = d$. This suggests that $f(d,\delta) = d$ is an efficient choice for D-optimality. Certainly it is known to be monotonic for this criterion.

6.2. We have not addressed the topic of convergence of iteration (4.1). So far only isolated results have been established in the literature, and mainly on monotonicity. Titterington (1976) describes a proof of monotonicity of $f(d,\delta) = d$ in the case of D-optimality, while Torsney (1983) establishes a sufficient condition for monotonicity of $f(d,\delta) = d^{\delta}$, $\delta = \delta_t = 1/(t+1)$ when the criterion $\varphi(p)$ is a homogeneous function of degree -t with positive derivatives, t>0. He further shows that this condition is satisfied by linear design criteria such as the c-optimal and A-optimal criteria. For these t=1 so that $\delta_t = \frac{1}{2}$. Also the case $f(d,\delta) = d$ sometimes proves to yield EM iterations which are therefore monotonic and convergent. See Dempster et al (1977). The EM algorithm is known to have notoriously slow convergence. This also seems to be the case with iteration (4.1). Silverman et al (1990) proposed a smoothed version of the EM algorithm to improve convergence in stereology and emission tomography problems, but convergence per se has not been proved. This too is the case with iteration (4.1). The extent of the difficulty is emphasised by the fact that Gaffke and Mather (1990) prove convergence of a wide class of algorithms for design problems but they cannot fit iteration (4.1) into their class. Of course convergence results must depend on properties of the criterion $\varphi(p)$, on the function $f(d,\delta)$ and on δ. We believe that if δ is sufficiently small convergence and probably monotonicity will be assured in a wide range of problems. Certainly this has happened in many examples.

In the absence of analytic progress we report some empirical results obtained when using $f(d,\delta) = d^{1/2}$ for constructing c-optimal designs under fairly testing conditions. The form of this criterion is $-c^T X^- c$ for a given vector c. Pukelsheim and Torsney (1990) report that there always exists a c-optimal design with a linearly independent support and given the support points there is an explicit solution for the optimal weights. This combines results of Fellman (1974) and Kitsos et al. (1988). Moreover iteration (4.1) with $f(d,\delta) = d^{1/2}$ will find this optimum in one step, starting from a design which assigns weight only to the optimal support points. More generally if an initial design $p^{(0)}$ has a linearly independent support, this particular case of (4.1) will identify the c-optimal design on this support in one step.

Consider $c = (1,2,3)^T$ in examples 1,2,3. In each case U contains four points, say v_1,v_2,v_3,v_4. If v_1,v_2,v_3,v_4 represent the four design points

of example 1, then the support of the c-optimal design is (v_2,v_3,v_4) with optimal weights ·072, ·214, ·714. In example 2 the fourth point is the only optimal support point. Finally if v_1,v_2,v_3,v_4 represent the four design points of example 3, the optimal support is (v_1,v_2,v_4) with weights ·2, ·2, ·6. We started iteration (4.1) with $f(d,\delta) = d^{1/2}$ from various initial designs $p^{(o)}$, which put small weight on at least one of these support points. These included permutations of $p^{(o)} = (\alpha,\alpha,\alpha,\beta)$, $p^{(o)} = (\alpha,\alpha,\beta,\beta)$ and $p^{(o)} = (\alpha,\beta,\beta,\beta)$ with $\beta \leq 10^{-12}$. At the first iteration the algorithm irresistably moves immediately to the optimal design on the subset of points receiving weight α. However the algorithm slowly moves away from this and converges to the global optimum. Similar results were found in the other two examples. It is hoped to produce analytic results in the future.

7. TABLES

In the following tables we report results when using three choices of $f(d,\delta)$ with $\delta = \delta^* = x^*/\sum p_i d_i$ (see section 5.2.2) in Examples 1-5 to calculate D-optimal designs. In particular we record for n=1,2,3,4 the number of iterations needed to achieve $F_j \leq 10^{-n}$, for all $j=1,\ldots,J$, where F_j are the vertex directional derivatives. We note that $\delta^* = x^*/k$ for D-optimality when $U \subset R^k$.

TABLE 1 $f(d,\delta) = \ell n(e+\delta d)$

Example	n=1	n=2	n=3	n=4
1	6	25	50	75
2	6	41	89	141
3	6	24	45	66
4	18	121	339	714
5	13	190	488	880

TABLE 2 $f(d,\delta) = \exp(\delta d)/[1+\exp(\delta d)]$

Example	n=1	n=2	n=3	n=4
1	7	29	57	86
2	7	48	101	161
3	6	28	52	76
4	20	139	388	815
5	15	217	557	1004

TABLE 3 $f(d,\delta) = c - \exp(-\delta d)$, c=1.0001

Example	n=1	n=2	n=3	n=4
1	1	7	14	22
2	3	13	27	43
3	2	7	13	19
4	6	39	109	229
5	5	61	157	283

8. REFERENCES

Atwood, C.L. (1976). Convergent design sequences for sufficiently regular optimality criteria. Annals of Statistics 4:1124-1138.

Atwood, C.L. (1980). Convergent design sequences for sufficiently regular optimality criteria, II: singular case. Annals of Statistics 8: 894-912.

Dempster, A.P. Laird, N.M. and Rubin, D.B. (1977). Maximum likelihood from incomplete data via the EM algorithm (with Discussion). JRSSB, 39:1-38.

Fellman, J., (1974). On the allocation of linear observations. Commentationes Physico-Mathematicae (Finska Vetenskaps Societeten) 44:27-77.

Fedorov, V.V. (1972). Theory of Optimal Experiments. Academic Press, New York.

Gaffke, N. and Mather, R. (1990). On a class of algorithms from experimental design theory. Report No. 196. Institut für Mathematik, Universität Augsburg, Germany.

Kitsos, C.P., Titterington, D.M. and Torsney, B. (1988). An optimal design problem in rhythmometry. Biometrics, 44:657-671.

Pukelsheim, F. & Torsney, B. (1991). Optimal weights for experimental designs on linearly independent support points. Annals of Statistics. (To appear).

Silverman, B.W., Jones, M.C., Wilson, J.D. and Nychka, D.W. (1990). A smoothed EM approach to indirect estimation problems with particular reference to stereology and emission tomography (with Discussion). JRSSB, 52:271-324.

Silvey, S.D., Titterington, D.M. and Torsney, B. (1978). An algorithm for optimal designs on a finite design space. Communications in Statistics A 7:1379-1389.

Titterington, D.M. (1976). Algorithms for computing D-optimal designs on a finite design space. Proceedings, Conference on Information Sciences and Systems, Dept. Elect. Eng., Johns Hopkins Univ., Baltimore MD:213-216.

Torsney, B. (1977). Contribution to discussion of 'Maximum Likelihood estimation via the EM algorithm' by Dempster et al., JRSSB, 39:26-27.

Torsney, B. (1981). Algorithms for a constrained optimization problem with applications in statistics and optimum design. Ph.D. Thesis, University of Glasgow.

Torsney, B. (1983). A moment inequality and monotonicity of an algorithm. Proceedings, International Symposium on Semi-Infinite Programming and Applications (Kortanek, K.O. and Fiacco, A.V. eds) at Univ. of Texas, Austin, Lecture Notes in Economics and Mathematical Systems 215:249-260.

Torsney, B. (1986). Moment inequalities via optimal design theory. Lin. Alg. & Its Applns. 82:237-253.

Torsney, B. (1988). Computing optimizing distributions with applications in design, estimation and image processing. Optimal Design and Analysis of Experiments (Y. Dodge, V.V. Fedorov and H.P. Wynn, Eds.) North Holland:361-370.

Whittle, P. (1973). Some general points in the theory of optimal experimental design. JRSSB 35:123-130.

Wu, C.F. (1978). Some iterative procedures for generating nonsingular optimal designs. Commnications in Statistics A 7:1399-1412.

Wynn, H.P. (1972). Results in the theory and construction of D-optimum experimental designs (with Discussion). JRSSB 34:133-147,170-186.

Part II:

REGRESSION ANALYSIS

Adaptive estimation in linear regression model and test of symmetry of residuals

Jan Ámos Víšek

Institute of Information Theory and Automation
Czechoslovak Academy of Sciences
Prague

1 Introduction

Studies of efficiency go back nearly to the first years of this century. Hence it is not suprising that on the Third Berkeley Symposium on Mathematical Statistics and Probability (in 1955) Charles Stein opened the question of possibility of efficient testing and estimation under (completely) unknown distribution (see Stein (1956) and for a possible solution Bickel (1982)). It is clear that any such procedure requires (explicit or implicit) adaptation to the unknown underlying distribution, or in another words, less or more explicit estimation of (density of) the unknown distribution (or some other function identifying the underlying distribution as for instance the logarithmic derivative). This yields - besides another difficulties - usually more time and space consuming procedures than those of classical statistics are. Naturally we expect that it will be paid back by some advantages, particularly by much better exploitation of information brought by data.

When we think about this matter we usually (unconsciously) have in mind a (possible) low efficiency of classical methods for "real" data. Really, already K. Pearson (1902) having collected under highly uniform conditions series of data found that the best approximation of their d. f. is Student t with 5 – 9 degrees of freedom and P. J. Huber came to conclusion that for some kind of high-quality data it may be even t_3. Together with the results of R. A. Fisher (1922) that the asymptotic efficiency of $(n-1)^{-1}\sum_{i=1}^{n}(x_i-\overline{x})^2$ is for t_9, t_5 and t_3 equal to 83 %, 40 % and 0, respectively, it seemingly justifies this idea. However the loss of efficiency of modern (appropriately selected robust) procedures is usually not so dramatic. E. g. for the mixture model $F(x) = (1-\varepsilon)\Phi(x) + \varepsilon\Phi(x/3)$ - Φ being standard normal distribution – the efficiency of 6 %-trimmed mean is not less than 96 % for any $\varepsilon \in [0, 0.1]$ although the efficiency of mean falls down to 70 % (for more complete discussion see Hampel et. al. (1986)).

So it seems that application of the adaptive procedures may be justified only in special cases e. g. when there is a suspicion that the distribution could be rather strange (or level of contamination considerably high). But then it is questionable wheather the assumptions under which the given adaptive procedure works hold. So it may seem at a first glance that (direct, i. e. without preprocessing steps) adaptive procedures may be more theoretical matter than practical tools. Nevertheless we shall try to show that at least in special cases adaptive procedures may be useful.

Present paper offers two methods of adaptive estimation of linear regression model. A common assumption for both of them is symmetry (of distribution of errors). Although the symmetry (or at least precise symmetry) doesn't take place so frequently as it is sometimes believed, if it can be assumed, it is advantage not only from technical point of view but it

may clarify also philosophy behind the mathematical theory. E.g. for location problem – under symmetry – the mean (if exists), median, modus (if unimodal distribution) and center of symmetry coincide and hence there is no problem what is to be understood under location parameter and estimated. Moreover the experiences of practitioners with symmetry are so good that sometimes they prefer to find (a simple) one-to-one transformation of data bringing them to symmetry and only then they apply an estimating procedure (naturally with succeeding retransformation). But even if we accept such kind of arguments we have to realize that the situation for location model is much simpler than for regression model because we may e. g. test whether the data are symmetric or not, or even we may estimate "a true" model.

Although today more and more people prefer such point of view that the objective existence of "a true model" (or if you want "objective nature laws" together with possibility of separation of them from the subjective role of observer) is only an illusion, the idea of "true model" – as something what may be (asymptotically) reached – is used very frequently as a pragmatic license. And for the location problem the situation with such license is not very complicated since there are tests which say which mathematical models are – with high probability – incompatible with given data and hence they can't serve as "true models". For the regression model the situation is more complicated because there is usually at least a few competing models and it is on user to select which he (or she) prefers. And not for all of them we have at hand tests reliably (and sensefully) disqualifying inappropriate models (especially for the whole family of (robust) methods one may invent a sequence of criteria to compare different models – see e. g. Ruppert & Carroll (1980)). Most of such criteria will be inspired – may be very loosely and through a long chain of considerations – by idea of "consistency", i.e. by idea to be as near as possible to the "true" model. Since most of new (robust) methods is (strongly or weakly) consistent under rather general conditions (see Marona & Yohai (1981)) – although their estimates of coefficients considerably differ (see e. g. estimates of regression model for Salinity data presented in Ruppert and Carroll (1980) and also bellow in this paper) – this asymptotic property may occur to be of little help for the finite sample situation. Then we may remember on the experience with the symmetry and to prefer such model which assures symmetry (in a reasonable level, i.e. in a such level which doesn't cause overdetermination). And we find (may be suprisingly) that the symmetry was used when deriving properties of regression analysis methods many times (see Bickel (1975), Rousseeuw and Yohai (1974), Ruppert and Carroll (1980), Yohai (1974)). Moreover, even if we can dispense with the symmetry some results may simplify under it (see Jurečková (1977) (and Huber (1969)) Remark after Corollary 3.1 or Hampel et. al. (1986)) or become more intuitively acceptable. Let us mention only one example. The regression quantile technique (as introduced by Koenker & Bassett (1978)) include as a special case L_1 estimate (as regression quantile for $\alpha = \frac{1}{2}$). But as Jurečková (1984) showed the difference of the estimate of intercept and its value (strongly) converge to $F^{-1}\left(\frac{1}{2}\right)$ which is zero e. g. for symmetric d.f.. (For more detailed discussion see Víšek (1990).) Moreover some (highly) robust techniques (as Least Median of Squares) are proved to be consistent under symmetry (Rousseeuw & Leroy (1987)) and hence it may be useful – after having used them, usually for the first rough fit of model, i.e. as a hint for smooth rejection of points – to test the symmetry of residuals (at least of a bulk of data). But residuals are dependent although identically distributed and hence the Wilcoxon test (as one possibility of test of symmetry) is out of game. That is why this paper proposes a special test for symmetry of residuals.

2 Notation

Let R be the real line and N the set of all positive integers. We shall consider a linear regression model

$$Y = X\beta^0 + e$$

where $Y = (Y_1, \ldots, Y_n)'$ is a response variable $X = \{x_{ij}\}_{i=1,j=1}^{n\ p}$ is a design matrix (in the case that the intercept is assumed we suppose $x_{i1} = 1$ for $i = 1, \ldots, n$), $\beta^0 = (\beta_1^0, \ldots, \beta_p^0)'$ vector of regression coefficients (unknown but fixed) and $e = (e_1, \ldots, e_n)'$ is a vector of i.i.d. (according to a distribution G) random variables. (We assume that $p \geq 2$.) G is assumed to allow absolutely continuous density g being symmetric. Moreover we suppose that Fisher information exists, is finite and denote it by $I(g)$.

Both estimators of regression coefficients as well as the test of symmetry will be based on kernel estimator of density of residuals. So we need a necessary notation for it. Let X_i denote i-th row of design matrix ($i = 1, \ldots, n$) and for any $\beta \in R^p$ let $e_i(\beta) = Y_i - X_i\beta$ be i-th residual; for $\beta = \beta^0$ let us write simply e_i (instead of $e_i(\beta^0)$). Let w be a symmetric and everywhere positive kernel and $\{c_n\}_{n=1}^{\infty} \downarrow 0$. Denote for any $y \in R$, $Y \in R^n$ and $\beta \in R^p$

$$g_n(y, Y, \beta) = \frac{1}{nc_n} \sum_{i=1}^{n} w\left(c_n^{-1}(y - e_i(\beta))\right)$$

the kernel estimator of density of residuals. We shall assume that w is symmetric, three times absolutely continuous and that there exist constants $K_1, \ldots, K_5$ such that

$$\sup_{y \in R} w(y) < K_1, \qquad \sup_{y \in R} \frac{|w'(y)|}{w(y)} < K_2,$$

$$\sup_{y \in R} \frac{|w''(y)|}{w(y)} < K_3, \qquad \sup_{y \in R} \frac{|w'''(y)|}{w(y)} < K_4,$$

$$\int_{-\infty}^{\infty} x\, w(x)dx = 0, \qquad \lim_{|x| \to \infty} x^4\, w(x) = 0$$

and for any $n \in N$

$$\max_{\substack{i=1,\ldots,n \\ j=1,\ldots,p}} |x_{ij}| < K_5.$$

3 Estimator based on Hellinger distance

For a sequence of positive numbers $\{a_n\}_{n=1}^{\infty} \nearrow \infty$ denote by $b_n(y)$ a symmetric differentiable function such that for all $y \in R$, $0 \leq b_n(y) \leq 1$ and

$$b_n(y) = \begin{cases} 1 & |y| \leq a_n, \\ 0 & |y| > a_n + c_n^4. \end{cases}$$

Definition 1. For any $Y \in R^n$ put

$$\hat{\beta}^n(Y) = \operatorname{argmax}_{\beta \in R^p} \int g_n^{\frac{1}{2}}(y, Y, \beta) g_n^{\frac{1}{2}}(-y, Y, \beta) b_n(y) dy.$$

If there is no such point then put $\hat{\beta}^n(y)$ equal to any $\tilde{\beta} \in R^p$ such that

$$\int g_n^{\frac{1}{2}}(y, Y, \tilde{\beta}) g_n^{\frac{1}{2}}(-y, Y, \tilde{\beta}) > \sup_{\beta \in R^p} \int g_n^{\frac{1}{2}}(y, Y, \beta) g_n^{\frac{1}{2}}(-y, Y, \beta) b_n(y) dy - \frac{1}{n}.$$

Denote for any $a, b \in R$ by $C_p(a, \beta^0) = \{\beta \in R^p : \|\beta - \beta^0\| > a\}$ and by

$$C_p\left(a, b, \beta^0\right) = C_p\left(a, \beta^0\right) \cap C_p^c\left(b, \beta^0\right).$$

Condition A. For any $\delta > 0$ there is $\Delta \in (0,1)$ and $K_\Delta \in R$ such that

i)

$$\limsup_{n\to\infty} \sup_{C_p(\delta, K_\Delta, \beta^0)} \int E^{\frac{1}{2}} g_n(y, Y, \beta) E^{\frac{1}{2}} g_n(-y, Y, \beta) b_n(y) dy < \Delta$$

and

ii)

$$\limsup_{n\to\infty} \sup_{C_p(K_\Delta, \beta^0)} \int g_n^{\frac{1}{2}}(y, Y, \beta) g_n^{\frac{1}{2}}(-y, Y, \beta) b_n(y) dy < \Delta \quad \text{in probability.}$$

Theorem 1. Let **Condition A** be fulfilled and

$$\lim_{n\to\infty} n c_n = \infty \qquad \text{and} \qquad \lim_{n\to\infty} n c_n^{4p} a_n^{-2p} = \infty.$$

Then $\hat{\beta}^n(Y)$ is (weakly) consistent estimator of β^0.

Theorem 2. Let there is $M \in R$ such that

$$\sup_{y\in R} |g'(y)| < M$$

and

$$\limsup_{n\to\infty} g(a_n)/c_n = 0.$$

Further let

$$\int t^2 w(t) dt < \infty$$

and **Condition A** be fulfilled. Then

$$n^{-\frac{1}{2}} I(g) \sum_{\ell=1}^{p} \left(\hat{\beta}_\ell^n - \beta_\ell^0\right) \sum_{i=1}^{n} x_{i\ell} = n^{-\frac{1}{2}} \sum_{i=1}^{n} g'\left(Y_i - X_i\beta^0\right) g^{-1}\left(Y_i - X_i\beta^0\right) + o_p(1).$$

Since the proofs of both Theorems are long (in both cases they are chains of simple but tedious approximations) we give only a hint of it in a form of sequence of lemmas proofs of which are either simple or references will be given. (We shall assume that assumptions of Theorem 1 and 2 hold in the rest of this chapter.)

Lemma 1. For any $\beta \in R^p$

$$\int \left[g_n^{\frac{1}{2}}(y, Y, \beta) - E^{\frac{1}{2}} g_n(y, Y, \beta)\right]^2 b_n(y) dy = O_p\left(n^{-1} c_n^{-1} a_n\right).$$

Lemma 2.

$$\int g_n^{\frac{1}{2}}(y, Y, \beta^0) \cdot g_n^{\frac{1}{2}}(-y, Y, \beta^0) b_n(y) dy \longrightarrow 1 \qquad \text{in probability.}$$

Lemma 3. For any $\beta \in R^p$ and $k = 1, \ldots, p$ we have

$$\frac{\partial}{\partial \beta_k} \int g_n^{\frac{1}{2}}(y, Y, \beta) g_n^{\frac{1}{2}}(-y, Y, \beta) b_n(y) dy =$$

$$= 2 \cdot \int \frac{\partial g_n^{\frac{1}{2}}(y, Y, \beta)}{\partial \beta_k} g_n^{\frac{1}{2}}(-y, Y, \beta) b_n(y) dy.$$

Lemma 4. For any $\beta \in R^p$ and $k = 1, \ldots, p$

$$\int \left[\frac{\partial}{\partial \beta_k} g_n^{\frac{1}{2}}(y, Y, \beta) - \frac{\partial}{\partial \beta_k} E^{\frac{1}{2}} g_n(y, Y, \beta) \right]^2 b_n(y) dy = O_p\left(n^{-1} c_n^{-3} a_n\right).$$

Lemma 5. For any $k, \ell = 1, \ldots, p$

$$\int \left\{ g_n^{\frac{1}{2}}(-y, Y, \beta^0) \cdot \frac{\partial^2}{\partial \beta_k \partial \beta_\ell} g_n^{\frac{1}{2}}(y, Y, \beta^0) - \right.$$

$$\left. - E^{\frac{1}{2}} g_n(-y, Y, \beta^0) \cdot \frac{\partial^2}{\partial \beta_k \partial \beta_\ell} E^{\frac{1}{2}} g_n(y, Y, \beta^0) \right\}^2 b_n(y) dy = O_p\left(n^{-1} c_n^{-6} a_n\right).$$

Lemma 6. For any $k, \ell = 1, \ldots, p$

$$\int \left\{ \frac{\partial g_n^{\frac{1}{2}}(y, Y, \beta)}{\partial \beta_k} \cdot \frac{\partial g_n^{\frac{1}{2}}(-y, Y, \beta)}{\partial \beta_\ell} - \right.$$

$$\left. - \frac{\partial}{\partial \beta_k} E^{\frac{1}{2}} g_n(y, Y, \beta) \cdot \frac{\partial}{\partial \beta_\ell} E^{\frac{1}{2}} g_n(-y, Y, \beta) \right\}^2 b_n(y) dy = O_p\left(n^{-1} c_n^{-3} a_n\right).$$

Lemma 7. For any $k, \ell = 1, \ldots, p$

$$\int \frac{\partial^2 E g_n(y, Y, \beta^0)}{\partial \beta_k \partial \beta_\ell} b_n(y) dy = o(1).$$

Lemma 8. For any $k = 1, \ldots, p$

$$\int \left| \left[\frac{\partial g_n^{\frac{1}{2}}(y, Y, \beta^0)}{\partial \beta_k} - \frac{\partial E^{\frac{1}{2}} g_n(y, Y, \beta^0)}{\partial \beta_k} \right] \times \right.$$

$$\left. \times \left[g_n^{\frac{1}{2}}(-y, Y, \beta^0) - E^{\frac{1}{2}} g_n(-y, Y, \beta^0) \right] b_n(y) \right| dy = O_p\left(n^{-1} c_n^{-2} a_n\right).$$

Lemma 9. For any $k = 1, \ldots, p$

$$n^{\frac{1}{2}} \int \left\{ \left[\frac{\partial g_n^{\frac{1}{2}}(y, Y, \beta^0)}{\partial \beta_k} - \frac{\partial E^{\frac{1}{2}} g_n(y, Y, \beta^0)}{\partial \beta_k} \right] E^{\frac{1}{2}} g_n(y, Y, \beta^0) \right.$$
$$\left. - \frac{\partial E^{\frac{1}{2}} g_n(y, Y, \beta^0)}{\partial \beta_k} \left[g_n^{\frac{1}{2}}(y, Y, \beta^0) - E^{\frac{1}{2}} g_n(y, Y, \beta^0) \right] \right\} b_n(y) = o_p(1).$$

Lemma 10. (Beran (1978))

$$\lim_{n \to \infty} c_n^{-3} \int \frac{\left[\int w'\left(c_n^{-1}(y - z)\right) g(z) dz \right]^2}{\int w\left(c_n^{-1}(y - z)\right) g(z) dz} dy = I(g)$$

Lemma 11. (Beran (1978))

$$n^{\frac{1}{2}} \int \frac{\partial E^{\frac{1}{2}} g_n(y, Y, \beta^0)}{\partial \beta_k} \left[g_n^{\frac{1}{2}}(y, Y, \beta^0) - E^{\frac{1}{2}} g_n(y, Y, \beta^0) \right] b_n(y) dy$$
$$= \frac{1}{2} n^{-\frac{1}{2}} \left[\frac{\sum_{i=1}^n x_{ik}}{n} \right] \sum_{i=1}^n g'\left(Y_i - X_i \beta^0\right) g^{-1}\left(Y_i - X_i \beta^0\right) + o_p(1).$$

For the full proofs of all assertions see Víšek (1990a). The proof of the Theorem 1 is based on idea of coverage of a compact ball (with radius K_Δ – see Condition A ii)) by balls of uniform continuity of the functional (from Definition 1). At centers of these balls – due to Condition A i) and Lemma 1 – the functional can be "made" enough small (except of ball with center at β^0). The proof of the Theorem 2 utilizes the fact that under its conditions (and common assumptions on g and w) we have for $\hat{\beta}^n$ (and $k = 1, \ldots, p$)

$$\int \left[\frac{\partial g_n^{\frac{1}{2}}(y, Y, \beta)}{\partial \beta_k} \right]_{\beta = \hat{\beta}^n} g_n^{\frac{1}{2}}(y, Y, \hat{\beta}^n) dy = 0$$

and using the standard technique of Taylor's expansion together with Lemmas 1 – 11 we arrive at the required assertion.

4 Maximum–likelihood–like estimator

In what follows let $\tilde{\beta}^n$ denote a preliminary estimator of regression coefficients and denote by $\tilde{e}_i$ residuals $e_i\left(\tilde{\beta}^n\right)$. For a sequence $\{a_n\}_{n=1}^\infty$ of a positive number, $a_n \nearrow \infty$ define

$$b_n(y) = \begin{cases} 1 & |y| \leq a_n, \\ 0 & |y| > a_n. \end{cases}$$

Condition B. Let for some $\delta \in \left[\frac{1}{4}, \frac{1}{2}\right]$

$$\lim_{n \to \infty} n^\delta c_n^4 = \infty \qquad \text{and} \qquad \lim_{n \to \infty} n^{4\delta - 1} c_n^6 = \infty.$$

Moreover let

$$n^{2\delta} E\|\tilde{\beta}^n - \beta^0\|^2 = o(1)$$

and preliminary estimator is assumed to be such that for any $j = 1, \dots n;\ i = 1, \dots, n,\ t \in R,\ s \in R$

$$P_g\left(\tilde{e}_i - E\left\{\tilde{e}_i \,|\, e_j = t\right\} < s \,|\, e_j = t\right) = P_g\left(\tilde{e}_i - E\left\{\tilde{e}_i \,|\, e_j = t\right\} > -s\right) + o_p(1).$$

Condition C. Let for any $a \in R$

$$\lim_{n\to\infty} \sup_{|b|<a} n^{-\frac{1}{2}} c_n^{-2} \int w^{-1}\left(c_n^{-1}(z+b-t)\right) g(t) g(z) dt dz = 0.$$

Further let there exist $\nu,\ D\ (\nu > 0,\ D > 0)$ such that for any $z_1, z_2 \in R,\ |z_1 - z_2| < \nu$ we have $w(z_1)/w(z_2) < D$. Let

$$\lim_{n\to\infty} \frac{1}{n} X'X = Q$$

where Q is a regular matrix.

Definition 2. For any sequence $\{d_n\}_{n=1}^{\infty} \downarrow 0$ denote by

$$\mathcal{G}\left(\{d_n\}_{n=1}^{\infty}\right) = \Bigg\{h;\ h \text{ is a density and for any} n \in N$$

$$P_h\left\{\max\left\{\sup_{y\in R}\left|g_n(y, Y, \beta^0) - h(y)\right|,\ \sup_{y\in R}\left|g_n(y, Y, \beta^0) - E_h g_n(y, Y, \beta^0)\right|\right\} > \frac{1}{2} d_n\right\} < d_n\Bigg\}.$$

Definition 3. For any $Y \in R^n$ put

$$\hat{\tilde{\beta}}^n(Y) = \operatorname{argmax}_{\beta\in R^p} \prod_{j=1}^{n} g_n\left(e_j(\beta), Y, \tilde{\beta}^n\right) b_n\left(\tilde{e}_j\right).$$

Again, if such point does not exist let $\hat{\tilde{\beta}}^n$ be any point $\tilde{\tilde{\beta}}$ for which

$$\prod_{j=1}^{n} g_n\left(e_j(\tilde{\tilde{\beta}}), Y, \tilde{\beta}^n\right) b_n\left(\tilde{e}_j\right) > \sup_{\beta\in R^p} \prod_{j=1}^{n} g_n\left(e_j(\beta), Y, \tilde{\beta}^n\right) b_n\left(\tilde{e}_j\right) - \frac{1}{n}.$$

Condition D. Let

$$\lim_{n\to\infty} \frac{d_n}{c_n} = \infty.$$

Further let us assume that there is a constant K_6 such that

$$P_g\left(\left\|\hat{\tilde{\beta}}^n\right\| > K_6\right) \overset{n\to\infty}{\longrightarrow} 0.$$

Let $g \in \mathcal{G}\left(\{d_n\}_{n=1}^{\infty}\right)$ and the above given sequence $\{a_n\}_{n=1}^{\infty}$ be chosen so (and g be of such type) that starting from some $n_0 \in N$ we have for any $n \geq n_0$

$$(-2a_n, 2a_n) \subset \left\{y \in R:\ g(y) > d_n^{\frac{1}{2}}\right\}.$$

Finally let

$$\lim_{n\to\infty} nc_n^6 a_n^{-2} = \infty.$$

Condition E. Let the density g and the kernel w be such that for any $t > 0$

$$\int [g'(t-y) - g'(t)]\, w(y)dy > 0$$

and let there is $M > 0$ such that

$$\sup_{y\in R} |g'(y)| < M.$$

Remark. Although the above given **Conditions B – E** may seem at a first glance rather restrictive they can be fulfilled for rather broad class of distributions. The details were described in Víšek (1990 b).

Theorem 3. Let **Conditions B – E** holds. Then $\hat{\beta}^n(Y)$ is (weakly) consistent estimator of β^0 and the following representation takes place for any $k = 1, \ldots, p$

$$n^{-\frac{1}{2}} \left\{ \left(\hat{\beta}^n - \beta^0 \right) X'X \right\}_k = n^{-\frac{1}{2}} I^{-1}(g) \sum_{j=1}^{n} x_{jk} \frac{c_n^{-1} \int w'\left(c_n^{-1}(e_j - z)\right) g(z)dz}{\int w\left(c_n^{-1}(e_j - z)\right) g(z)dz} + o_p(1).$$

Corollary.

$$\mathcal{L}\left(n^{-\frac{1}{2}} \left(\hat{\beta}^n - \beta^0 \right) X'X \right) \xrightarrow{n\to\infty} N\left(O, Q \cdot I^{-1}(g)\right).$$

We give again some hint for the proof of Theorem 3 and of Corollary. (We shall again assume that the assumptions of Theorem 3 hold through this chapter.)

Lemma 12. Let Q be a regular and symmetric matrix. For any $\omega > 0$ denote $Z_\omega = \{z \in R^p : \|z\| = \omega\}$. Then

$$\min_{z\in Z_\omega} z'Qz > 0.$$

Lemma 13. Let $\mathcal{V}$ be a matrix $\{v_{k\ell}\}_{k=1,\ell=1}^{n\quad p}$ such that there is a $C > 0$ such that for any $n \in N$

$$\max_{\substack{k=1,\ldots,n \\ \ell=1,\ldots,p}} |v_{k\ell}| < C$$

and $\lim_{n\to\infty} \frac{1}{n}\mathcal{V}'\mathcal{V} = Q$ where Q is a regular matrix. Then for any $\omega > 0$ there are $\lambda > 0$, $\tau > 0$ and $n_0 \in N$ such that for any $z \in R^p$, $\|z\| \geq \omega$ and $n \geq n_0$ we have

$$\#\left\{ k : k \in \{1, \ldots, n\};\ \left| \sum_{\ell=1}^{p} v_{k\ell} z_\ell \right| > \lambda \right\} \geq n \cdot \tau$$

(where $\# A$ denotes the number of elements of the set A).

Lemma 14. Let $f(u)$ be a convex function on $(0,\infty)$ and g_1, g_2 densities on $(-\infty,\infty)$ such that $g_2(x)/g_1(x)$ is increasing on $(-\infty,\infty)$. Then there is a nondecreasing function $\varphi(u)$ on $(0,\infty)$ such that

$$E_{g_1} f\left(\frac{g_2}{g_1}\right) = f(1) + \int_0^1 (t-1)d\varphi(t) + \frac{1}{2}\int_0^\infty \left\{ 1 - t + E_{g_1}\left| \frac{g_2}{g_1} - t \right| \right\} d\varphi(t).$$

Lemma 15. For any θ_1, θ_2, $0 < \theta_1 < \theta_2$ we have

$$E_g \log \frac{c_n^{-1} \int w\left(c_n^{-1}(t-\theta_1-z)\right) g(z)dz}{g(t)} \geq E_g \log \frac{c_n^{-1} \int w\left(c_n^{-1}(t-\theta_2-z)\right) g(z)dz}{g(t)}.$$

Lemma 16. (Csőrgő, Révész (1981) Lemma 6.1.2 and Theorem 6.2.1.)

$$\sup_{y \in R} \left| E g_n(y, Y, \beta^0) - g(y) \right| = O(c_n^2),$$
$$\sup_{y \in R} \operatorname{var} c_n^{-1} w\left(c_n^{-1}(y-z)\right) = c_n^{-1}$$

where variation is taken over $z \in R$. If moreover for any $y \in R$

$$\lim_{z \to \infty} c_n^{-1} w\left(c_n^{-1}(y-z)\right) \left[G(z) \log \log G^{-1}(z)\right]^{\frac{1}{2}} =$$
$$= \lim_{z \to -\infty} c_n^{-1} w\left(c_n^{-1}(y-z)\right) \left[(1-G(z)) \log \log (1-G(z))^{-1}\right]^{\frac{1}{2}} = 0$$

then

$$\lim_{n \to \infty} \sup_{y \in R} \left| g_n(y, Y, \beta^0) - g(y) \right| = 0 \qquad \text{a. e. g.}$$

Lemma 17.

$$n^{-1} c_n^{-3} \sum_{i=1}^{n} \int \left[w''\left(c_n^{-1}(y-e_i)\right) - E w''\left(c_n^{-1}(y-e_i)\right) \right] b_n(y)dy = o_p(1)$$

(let us recall $e_i = e_i(\beta^0) = Y_i - X_i \beta^0$).

Lemma 18.

$$\int \left[\frac{d^2 E g_n(z, Y, \beta^0)}{dz^2} \right]_{z=y} b_n(y)dy = o(1).$$

Lemma 19. For any $k, \ell = 1, \ldots, p$ we have

$$n^{-1} c_n^{-2} \sum_{j=1}^{n} x_{jk} x_{j\ell} \left[\frac{\sum_{i=1}^{n} w''\left(c_n^{-1}(e_j - \tilde{e}_i)\right)}{\sum_{i=1}^{n} w\left(c_n^{-1}(e_j - \tilde{e}_i)\right)} b_n(\tilde{e}_j) - \right.$$
$$\left. - c_n^{-1} \int \int w''\left(c_n^{-1}(y-z)\right) g(z) b_n(y) dz dy \right] = o_p(1)$$

and

$$n^{-1} c_n^{-2} \sum_{j=1}^{n} x_{jk} x_{j\ell} \left[\left\{ \frac{\sum_{i=1}^{n} w'\left(c_n^{-1}(e_j - \tilde{e}_i)\right)}{\sum_{i=1}^{n} w\left(c_n^{-1}(e_j - \tilde{e}_i)\right)} \right\}^2 b_n(\tilde{e}_j) - \right.$$
$$\left. - c_n^{-1} \int \frac{\left[\int w'\left(c_n^{-1}(y-z)\right) g(z)dz\right]^2}{\int w\left(c_n^{-1}(y-z)\right) g(z)dz} b_n(y)dy \right] = o_p(1).$$

Lemma 20. For any $k = 1, \ldots, p$ we have

$$n^{-\frac{1}{2}} c_n^{-1} \sum_{j=1}^{n} x_{jk} \left[\frac{\sum_{i=1}^{n} w'(c_n^{-1}(e_j - \tilde{e}_i))}{\sum_{i=1}^{n} w(c_n^{-1}(e_j - \tilde{e}_i))} - \right.$$
$$\left. - \frac{\int w'(c_n^{-1}(e_j - z)) g(z) dz}{\int w(c_n^{-1}(e_j - z)) g(z) dz} \right] b_n(e_j) = o_p(1).$$

Lemma 21. The asymptotic distribution of

$$\left\{ n^{-\frac{1}{2}} c_n^{-1} \sum_{j=1}^{n} x_{jk} \frac{\int w'(c_n^{-1}(e_j - z)) g(z) dz}{\int w(c_n^{-1}(e_j - z)) g(z) dz} b_n(e_j) \right\}_{k=1,\ldots,p}$$

is $N(O, Q \cdot I(g))$.

Full proofs of all assertions may be found in Víšek (1990 b). The proofs of Theorem 3 and of Corollary use the same technique as the proofs of Theorem 1 and 2 but the approximations are now based also on Lemmas 12 - 21.

5 Test of symmetry of residuals

In this chapter we shall propose a measure of symmetry of residuals based on an idea similar to Hellinger distance is based on.

It was mentioned several times that robust statistics is the statistics of the bulk of data and the rest - possibly outliers - should be (smoothly) rejected (e. g. Hampel et. al. (1986)). The above proposed methods also "reject" (by means of functions $b_n(y)$ and hence not smoothly) some part of observational space. But this is a technical matter just allowing to cope with tails of the estimator of density in the region where we have no data. Hence this rejection doesn't lead - in applications - to rejection of any data. Nevertheless it is clear that from the idea of adaptation it follows that some data (being in the tails of estimated density) are - in some sense - "smoothly rejected" since they are in the region of small values of estimate of density. The idea of "smooth rejection" or "construction a model for the main mass of data" may be emphasized by considering as a measure of symmetry of residuals the following statistics

$$\tilde{H}_n(Y, \beta) = n \cdot \int_{-a_n}^{a_n} \left[g_n^{\frac{1}{2}}(y, Y, \beta) - g_n^{\frac{1}{2}}(-y, Y, \beta) \right]^2 g_n(y, Y, \beta) dy$$

where we assume $\{a_n\}_{n=1}^{\infty} \nearrow \infty$ and

$$\limsup n^{-1} c_n^{-4} a_n = 0.$$

It is clear that although $\tilde{H}_n(Y, \beta)$ seems to be "asymmetric" for $\tilde{\tilde{H}}_n(Y, \beta) = n \int_{-a_n}^{a_n} \left[g_n^{\frac{1}{2}}(y, Y, \beta) - g_n^{\frac{1}{2}}(-y, Y, \beta) \right]^2 g_n(-y, Y, \beta) dy$ we have from the Lemma 24 $\tilde{H}_n(Y, \beta) - \tilde{\tilde{H}}_n(Y, \beta) = o_p(1)$.

Through this chapter we shall assume that there is $V \in R$ such that

$$\sup_{y \in R} g(y) < V < \infty.$$

Theorem 4. The asymptotic distribution of

$$\Delta_n^{-1}\left\{\tilde{H}_n(Y,\beta^0) - m_n\right\}$$

where

$$m_n = \frac{1}{2}\cdot c_n^{-1}\int_{-\infty}^{\infty} w^2(z)dz$$

and

$$\Delta_n^2 = \frac{1}{2}c_n^{-1}\int_{-\infty}^{\infty} g^2(r)dr\int_{-\infty}^{\infty}\left\{\int_{-\infty}^{\infty} w(z)w(v+z)dz\right\}^2 dv$$

is $N(0,1)$.

For the proof of Theorem we prepare a few lemmas. (We shall utilize the function $b_n(y)$ from the previous chapter, i.e. $b_n(y) = 1$ for $|y| \leq a_n$ and equal to zero otherwise. Let us recall also that we have assumed $\sup_{x\in R} w(x) < K_1$.)

Lemma 22.

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} w(z)w\left(z - 2c_n^{-1}t\right) g\left(t - c_n z\right) b_n\left(t - c_n z\right) dtdz = o(1).$$

Proof. Fix an $\epsilon > 0$, find T so that for $|z| > T$ $w(z) < \epsilon$ and $\int_{|z|>T} w(z)dz < \epsilon\cdot K_1^{-1}$ and finally select $n_0 \in N$ such that for $n \geq n_0$ $c_n < \{T^{-2}, 4\epsilon^2 K_1^{-2}V^{-2}\}$. Then for $n \geq n_0$ and $|t| > c_n^{\frac{1}{2}}$ we have $2|c_n^{-1}t| > 2T$, i.e. for $|z| < T$ $|z - c_n^{-1}t| > T$ and it implies that

$$\begin{aligned}&\int_{|z|<T} w(z)\int_{|t|>c_n^{\frac{1}{2}}} w\left(z - 2c_n^{-1}t\right) g\left(t - c_n z\right) dtdz\\ \leq\ & \epsilon\int_{|z|<T} w(z)\int_{|t|>c_n^{\frac{1}{2}}} g\left(t - c_n z\right) dtdz \leq \epsilon\end{aligned}$$

and also

$$\begin{aligned}&\int_{|z|>T} w(z)\int_{|t|>c_n^{\frac{1}{2}}} w\left(z - 2c_n^{-1}t\right) g\left(t - c_n z\right) dtdz\\ \leq\ & K_1\int_{|z|>T} w(z)\left\{\int_{-\infty}^{\infty} g(y)d(y)\right\} dz \leq \epsilon.\end{aligned}$$

On the other hand

$$\begin{aligned}&\int_{-\infty}^{\infty} w(z)\int_{|t|<c_n^{\frac{1}{2}}} w\left(z - 2c_n^{-1}t\right) g\left(t - c_n z\right) dtdz\\ \leq\ & V\cdot K_1\cdot 2c_n^{\frac{1}{2}}\cdot\int_{-\infty}^{\infty} w(z)dz = 2\cdot V\cdot K_1\cdot c_n^{\frac{1}{2}} < \epsilon.\end{aligned}$$

Lemma 23. The asymptotic distribution of

$$\tilde{\Delta}_n^{-1}\left\{\int_{-\infty}^{\infty}\left[\sqrt{n}\left(g_n(y,Y,\beta^0) - g_n(-y,Y,\beta^0)\right)\right]^2 b_n(y)dy - \tilde{m}_n\right\}$$

is $N(0,1)$ where $\tilde{m}_n = 2 \cdot c_n^{-1} \int_{-\infty}^{\infty} w^2(z)dz$ and

$$\tilde{\Delta}_n = 8 \cdot c_n^{-1} \int_{-\infty}^{\infty} g^2(r)dr \int_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} w(z)w(v+z)dz \right\}^2 dv.$$

Proof: Let $G_n(y)$ denote empirical distribution function and put $B_n(t) = \sqrt{n}\,[G_n(\text{inv}G(t)) - t]$. Moreover denote $\psi_n(x,y) = c_n^{-1}\{w(c_n^{-1}(x-y)) - w(c_n^{-1}(x+y))\}$. Then we have

$$\sqrt{n}\left\{g_n(y,Y,\beta^0) - g_n(-y,Y,\beta^0)\right\} =$$
$$n^{-\frac{1}{2}}\left\{\int_0^1 B_n(t)d_t\psi_n(y,\text{inv}\,G(t)) - \int_0^1 B_n(t)d_t\psi_n(-y,\text{inv}\,G(t))\right\}$$

(see Csőrgő, Révész p. 223). Now, following again Csőrgő, Révész, p. 227, denote

$$\xi_n(x,y) = \psi_n(x,y) - \psi_n(-x,y)$$

and put

$$\Gamma_n^*(x) = \int_0^1 \xi_n(x,y)dW(y)$$

where W is the Wiener process. Finally let $R^*(t,s) = E\Gamma^*(t)\Gamma^*(s)$. Then we have

$$R^*(t,s) = \int_{-\infty}^{\infty} \xi_n(t,y)\xi_n(s,y)g(y)dy$$

and denote

$$\tilde{m}_n = \int_{-\infty}^{\infty} R_n^*(t,t)dt \qquad \text{and} \qquad \Delta_n^2 = 2 \cdot \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} [R^*(t,s)]^2\,dtds.$$

Then we find that

$$\begin{aligned}
\tilde{m}_n &= 2 \cdot c_n^{-1} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left\{w^2(c_n^{-1}(t-y)) - w(c_n^{-1}(t-y))\,w(c_n^{-1}(t+y))\right\} g(y)dydt = \\
&= 2 \cdot c_n^{-1} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left\{w^2(z) - w(z)w(z - 2c_n^{-1}t)\right\} g(t - c_n z)\,dtdz = \\
&= 2 \cdot c_n^{-1}\left\{\int_{-\infty}^{\infty} w^2(z)dz + o(1)\right\}
\end{aligned}$$

the last step being implied by the previous lemma. Similarly for $\tilde{\Delta}_n^2$ we obtain successively

$$\begin{aligned}
&\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left\{c_n^{-2}\int_{-\infty}^{\infty} w(c_n^{-1}(t-y))\,w(c_n^{-1}(s-y))\,g(y)dy\right\}^2 dtds \\
= \;& c_n^{-1}\int_{-\infty}^{\infty} g^2(r)dr \int_{-\infty}^{\infty}\left\{\int_{-\infty}^{\infty} w(z)w(v+z)dz\right\}^2 dv
\end{aligned}$$

and evaluation of

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left\{c_n^{-2}\int_{-\infty}^{\infty} w(c_n^{-1}(t-y))\,w(c_n^{-1}(-s-y))\,g(y)dy\right\}^2 dtds$$

gives the same result. To be able to use Csőrgő, Révész, Theorem 6.1.4 we need to verify 6.1.14 of their book. We may write for any $h(t) \in L_2$

$$\begin{aligned}
&\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty}\left\{c_n^{-2}\int_{-\infty}^{\infty} w(c_n^{-1}(t-y))\,w(c_n^{-1}(s-y))\,g(y)dy\right\}h(t)dt\right]^2 ds \\
= \;& \int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} w(z)w(v+z)g(s - c_n v - c_n z)\,dzh(s - c_n v)\,dv\right]^2 ds = O(1)
\end{aligned}$$

and the proof follows (compare Csőrgő, Révész, 6.1.24).

Lemma 24.

$$n \cdot \int_{-a_n}^{a_n} \left[g_n^{\frac{1}{2}}(y,Y,\beta^0) - g_n^{\frac{1}{2}}(-y,Y,\beta^0) \right]^2 \left[g_n(y,Y,\beta^0) - Eg_n(y,Y,\beta^0) \right] dy = O_p\left(n^{-\frac{1}{2}} c_n^{-2} a_n \right)$$

and

$$n \int_{-a_n}^{a_n} \left[g_n^{\frac{1}{2}}(y,Y,\beta^0) - E^{\frac{1}{2}} g_n(y,Y,\beta^0) \right]^2 \left[g_n^{\frac{1}{2}}(-y,Y,\beta^0) - E^{\frac{1}{2}} g_n(-y,Y,\beta^0) \right]^2 dy = O_p\left(n^{-1} c_n^{-2} a_n \right).$$

Proof: By the Schwarz inequality we find an upper bound of the squared value of the left-hand-side (using the fact that $Eg_n(y,Y,\beta^0) = Eg_n(-y,Y,\beta^0)$) in a form

$$n^2 \int_{-a_n}^{a_n} \left[g_n^{\frac{1}{2}}(y,Y,\beta^0) - E^{\frac{1}{2}} g_n(y,Y,\beta^0) - g_n^{\frac{1}{2}}(-y,Y,\beta^0) + E^{\frac{1}{2}} g_n(y,Y,\beta^0) \right]^4 \cdot Eg_n(y,Y,\beta^0) dy \times$$
$$\times \int_{-a_n}^{a_n} \left[g_n(y,Y,\beta^0) - Eg_n(y,Y,\beta^0) \right]^2 E^{-1} g_n(y,Y,\beta^0) dy. \tag{1}$$

Now the first member may be bounded by

$$8 \cdot \int_{-a_n}^{a_n} \left[\left[g_n^{\frac{1}{2}}(y,Y,\beta^0) - E^{\frac{1}{2}} g_n(y,Y,\beta^0) \right]^4 + \left[g_n^{\frac{1}{2}}(-y,Y,\beta^0) - E^{\frac{1}{2}} g_n(-y,Y,\beta^0) \right]^4 \right] Eg_n(y,Y,\beta^0) dy.$$

We shall use inequality $(a-b)^2 \le b^{-2}(a^2-b^2)^2$ which holds for $a \ge 0$ and $b > 0$. We obtain again upper bound for the first summand of the last expression

$$8 \int_{-a_n}^{a_n} E^{-1} g_n(y,Y,\beta^0) \left[g_n(y,Y,\beta^0) - Eg_n(y,Y,\beta^0) \right]^4 dy \le$$
$$\le \quad 8 \cdot \int_{-a_n}^{a_n} E^{-1} g_n \left\{ \frac{1}{n^3 c_n^4} E[w - Ew]^4 + \frac{6}{n^2 c_n^4} \left\{ E[w - Ew]^2 \right\}^2 \right\} dy.$$

Now

$$E[w - Ew]^4 \le E[w - Ew]^2 [w + Ew]^2 \le 4 \left[\sup_{z \in R} w(z) \right]^2 E[w - Ew]^2$$
$$\le \quad 4 \cdot \sup_{z \in R}{}^2 w(z) Ew^2 \le 4 \cdot \sup_{z \in R}{}^3 Ew = 4 \cdot c_n \cdot \sup_{z \in R}{}^3 w(z) Eg_n.$$

In a similar way we arrive at

$$\left\{ E[w - Ew]^2 \right\}^2 \le c_n \sup_{z \in R}{}^3 w(z) Eg_n.$$

Hence the first member of (1) (taking into account also n^2) has order $O_p(c_n^{-3} a_n)$. For the second member we may derive (along similar lines) the order $O_p(n^{-1} c_n^{-1} a_n)$. Taking now into account the fact that we have investigated the squared upper bound we obtain the first assertion of Lemma. The proof of the second one is similar.

Proof of Theorem 4: Due to previous Lemma we have

$$\tilde{H}_n(Y,\beta^0) = n \int_{-a_n}^{a_n} \left[g_n^{\frac{1}{2}}(y,Y,\beta^0) - g_n^{\frac{1}{2}}(-y,Y,\beta^0) \right]^2 Eg_n(y,Y,\beta^0) dy + O_p\left(n^{-\frac{1}{2}} c_n^{-2} a_n \right).$$

Making use of equality

$$g_n^{\frac{1}{2}}(y,Y,\beta) - E^{\frac{1}{2}}g_n(y,Y,\beta) = \frac{1}{2}\left\{g_n(y,Y,\beta) - Eg_n(y,Y,\beta) - \right.$$

$$\left. - \left[g_n^{\frac{1}{2}}(y,Y,\beta) - E^{\frac{1}{2}}g_n(y,Y,\beta)\right]^2\right\} E^{-\frac{1}{2}}g_n(y,Y,\beta)$$

and the fact that (see the proof of previous Lemma)

$$\int_{-a_n}^{a_n}\left[g_n(y,Y,\beta^0) - Eg_n(y,Y,\beta^0)\right]\left[g_n^{\frac{1}{2}}(y,Y,\beta^0) - E^{\frac{1}{2}}g_n(y,Y,\beta^0)\right]^2 dy = O_p\left(n^{-\frac{1}{2}}c_n^{-2}a_n\right)$$

as well as

$$\int_{-a_n}^{a_n}\left[g_n^{\frac{1}{2}}(y,Y,\beta^0) - E^{\frac{1}{2}}g_n(y,Y,\beta^0)\right]^2\left[g_n^{\frac{1}{2}}(-y,Y,\beta^0) - E^{\frac{1}{2}}g_n(-y,Y,\beta^0)\right]^2 dy = O_p\left(n^{-1}c_n^{-2}a_n\right)$$

we arrive at

$$\tilde{H}_n(Y,\beta^0) = \frac{n}{4}\int_{-a_n}^{a_n}\left[g_n(y,Y,\beta^0) - g_n(-y,Y,\beta^0)\right]^2 dy + O_p\left(n^{-\frac{1}{2}}c_n^{-2}a_n\right).$$

Now the proof follows from the Lemma 23.

Remark. Unfortunately the practical experiences with $\tilde{H}_n$ has revealed that "smooth rejection" by means of $g_n(y,Y,\beta)$ is not the luckiest choice. The better is to take as a measure of symmetry

$$H_n(Y,\beta) = n\int_{-a_n}^{a_n}\left[g_n^{\frac{1}{2}}(y,Y,\beta) - g_n^{\frac{1}{2}}(-y,Y,\beta)\right]^2 g_n^{\frac{1}{2}}(y,Y,\beta)dy.$$

The only difference is that we are not able to give explicite expressions for the moments of this statistics and hence the moments have to be estimated from data (by numerical integration). An analogy of the Theorem 4 can be given in the form:

Theorem 4'. The asymptotic distribution of

$$\Delta_n^{-1}\left\{H_n(Y,\beta^0) - m_n\right\}$$

where

$$m_n = \frac{1}{2}c_n^{-\frac{3}{2}}\int\frac{\int w^2\left(c_n^{-1}(z-y)\right)g(y)dy}{\left[\int w\left(c_n^{-1}(z-y)\right)g(y)dy\right]^{\frac{1}{2}}}dz$$

and

$$\Delta_n^2 = \frac{1}{2}c_n^{-2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\left\{\int w\left(c_n^{-1}(z-y)\right)w\left(c_n^{-1}(s-y)\right)g(y)dy\right\}^2}{\left\{\int w\left(c_n^{-1}(z-y)\right)g(y)dy\int w\left(c_n^{-1}(s-y)\right)g(y)dy\right\}^{\frac{1}{2}}}dsdz$$

is $N(0,1)$.

The proof may be carried out along the similar lines as the proof of the Theorem 4.

Remark. To use as a measure of symmetry just the Hellinger distance

$$HD_n(Y,\beta) = n\cdot\int_{-a_n}^{a_n}\left[g_n^{\frac{1}{2}}(y,Y,\beta) - g_n^{\frac{1}{2}}(-y,Y,\beta)\right]^2 dy$$

brings some difficulties since e. g.

$$\int\frac{\int w^2\left(c_n^{-1}(x-y)\right)g(y)dy}{\int w\left(c_n^{-1}(x-y)\right)g(y)dy}dx$$

may be infinite (e. g. for normal as well as exponential kernel and $g(y) = \frac{1}{2}\exp\{-|x|\}$ this integral is really infinite; on the other hand for normal kernel and normal density it is equal to $c_n^{-1}\left(1+c_n^2\right)$).

6 Numerical illustration

In this section we illustrate on the numerical examples the above given results. Two sets of data where used. The first is known from literature as Salinity Data (see Brownlee (1965) or Rousseeuw, Leroy (1987) and for results also Ruppert, Carroll (1980) and again Rousseeuw, Leroy (1987)). The second sample of data was simulated.

Example 1. Let us explain notation of the first table. The first column contains codes of methods: LS – Least Squares; L_1 – Least Absolute Deviations; $\hat{\beta}_{KB}(\alpha)$ – Trimmed Least Squares i.e. after trimming off points "under" 100α % regrenssion quantile (of Koenker & Bassett (1978)) as well as points "above" $100\,(1-\alpha)$ % regression quantile the LS were applied; $\hat{\beta}_{PE}(RQ10)$ – finding 10 % and 90 % regression quantiles (β_{10} and β_{90}), the preliminary estimate $\tilde{\beta} = \frac{1}{2}\,(\beta_{10} + \beta_{90})$ was considered for which residuals were evaluated, then 10% of the smallest and 10 % of the largest residuals (or more precisely points with these residuals) were cut off and finally LS were applied; Huber – M–estimate with $\psi(x) = \mathrm{sign}x \cdot \min\{|x|, 1.25\}$ (1.483.MAD as a scale estimate was used); Andrews – M–estimate with $\psi(x) = \sin(x).\ I_{\{|x|<\pi\}}$ (MAD as a scale estimate was used); LMS – Least Median of Squares; LTS – Least Trimmed Squares (i.e. $\hat{\beta} = \mathrm{argmin}\left\{\sum_{i=1}^{h}(Y - X\beta)^2_{i:n},\ h = [\frac{n}{2}] + \left[\frac{p+1}{2}\right]\right\}$); Adaptive – adaptive estimator based on Hellinger distance was used as a preliminary estimate for Maximum–likelihood–like estimator. The next four columns present values of estimate of corresponding regression coefficients (i.e. for Intercept, Lagged Salinity, Trend and Discharge). The sixth column gathers values of medians of absolute values of residuals (MAD). The seventh one offers values of interquartile range, last but one the values of $H_n(Y,\beta)$ and finally the last one corresponding values of standard normal distribution (for $H_n(Y,\beta)$).

TAB. 1. SALINITY DATA

CODE	INTER-CEPT	SALLAG	TREND	DIS-CHARGE	MAD	IQR	$H_n(Y,\beta)$	P-value
LS	9.59	.777	-.026	-.295	.72	1.38	.096	.538
L_1	14.21	.740	-.111	-.458	.50	.98	.857	.804
$\hat{\beta}_{KB}(.15)$	9.69	.800	-.128	-.290	.67	1.36	.251	.599
$\hat{\beta}_{PE}(RQ10)$	14.49	.774	-.160	-.488	.60	1.05	.541	.704
Huber	13.36	.756	-.094	-.439	.56	1.02	.900	.816
Andrews	17.22	.733	-.196	-.578	.47	.83	.596	.724
LMS	36.70	.365	-.703	-1.298	.36	1.78	1.175	.880
LTS	35.54	.436	-.061	-1.277	.47	1.38	2.522	.994
Adaptive	9.59	.777	-0.30	-.294	.71	1.37	.086	.527

Let us mention that the data are such that even LS applied on the whole sample has coefficient of determination equal to 82,6 %. The use of a robust method for the estimation of model may be justified by (considerable) decrease of dispersion of the main part of residuals. On the other hand the prize we have paid for it is a "decline" of symmetry of residuals (on which e.g. consistency of LMS is based on).

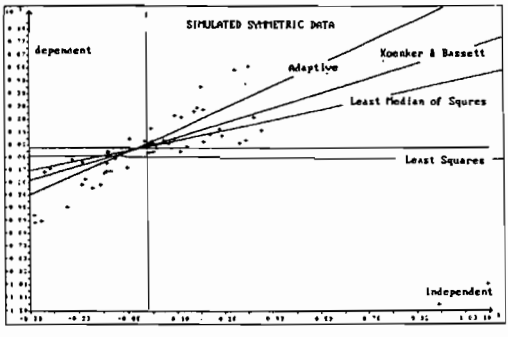
Example 2. Simulated Symmetric Data. The regression model with the zero intercept and slope equal to one was considered. The sample of 56 number from $N(0, 1.3)$ was repeatedly (250 times) generated and the sample with the smallest value of Hellinger distance between the kernel estimate of density of generated data and the kernel estimate of density of data with

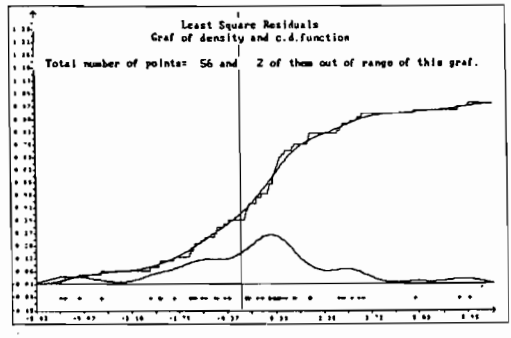
opposite signs was used as a "noise" to create simulated data (data are presented (below) only graphically but available from the author of the present paper). Notation in table is the same as above. The only difference is in the code notation $\hat{\beta}_{KB}(.10WIN)$ which means that the winsorising was used instead of the trimming of points.

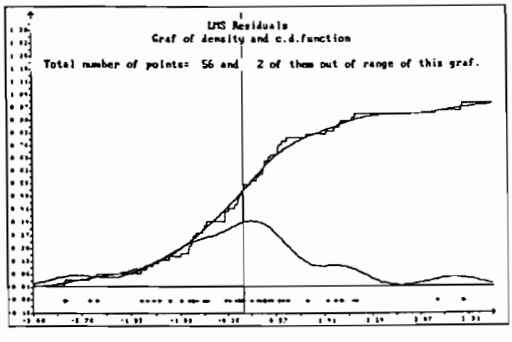
TAB. 2. SIMULATED SYMMETRIC DATA

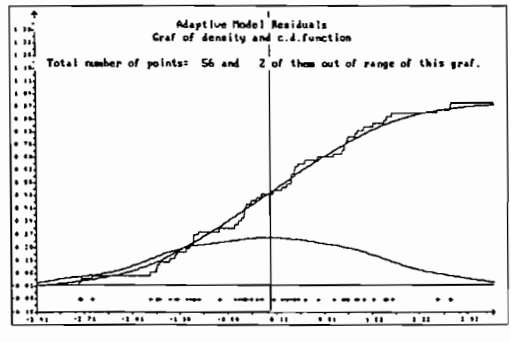
CODE	INTERCEPT	Slope	MAD	IQR	$H_n(Y,\beta)$	P-value
LS	-.375	-.019	1.26	2.36	7.721	1.000
L_1	-.017	.500	.61	1.44	3.772	.999
$\hat{\beta}_{KB}(.10)$	-.025	.668	.79	1.53	1.500	.933
$\hat{\beta}_{KB}(.10WIN)$	-.227	.588	.73	1.44	4.392	1.000
$\hat{\beta}_{PE}(RQ,.10)$	-.263	.661	.77	1.54	4.856	1.000
LMS	.056	.466	.61	1.44	3.067	.999
LTS	.007	.638	.79	1.52	1.530	.937
Adaptive	.001	1.000	1.10	2.19	-.507	.306

TAB. 2 shows that the only method which estimated true model was the adaptive one – due to fact that is had fully utilized the information of symmetry of residuals.









7 Conclusion

The above proposed methods are a little more time consuming than the common (even robust) ones. But as the above example proofs the required extratime may pay back.

The proposed measure of symmetry may be also used as a characteristic of stability of model (an analogy of the coefficient of determination). Its drawback is that the moments of asymptotic distribution are not very easy evaluable. In the present study normal approximations were used. The problem deserves some further studies. The author intents to carry out such study in the next paper.

REFERENCES

Beran, R. (1978) : An efficient and robust adaptive estimator of location, AS 6, pp. 292–313.

Bickel, P. J. (1982) : The 1980 Wald Memorial Lecture: On adaptive estimation, Ann. Statist. 10, pp. 647–671.

Brownlee, K. A. (1965) : Statistical Theory and Methodology in Science and Engineering, 2nd ed., John Wiley & Sons, New York.

Csőrgő, M. and Révész, P. (1981) : Strong Approximations in Probability and Statistics, Akadémiai Kiadó, Budapest.

Fisher, R. A. (1922) : On the Mathematical foundations of theoretical statistics, Philos. Trans. Roy. Soc. London Ser. A 222, pp. 309–368.

Hampel, F. R.; Ronchetti E. M.; Rousseeuw, P. J.; Stahel, W. A. (1986) : Robust Statistics, The Approach Based on Influence Functions, J. Wiley & Sons, New York.

Jurečková, J. (1984) : Regression quantiles and trimmed least squares estimators under a general design, Kybernetika 20, pp. 345–357.

Koenker, R. and Bassett, G. (1978) : Regression quantiles, Econometrika 46, pp. 33–50.

Maronna, R. A. and Yohai, V. J. (1981) : Asymptotic Behaviour of General M–estimates for Regression and Scale with Random Carriers. Z. Wahrscheinlichkeitsteorie verw. Gebiete 58, pp. 7–20.

Pearson, K. (1902) : On the mathematical theory of errors of judgement, with special reference to the personal equation, Philos. Trans. Roy. Soc. Ser. A 198, pp. 235–299.

Rousseeuw, P. J. and Leroy, A. M. (1987) : Robust Regression and Outlier Detection, J. Wiley & Sons, New York.

Rousseeuw, P. and Yohai, V. (1984) : Robust regression by means of S–estimates, in Robust and Nonlinear Time Series Analysis (eds. J. Franke, W. Härdle and D. Martin), Lecture Notes in Statistics No. 26, Springer Verlag, pp. 256–272.

Ruppert, D. and Carroll, R. J. (1980) : Trimmed least squares estimation in the linear model, J. American Statist. Ass. 75, pp. 828–838.

Stein, C. (1956) : Efficient nonparametric testing and estimation, Proc. Third Berkeley Symp. Math. Statist. Prob. University of California Press, 1 pp. 187–196.

Víšek, J. Á. (1990) : What is adaptivity of regression analysis intended for?, Proceedings of ROBUST'90, published by Union of Czechoslovak mathematicians and physicists.

Víšek, J. Á. (1990a) : Adaptive estimation in linear regression model, research report IITA – CSAS[1].

Víšek, J. Á. (1990b) : Adaptive maximum–likelihood–like estimation of regression model, research report IITA – CSAS.

Yohai, V. J. (1974) : Robust estimation in the linear model, Ann. Statist. 2, pp. 562–567.

[1]Institute of Information Theory and Automation, Czechoslovak Academy of Sciences

LEAST SQUARES ESTIMATION IN ALMOST-LINEAR REGRESSION MODEL

Boris P. Kovachev
Laboratory of Computational Stochastics, Institute of Mathematics,
Bulgarian Academy of Sciences, 1113 Sofia, BULGARIA

1. INTRODUCTION

Efron (1975) introduces basic geometrical structures of one-parameter curved exponential families. Bates and Watts (1980) discuss the effect of parameter transformations in non-linear regression model and introduce intrinsic and parameter-effect curvature in order to elucidate its non-linearity. The higher-order geometrical asymptotic theory of statistical estimators however is constructed only for exponential families of distributions (Amari 1982,1985). The explanation is that the regular family of distributions is exponential if and only if a finite-dimensional sufficient statistic exists.

The almost-linear regression models (ALRM) are introduced by Kovachev (1989a). It is proved that a finite-dimensional sufficient statistic exists for a non-linear regression model with normal distributed error iff it is ALRM, (Kovachev 1988). We put ourselves the task to show that in the class of all regression models the almost-linear model plays the same role as the exponential families in the class of all probability distributions. In that sense the linear regression models correspond to exponential-type distributions.

As it is shown by Kovachev (1989b) even in case of error with non-Gaussian distribution ALRM has characteristics which enable to construct suitable differential- geometrical structures. The ideas are similar to those developed by Amari (1985) for curved exponential families. The structures so defined lead to some higher- order asymptotic properties of the estimators. In the present paper first-, second- and third- order efficiency of the least squares estimator (LSE) in ALRM are derived. An accelerated double- step least squares estimation procedure for ALRM based on its geometrical structure is proposed.

2. THE MODEL

Let $y_1, y_2, ..., y_N$ be independent random variables which can be expressed as

$$y_i = r(p_i, u) + \varepsilon_i \qquad (1)$$

where $r(p, u)$ is a regression function of the predictors $p_1, p_2, ..., p_N$ and of the vector

parameter $u = (u_1, ..., u_m)' \epsilon U \subset R^m$. $\varepsilon_1, \varepsilon_2, ..., \varepsilon_N$ are independent random variables which satisfy the conditions:

$$E\varepsilon_i = 0, \quad E\varepsilon_i^2 = \sigma_i^2, \quad E\varepsilon_i^3 = 0, \quad i = 1, 2, ..., N. \tag{2}$$

The variances σ_i, $i = 1, 2, ..., N$ are supposed to be uniformly bounded by some positive constant. By putting $y^N = (y_1, y_2, ..., y_N)'$, $r^N(u) = (r(p_1, u), ..., r(p_N, u))'$ and $\varepsilon^N = (\varepsilon_1, \varepsilon_2, ..., \varepsilon_N)'$ we obtain from (1) the common vector form of the nonlinear regression model

$$y^N = r^N(u) + \varepsilon^N \tag{3}$$

Let for every fixed N the set $\Im_N = \{r^N(u), u \epsilon U\}$ be the linear hull of the regression function and let $n_N = dim(\Im_N)$.

Definition 1. *The number* $n = \lim_{N \to \infty} n_N$ *(finite or* $+\infty$*) is called rank of the regression model (3).*

Definition 2. *If* $n < +\infty$ *the model (3) is called ALRM.*

It is proved by Kovachev (1989b) that the common vector form of ALRM is given by:

$$y^N = A^N . \eta(u) + \varepsilon^N \tag{4}$$

where A^N is an $(N \times n)$ matrix with full rank n and $\eta(u)$ is a n-dimensional vector function of the parameter $u = (u_1, ..., u_p)'$ which does not depend on N. Let Σ^N be the covariance matrix of the random vector ε^N and let

$$y^N = A^N . \eta + \varepsilon^N \tag{5}$$

be the correspondent to (4) linear regression model, where $\eta = (\eta_1, ..., \eta_n)'$ is its n-dimensional vector parameter. In the following we shall not write the upper index N remembering that y, A, ε and Σ depend on it.

Since the matrix A has a full rank then $G = A'\Sigma^{-1}A$ is symmetric and positive-definite. For the elements of G we introduce the following notations: $G = (g^{ij})$, $G^{-1} = (g_{ij})$, $d^i = (g^{ii})^{1/2}$, $i, j = 1, 2, ..., n$. The least squares estimator $\hat{\eta}$ of the parameter η in the linear model (5) based on the observations $y_1, y_2, ..., y_N$ is given by

$$\hat{\eta} = G^{-1} A' \Sigma^{-1} y \tag{6}$$

As it is mentioned above if the random vector ε has normal distribution then the LSE $\hat{\eta}$ is sufficient statistic for the parameter u in the model (4). Moreover in that case G is the Fisher information matrix for the parameter η in (5). That enables to project ALRM without information losses. As it is seen below the projection is formally clear even in case of an arbitrary error ε satisfying the conditions (2).

3. PROJECTION

In order to study the relations between a geometrical structure of ALRM (4) and its asymptotic properties (as $N \to \infty$) we have to project it in finite- dimensional Euclidean space.
Let' denote $e = G^{-1}A'\Sigma^{-1}\varepsilon$. e is n-dimensional random vector $e = (e_1, e_2, ..., e_n)'$ with

$$Ee_i = 0, \quad Ee_ie_j = g_{ij}, \quad Ee_ie_je_k = 0, \quad i,j,k = 1,2,...,n.$$

which follows directly from (2).

Definition 3. *The model*

$$x = \eta(u) + e, \quad x = (x_1, ..., x_n)' \tag{7}$$

is called a projection of ALRM (4).

Let $\check{u}$ be the LSE in the model (4) and let $\hat{u}$ be the LSE in its projection (7).

Proposition 1. *The estimators $\check{u}$ and $\hat{u}$ coincide.*

Proof. The LSE $\check{u}$ is the solution of the equations

$$(\partial/\partial u_a \eta(u))'(A'\Sigma^{-1}y - G\eta(u)) = 0, \quad a = 1,2,...,m$$

In the model (7) $\hat{u}$ is given by $\min_u(\hat{\eta} - \eta(u))'G(\hat{\eta} - \eta(u))$ i.e. $\hat{u}$ is the solution of the equations

$$(\partial/\partial u_a \eta(u))'(G\hat{\eta} - G\eta(u)) = 0, \quad a = 1,2,...,m \tag{8}$$

Now (6) completes the proof. ∎

The statement of the proposition above is important from computational point of view. It enables us to construct a double-step least squares estimation procedure for almost-linear models:

(i) Linear regression in (5) and producing the estimator $\hat{\eta}$.

(ii) Non-linear regression in the projection (7) by taking observations at $\hat{\eta}$.

If the model is an almost-linear one and $N \gg n$ the two-step procedure (i)-(ii) given above is much more effective than the direct estimation in (2).

Furthermore we shall study the projected model (7) and the estimators of u which are functions of the $\hat{\eta}$. It is necessary to assume some asymptotic properties of the LSE $\hat{\eta}$. Let $\eta^0 = (\eta_1^0, ..., \eta_n^0)'$ be the true value of η and $\tilde{\eta}_i = d^i(\hat{\eta}_i - \eta_i^0), i = 1,2,...,n$. Under simple conditions on G given by Eicker (1963) the estimator $\hat{\eta}$ is proved to have the following properties:

A1 $\hat{\eta}$ is consistent, i.e. $\lim_{N\to\infty} = \eta^0$;

A2 $\tilde{\eta} = (\tilde{\eta}_1, ..., \tilde{\eta}_n)$ is asymptotically normal distributed with zero mean and covariance matrix I_n.

4. GEOMETRICAL STRUCTURE OF ALRM

Let us consider the linear model

$$x = \eta + e, \quad x = (x_1, ..., x_n)' \tag{9}$$

and the functions

$$l(x, \eta) = x'G\eta - \Phi(\eta), \quad l(x, \theta) = x'\theta - \Psi(\theta)$$

where

$$\theta = G\eta, \quad \Phi(\eta) = \frac{1}{2}\eta' G\eta, \quad \Psi(\theta) = \frac{1}{2}\theta' G^{-1}\theta$$

The set of functions $S = \{l(x, \eta); \eta \epsilon R^n\}$ is a linear manifold with natural part of dual coordinate systems η and θ which is isomorphic to the n-dimensional Euclidean space. The tangent vectors at point θ_0 are given by $\partial_i = \partial/\partial\theta^i$ for θ -coordinate system and by $\partial^i = \partial/\partial\eta_i$ for η -coordinate system respectively. The tangent space T_{θ_0} at a point θ_0 is a vector space spanned on $\{\partial_i\}$ or $\{\partial^i\}$. In the following we adopt Einstein summation convention without using summation symbol.

The set

$$T^{(1)}_{\theta_0} = \{A(x); A(x) = A^i \partial_i l(x, \theta_0)\}$$

is a linear space of random variables which is naturally isomorphic to T_{θ_0}.

Definition 4. *$T^{(1)}_{\theta_0}$ is called 1-representation of the tangent space T_{θ_0}.*

Let us introduce the inner product of two tangent vectors of T_θ via their 1-representation by the following way. For every $A, B \epsilon T_\theta, < A, B >= EA(x)B(x)$. .

Proposition 2. *The metric tensor in T_θ is exactly the covariance of the random variable e.*

Proof. By definition $E\partial_i l(x, \theta) = E(x_i - \partial_i \Psi(\theta))$, but $\partial_i \Psi(\theta) = g_{ij}\theta^j = \eta_i$. Therefore

$$E\partial_i l(x, \theta) = 0, i = 1, 2, ..., n$$

and

$$< \partial_i, \partial_j >= Cov(\partial_i l(x, \theta), \partial_j l(x, \theta))$$

Hence

$$< \partial_i, \partial_j >= g_{ij} \tag{10}$$

which completes the proof.∎

Corollary 1. *The metric tensor in T_η is given by*

$$< \partial^i, \partial^j >= g^{ij} \tag{11}$$

Proof. The statement follows directly from the definition of g^{ij}. ∎

Corollary 2. *Let the random variable ε in the model (3) be normally distributed. Then the metric tensor G is exactly Fisher information matrix for the parameter η in the model (9).* ∎

In the non-Gaussian case we can define G to be the information matrix for the parameter η in the model (4).

Note. G^{-1} is the information matrix for the parameter θ.

Corollary 3. The two bases $\{\partial_i\}$ and $\{\partial^i\}$ are biorthogonal.

Proof. The two bases $\{\partial_i\}$ and $\{\partial^i\}$ are connected by $\partial_i = (\partial\eta_h/\partial\theta^i)\partial^h$ and $\partial^j = (\partial\theta^k/\partial\eta_j)\partial_k$ Since $\partial\eta_k/\partial\theta^i = g_{ki}$ and $\partial\theta^h/\partial\eta_j = g^{kj}$ then we obtain from (11)

$$< \partial_i, \partial^j >= g_{ki}g^{jk} = \delta_i^j$$

where δ_i^j is Kroneker symbol. ∎

Corollary 4. $< \partial_i, \partial_j >= \partial_i\partial_j\Psi(\theta)$ and $< \partial^i, \partial^j >= \partial^i\partial^j\Phi(\eta)$.

The proof follows from (10),(11). ∎

Using corollaries 3 and 4 we can say that the coordinate systems θ and η are mutually dual and $\Psi(\theta)$ and $\Phi(\theta)$ are their potential functions.

Definition 5. *For the linear model (9) θ and η are called natural and expectation coordinate systems respectively.*

Let $l(x,u) = l(x,\eta(u))$ and $M = \{l(x,u); u\epsilon U\}$. The parameter $u = (u_a), a = 1,2,...,m$ defines a coordinate system of M . Let the mapping $\eta = \eta(u)$ be smooth and the Jacobian matrix $B_{ai} = \partial\eta_i(u)/\partial u_a, a = 1,2,...,m, i = 1,2,...,n$ has a full rank m for all $u\epsilon U$. Then the equation $\eta = \eta(u)$ gives a parametric representation of M as a smooth manifold imbedded in R^n. The tangent space $T_u(M)$ of M is a vector space spanned on the m vectors $\partial_a = \partial/\partial u_a$. Since $\partial_a = B_{ai}\partial^i$ it follows that ∂_a is a linear combination of ∂^i and the tangent space $T_u(M)$ is a subspace of $T_{\eta(u)}$. The metric tensor of $T_u(M)$ is given by

$$g_{ab}(u) =< \partial_a, \partial_b >= B_{ai}B_{bj}g^{ij} \tag{12}$$

Proposition 3. *(g_{ab}) is Fisher information matrix for the parameter u in the model (7).*

Proof. Follows directly from Proposition 2. ∎

Let $\hat{u} = \hat{u}(\hat{\eta})$ be an estimator of u in the model (7). Let $B_\varepsilon(u) = \{\eta; \hat{u}(\eta) = u\}$ and $A_\varepsilon(u) = \{l(x,\eta); \eta\epsilon B\}$. Let $A(\hat{u}) = \{A_\varepsilon(u); u\epsilon U\}$. $A(\hat{u})$ is a family of $(n-m)$-dimensional submanifolds of R^n.

Definition 6. *The estimator $\hat{u}$ is said to be regular if the family $A(\hat{u})$ form a local foliation of R^n in a neighborhood of M.*

Let $v = (v_\lambda), \lambda = m+1,...,n$ be a coordinate system of $A_\varepsilon(u)$ and let the origin $v = 0$ coincide with $\eta(u)$ .If the estimator $\hat{u}$ is regular $w = (u_a, v_\lambda), a = 1,...,m, \lambda = m+1,...,n$

is a coordinate system of R^n in a neighborhood of M. Let $w = (w_\alpha), \alpha = 1, 2, ..., n$ and let $\partial_\alpha = \partial/\partial w_\alpha$. The metric tensor $g_{\alpha\beta} =< \partial_\alpha, \partial_\beta >$ decomposes into four parts:

$$(g_{\alpha\beta}) = \begin{pmatrix} g_{ab} & g_{a\lambda} \\ g_{\mu b} & g_{\mu\lambda} \end{pmatrix} \tag{13}$$

where $\alpha, \beta = 1, 2, ..., n; \quad a, b = 1, 2, ..., m; \quad \lambda, \mu = m+1, ..., n.$

Definition 7. *The family $A(\bar{u})$ is ancillary family associated with the estimator $\bar{u}$.*

The theorems below proved by Kovachev (1989a) clarify that there is one-to-one correspondence between the statistical properties of an estimator and the geometry of its ancillary family.

Theorem 1. *Let $\bar{u}$ be a regular estimator and* **A1** *holds. $\bar{u}$ is consistent iff the point $\eta(u) \epsilon B_{\bar{u}}(u)$ for every $u \epsilon U$.* ∎

Theorem 2. *Let the conditions* **A1** *and* **A2** *hold. The regular consistent estimator $\bar{u}$ is first- order efficient if and only if its ancillary family is orthogonal to M in every crosspoint.* ∎

Note. It means that the mixed part in the decomposition of the metric tensor (13) vanishes, i.e. $g_{a\lambda} = 0, a = 1, ..., m; \ \lambda = m+1, ..., n$

Let $H_{ab\lambda}(u)$ be the Euler- Schouten curvature tensor i.e the imbedded curvature of M in R^n and $H_{\lambda\mu a}(u)$ be the imbedded curvature of $B_{\bar{u}}(u)$. Let Δg_{ab} be the asymptotic information losses of the first- order efficient estimator $\bar{u}$ given by:

$$\Delta g_{ab}(\bar{u}) = lim_{N \to \infty} E|Cov(\partial_a l(x, u), \partial_b l(x, u) \mid \bar{u})|$$

Theorem 3. *Let the conditions* **A1** *and* **A2** *hold. The asymptotic information losses of a regular first- order efficient estimator are given by*

$$\Delta g_{ab}(\bar{u}) = (H^M_{ab})^2 + \frac{1}{2}(H^A_{ab})^2$$

where $(H^M_{ab})^2$ is the sum of squares of the components $(H_{ab\lambda}(u))$ and $(H^A_{ab})^2$ is sum of squares of $(H_{\lambda\mu a}(u))$. ∎

Corollary 5. *A regular first- order efficient estimator is second- order efficient iff $B_{\bar{u}}(u)$ is flat in the neighbourhood of M, i.e. iff $(H^A_{ab}) = 0, a, b = 1, ..., m.$* ∎

5. LEAST SQUARES ESTIMATION

Let $\hat{u}$ be the LSE for the model (7). It was already pointed out that $\hat{u}$ is a solution of (8). **Theorem 4.** *Let $\hat{u}$ be the LSE for the model (7). Then for every $u \epsilon U$, $B_{\hat{u}}(u)$ and $A_{\hat{u}}(u)$ have the properties:*

(i) $\eta(u) \epsilon B_{\hat{u}}(u)$

(ii) $A_{\hat{u}}(u)$ is orthogonal to M at point $\eta(u)$.

(iii) $B_{\hat{u}}(u)$ is an (n-m)-dimensional linear subspace of R^n

Proof. By (8) we obtain that

$$B_{\hat{u}}(u) = \{\eta \epsilon R^n \mid (\partial_a \eta(u))' G(\eta - \eta(u)) = 0\} \qquad (14)$$

Hence $\eta(u) \epsilon B_{\hat{u}}(u)$. For every fixed u the set $B_{\hat{u}}(u)$ is the set of solutions of a homogeneous linear system of equations with rank m . Therefore (iii) holds. By (14) and (11) we obtain further that

$$< \eta - \eta(u), \partial_a \eta(u) >= 0, a = 1, 2, ..., m$$

Hence the tangent space $T_{\hat{u}}(A)$ of $A_{\hat{u}}(u)$ is orthogonal to the tangent space $T_{\hat{u}}(M)$ at a point $\eta(u)$. Finally we obtain from (13) that the mixed part $(g_{a\lambda}), a = 1, 2, ..., m, \lambda = m + 1, ..., n$ of the metric tensor $(g_{\alpha\beta}), \alpha, \beta = 1, 2, ..., n$ vanishes. Thus (ii) holds. ∎

Corollary 6. *Let $\hat{\eta}$ be a consistent estimator of η in the linear model (5). Then $\hat{u}$ is consistent, first order and second order efficient estimator of in the model (7).* ∎

5. REFERENCES

Amari, S.(1982). Differential geometry of curved exponential families-curvatures and information loss. Ann. Stat. **10**.

Amari, S.(1985). Differential geometrical methods in Statistics, Spinger-Verlag, Berlin.

Bates, D.M., Watts, B.G. (1980). Relative curvature measures of non-linearity. J. Roy. Stat. Soc. **B40**.

Efron, B., (1975). Defining the curvature of a statistical problem (with application to second order efficiency). Ann. Stat. **3**.

Efron, B., (1978). The geometry of exponential families. Ann. Stat.**6**.

Eicker, F., (1963). Asymptotic normality and consistency of least squares estimators for families of linear regressions. Ann. Math. Statist.,**34**.

Kovachev, B.P. (1988). Sufficient statistics in non-linear regression model. Proc. of Seventh Spring Conf. of the Union of Bulg. Mathematicians, April 1988.

Kovachev, B.P. (1989a). Asymptotic properties of estimators in almost- linear regression model. Compt. Rend. Acad. bulg. Sci., **42**, 3.

Kovachev, B.P. (1989b). Asymptotic expansions for a family of non-linear regression models. Compt. Rend. Acad. bulg. Sci., **42**, 5.

BOOTSTRAP AND ESTIMATION OF NONLINEAR PARAMETERS

Henning Läuter, Berlin

Bootstrap methods are widely used in many fields of statistics. Efron published in 1979 his pioneer work on jackknife and general resampling methods. He discussed advantages and disadvantages for such procedures. The resampling methods are popular in such a high way because of the possibilities for approximating unknown distributions and for increasing the efficiency of statistical procedures. Of course not in all situations bootstrap and other resampling methods will improve statistical decisions. This is the reason for investigating the resampling methods from the theoretical point of view. One has to justify the use of these methods.

We will consider the nonlinear estimation. Mostly in such problems the usual methods known from linear models are used in a very direct way. But one can increase the efficiency of nonlinear procedures by explicite using the special structure of the nonlinearities. We will discuss the conditional unbiasedness of estimators and will improve the maximum-likelihood or least squares estimators in special models with the help of a bootstrap principle. As examples we consider the estimation of an exponential parameter and the estimation of the error rate in discriminant analysis.

1. ESTIMATION OF NONLINEAR PARAMETERS

Let y be a random variable with a distribution Q_o, $Q_o \in \mathcal{P}$. $\mathcal{P}$ is a known class of distributions. $\lambda(Q) \in R^1$ is a parameter to be estimated. If $\hat{\lambda}$ is an estimate for $\lambda(Q)$ then $\hat{\lambda}$ is unbiased if

$$E_Q \hat{\lambda}(y) = \lambda(Q) \quad \text{for all } Q \in \mathcal{P}. \tag{1}$$

Here $E_Q \hat{\lambda}(y) = \int \hat{\lambda}(z) Q(dz)$. In special problems we need for $\hat{\lambda}$ instead of (1) only

$$E_{Q_o} \hat{\lambda}(y) = \lambda(Q_o) \tag{2}$$

but Q_o is unknown. An outway from this is to work with approximations $\hat{Q}$ for Q_o and those approximations are to be constructed with resampling methods. For example let us consider the linear model $y=X\beta+\epsilon$ under the standard assumptions: $X:nxk$, $\beta \epsilon R^k$, $E\epsilon=0$, Cov $\epsilon=\sigma^2 I$. And for $\epsilon=(\epsilon_1,\ldots,\epsilon_n)'$ we assume $\epsilon_i \sim F$. Then we have the residuals $\hat{\epsilon}=y-X\hat{\beta}$ for the least squares estimator $\hat{\beta}=(X'X)^{-}X'y$. Because in general $\hat{\mu}=\frac{1}{n}\Sigma \epsilon_i \neq 0$ we construct the centered residuals

$$\epsilon_1 - \hat{\mu},\ldots,\epsilon_n - \hat{\mu}$$

with the empirical distribution function $\hat{F}$. Here we have $\int x d\hat{F} = 0$. Now for given y let $\epsilon_1^*,\ldots,\epsilon_n^*$ be conditionally independent with $\epsilon_i^* \sim F$. We denote $\epsilon^*=(\epsilon_1^*,\ldots,\epsilon_n^*)'$ and consider the bootstrap model

$$y^*=X\hat{\beta}+\epsilon^*.$$

The ϵ^* is obtained by resampling the centered residuals. Therefore the y^* is generated from the data using the regression model with $X\hat{\beta}$ as the expectation and $\hat{F}$ as the distribution of the components in ϵ^*. The asymptotic properties of estimations in the bootstrapped model is investigated by several authors, especially we mention Efron (1979), Bickel & Freedman (1981), Freedman (1981).

In this example $\hat{F}$ is an approximation of the unknown distribution F. The condition (3) can be interpreted as the validity of

$$E_Q \hat{\lambda} = \lambda(Q)$$

for all Q from a neighbourhood of Q_0. The approximations $\hat{Q}=\hat{Q}_y$ of Q_0 are elements of another neighbourhood of Q_0 and hence one could demand

$$E_{\hat{Q}_y}\hat{\lambda} = \quad (\hat{Q}_y)$$

instead of (1). These $\hat{Q}_y$ are based on the sample and insofar in real practical problems the family of the $\hat{Q}_y$ is more natural than a given family $\mathcal{P}$.

Definition: The estimator $\hat{\lambda}$ is called conditioned unbiased (CUE) if for almost all z

$$E_{\hat{Q}_z}\hat{\lambda} = \lambda(\hat{Q}_z)$$

with

$$E_{\hat{Q}_z}\hat{\lambda} = E\{\quad \hat{\lambda}(y_1^*,\ldots,y_n^*) \mid y=z\},$$

$$y^* = (y_1^*,\ldots,y_n^*) \sim \quad \hat{Q}_z.$$

We give now two examples for such CUE.

Example 1: Let $y_1,\ldots,y_n$ be i.i.d. variables with $Ey_i=\mu$ and $\lambda(Q)=\mu$. We use $\hat{\lambda}(y)=\frac{1}{n}\Sigma\, y_i=\bar{y}$ and we denote by $\hat{F}$ the empirical distribution of the residuals. As before $\epsilon_1^*,\ldots,\epsilon_n^*$ are i.i.d. variables with the distribution $\hat{F}$. Then the bootstrapped model is

$$y_i^* = \bar{y} + \epsilon_i^*, \quad i=1,\ldots,n$$

and we have $(y_1^*,\ldots,y_n^*) \sim \hat{Q}_y$. Then $\lambda(\hat{Q}_y)=\bar{y}$ and $E_{\hat{Q}_y}y_i^*=\bar{y}$, $i=1,\ldots,n$. Furthermore there is $\hat{\lambda}(y_1^*,\ldots,y_n^*)=\bar{y}^*$ and

$$E\{\quad \hat{\lambda}(y_1^*,\ldots,y_n^*) \mid y=z\} = \bar{z} = \lambda(\hat{Q}_z).$$

This means that the sample mean is CUE.

Example 2: For k distributions $Q_1,\ldots,Q_k$ the parameter $\lambda(Q)=\lambda(Q_1,\ldots,Q_k)$ is to be estimated,

$$\lambda(Q) = \int\ldots\int \varphi(x_{11},\ldots,x_{1m_1},x_{21},\ldots,x_{km_k}) \prod_{i=1}^{k} Q_i(d\,X_i)$$

with $x_{ij}\in \mathbb{R}^p$, $X_i=(x_{i1},\ldots,x_{im_i})$, $Q_i(d\,X_i) = \prod_{j=1}^{m_i} P_i(dx_{ij})$. Here φ is symmetrically in each of the k tupels $x_{i1},\ldots,x_{im_i}$. If there are given samples $y_{i1},\ldots,y_{in_i}$ of P_i, $n_i>m_i$, and if $\hat{Q}_i$ is the empirical distribution of all subsamples of $y_{i1},\ldots,y_{in_i}$ of the size m_i without replacement then the usual U-statistics $\hat{\lambda}$ can be represented by

$$\hat{\lambda} = \int\ldots\int \varphi(X_1,\ldots,X_k) \prod_{i=1}^{k} \hat{Q}_i(d\,X_i) = \lambda(\hat{Q}_1,\ldots,\hat{Q}_k) = \lambda(\hat{Q}).$$

From this $E_{\hat{Q}}\varphi=\lambda(\hat{Q})$ follows. Hence the kernel φ of the functional λ is CUE.

In general it is difficult to find a CUE for special estimation problems. But one can determine a first corrected approximation starting with a given estimator $\hat{\lambda}$. For this one has two possibilities:

- Multiplicative correction
  We define the estimator $\hat{\lambda}_m$ by

$$\frac{\hat{\lambda}_m(y)}{\hat{\lambda}(y)} = \frac{\lambda(\hat{Q}_y)}{E_{\hat{Q}_y}\hat{\lambda}} .$$

- Additive correction
  We define $\hat{\lambda}_a$ by

$$\hat{\lambda}_a(y) - \hat{\lambda}(y) = \lambda(\hat{Q}_y) - E_{\hat{Q}_y}\hat{\lambda} .$$

In both variants we transmit the relations in the sample expressed by $\hat{Q}_y$ to the whole populations. E.g. $\lambda(\hat{Q}_y)-E_{\hat{Q}_y}\hat{\lambda}$ gives us the negative bias of $\hat{\lambda}$ assuming $\hat{Q}_y$ is the "true" distribution. Then it is naturally to correct $\hat{\lambda}$ in the given way and to work with $\hat{\lambda}_a$ instead of $\hat{\lambda}$. The same arguments hold for $\hat{\lambda}_m$.

The power of these corrected estimates is to be studied for special models.

2. ESTIMATION OF A NONLINEAR PARAMETER IN LINEAR MODELS

Let $y_1,\ldots,y_n$ be independently normally distributed according to $N(\beta,1)$. We estimate $\lambda(Q)=e^{\beta}$ and use the maximum-likelihood estimator $\hat{\lambda}=e^{\hat{\beta}}$ with $\hat{\beta}=\bar{y}$. Then $\lambda(\hat{Q}_y)=\hat{\lambda}$ if $\hat{Q}_y$ is the empirical distribution function. We denote

$$c(z) = E\{e^{\bar{y}^*}|y=z\}$$

and find by a multiplicative correction

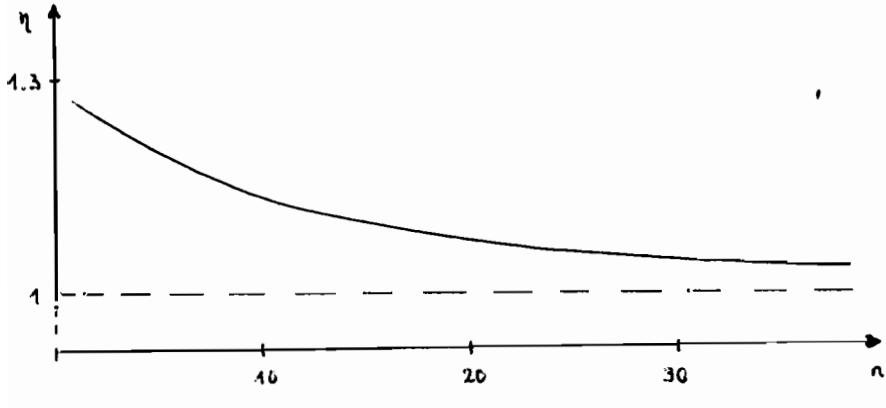
$$\hat{\lambda}_m(y) = \frac{e^{\bar{y}}}{c(y)}\hat{\lambda} = \frac{e^{2\bar{y}}}{c(y)} .$$

Then we have $c(y)=(\frac{1}{n}\sum e^{\frac{1}{n}y_i})^n$. Furthermore $(e^{\hat{\beta}})^{\frac{1}{n}}$ and $c(y)^{\frac{1}{n}}$ are the geometric and arithmetic means of $e^{\frac{1}{n}y_1},\ldots,e^{\frac{1}{n}y_n}$ and therefore $e^{\hat{\beta}} < c(y)$ holds. This means that $\hat{\lambda}_m < \hat{\lambda}$ with the strinkage factor $\frac{e^{\bar{y}}}{c(y)}$. One finds that $\frac{e^{\bar{y}}}{c(y)}$ is independent of β. We check that

$$\text{MSE } \hat{\lambda}_m = E(\hat{\lambda}_m - \lambda(Q))^2 = e^{2\beta}\, E\left(\frac{e^{2\bar{\epsilon}}}{c(\epsilon)} - 1\right)^2,$$

$$\text{MSE } \hat{\lambda} = e^{2\beta}E(e^{\bar{\epsilon}}-1)^2.$$

For $\eta = \text{MSE } \hat{\lambda}/\text{MSE } \hat{\lambda}_m$ we get the following plot.



3. ESTIMATION OF THE ERROR RATE IN DISCRIMINANT ANALYSIS

We consider k classes with unkonown distributions $P_1,\ldots,P_k$. For any P_i there is given a sample $y_{i1},\ldots,y_{in_i}$ of size n_i. By $Y=(y_{11},\ldots,y_{kn_k})$ we denote the total sample matrix. A discriminant procedure is defined by k nonnegative functions $g_1(y|Y),\ldots,g_k(y|Y)$ with $\sum_i g_i(y|Y)=1$ and $g_i(y|Y)$ is the probability for assigning y to P_i. The probability for misclassification from the i-th into the j-th class is given by

$$f_{j|i} = \int g_j(x|Y)\, P_i(dx).$$

Let $q_1,\ldots,q_k$ be prior probabilities for the classes. With the total probability for misclassification

$$f(P|Y) = \sum_{i=1} q_i \sum_{\substack{j=1 \\ j\neq i}} f_{j|i}$$

the error rate of the discriminant procedure $g(y|Y)=(g_1(y|Y),\ldots,g_k(y|Y))$ is defined by $F(P)=E\, f(P|Y)$.

We look for the estimation of F(P). We mention here the results of Smith (1947), Lachenbruch & Mickey (1968), Schaafsma & van Vark (1977), McLachlan (1977), Efron (1979), Ahrens & J. Läuter (1981), H. Läuter (1985). Here one finds results on the cross-validation and the bootstrap estimator for F(P).

The cross-validation estimator is an almost unbiased estimator. By $Y_{(il)}$ we denote the px(n-1) sample matrix of all $y_{11},\ldots y_{kn_k}$ besides y_{il}. Here $n=n_1+\ldots+n_k$. The cross validation estimator is defined by

$$f = \sum_{i=1}^{k} \frac{q_i}{n_i} \sum_{\substack{j=1 \\ j\neq i}}^{k} \sum_{l=1}^{n_i} g_j(y_{il}|Y_{(il)}) \cdot$$

The bootstrap estimator has a small variance. By $\hat{P}_i$ we denote the empirical distribution of $y_{i1},\ldots,y_{in_i}$ and $\hat{P}=(\hat{P}_1,\ldots,\hat{P}_k)$. Then the bootstrap estimator is given by $f^*=F(\hat{P})$.

If one compares these two estimators then the following results are known:

$$|E\,\bar{f} - F(P)| \leq |E\,f^* - F(P)|,$$

$$\text{Var } f^* \leq \text{Var } \bar{f},$$

$$\text{MSE } f^* \leq \text{MSE } \bar{f} \qquad \text{for "small" dimensions or "large" } n_i,$$

$$\text{MSE } \bar{f} \leq \text{MSE } f^* \qquad \text{for "high" dimensions or "small" } n_i.$$

An alternative estimator to $\bar{f}$ and f^* is a corrected estimator according to the discussions in section 1. We choose $\hat{\lambda} = f^*$ and $E_P\bar{f}$ is to be estimated. Then $\hat{\lambda}_m$ is defined by

$$\hat{\lambda}_m = \frac{E_{\hat{P}}\bar{f}}{E_{\hat{P}}f^*}\, f^* .$$

The comparison of $\hat{\lambda}_m$ with $\bar{f}$ and f^* was done by simulations. We considered k=2, p=10, $P_i=(\mu_i, \Sigma)$ and $n_1=n_2=20$. We choose as discriminant procedure the maximum likelihood rule, i.e. if $\hat{\mu}_1$, $\hat{\mu}_2$, S are the usual unbiased estimators for μ_1, μ_2, Σ then $g_1(x|Y)=1$ if $(x-\mu_1)'S^{-1}(x-\mu_1) \leq (x-\mu_2)_S^{-1}(x-\mu_2)$. Then F(P) is a function of $\Delta^2=(\mu_1-\mu_2)'\Sigma^{-1}(\mu_1-\mu_2)$. In the table the values were computed on the basis of 100 repetitions.

Δ	0	.5	1.	2.	4.
F(P)	.5	.455	.379	.226	.053
E $\bar{f}$	.5	.459	.378	.195	.041
E f^*	.32	.296	.343	.135	.028
100·Var $\bar{f}$	1.07	1.03	.768	.412	.134
100·Var f^*	.18	.281	.20	.224	.028
E $\hat{\lambda}_m$	.5	.458	.371	.201	.037
100·Var $\hat{\lambda}_m$	.758	.787	.733	.427	.099
100 MSE $\bar{f}$	1.07	1.03	.768	.506	.145
100 MSE f^*	3.42	2.84	2.15	1.03	.084
100 MSE $\hat{\lambda}_m$	.758	.788	.739	.48	.123

Here is obviously that Var $\hat{\lambda}_m >$ Var f^*, bias $\hat{\lambda}_m <$ bias f^*, MSE $\hat{\lambda}_m <$ MSE f^*, MSE $\hat{\lambda}_m <$ MSE $\bar{f}$ hold. This means that the corrected bootstrap estimator for F(P) is bias reduced and in the result this new estimator is the best of the considered ones.

REFERENCES

Ahrens, H., J. Läuter (1981). Mehrdimensionale Varianzanalyse. Akademie-Verlag Berlin.

Bickel, P.J., D.A. Freedmann (1981). Some asymptotic theory for the bootstrap. Ann. Statist. 9, 1196-1217.

Efron, B. (1979). Bootstrap methods: Another look at the jackknife. Ann. Statistt. 7, 1-26.

Freedman, D.A. (1981). Bootstrapping regression models. Ann. Statist. 9, 1218-1228.

Lachenbruch, P.A., M.R. Mickey (1968). Estimation of error rates in discriminant analysis. Technometrics 10, 1-11.

Läuter, H. (1985). An efficient estimator for the error rate in discriminant analysis. Statistics 16, 107-119.

McLachlan, G.J. (1974). An asymptotic unbiased technique for estimating the error rates in discriminant analysis. Biometrics 30, 239-249.

Schaafsma, W., G.N. Van Vark (1977). Classification and discriminant problems with applications, Part 1. Statist. Neerlandica 31, 25-45.

Smith, C.A.B. (1947). Some examples of discrimination. Ann. Eugen. 13, 272-282.

STATISTICAL INFERENCE FOR L_1 REGRESSION

S.Hadživuković and E.Nikolić-Djorić
University of Novi Sad,Yugoslavia

1. Introduction

The least squares method is a common procedure in the regression analysis. Its statistical inference is based on the theory with relatively sound assumptions. The method is optimal in the sense it provides the maximum likelihood estimator of the estimated parameters assuming the normal distributions of errors. There are now numerous computer packages for regression analysis.

The regression based on the least squares is sensitive to the outliers in errors. If there is only one outlier in data, the estimate of parameters may be distorted. The outliers are more difficult to spot in the regression than in case of simple location. Box (1953) introduced the word robustness and since then many papers have been published on the subject. More references are given by Dodge (1987).

The best known alternative to the least squares is the least absolute errors regression method. This method is based on the assumption of the absolute error loss function (L_1 - norm) which is less sensitive than the least squares method, but more flexibile. It gives the maximum likelihood in case errors follow the Laplace distribution. The wider explanation of robust estimation is given by Huber (1987). However, the main feature of the least absolute errors regression, which makes it different from other robust methods of regression, is that it does not require "a rejection parameter". The least absolute errors regression has several abbreviated forms in use: MSAE, LAE, MAE, LAD, LAV and MAD. The most often used expressions are LAV (Least Absolute Values) and MAD (Minimum Absolute Deviations).

Generally speaking, the LAV method can be recommended whenever errors have the form of the Laplace or Cauchy distributions (Rice, White, 1964), when the mixture of a normal and uniform distribution is present (Blattberg, Sargent, 1971), or in case of the contaminated normal distributions (Ekblom, 1974).

2. Computational Procedure

The standard linear regression model has the form

$$\mathbf{Y} = \mathbf{X}\beta + \epsilon \tag{1}$$

where $\mathbf{Y}$ is a $N \times 1$ vector of the dependent (response) variable; $\mathbf{X}$ is a $N \times$k matrix of independent (predictor) variables (the intercept term is included); β is a $k \times 1$ vector of parameters and ϵ is a $N \times 1$ vector of errors. The estimate of the dependent variable of the model (1) is

$$\hat{\mathbf{Y}} = \mathbf{X}\mathbf{b} \tag{2}$$

where $\hat{\mathbf{Y}}$ is a $N \times 1$ vector of estimated dependent variable; $\mathbf{b}$ is a $k \times 1$ vector of the estimated parameters. It is assumed that the vector ϵ is normally distributed and $E(\epsilon) = \mathbf{0}$, $E(\epsilon'\epsilon) = \sigma^2 \mathbf{I}$, $\sigma^2 < +\infty$ and $\lim_{N \to +\infty} 1/N\,(\mathbf{X}'\mathbf{X})$ is a definite nonsingular matrix. In this assumption the estimates of β and σ^2 based on the OLS (Ordinary Least Squares) are maximum likelihood estimates.

The LAV estimation minimizes the sum of the absolute deviations formulated as

$$min \sum_{i=1}^{N} |Y_i - \mathbf{X_i b}| \tag{3}$$

where Y_i is i-th unity of the vector $\mathbf{Y}$; $\mathbf{X_i}$ is i-th row of the matrix $\mathbf{X}$.

As long ago as 1757, Boscovich studied the simple model based on (3). He set the conditional under which the sum of positive and negative errors from the fitted line should have equal values. Later, Edgeworth (1888) used the LAV for the estimation of parameters in simple linear regression. Karst (1958) introduced the intuitively iterative algorithm. Several algorithms have been developed (Sharpe, 1971; Rao, Srinivasan, 1972; Appa, Smith, 1973; Sposito, Smiths, 1976 etc.). A number of the computer's programs have been published dealing with the simple linear regression (Sadovsky, 1974; Sposito, Kennedy, Gentle, 1977; Armstrong, Kung, 1978 etc.).

Rhodes (1930) and Singleton (1940) introduced the L_1-norm in the multiple linear regression. Charnes, Cooper, Ferguson (1955) showed that the LAV is the equivalent to the linear programming. That was followed by the development of a number of algorithms for the LAV solutions. Wagner (1959) has developed the LAV as a dual problem of linear programming, so

$$min\ \mathbf{1}'(\mathbf{e}^+ + \mathbf{e}^-)$$

subject to

$$\mathbf{Xb} + \mathbf{Ie}^+ - \mathbf{Ie}^- = \mathbf{Y} \qquad \text{and} \qquad \mathbf{e}^+\mathbf{e}^- \geq \mathbf{0} \tag{4}$$

where $\mathbf{b}$ is unrestricted in sign; $\mathbf{e}^+$ and $\mathbf{e}^-$ are $N \times 1$ vectors of over and under prediction of $\mathbf{Y}$; $\mathbf{1}$ is a $N \times 1$ vector; $\mathbf{I}$ is a $N \times N$ identity matrix. There are also a number of modified simplex methods in addition to other methods of mathematical programming (Barrodal, Young, 1966; Davies, 1967; Usow, 1967; Robers, Ben-Izrael, 1969; Abdelmalek, 1971). To solve the LAV problems an efficient algorithm was introduced by Barrodal, Roberts, 1973. A program on the base of this algorithm is included in the IMSL library of programs. Bloomfield, Steiger (1980) and Wesolovsky (1981) introduced the algorithms which accelerate the computational solution of problems.

A review of algorithms for the LAV estimations were given by Dielman (1984); Narula (1987) and Dodge (1987). A significant practical contribution was presented by Gentle, Narula and Sposito (1987) giving advantage to the algorithms introduced by Armstrong, Frome, Kung (1979).

There have been some procedures developed to deal with a number of specific problems. These procedures, principally are more efficient than the unmodified algorithms used to obtain the LAV. Thus, to solve the problem Armstrong, Hultz (1977) used the restricted LAV by an extension of the interval linear programming. Armstrong, Elam, Hultz (1977) used the LAV estimation in two-way classification models etc.

Although the robust regression procedure has given many satisfactory results, there is a relatively small number of program packages. One program package BLINWDR for the robust regression has been developed by Dutter (1987); another, ROBSYS is by Marazzi (1987).

3. Distribution of LAV regression estimates

The inference of the regression parameters of the LAV estimates is based on their behaviour in both the small sample and the limiting case. The lack of an adequate theory of statistical inference can explain why the robust regression was not used more extensively in the past. The recent contribution in this area was helpful to bridge the gap. Thus, Rosenberg, Carlson (1977) concluded that if the errors follow symetric distribution, the LAV estimation of the regression parameters **b** follow the multinormal distribution with expectation β and variance-covariance matrix $\lambda^2/N\ (\mathbf{X'X})^{-1}$ where λ^2/N is the variance of median for the size of sample N. Basset, Koenker (1978) developed the asymptotic theory of the LAV estimates of regression parameters. It has been proved that in the model with independent and indentical distributed errors, the LAV estimates of **b** are unbiased, consistent and follow the normal distribution asymptotically

$$\sqrt{N}\ (\mathbf{b} - \beta) \rightarrow \mathbf{N}(0,\ [2\mathbf{f}(0)]^{-2}\mathbf{Q}^{-1}) \tag{5}$$

where $\lim_{N\rightarrow\infty} 1/N\ (\mathbf{X'X}) = \mathbf{Q}$; $\mathbf{f}(0)$ is the value of density at the median and $[2f(0)]^{-2}/N$ is asymptotic variance of the sample median.

The relation (5) shows that the L_1 norm is more efficient than the OLS estimator in case when the distribution of errors of the median is more precise compared with the aritmetic mean. Cox, Hinkly (1974) introduced the unbiased estimate for the parameter $\lambda = [2f(0)]^{-1}$. That is

$$\hat{\lambda} = \frac{\hat{f}}{2}$$

where

$$\hat{f} = \frac{e(t) - e(s)}{(t - s)/N} \tag{6}$$

$e(i)$, $(i = 1, ..., N)$ are residuals of the regression model on the base of L_1; t and s are indexes which are symetric in relation to the median.

The $(1 - \alpha)\%$ confidence interval is

$$\mathbf{r'b} \pm \mathbf{z}_{\alpha/2}\,\lambda[\mathbf{r'}\,(\mathbf{X'X})^{-1}\,\mathbf{r}]^{-1/2} \tag{7}$$

where $\mathbf{r'b}$ is a $1 \times k$ arbitrary vector and $z_{\alpha/2}$ is the percentile from the standard normal distribution. The estimate is satisfactory when the errors follow a normal distribution and in case of more than 20 sample units. If it is a Laplace distribution, for a satisfactory confidence interval, the size of sample should be at least 100 units, and for a Cauchy distribution at least 150 unites.

The bootstrap estimation is an alternative way to construct the confidence interval (Stangenhaus, 1987). The bootstrap estimates of regression coefficients and standard deviations of estimates on the base of B samples are given by

$$b_i^* = \frac{\sum_{k=0}^{B} b_i^*(k)}{B} \tag{8}$$

$$s_{bi} = \left[\frac{\sum_{k=0}^{B}\{b_i^*(k) - b_i^*\}^2}{B - 1}\right]^{-1/2} \tag{9}$$

The value $b_i^*(k)$ is i-th component of vector $\mathbf{b}^*$ obtained from L_1 regression model

$$\mathbf{Y}^* = \mathbf{Xb} + \mathbf{e}^* \tag{10}$$

where $\mathbf{e}^* = (e_1^*, e_2^*, ..., e_N^*)$ is the sample without replacement of size N from population of residuals $(e_1, e_2, ..., e_N)$ of L_1 (1). The empirical study (Stangenhaus, 1987) shows that standard deviations of regression coefficients obtained by bootstrap method are closed to Monte Carlo results for normal, contaminated normal and Laplace distributions referring to the sample size of 20,30 and 50 units and for the Cauchy distribution, size 50. The confidence intervals on the base of bootstrap is close to Monte Carlo results only in the normal distribution.

4. Empirical Study

The aim of this empirical study was to examine:

- the effect of discrepancy of normal distribution on standard deviation and confidence interval of the OLS regression estimates;
- the comparison of precision of L_1 regression estimates with corresponding OLS values;
- the comparison of standard deviation and confidence interval of L_1 regression estimates on the base of asymptotic results (5) and bootstrap sampling (8), (9) with Monte Carlo results.

In this study the linear regression model was used with two independent variables

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \epsilon_i \qquad (i = 1, 2, ..., N) \tag{11}$$

The regressors of the model were independent of the errors and were generated independently from uniform distribution U(10,20) and fixed in this study. The values of the regression coefficients were $\beta_0 = 3$, $\beta_1 = 2$ and $\beta_2 = 1$. The disturbances ϵ_i were random samples of size 30 and 50 from the following distributions

- Normal distribution, $\mathbf{N}(0,1)$

$$f(x) = 1/\sqrt{2\pi}\, e^{-1/2x^2} \qquad (-\infty < x < +\infty)\,; \tag{12}$$

- Five values of errors are from $\mathbf{N}(0,20)$ and the rest from $\mathbf{N}(0,1)$;
- Exponential distribution

$$f(x) = e^{-x} \qquad (x \geq 0)\,; \tag{13}$$

- Lognormal distribution

$$f(x) = 1/\sqrt{2\pi}\, e^{-(\ln x)^2/2} \qquad (x \geq 0) \tag{14}$$

- "Student's" or the t-distribution for one degree of freedom (Cauchy) and three degrees of freedom

$$f(x) = \frac{\Gamma\left(\frac{n+1}{2}\right)}{\sqrt{n\pi}\,\Gamma\left(\frac{n}{2}\right)} (1 + x^2)^{-\frac{n+1}{2}} \qquad (-\infty < x < +\infty) \tag{15}$$

All distributions were generated by the use of random generation function for the uniform and normal distributions from the Economics Computer Program SHAZAM. Also, all necessary programs are writen using instructions of this program package. The possibility to use the random number generation and the presence of routine for OLS as well as L_1 estimation make this program very helpful in this kind of simulation studies. The SHAZAM program computes L_1 regression estimates on the base of regression quantiles method (Koenker, Basset, 1978; Koenker, D'Orey, 1987) by minimizing the function

$$\theta \sum_{\mathbf{Y} \geq \mathbf{X}\beta} |\mathbf{Y} - \mathbf{X}\beta| + (1 - \theta) \sum_{\mathbf{Y} < \mathbf{X}\beta} |\mathbf{Y} - \mathbf{X}\beta| \tag{16}$$

where $\theta = 0.5$. The variance-covariance matrix for L_1 estimates is computed using relation (5).

In this experiment for each distribution of errors, 500 samples of size 30 and 50 were generated. The mean values and standard deviations of OLS and L_1 estimates were computed and used for construction of 95% confidence interval for regression parameters.

In order to compute bootstrap estimates of L_1 regression coefficients, 100 bootstrap samples were obtained for each considered error distribution and each sample size by resampling the estimated L_1 errors and computing Y_i^* using relation (10). Mean values and standard deviations for L_1 regression coefficients on the base of 100 samples (Y_i^*, X_{1i}, X_{2i}) were used to construct the confidece interval for regression parameters, $b_i^* \pm 1.96\, s_{b_i^*}$.

5. Results

The results of Monte Carlo simulation for the OLS regression are present in Table 1. They show that the presence of outliers have affected the standard deviation of the OLS regression estimates. The value of the standard deviations for the normal distribution of errors with five values of outliers $\mathbf{N(0,5)}$ are about two times bigger than in standard normal case and six to ten times when $\mathbf{N(0,20)}$. The distortion from the normal distribution also affects the precision of estimates. For the exponential distribution with skewness $\beta_1 = 2$ and kurtosis $\beta_2 = 9$ the effect is almost negligible. For the lognormal distribution

Monte Carlo results for OLS

Table 1

Error distribution		$N = 30$			$N = 50$		
		Coefficient	Standard deviation	Confidence interval	Coefficient	Standard deviation	Confidence interval
Normal	b_0	3.0365	1.4615	(0.172 , 5.901)	3.0375	1.0163	(1.045 , 5.030)
	b_1	1.9977	0.0618	(1.877 , 2.119)	1.9980	0.0505	(1.899 , 2.097)
	b_2	0.9994	0.0666	(0.869 , 1.130)	0.9998	0.0456	(0.910 , 1.089)
Normal with five values $\mathbf{N(0,5)}$	b_0	3.0958	2.2103	(-1.236 , 7.428)	3.0832	2.3626	(-1.548 , 7.714)
	b_1	1.9982	0.1326	(1.738 , 2.258)	2.0096	0.1478	(1.720 , 2.299)
	b_2	0.9956	0.1378	(0.726 , 1.266)	0.9869	0.1037	(0.784 , 1.190)
Normal with five values $\mathbf{N(0,20)}$	b_0	3.3166	13.5510	(-23.243 , 29.877)	3.0753	6.9883	(-10.622 , 16.773)
	b_1	1.9971	0.6220	(0.778 , 3.216)	2.0118	0.3006	(1.423 , 2.601)
	b_2	0.9869	0.4745	(0.057 , 1.917)	0.9710	0.3034	(0.386 , 1.576)
Exponential	b_0	3.9255	1.3792	(1.222 , 6.629)	4.0007	1.0886	(1.867 , 6.134)
	b_1	2.0020	0.0719	(1.861 , 2.143)	1.9999	0.0535	(1.895 , 2.105)
	b_2	1.0032	0.0564	(0.893 , 1.114)	1.0002	0.0477	(0.907 , 1.097)
Lognormal	b_0	4.3936	2.7784	(-1.052 , 9.839)	4.6270	2.1976	(0.319 , 8.934)
	b_1	2.0045	0.1205	(1.768 , 2.241)	2.0018	0.1113	(1.784 , 2.220)
	b_2	1.0116	0.1550	(0.708 , 1.315)	1.0007	0.1125	(0.780 , 1.221)
Caushy	b_0	5.1985	71.5960	(-135.130 , 145.527)	1.3498	76.1140	(-147.834 , 150.533)
	b_1	2.1174	3.9894	(-5.702 , 9.937)	2.1275	4.8598	(-7.398 , 11.653)
	b_2	0.7458	3.9579	(-7.012 , 8.503)	1.0321	3.8315	(-6.478 , 8.542)
Student	b_0	3.0425	2.7653	(-2.378 , 8.463)	2.9924	1.6666	(-0.274 , 6.259)
	b_1	1.9986	0.1023	(0.179 , 2.199)	1.9987	0.08053	(1.841 , 2.157)
	b_2	0.9986	0.1221	(0.759 , 1.238)	1.0020	0.09219	(0.821 , 1.183)

which is more skewed and more leptokurtic ($\beta_1 = 4$, $\beta_2 = 41$), the standard deviations of the OLS estimates are nearly two times bigger than in the case of standard distribution of errors. The values of standard deviations of the OLS estimates are similar when errors follow the t-distribution. In this example the basis is three degrees of freedom. The biggest standard deviations of estimates are obtained by the Cauchy distribution (a special case of the t-distribution based on one degree of freedom).

Monte Carlo results for L_1 regression

Table 2

Error distribution		$N = 30$			$N = 50$		
		Coefficient	Standard deviation	Confidence interval	Coefficient	Standard deviation	Confidence interval
Normal	b_0	2.9058	2.0067	(-1.027 , 6.839)	2.9875	1.2408	(0.566 , 5.420)
	b_1	2.0013	0.0841	(1.837 , 2.166)	1.9989	0.0550	(1.891 , 2.107)
	b_2	1.0052	0.0840	(0.841 , 1.170)	1.0017	0.0652	(0.874 , 1.130)
Normal with five values N(0,5)	b_0	2.7951	2.0067	(-1.138 , 6.728)	2.9679	1.4755	(0.076 , 5.860)
	b_1	2.0104	0.1069	(1.801 , 2.220)	2.0029	0.0585	(1.888 , 2.118)
	b_2	1.0030	0.0859	(0.835 , 1.171)	0.9992	0.0709	(0.860 , 1.138)
Normal with five values N(0,20)	b_0	3.0448	2.3143	(-1.491 , 7.581)	3.0966	1.4245	(0.305 , 5.889)
	b_1	1.9974	0.1079	(1.786 , 2.209)	1.9975	0.0681	(1.864 , 2.131)
	b_2	1.0003	0.1087	(0.787 , 1.213)	0.9963	0.0629	(0.873 , 1.120)
Exponential	b_0	3.7860	1.7109	(0.443 , 7.139)	3.7796	1.1203	(1.584 , 5.975)
	b_1	2.0005	0.0643	(1.875 , 2.127)	1.9978	0.0483	(1.903 , 2.093)
	b_2	0.9960	0.0660	(0.867 , 1.125)	0.9981	0.0550	(0.890 , 1.106)
Lognormal	b_0	4.1311	1.9821	(0.246 , 8.016)	3.9574	1.3415	(1.328 , 6.587)
	b_1	1.9944	0.0876	(1.823 , 2.166)	2.0082	0.0648	(1.881 , 2.135)
	b_2	1.0015	0.0810	(0.843 , 1.160)	0.9978	0.0586	(0.883 , 1.113)
Caushy	b_0	2.9619	3.1423	(-3.197 , 9.121)	3.0455	1.9570	(-0.790 , 6.881)
	b_1	2.0016	0.1254	(1.756 , 2.247)	1.9953	0.0752	(1.848 , 2.143)
	b_2	1.0021	0.1376	(0.732 , 1.272)	1.0023	0.0954	(0.815 , 1.189)
Student	b_0	3.0599	1.7635	(-0.367 , 6.516)	2.9611	1.3497	(0.316 , 5.607)
	b_1	1.9997	0.0928	(1.818 , 2.182)	1.9985	0.0677	(1.866 , 2.131)
	b_2	0.9961	0.0814	(0.837 , 1.156)	1.0037	0.0803	(0.846 , 1.161)

Comparing the resultats of Table 1 with Table 2, which presents Monte Carlo effects for L_1 regression, one can see that the OLS gives slightly more precise estimates compared with L_1 but only when the errors are normally distributed. When the errors follow the exponential distribution, the precision achieved from the OLS and L_1 are nearly the same. In all other considered cases, the standard deviations of the OLS regression estimates are bigger in comparison to corresponding L_1 values. The greatest difference in precision between these two methods of estimation is when some units are significantly discrepant from the standard normal distribution and when the errors follow the Caushy distribution. The increase of the sample size gives in all cases better precision of L_1 estimates. The distribution of L_1 estimates for sample sizes of $N = 30$ and $N = 50$ was close to the normal distribution in all cases except the t-distribution.

The confidence interval for the t-distribution should be improved by using some transformations or by the application of percentile method for the confidence intervals which require more Monte Carlo simulations.

Table 3 presents L_1 regression estimates on the basis of one regression equation in seven different presumed values of the error distribution. Standard deviations of estimates calculated by SHAZAM program are used to construct the confidence intervals based on the normal distribution.

Table 4 shows the mean values, standard deviations and standard normal intervals of L_1 estimates of regression coefficients using 100 bootstrap samples. The obtained results show that the values of standard deviations on the basis of bootstrap sampling are close to Monte Carlo results for all distributions and all considered sample sizes. The confidence intervals calculated by the routine of program SHAZAM are close to bootstrap intervals and the intervals obtained by Monte Carlo simulation, especially for coefficients β_1 and β_2 .

Standard deviations and confidence intervals for L_1 regression coefficients on the base of asympthotic distributions

Table 3

Error distribution		$N = 30$			$N = 50$		
		Coefficient	Standard deviation	Confidence interval	Coefficient	Standard deviation	Confidence interval
Normal	b_0	5.2648	0.7196	(3.854 , 6.675)	2.6107	1.3827	(-0.099 , 5.376)
	b_1	1.9463	0.0355	(1.877 , 2.016)	2.0584	0.0565	(1.948 , 2.169)
	b_2	0.8916	0.0306	(0.832 , 0.952)	0.9828	0.0599	(0.865 , 1.100)
Normal with five values N(0,5)	b_0	3.8916	1.6902	(0.579 , 7.204)	3.4315	1.4265	(0.636 , 6.227)
	b_1	1.9500	0.0750	(1.803 , 2.097)	2.0778	0.0738	(1.933 , 2.222)
	b_2	0.9988	0.0780	(0.846 , 1.152)	0.8854	0.0756	(0.737 , 1.034)
Normal with five values N(0,20)	b_0	3.1839	1.9586	(-0.655 , 7.023)	3.7107	1.6221	(0.531 , 6.890)
	b_1	2.0385	0.0850	(1.872 , 2.205)	1.9349	0.0732	(1.791 , 2.078)
	b_2	0.9615	0.0825	(0.800 , 1.123)	1.0198	0.0830	(0.857 , 1.183)
Exponential	b_0	4.3679	1.1626	(2.089 , 6.647)	2.9732	0.9157	(1.179 , 4.768)
	b_1	1.9927	0.0598	(1.876 , 2.110)	2.0822	0.0446	(1.995 , 2.170)
	b_2	0.9461	0.0554	(0.838 , 1.055)	0.9681	0.0410	(0.888 , 1.049)
Lognormal	b_0	4.5536	1.7335	(-1.156 , 7.951)	6.0502	1.4352	(3.237 , 8.863)
	b_1	1.9853	0.0777	(1.833 , 2.138)	1.9359	0.0694	(1.800 , 2.072)
	b_2	0.9623	0.0936	(0.779 , 1.146)	0.9359	0.0656	(0.807 , 1.065)
Caushy	b_0	1.5799	2.8345	(-3.976 , 7.136)	4.0111	2.0635	(-0.033 , 8.055)
	b_1	2.0630	0.1461	(1.777 , 2.349)	1.9494	0.0835	(1.786 , 2.113)
	b_2	1.0202	0.1199	(0.785 , 1.255)	0.9884	0.0920	(0.808 , 1.169)
Student	b_0	4.2123	1.3159	(1.633 , 6.791)	3.9405	1.3775	(1.241 , 6.640)
	b_1	2.0465	0.0783	(1.893 , 2.354)	1.9717	0.0589	(1.856 , 2.087)
	b_2	0.8640	0.0643	(0.738 , 0.990)	0.9600	0.0590	(0.844 , 1.076)

Standard deviations and confidence intervals for L_1 regression coefficients on the base of bootstrap sampling

Table 4

Error distribution		$N = 30$			$N = 50$		
		Coefficient	Standard deviation	Confidence interval	Coefficient	Standard deviation	Confidence interval
Normal	b_0	5.2604	2.0580	(1.227 , 9.294)	2.3911	1.4650	(-0.480 , 5.263)
	b_1	1.9468	0.0972	(1.756 , 2.137)	2.0694	0.0561	(1.960 , 2.179)
	b_2	0.8932	0.0869	(0.723 , 1.063)	0.9870	0.0569	(0.876 , 1.099)
Normal with five values N(0, 5)	b_0	3.8486	1.7093	(0.498 , 7.199)	3.6506	1.4394	(0.829 , 6.472)
	b_1	1.9577	0.0831	(1.795 , 2.121)	2.0703	0.0665	(1.940 , 2.201)
	b_2	0.9943	0.0856	(0.827 , 1.162)	0.8827	0.0770	(0.732 , 1.034)
Normal with five values N(0, 20)	b_0	3.1575	1.5842	(0.053 , 6.263)	3.8304	1.5712	(0.751 , 6.910)
	b_1	2.0402	0.0878	(1.868 , 2.212)	1.9311	0.0703	(1.793 , 2.069)
	b_2	0.9609	0.0739	(0.816 , 1.106)	1.0128	0.0811	(0.854 , 1.172)
Exponential	b_0	4.4933	1.0407	(2.454 , 6.533)	2.8880	1.0926	(0.747 , 5.029)
	b_1	1.9931	0.0570	(1.881 , 2.105)	2.0836	0.0560	(1.974 , 2.193)
	b_2	0.9484	0.0511	(0.848 , 1.048)	0.9713	0.0480	(0.877 , 1.065)
Lognormal	b_0	4.6388	1.3312	(2.030 , 7.248)	6.0839	1.4834	(3.176 , 8.991)
	b_1	1.9854	0.0621	(1.864 , 2.110)	1.9393	0.0652	(1.812 , 2.067)
	b_2	0.9677	0.0768	(0.817 , 1.118)	0.9476	0.0606	(0.829 , 1.066)
Caushy	b_0	1.4528	2.5917	(-3.627 , 6.533)	3.9112	2.0955	(-0.196 , 8.018)
	b_1	2.0650	0.1448	(1.781 , 2.349)	1.9535	0.0758	(1.805 , 2.102)
	b_2	1.0312	0.1168	(0.802 , 1.260)	0.9877	0.1050	(0.782 , 1.193)
Student	b_0	4.4428	1.3028	(1.890 , 6.996)	4.2515	1.5238	(1.265 , 7.238)
	b_1	2.0474	0.0910	(1.869 , 2.226)	1.9628	0.0630	(1.839 , 2.086)
	b_2	0.8468	0.0821	(0.686 , 1.008)	0.9513	0.0718	(0.810 , 1.092)

6. Conclusion

This empirical study, as expected, shows that the standard deviations of the OLS regression estimates are more sensitive than L_1 estimates to outliers and discrepencies which can appear in the normal distribution. The standard deviations for L_1 estimates of regression coefficients are stable for all considered distributions of errors. Thus, the results justify the application of L_1 regression when some observations are discrepant from the normal distribution. The L_1 regression also gave, more precise results in case of a heavy tailed (Student's), highly skewed and leptokurtic distributions (lognormal). The results suggest that skewness of distribution of errors may bias the constant terms of L_1 regression. More empirical study should be done to investigate the effect of biased regression coefficients in the skew distribution in the small sample.

The standard normal confidence intervals for L_1 estimates of β_1 and β_2 based on bootstrap sampling, are close to Monte Carlo results. The confidence intervals for the t-distribution should be corrected when the sample sizes are not sufficient for the convergence of regression estimates to normal distribution of

errors (in this example $N = 30$ and $N = 50$). The confidence intervals obtained by SHAZAM program are close to the results obtained by bootstrap sampling.

It can be concluded that both bootstrap and SHAZAM procedures give satisfactory estimates of standard deviations for L_1 regression coefficients. Futher investigations should be done in order to find out the nearness of the bootstrap estimates of regression coefficients to the normal distribution of errors.

7. References

Abdelmalek, N.N. (1971). Linear L_1 approximation for a discrete point set and L_1 solutions of over determined linear equations. J.Assoc.Compt.Mach., 18:41-47.

Appa, G. and Smith, C. (1973). On L_1 and Chebychev estimation. Math. Programming, 5:73-87.

Armstrong, R. D. and Hultz, J. W. (1977). An algorithm for a restricted discrete approximation problem in the L_1 norm. S.I.A.M.J. Numer. Anal., 14:555-565.

Armstrong, R. D., Elam, J. J. and Hultz, J. W. (1977). Obtaining least absolute value estimates for a two-way classification model. Commun. Statist., B6:365-381.

Armstrong, R. D. and Kung, D. S. (1978). Algorithm AS 132: Least absolute value estimates for a simple linear regression problem. Appl. Stat., 27:363-366.

Armstrong, R. D., Frame, E. L. and Kung, D. S. (1979). A revised simplex algorithm for the absolute deviation curve fitting problem. Commun. Statist., B8:175-190.

Barrodale, I. and Young, A. (1966). Algorithms for best L_1 and L_∞ linear approximations on a discrete set. Numerische Mathematik, 8:295-306.

Barrodale, I. and Roberts, F. D. K. (1973). An improved algorithm for L_1 linear approximation. S.I.A.M.J. Numer. Anal., 10:839-848.

Basset, G. W. and Koenker, R. (1978). Asymptotic theory of least absolute error regression. JASA, 73:618-622.

Blattberg, R. and Sargent, T. (1971). Regression with non-gaussian stabile disturbances: Some sampling results. Econometrica, 39:501-510.

Bloomfield,P. and Steiger, W. (1980). Least absolute deviations curve-fitting. S.I.A.M.J. Sci. Stat. Comput., 1:290-301.

Boscovich, R. J. (1757). De litteraria expeditione per pontificiam ditionem, et synopsis amplioris operis, ac habentur plura eius ex exemplaria etiam sensorus impressa. Bononiensi Scientiarum et Artium Instituto Atique Academia Commentarii, 4:353-396.

Box, G. E. P. (1953). Non-normality and tests on variances. Biometrica, 40:318-335.

Charnes, A., Cooper, W. W. and Ferguson, R. O. (1955). Optimal estimation of executive compensation by linear programming. Manag. Sci., 1:138-150.

Davies, M. (1967). Linear approximation using the criterion of least total deviations. J.R. Stat. Soc.(B), 29:101-109.

Dielman, T. E. (1984). Least absolute value estimation in regression models: An annotated bibliography. Comm. Statist., 13:513-541.

Dodge, Y. (1987). An introduction to statistical data analysis L_1 - norm based. Els. Sci. Publ. B. V. (North Holland), 1-16.

Dutter, R. (1987). BLINWDR: A fortran program for robust and bounded influence regression. Els. Sci. Publ. B. V. (North Holland), 139-144.

Edgeworth, F. Y. (1988). On a new method of reducing observations relating to several quantities. Phil. Mag. (5 th Series), 25:184-191.

Ekblom, H. (1974). L_p methods for robust regression. BIT, 14:22-32.

Gentle, J. E., Narula, S.C. and Sposito, V. A. (1987). Algorithms for unconstrained L_1 linear regression. Els. Sci. Publ. B. V. (North Holland), 83-94.

Huber, P. J. (1987). The place of the L_1 norm in robust estimation. Els. Sci. Publ. B. V. (North Holland), 23-33.

Karst, O. J. (1958) Linear curve fitting using least deviations. JASA, 53:118-132.

Koenker, R. and Basset, G. W. (1978). Regression quantiles. Econometrica, 46:33-50.

Koenker, R. and D'Orey, V. (1987). Computing regression quantiles. Appl. Stat., 36:383:394.

Marazi, A. (1987). Solving bounded influence regression problems with ROBSYS. Els. Sci. Publ. B. V. (North Holland), 145-161.

Narula, S. C. (1987). The minimum sum of absolute errors regression. J. Quality Tech., 19:37-45.

Rao, M. R. and Srinivasan, V. (1972). A note on Sharpe's algorithm for minimizing the sum of absolute deviations in simple regression problem. Manag. Sci., 19:222-225.

Rhodes, E. C. (1930). Reducing observations by the method of minimum deviations. Phil. Mag. (7th Series), 9:974-992.

Rice, J. R. and White, J. S. (1964). Norms for smoothing and estimation. S.I.A.M. Rev., 6:243-256.

Robers, P. D. and Ben-Izrael, A. (1969). An interval programming algorithm for discrete linear L_1 approximation problem. J. Approx. Theory, 2:323-336

Rosenberg, B. and Carlson, D. (1977). A simple approximation of the sampling distribution of least absolute residual regression estimates. Commun. Statist., B6:421-437.

Sadovski, A. N. (1974). Algorithm AS74:L_1 -norm fit of a straight line. Appl. Stat., 23:224-248.

Sharp, W. E. (1971). Mean-absolute-deviation characteristic lines for securities and portfolios. Mang. Sci., 18:B1-B13.

Singelton, R. R. (1940). A method of minimizing the sum of absolute values of deviations. Ann. Math. Statist., 11:301-310.

Sposito, V. A. and Smith, W. C. (1976). On a sufficient and a necessary condition for L_1 estimation. Apl. Stat., 25:154-157.

Sposito, V. A., Kennedy, W. J. and Gentle, J. E. (1977). Algorithm AS110:L_p norm fit of a straight line. Appl. Stat., 26:114-118.

Stangenhause, G. (1987). Bootstrap and inference procedures for L_1 regression. Els. Sci. Publ. B. W. (North Holland), 323-332.

Usov, K. H. (1967). On L_1 approximation II. Computation for discrete functions and discretization effects. S.I.A.M.J. Numer. Anal., 4:233-244.

Wagner, H. M. (1959). Linear programming techniques for regression analysis. JASA, 54:206-212.

Wesolowsky, G. O. (1981). A new descent algorithm for the least absolute value regression problem. Comm. Statist., B10:479-491.

ON A COMPUTER PROGRAM FOR THE SELECTION OF VARIABLES AND MODELS IN REGRESSION ANALYSIS

B. Droge

Department of Mathematics, Humboldt University
P.O. Box 1297, O-1086 Berlin, Germany

1 INTRODUCTION

We consider the problem where an output (or response) variable depends in some nondeterministic manner on some input (or explanatory) variables, and we aim at describing this dependence by an approximate function on the basis of observations. In particular, we assume to have the following regression model, which includes the case of possibly replicated observations:

$$y_{ij} = f(x_i) + \varepsilon_{ij}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n_i, \quad \sum_{i=1}^{m} n_i = n.$$

Here the ε_{ij} are zero mean, uncorrelated random errors with possibly heteroscedastic variances σ_i^2, $x_i = (x_i^1, \ldots, x_i^k)$ is the vector of, e.g., k input variables $x^1, \ldots, x^k$ at the i-th design point, and f is the unknown regression function that we want to approximate in order to predict future values of the response variable, for example.

In such a situation it is common to select a model which depends only on some of the explanatory variables, and which is known up to a finite number of parameters. Then, these parameters are estimated on the basis of the observations to obtain an approximation for the regression function.

It is widely accepted by the statistical community that the process of extracting a convenient model should be a stepwise procedure depending on the intended use of the model, which requires a maximal exploitation of the knowledge of the problem environment and of the theory in the relevant field of application, together with the use of modern statistical methodology including regression diagnostics, transformations, and sensitivity analysis, as presented, for example, in the books of Atkinson (1985), Belsley et al. (1980), Cook and Weisberg (1982), and Daniel and Wood (1980). In conclusion, model selection is a more complex problem than merely comparing models by some criterion. At each stage of the procedure the model candidates have to be examined carefully as well as the role of explanatory variables and their interactions, the sensitivity of the parameter estimates, the influence of the observations and sensible model corrections suggested by the data. This makes it undoubtlessly desirable that, in problems associated with the search for an appropriate model, a specialist in the corresponding field should cooperate

with a professional statistician unless he has a profound statistical education.

In spite of the above considerations we believe that there is a need for some reliable semi-automatic procedure of model selection in which the user comes into action at a few well-defined stages of the process and which proposes some models for a more detailed investigation by the user. This was the starting point for our work.

We have developed a general strategy for model selection, and we have implemented a first FORTRAN 77-version of this on an ATARI-ST computer. Preliminary ideas of the strategy have been discussed in Bunke (1984).

The primary purpose of this paper is to introduce those concepts and methods associated with the selection of variables and models in regression analysis which have been used in the implemented strategy. The main steps of this strategy are treated in Section 2 and can be headed as follows:

- data pre-processing
- basic model choice
- transformation and elimination of variables
- second model choice
- nonparametric kernel estimates as competitors
- estimation of model error
- sensitivity analysis.

Due to space restrictions, however, the paper does not contain details concerning motivations, theoretical justifications and computational aspects for the used methods and algorithms as well as illustrating examples and a general comparison and discussion of existing model selection procedures. The paper is also not thought as a user's guide.

Most parts of the computer program, entitled SELEKT, have been developed by students of our department under the guidance of the author. The corresponding algorithms are described and discussed in the diploma theses of Schultz (1986), Sohn (1987), Kinast (1988) and Neubert (1989).

2 THE MAIN STEPS OF THE IMPLEMENTED MODEL SELECTION PROCEDURE

First of all it is necessary to classify the explanatory variables into the following categories:

(a) *Obligatory variables*, which the analyst may wish to force into the final model, say, $x^1, \ldots, x^a$. The number of these variables should not exceed 2, i.e. $0 \leq a \leq 2$.

(b) *Basic variables*, which are preliminarily considered to be most important, say $x^1, \ldots, x^b$. Here we assume $a \leq b \leq 4$.

(c) *Important variables* $x^1, \ldots, x^c$, where $\max(1, b) \leq c$.

(d) *Remaining variables*: $x^{c+1}, \ldots, x^k$.

Furthermore, the user has the possibility to put different weights on the design points in order to compute weighted instead of ordinary least squares estimators of the model parameters, for instance. However, in the following we will give all formulae without weights to simplify the notation.

2.1 Data pre-processing

Before starting with the selection of variables and models, the data should be pre-processed in several ways. Most of the data pre-processing methods discussed here are optional in the program.

First, the explanatory variables are standardized by

$$\tilde{x}_j^i = (x_j^i - \bar{x}^i)/s_i, \qquad i = 1,\dots,k, \qquad j = 1,\dots,m,$$

with

$$\bar{x}^i = m^{-1}\sum_{j=1}^{m} x_j^i$$

and

$$s_i^2 = (m-1)^{-1}\sum_{j=1}^{m}(x_j^i - \bar{x}^i)^2.$$

Reasons for this being a good statistical practice may be found e.g. in Snee (1983). In the sequel we omit the tilde in the denotation of standardized variables.

Then a polynomial model containing the important variables $x^1,\dots,x^c$ and having an order not greater than three is fitted to the data, where the number p of parameters of the model is required to fulfil the condition $p \le p_{\max} := \min(m, n/5)$. Let $g_1(x),\dots,g_p(x)$ denote the resulting new variables. This means, if $p_{\max} \le c$, then the first $p_{\max}$ important variables are included in the model: $g_i(x) = x^i$ for $i = 1,\dots,p = p_{\max}$. If $c < p_{\max}$, then, in addition to the linear terms in the important variables $x^1,\dots,x^c$, quadratic terms (such as $(x^j)^2$) and two-fold interactions (e.g. $x^j x^k$) are among the functions $g_i(x)$.

To simplify notation, let $n = m$, and $y = (y_1,\dots,y_n)'$ the vector of observations. Furthermore, we denote by

$$G = (\!(g_j(x_i))\!)_{i=1,\dots,n}^{j=1,\dots,p}$$

the corresponding design matrix, and by

$$P = (\!(p_{ij})\!)_{i,j=1,\dots,n}$$

the projection onto the range space of G. Then, the i-th fitted data point is

$$\hat{y}_i = \sum_{j=1}^{p} \hat{\beta}_j g_j(x_i),$$

where the $\hat{\beta}_j$ are the least squares estimators of the regression coefficients β_j:

$$\hat{\beta} = (\hat{\beta}_1,\dots,\hat{\beta}_p)' = \arg\min_{\beta_1,\dots,\beta_p} \sum_{i=1}^{n}(y_i - \sum_{j=1}^{p}\beta_j g_j(x_i))^2.$$

Thus,

$$\hat{y} = (\hat{y}_1, \ldots, \hat{y}_n)' = Py,$$

and

$$\hat{\sigma}^2 = (n-p)^{-1} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{1}$$

would be an unbiased variance estimator in case of a homogeneous error variance.

Considering the standardized residuals

$$r_i = (y_i - \hat{y}_i)/\hat{\sigma}(1 - p_{ii}) \qquad (i = 1, \ldots, n),$$

it is now possible to *detect potential outliers* in the observations. For this, we compute a critical value r_o for testing

$$H : \mathbf{E}r_i = 0 \quad \text{(for all i) against} \quad K : \exists i : \ \mathbf{E}r_i \neq 0$$

under the assumption of normally distributed observations and homogeneous variances. The test would reject the hypothesis if $r := \max_i |r_i| > r_o$.
Observing that the $\xi_i := r_i^2/(n-k)$ are identically beta-distributed with parameters $1/2$ and $(n-p-1)/2$, and using a Bonferroni inequality, we obtain, for the critical value of the ξ_i, say ξ_o, an approximate requirement

$$\mathbf{P}(\max_i \xi_i > \xi_o) \leq \sum_{i=1}^{n} \mathbf{P}(\xi_i > \xi_o) = \alpha,$$

where the significance level α may be chosen by the user (the program uses $\alpha = 0{,}05$ as standard value). As in Cran et al. (1977) we determine the point ξ_o by numerical methods with

$$\frac{1}{b\left(\frac{1}{2}, \frac{n-p-1}{2}\right)} \int_0^{\xi_o} \xi^{1/2}(1-\xi)^{(n-p-1)/2} d\xi = 1 - \alpha/n,$$

where $b(\cdot,\cdot)$ denotes the beta function. An upper bound for the critical value of the above test problem is then given by $r_o = \sqrt{\xi_o(n-p)}$. Finally, in a residual plot all observations with $|r_i| > r_o$ are marked as potential outliers, and, at the screen, the user can select those observations which he intends to delete from the data.

A further useful data pre-processing tool are *Box-Cox transformations* (see Box and Cox (1964). The use of such transformations tends to make the data more normal and homogeneous at least in an asymptotic sense, see Bunke (1982), where it is shown that such transformations try to minimize the Kullback information distance between the distribution of the transformed observations and a normal distribution with homogeneous variance. Indeed, such transformations seem to make the data rather normal than homogeneous.

Nevertheless, our program provides the user with the option to try transformations of the Box-Cox type

$$y_i^{\lambda} = \begin{cases} [(y_i + a)^{\lambda} - 1]/\lambda & , \text{if } \lambda \neq 0 \\ \ln(y_i + a) & , \text{if } \lambda = 0, \end{cases}$$

where $a = 1 - \min_{i=1,\ldots,n} y_i$.
As possible values for λ we admit $0, \pm 1/2, \pm 1$ and ± 2. The proposed transformation is that which maximizes the log-likelihood function. However, the user can decide whether he wishes to perform the transformation or not. For making this decision, he can look at the log-likelihood values and both the original and the transformed data.

For the next steps of the model selection procedure it is necessary to have *estimates of the error variances.* The user can decide between the assumption of a homogeneous or heteroscedastic variances. This may be done, for example, on the basis of the residual plots obtained in the outlier detection step.

In case the decision is to work with a homogeneous error variance, the estimator (1) will be used. In the other case, we define estimates of the heteroscedastic variances as follows: Let

$$D_{ij} = \sum_{k=1}^{p} |\hat{\beta}_k| |g_k(x_i) - g_k(x_j)| \tag{2}$$

denote the distance between two design points x_i and x_j in the sense of Daniel and Wood (1980), and let

$$j_i = \arg\min_j D_{ij}$$

denote the index belonging to that design point which is nearest to x_i in the sense of (2). Then, an estimator of σ_i^2 is defined by

$$\hat{\sigma}_i^2 = \alpha_i w_i + (1 - \alpha_i) v_i, \qquad i = 1, \ldots, m,$$

where w_i is a variance estimator basing on the replicated observations (if they exist) in some neighbourhood $U(x_i)$ of x_i in the sense of (2),

$$w_i = (N_i - d_i)^{-1} \sum_{j: x_j \in U(x_i)} \sum_{k=1}^{n_j} (y_{jk} - \bar{y}_j)^2,$$

with

$$N_i = \sum_{j: x_j \in U(x_i)} n_j, \qquad d_i = \#\{j |\, x_j \in U(x_i)\}, \qquad \bar{y}_j = n_j^{-1} \sum_{k=1}^{n_j} y_{jk},$$

and the estimation part v_i is constructed from the variation between different means in the neighbourhood of x_i,

$$v_j = \sum_{k=1}^{r_i} b_j (n_k^{-1} + n_{j_k}^{-1})^{-1} (\bar{y}_k - \bar{y}_{j_k})^2,$$

where r_i is the number of different pairs of neighbours in $U(x_i)$. The coefficients b_j and α_j are chosen in some sub-optimal manner, i.e. in such a way that, in estimating the local variances, the MSE is minimized under some conditions, for details we refer to Sohn (1987). In the program the neighbourhoods $U(x_i)$ have been chosen with a fixed size defined by $\max(5, n/5)$.

2.2 Basic model choice

After the data have been pre-processed, a first model will be selected in a so-called basic model choice step, which consists of two parts.

(a) We compare various *pseudo-linear regression models* including the basic variables, where each competitor involves the obligatory variables if there are some. Each variable can enter the model through a transformation, but we allow only one transformation for a variable. The following transformations are possible, where $x_{\max}$ and $x_{\min}$ denote the maximum and minimum value, respectively, of the corresponding variable x:

$$\begin{aligned} T_1(x) &= x\,, \\ T_2(x) &= (x+a)^{-1}\,, \qquad a = \tfrac{1}{9}x_{\max} - \tfrac{10}{9}x_{\min}, \\ T_3(x) &= \ln(x+b)\,, \qquad b = \tfrac{1}{2}\cdot 10^{-s}(x_{\max} - x_{\min}) - x_{\min}, \\ T_4(x) &= e^{cx}\,, \qquad c = \ln 10/(x_{\max} - x_{\min}). \end{aligned}$$

Note that the transformations T_2, T_3 and T_4 are defined in such a way that they have a clear nonlinearity in the following sense:

$$\frac{T_i(x_{\max}) - T_i(x_*)}{T_i(x_*) - T_i(x_{\min})} = 10 \quad \text{or} \quad \frac{1}{10},$$

where $x_* = (x_{\min} + x_{\max})/2$.

Then, any model candidate can be described by some set M and is of the form:

$$g_{\beta_M}(x^1, \ldots, x^b) = \sum_{\tau \in M} \beta_\tau g_\tau(x^1, \ldots, x^b), \tag{3a}$$

where $M \subseteq \mathcal{T}$,

$$\mathcal{T} = \{\tau = (\tau_1, \ldots, \tau_b) |\ \tau_i \in \{0,1,2\},\ \sum_{i=1}^{b} \tau_i \le 2\} \tag{3b}$$

and

$$g_\tau(x^1, \ldots, x^b) = \prod_{i=1}^{b} g^i_{\tau_i}(x^i), \qquad g^i_{\tau_i}(x^i) = [t_i(x^i)]^{\tau_i}, \qquad t_i \in \{T_1, \ldots, T_4\}. \tag{3c}$$

Note that (3b) controls that at most quadratic terms of the transformed variables and only two-fold interactions between them can enter the model. The program provides only model candidates M that contain all (possibly transformed) obligatory variables at least with a linear term. Quadratic terms are only included when linear terms of the corresponding variables already occur. The parameter $\beta_M = (\beta_\tau)_{\tau \in M}$ is always estimated by least squares:

$$\hat{\beta}_M = \arg\min_{\beta_M} \sum_{i=1}^{n} (y_i - g_{\beta_M}(x_i))^2. \tag{4a}$$

Here $x_i = (x_i^1, \ldots, x_i^b)$. Hence,

$$\hat{y}_M := (g_{\hat{\beta}_M}(x_1), \ldots, g_{\hat{\beta}_M}(x_n))' = P_M y, \tag{4b}$$

where P_M is the projection onto the column space of the design matrix associated with M. Note that, for simplicity, the formulae in (4) are only given for the case of $m = n$ and no weights are desired by the user.

The competitive models are compared by an estimate of some risk for estimating the regression function, as discussed in detail by Bunke and Droge (1984). For presenting such an estimate, let

$$MSE(M) = E\{\frac{1}{n}\sum_{i=1}^{n}(f(x_i) - g_{\beta_M}(x_i))^2\} \tag{5}$$

be the mean squared error (MSE) for estimating the regression function using the model M. Then an MSE estimate is given by

$$\widehat{MSE}(M) = \frac{1}{n}\sum_{i=1}^{n}(y_i - g_{\hat{\beta}_M}(x_i))^2 - \frac{1}{n}\mathrm{tr}[(I - 2P_M)\hat{\Sigma}], \tag{6}$$

where $\hat{\Sigma}$ is an estimate of $\Sigma = \mathrm{diag}[\sigma_1^2, \ldots, \sigma_n^2]$ as introduced in Section 2.2. Clearly, (6) would be an unbiased estimate of (5) if $\mathbf{E}\hat{\Sigma} = \Sigma$. Now we select a first model M_1' by minimizing the estimated risk (6):

$$M_1' = \arg\min_{M \subset \mathcal{I}} \widehat{MSE}(M).$$

Although not explicitly expressed, this minimization process is also directed to the choice of appropriate transformations for the basic variables included in the model.

(b) Alternatively to the polynomial model in (a) we also consider *multivariate B-splines* as possible basic models. Looking at the construction of the polynomial models in (a), we observe that it is similar to the construction of a basis in certain linear spaces of functions of variables $x^1, \ldots, x^b$ starting with a basis in each of the linear spaces corresponding to functions in one of the variables ($g^i_{\tau_i}$, $\tau_i = 0, 1, 2$). Hence, if for each i the functions $g^i_o, \ldots, g^i_{r_i}$ are the B-splines of order ω_i in the argument x^i according to a fixed set of, e.g., k_i knots (cf. de Boor (1978)), then

$$\begin{aligned} &\{g_\tau(x^1, \ldots, x^b) = \prod_{i=1}^{b} g^i_{\tau_i}(x^i) |\ \tau \in M^*\}, \\ &\quad \text{with} \quad M^* = \{\tau = (\tau_1, \ldots, \tau_b) |\ 0 \le \tau_i \le r_i\} \\ &\quad \text{and} \quad r_i = \omega_i + k_i - 1, \end{aligned} \tag{7}$$

is a basis of the space of multivariate splines with corresponding order and knots. Therefore, a multivariate B-spline can be defined by

$$g_{\beta_{M^*}}(x^1, \ldots, x^b) = \sum_{\tau \in M^*} \beta_\tau g_\tau(x^1, \ldots, x^b), \tag{8}$$

see Bunke (1984). We remark that this multivariate spline is a spline of order ω_i with certain knots as a function of x^i if the other explanatory variables are kept fixed.

The orders of the splines, ω_i, as well as the number k_i, and the position of knots in each variable are selected by minimizing the criterion $\widehat{MSE}$ in (6). Depending on the number of basic variables, the possible number of knots and orders is chosen in such a way that at most 200 or 300 models have to be compared. The maximum order of the splines is four, i.e. $\omega_i \le 4$, whereas the number of inner knots for each variable does not

exceed two. The knots are selected from a set of potential knots, which are defined by various procedures:

(i) In case of only one basic variable, we choose, roughly speaking, the potential knots sequentially in such a way that there are at least five design points between two knots. This number will be increased by shifting the larger knot as long as the "spread" of the responses observed between the knots does not exceed the "average spread" of observations belonging to five consecutive design points. The resulting partition of the data is hoped to provide similar response variabilities in the different intervals, for details see Willig (1982).

(ii) If there are more than one basic variable, we distribute the potential knots equidistantly in each direction. This is done in two different ways. On the one hand, we set comparatively few potential knots and select among all combinations of knots (0, 1, or 2 in each direction). On the other hand, we set many potential knots and select at most one inner knot in each direction.

Minimizing the criterion $\widehat{MSE}$ for the multivariate B-splines (8) over the admitted combinations of knots and orders of splines yields a second model of interest, which is characterized by some set of type (7), say, M_1^*. As an immediate consequence of the minimal requirements concerning the orders and numbers of knots outlined above, we obtain for M_1^* that $r_i \leq 5$ for $i = 1, \ldots, b$.

Finally, we arrive at the so-called *basic model* M_1, which is either M_1' or M_1^*, depending on the corresponding $\widehat{MSE}$-values.

Notice that, if necessary, at several stages the program uses additional restrictions not described here to ensure that the number of model candidates to be compared in this step does not exceed a certain value, say, 300.

2.3 Transformation and elimination of variables

The aim of this step is to provide a second model, say M_2, which is obtained by a *backward elimination of variables*, starting with a rough large model depending on all (possibly transformed) explanatory variables and minimizing the criterion $\widehat{MSE}$ at each step. The elimination procedure stops when the number of explanatory variables in the achieved model M_2 is as small as possible, provided that the corresponding $\widehat{MSE}$-value is still in a neighbourhood of the minimum value $\widehat{MSE}_{\min}$, say

$$\widehat{MSE}(M_2) \leq \widehat{MSE}_{\min} + \gamma[\widehat{MSE}(M_1) - \widehat{MSE}_{\min}].$$

The program uses $\gamma = 0.1$. Backward elimination is preferred to forward selection because of the higher chance for including interactions in the model.

The large starting model has the structure

$$g_{\beta_{M_1}}(x^1, \ldots, x^b) + \sum_{j=b+1}^{k} \{\gamma_j t_j(x^j) + \delta_j [t_j(x^j)]^2 + \sum_{i=1}^{b} \kappa_{ij} t_i(x^i) t_j(x^j)\}, \tag{9}$$

i.e. it extends the basic model by adding linear and quadratic terms for effects of non-basic variables as well as simple interaction terms between basic and non-basic variables. To secure parameter identifiability it may be necessary to omit some or all of the quadratic (and interaction) terms. As expressed by the notation, all variables may enter the model

(9) by some transformations $t_i \in \{T_1, T_2, T_3, T_4\}$. For the basic variables we use always the same transformations t_i $(i = 1, \ldots, b)$ as they occur in the basic model M_1. Due to computational aspects, the *convenient transformations for the non-basic variables* are chosen separately for each variable by adding to M_1 a linear, a quadratic and interaction terms in the transformed value of the non-basic variable and minimizing the criterion $\widehat{MSE}$ over the class of admitted transformations. This means, for example, that the "optimal" transformation t_j for the non-basic variable x^j , $b < j \leq k$, is obtained by minimizing the $\widehat{MSE}$-values for the models

$$g_{\beta_{M_1}}(x^1, \ldots, x^b) + \gamma_j t(x^j) + \delta_j [t(x^j)]^2 + \sum_{i=1}^{b} \kappa_{ij} t_i(x^i) t(x^j)$$

over $t \in \{T_1, \ldots, T_4\}$.

2.4 Second model choice

Using the variables included in the model M_2, finer models than in Section 2.3 can be constructed and compared by the $\widehat{MSE}$-criterion in the same way as it was done in the basic model choice step 2.2, provided the number of explanatory variables allows this. This results in a model M_3. Notice that in many cases the computational effort for this step will not be too high, since the $\widehat{MSE}$-values for an essential part of the models to be compared have been already calculated in previous steps.

2.5 Nonparametric kernel estimates as competitors

In addition to the polynomial and spline models considered until now, the user has the possibility to compute nonparametric kernel estimates of the regression function. These kernel estimates may be constructed on the basis of those variables which are included in one of the models obtained in the previous steps.

Let d be the number of variables to be considered. Then we calculate the following Nadaraya-Watson type kernel estimate:

$$\hat{f}(x) = \sum_{i=1}^{n} K(h^{-1} \|x - x_i\|_B) y_i / \sum_{i=1}^{n} K(h^{-1} \|x - x_i\|_B), \tag{10}$$

where $x \in \mathbb{R}^d$, K is the kernel, h is the bandwidth, x_i is the vector of the d explanatory variables of the model at the i-th design point and $\|z\|_B^2 = z'Bz$ for a d-vector z and a $d \times d$ (weighting) matrix B. The user of the program can decide between the standard choice $B = I_d$ and $B = \mathrm{diag}[|b_1|, \ldots, |b_d|]$, where the b_i denote the estimated regression coefficients of the included variables in a linear regression model. The last definition of B allows to weight the different variables in accordance with their linear influence on the response variable. Notice that the estimator (10) coincides with the multivariate Nadaraya-Watson kernel estimator using a product kernel if we choose a normal kernel.

Again, the smoothing parameter (bandwidth) h and an appropriate kernel K are selected by minimizing the criterion $\widehat{MSE}$. As possible kernels we admit the moving average, triangular, normal, and truncated normal kernel.

2.6 Estimation of the model error

As described in the previous sections, the program provides several models that may be of interest. As an assessment of their performance, the corresponding values of the MSE-estimates are calculated. Additionally, it is instructive to have information on the systematic model error (bias) of the different models,

$$\Delta_M = \min_{\beta} \frac{1}{n} \sum_{i=1}^{n} [f(x_i) - g_{\beta_M}(x_i)]^2, \tag{11}$$

where M is one of the models M_1, M_2 or M_3. Δ_M describes the quality of the model in view of future replicated observations at the same design points. The program yields both, an estimate $\hat{\Delta}_M$ and a joint upper confidence limit $\bar{\Delta}_M$ for Δ_M, which are defined by

$$\hat{\Delta}_M = \frac{1}{n}\|y - P_M y\|^2 - \frac{1}{n}\mathrm{tr}[(I - P_M)\hat{\Sigma}] \tag{12}$$

and

$$\bar{\Delta}_M = \{\sqrt{\lambda_{\max}(A)} \cdot \sqrt{\chi^2_{n,\pi}} + n^{-\frac{1}{2}}\|y - P_M y\|\}^2, \tag{13}$$

where $\lambda_{\max}(A)$ is the largest eigenvalue of $A = n^{-1}\hat{\Sigma}^{1/2}(I - P_M)\hat{\Sigma}^{1/2}$, π the confidence level to be chosen by the user (the standard value is $\pi = 0.9$), and $\chi^2_{n,\pi}$ the π- quantile of the χ^2-distribution with n degrees of freedom. Clearly, (12) is an unbiased estimator of (11) if $\mathbf{E}\hat{\Sigma} = \Sigma$, whereas (13) can be derived by asymptotic considerations. For details we refer to Bunke and Grabowski (1978).

2.7 Sensitivity analysis

The sensitivity analysis for the models proposed in the different steps can be performed using various plots and statistics. In particular, our program generates plots of the standardized residuals r_j versus the fitted values $\hat{y}_j$ and single explanatory variables x^i_j, respectively. Furthermore, we can generate tables containing, for each data set i, the corresponding observations y_i, the diagonal elements of the hat matrix p_{ii} (leverage values), the standardized residuals r_i, and Cook's distance (see e.g. Cook and Weisberg (1982)),

$$D_i = \frac{p_{ii} r_i^2}{d(1 - p_{ii})},$$

where d is the model dimension (trace of the hat matrix). The results could suggest a renewed application of some steps after a certain manipulation such as the elimination of some observations or explanatory variables, if e.g. the plots exhibit patterns or trends.

3 CONCLUDING COMMENTS

The implemented strategy is only one of several possible variants. However, it is based on a series of theoretical and intuitive justifications, which could not be presented here in detail. Some of these possible modifications have already been discussed in Bunke (1984). For example, it would be useful for the user to have the opportunity to propose special model candidates or at least to try some specific transformations of explanatory variables, which could be suggested by the sensitivity analysis. The consideration of nonlinear regression models and its comparison by a criterion as proposed in Droge (1987) could

improve the strategy, too. Further modifications may be concerned with the algorithms for searching convenient transformations of the non-basic variables, and for estimating the heteroscedastic error variances, etc. All in all, the kind of necessary adjustments will mainly be determined by further applications of the program to both, real data and simulation experiments.

ACKNOWLEDGEMENT

I am very grateful to Professor O. Bunke, who initiated the work and gave a first proposal for a strategy. The whole process of refining and implementing the strategy was accompanied by stimulating discussions with him.

REFERENCES

Atkinson, A.C. (1985). *Plots, Transformations, and Regression.* University Press, Oxford.

Belsley, D. A., Kuh,E. and Welsch, R.E. (1980). *Regression Diagnostics: Identifying Influential Data and Sources of Collinearity.* Wiley, New, York.

Box, G.E.P. and Cox, D.R. (1964). An analysis of transformations. *J. Roy. Statist. Soc., B* **26**, 211-252.

Bunke, O. (1982). The roles of transformations and response functions chosen by maximum likelihood. *Math. Operationsforsch. u. Statist., ser. statist.*, **13**, 395-404.

Bunke, O. (1984). Selecting variables and models in regression analysis: Some tools and suggestions for a strategy. Preprint No. 68, Humboldt University, Department of Mathematics, Berlin.

Bunke, O. and Droge. B. (1984). Bootstrap and cross-validation estimates of the prediction error for linear regression models. *Ann. Statist.* **12**, 1400-1424.

Bunke, O. and Grabowski, B. (1978). A procedure for model choice or variable selection with controlled model specification error. *Math. Operationsforsch. u. Statist., ser. statist.*, **9**, 483-497.

Cook, R.D. and Weisberg, S. (1982). *Influence and Residuals in Regression.* Chapman and Hall, London.

Cran, G.W., Martin, K.J. and Thomas, G.E. (1977). Remark ASR19 and Algorithm AS109: a remark on Algorithm AS63: the incomplete integral, AS64: inverse of the incomplete beta function ratio. *Appl. Statist.* **26**, 111-114.

Daniel, C. and Wood, F.S. (1980). *Fitting Equations to Data.* 2nd ed., Wiley, New York.

De Boor, C. (1978). *A Practical Guide to Splines.* Springer Verlag, New York.

Droge, B. (1987). A note on estimating the MSEP in nonlinear regression. *Statistics* **18**, 499-520.

Kinast, E. (1988). Algorithmen zur Datenvorbehandlung im Rahmen der Modellwahl und ihre rechentechnische Realisierung auf dem ATARI ST. Diploma-thesis, Humboldt University, Department of Mathematics, Berlin.

Neubert, S. (1989). SELEKT - Ein Programm zur Wahl von Regressionsmodellen. Diploma-thesis, Humboldt University, Department of Mathematics, Berlin.

Schultz, U. (1986). Ausgleich von Regressionsdaten durch multivariate Splines oder Kernschätzungen als alternative Basismodelle - Erstellung von Unterprogrammen zur Wahl solcher Modelle. Diploma-thesis, Humboldt Universtiy, Department of Mathematics, Berlin.

Snee, R.D. (1983). Discussion on the paper "Developments in linear regression methodology: 1959-1982" by R.R. Hocking. *Technometrics* **25**, 230-237.

Sohn, S. (1987). Untersuchung von Eigenschaften lokaler Varianschätzungen und rechentechnische Realisierung von Programmen zur Wahl von Regressionsmodellen. Diploma-thesis, Humboldt University, Department of Mathematics, Berlin.

Willig, R. (1982). Ein Programm zum Ausgleich von Regressionsdaten durch kubische Splines mit einem Knotenwahlalgorithmus. Diploma-thesis, Humboldt University, Department of Mathematics, Berlin.

Part III:

QUALITY ENGINEERING AND APPLICATIONS

QUALITY IMPROVEMENT THROUGH DESIGN OF EXPERIMENTS WITH BOTH PRODUCT PARAMETERS AND EXTERNAL NOISE FACTORS

I.N. Vuchkov, L.N. Boyadjieva *

1 INTRODUCTION

This paper presents a model-based approach to the Taguchi (1986) method of quality improvement through design of experiments. It is an extension of authors results (Vuchkov, Boyadjieva (1988)).

Consider a product with performance characteristic η. Assume that all factors influencing η can be divided into following groups:

- Product or/and process parameters $\underline{p} = (p_1, p_2 \dots p_m)$. They can be kept to given values when experiments are carried out, but in mass production they are subject to errors $\underline{e} = (e_1, e_2 \dots e_m)^T$. The errors are due to tolerances of the components and manufacturing imperfections. For example in an electronic circuit the values of resistors and capacitors vary within some tolerance limits around the nominals. In a chemical process the temperature, pressure, etc. can be set with random errors. That is why in the real production the true values of product or process parameters can be presented by the elements of a random vector $\underline{p} + \underline{e}$.

- External noise factors $\underline{x} = (x_1, x_2 \dots x_l)^T$. In design stage they can be varied within given intervals, but during the mass production and use of product they are uncontrollable and their values are random. For example for an electronic device such factors are temperature, humidity, vibrations, etc.

- Random noise v. It takes into account random disturbances, which are not included in $\underline{x}$ and $\underline{e}$.

Assume that $\underline{e}$, $\underline{x}$ and v are independently and normally distributed with zero expectations and following covariance matrices:

$$\Sigma_e = \mathrm{diag}(\sigma_1^2, \sigma_2^2, \dots, \sigma_m^2),$$

*Sofia University of Technology, 1156 Sofia, Bulgaria

$$\Sigma_x = \mathrm{diag}[\sigma^2(x_1), \sigma^2(x_2), \ldots, \sigma^2(x_l)],$$

The variance of random noise is σ_v^2.

Because of normality of distributions third order moments of $\underline{e}$, $\underline{x}$ and v are equal to zero:

$$E(e_i^3) = E(x_j^3) = E(v^3) = 0, \quad i = 1, 2, \ldots, m, \quad j = 1, 2, \ldots, l.$$

Fourth order moments are equal correspondingly to $E(e_i^4) = 3\sigma_i^4$, $E(x_i^4) = 3\sigma^4(x_i)$ and $E(v^4) = 3\sigma_v^4$.

Assuming that during the experiment product or process parameters and external noise factors can be set to given values without errors, the performance characteristic's value is:

$$y = \eta(\underline{p}, \underline{x}) + v,$$

where $\eta(\underline{p}, \underline{x})$ is nonrandom.

After shipping the product's performance characteristic is

$$y = \eta(\underline{p} + \underline{e}, \underline{x}) + v, \tag{1}$$

where $\eta(\underline{p} + \underline{e}, \underline{x})$ is random, because $\underline{e}$ and $\underline{x}$ are random vectors.

We consider a model-based approach to quality improvement which comprises:

- Model building of the performance characteristic and its variance in production process and exploitation of the product.
- Optimization procedures, which ensure minimization of variance while keeping the performance characteristic close to a target.

2 MODELS OF THE PERFORMANCE CHARACTERISTIC AND ITS VARIANCE

Suppose an experiment is carried out with both parameters and external noise factors. Any response surface design can be used for this purpose. The total number of columns in the design matrix is $m + l$, with first m of them corresponding to parameters and the remaining l columns - to external noise factors. If the design matrix is written in coded factors, for example $-1 \le p_i \le 1$, $i = 1, 2, \ldots, m$ and $-1 \le x_i \le 1$, $i = 1, 2, \ldots, l$, then the moments of the distribution of $\underline{e}$ and $\underline{x}$ must correspond to their coded values.

Assume that during the experiment the values of p_i and x_i can be set to the levels given in the design matrix without errors. Consider the most impportant case when the results of this experiment can be described by second order polynomial:

$$y(\underline{p}, \underline{x}) = \eta(\underline{p}, \underline{x}) + v = \beta_o + \sum_{i=1}^{m} \beta_i p_i + \sum_{i=1}^{m} \sum_{j=1}^{m} \beta_{ij} p_i p_j + \sum_{i=1}^{l} \alpha_i x_i + \sum_{i=1}^{l} \sum_{j=1}^{l} \alpha_{ij} x_i x_j + \sum_{i=1}^{m} \sum_{j=1}^{l} \gamma_{ij} p_j x_j + v. \tag{2}$$

This equation can also be presented in the form

$$y(\underline{p},\underline{x}) = \beta_o + \underline{\beta}^T\underline{p} + \underline{p}^T\mathcal{B}\underline{p} + \underline{\alpha}^T p + \underline{x}^T\mathcal{A}\underline{x} + \underline{p}^T\mathcal{T}\underline{x} + v \tag{3}$$

where:

$$\underline{\alpha} = (\alpha_1, \alpha_2 \ldots \alpha_l)^T; \underline{\beta} = (\beta_1, \beta_2 \ldots \beta_m)^T,$$

$\mathcal{A}$ is $l \times l$ matrix with elements

$$\mathcal{A}_{ij} = \begin{cases} \alpha_{ij}/2 & \text{for } i \neq j \\ \alpha_{ii} & \text{for } i = j \end{cases}.$$

$\mathcal{B}$ is $m \times m$ matrix with elements

$$\mathcal{B}_{ij} = \begin{cases} \beta_{ij}/2 & \text{for } i \neq j \\ \beta_{ii} & \text{for } i = j \end{cases},$$

and $\mathcal{T}$ is $m \times l$ matrix with elements γ_{ij}, $i = 1, 2, \ldots, m$; $j = 1, 2, \ldots, l$.

In mass production errors e_i occur in product parameters p_i and external noise factors x_i are random. That is why for this case following model must be used instead of (3):

$$y(\underline{p},\underline{x}) = \eta(\underline{p}+\underline{e},\underline{x}) = \beta_o + \underline{\beta}^T(\underline{p}+\underline{e}) + (\underline{p}+\underline{e})^T\mathcal{B}(\underline{p}+\underline{e}) + \underline{\alpha}^T\underline{x} + \underline{x}^T\mathcal{A}\underline{x} + (\underline{p}+\underline{e})^T\mathcal{T}\underline{x} + v. \tag{4}$$

Taking expectation with respect to $\underline{e}$ and $\underline{x}$ one can find following model of the mean value of the performance characteristic:

$$\tilde{y}(\underline{p}) = E[y(\underline{p},\underline{x})] = \beta_o + \underline{\beta}^T\underline{p} + \underline{p}^T\mathcal{B}\underline{p} + \operatorname{tr}\mathcal{B}\Sigma_e + \operatorname{tr}\mathcal{A}\Sigma_x. \tag{5}$$

One can see that $y(\underline{p})$ depends on values of parameters $\underline{p}$ and on second order moments of $\underline{e}$ and $\underline{x}$. The coefficients of model (2) have to be also known. They can be estimated on the basis of the experiment and substituted in (5).

Using (4) one can find also a model of variance of the performance characteristic:

$$\sigma^2(p) = \operatorname{var}[y(\underline{p},\underline{x})] = (\underline{\beta}+2\mathcal{B}\underline{p})^T\Sigma_e(\underline{\beta}+2\mathcal{B}\underline{p}) + (\underline{\alpha}+\mathcal{T}^T\underline{p})^T\Sigma_x(\underline{\alpha}+\mathcal{T}^T\underline{p}) + \operatorname{tr}\mathcal{T}\Sigma_x\mathcal{T}^T\Sigma_e + HM + \sigma_v^2 \tag{6}$$

where the influence of high order terms is described by

$$HM = 2\sum_{i=1}^{m}\beta_{ii}^2\sigma_i^4 + \sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\beta_{ij}^2\sigma_i^2\sigma_j^2 + 2\sum_{i=1}^{l}\alpha_{ii}^2\sigma^4(x_i) + \sum_{i=1}^{l-1}\sum_{j=i+1}^{l}\alpha_{ij}^2\sigma^2(x_i)\sigma^2(x_j). \tag{7}$$

The proofs of equations (5) and (6) are given in the appendix.

Let b_o, $\underline{a}$, $\underline{b}$, A, B, C correspond to β_o, $\underline{\alpha}$, $\underline{\beta}$, $\mathcal{A}$, $\mathcal{B}$, $\mathcal{T}$ in which estimates are substituted for the regression coefficients. Then the quadratic forms (5) and (6) can be written as follows:

$$\hat{y}(\underline{p}) = \underline{p}^T\underline{b} + \underline{p}^T B\underline{p} + d_1, \tag{8}$$

$$\hat{\sigma}^2(\underline{p}) = \underline{p}^T\underline{\theta} + \underline{p}^T D\underline{p} + d_2, \tag{9}$$

where

$$d_1 = b_o + \operatorname{tr} B\Sigma_e + \operatorname{tr} A\Sigma_x,$$

$$d_2 = (\underline{b}^T, \underline{a}^T) \begin{pmatrix} \Sigma_e & 0 \\ 0 & \Sigma_x \end{pmatrix} \begin{pmatrix} \underline{b} \\ \underline{a} \end{pmatrix} + \operatorname{tr} C\Sigma_x C^T \Sigma_e + HM + \sigma_v^2,$$

$$\theta^T = 2(\underline{b}^T, \underline{a}^T) \begin{pmatrix} \Sigma_e & 0 \\ 0 & \Sigma_x \end{pmatrix} \begin{pmatrix} 2B \\ C^T \end{pmatrix},$$

$$D = (2B^T, C) \begin{pmatrix} \Sigma_e & 0 \\ 0 & \Sigma_x \end{pmatrix} \begin{pmatrix} 2B \\ C^T \end{pmatrix}.$$

3 OPTIMIZATION PROCEDURES FOR QUALITY IMPROVEMENT

3.1 Optimality criteria

As an optimality criterion one can use Taguchi's (1986) loss function: $L = k(y-\tau)^2$, where k is a constant and τ is the target value. Denote $m_y = E(y)$ and $\sigma_y^2 = E[(y - m_y)^2]$. One can find:

$$E(L) = kE[(y - m_y + m_y - \tau)^2] = k[(m_y - \tau)^2 + \sigma_y^2].$$

Substituting $\hat{y}$ and $\hat{\sigma}^2$ for σ_y^2 one can find

$$E(\hat{L}) = k[(\hat{y} - \tau)^2 + \hat{\sigma}^2)]. \tag{10}$$

$\hat{y}$ and $\hat{\sigma}^2$ can be computed by use of models (8) and (9). Then the quality improvement problem is to find such values of $p_1, p_2, \ldots, p_m$, which minimize $E(\hat{L})$. Similar criteria can be used for "the smaller the better" problem and "the largest the better" problem (see Taguchi (1986) and Kackar (1985)). For example if $y \geq 0$, then for "the smaller the better" problem one can put $\tau = 0$ in (10) and to obtain $E(\hat{L}) = k(\hat{y}^2 + \hat{\sigma}^2)$. For "the largest the better" problem following formula can be used (see Taguchi (1984)):

$$E(\hat{L}) = \frac{k}{\hat{y}^2}(1 + \frac{3\hat{\sigma}^2}{\hat{y}^2}).$$

Another definition of the optimization problem is as follows: minimize $\hat{\sigma}^2$ under the condition that $\hat{y} = \tau$.

Signal to noise ratio can also be used as a performance characteristic (see Taguchi (1986)) and then the optimization problem is to maximize signal to noise ratio.

For solving optimization problem one can use numerical methods. However taking into account that (8) and (9) are quadratic forms some simple analytic solution can be found. Further on we use the conditional optimization criterion.

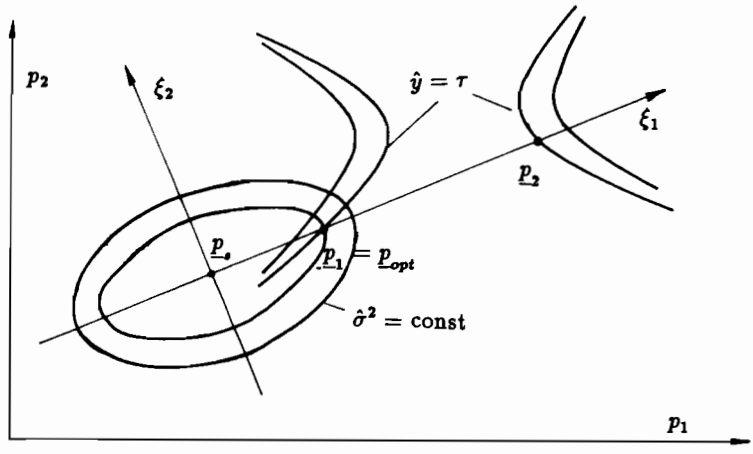


Figure 1: The idea of the geometric solution

3.2 A geometric solution of unconstrained conditional optimization problem

The matrix D is positive definite because Σ_e and Σ_x are positive definite too. Consequently the contours of equal values of $\hat{\sigma}^2$ are ellipses or ellipsoids. A simple solution of the conditional optimization problem exists if the contour defined by $\hat{y} = \tau$ intersects the largest axis of these ellipsoids.

The stationary point $\underline{p}_*$ of (9) can be found by putting first derivative of $\hat{\sigma}^2$ equal to zero:

$$\frac{\partial \hat{\sigma}^2}{\partial \underline{p}} = \underline{\theta} + 2D\underline{p} = \underline{0}$$

and

$$\underline{p}_* = -\frac{1}{2}D^{-1}\underline{\theta}. \tag{11}$$

The second derivative of σ^2 is $2D$. This is a positive definite matrix and consequently the stationary point corresponds to minimum of $\hat{\sigma}^2$.

In order to take into account the condition $\hat{y} = \tau$ one can use a canonical form of $\hat{\sigma}^2$ ((3.2)). Then two solutions $\underline{p}_1$ and $\underline{p}_2$ can be found as points in which the largest axe of $\hat{\sigma}^2$ contours intersects the contour defined by $\hat{y} = \tau$. The final solution is this one which is nearest to $\underline{p}_*$. Note that this method does not work if $\hat{y} = \tau$ does not intersect the largest axis of $\hat{\sigma}^2$ contours.

Denote by $\lambda_1, \lambda_2, \ldots, \lambda_m$ the eigenvalues of D and by $T-$ the corresponding matrix of eigenvectors. Substituting $\underline{p}_2$ from (11) in (9) one can obtain the value of variance in the stationary point:

$$\hat{\sigma}_* = d_2 + \frac{1}{2}\underline{p}_*^T\underline{\theta}. \tag{12}$$

Following canonical form of $\hat{\sigma}^2$ can be written:

$$\hat{\sigma}^2 = \hat{\sigma}_*^2 + \underline{\xi}^T \Lambda \underline{\xi}, \tag{13}$$

where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m)$ and

$$\underline{\xi} = T^T(\underline{p} - \underline{p}_*) = T^{-1}(\underline{p} - \underline{p}_*). \tag{14}$$

Consider the value

$$\hat{\sigma}_1^2 = \hat{\sigma}^2 - \hat{\sigma}_*^2 = \underline{\xi}^T \Lambda \underline{\xi} = \lambda_1 \xi_1^2 + \lambda_2 \xi_2^2 + \ldots + \lambda_m \xi_m^2. \tag{15}$$

Denote $\lambda_* = \min \lambda_i$, $i = 1, 2, \ldots, m$. The minimal value of $\hat{\sigma}_1^2$ is in the direction of ξ_* axis and is equal to

$$\hat{\sigma}_{1*}^2 = \lambda_* \xi_*^2. \tag{16}$$

In the stationary point $\underline{p} = \underline{p}_*$ and from (14) and (16) follows that $\underline{\xi}_* = \underline{0}$ and $\hat{\sigma}_{1*}^2 = 0$.

Taking into account that $T^T = T^{-1}$ one can obtain from (14) following equation:

$$\underline{p}_* = T\underline{\xi}_* + \underline{p}_*. \tag{17}$$

For any point on the ξ-axis only one coordinate of $\underline{\xi}_*$ is nonzero. Denote it ξ_* and rewrite (17) as follows:

$$\underline{p}_* = \underline{t}_* \xi_* + \underline{p}_*, \tag{18}$$

where $\underline{t}_*$ is the eigenvector which corresponds to $\lambda_* = \lambda_{min}$.

The optimal value of ξ_* can be found by substitution of $\underline{p}_*$ for $\underline{p}$ in equation $\hat{y} = \tau$. We use for this purpose the relationships (8) and (18) .

$$\xi_* \underline{t}_*^T \underline{b} + \underline{p}_*^T \underline{b} + \xi_*^2 \underline{t}_*^T B \underline{t}_* + 2\xi_* \underline{t}_*^T B \underline{p}_* + \underline{p}_*^T B \underline{p}_* + d_1 - \tau = 0$$

This equation can be rewritten in the form:

$$\rho_1 \xi_*^2 + \rho_2 \xi_* + \rho_3 = 0 \tag{19}$$

where

$$\begin{aligned} \rho_1 &= \underline{t}_*^T B \underline{t}_*, \\ \rho_2 &= \underline{t}_*^T \underline{b} + 2\underline{t}_*^T B \underline{p}_* = \underline{t}_*^T (\underline{b} + 2B\underline{p}_*), \\ \rho_3 &= d_1 - \tau + \underline{p}_*^T \underline{b} + \underline{p}_*^T B \underline{p}_*. \end{aligned}$$

The solution of (19) is

$$\xi_{*1,2} = \frac{-\rho_2 \pm \sqrt{\rho_2 - 4\rho_1\rho_3}}{2\rho_1}. \tag{20}$$

This solution exists if and only if $\rho_2^2 - 4\rho_1\rho_3 \geq 0$.

When $\rho_2^2 - 4\rho_1\rho_3 < 0$ the contour of $\hat{y} = \tau$ does not intersect the largest axis ξ_*.

When (20) exists two solutions are possible. The smaller one minimizes the variance. Suppose for example that $| \xi_{*1} | < | \xi_{*2} |$. Then the minimal value of variance is

$$\hat{\sigma}_{1*}^2 = \lambda_* \xi_{1*}^2. \tag{21}$$

It can be obtained for

$$\underline{p}_{1*} = \underline{t}_* \xi_{1*} + \underline{p}_*. \tag{22}$$

3.3 Optimization by use of Lagrange multipliers

If (20) does not exist then the solution can be found by use of Lagrange mutlipliers. Some ideas of Myers and Carter (1973) are used in this section.

Consider following function

$$\phi = \hat{\sigma}^2(\underline{p}) - \mu(\hat{y} - \tau) = \underline{p}^T\underline{\theta} + \underline{p}^T D\underline{p} + d_2 - \mu(\underline{p}^T\underline{b} + \underline{p}^T B\underline{p} + d_1),$$

where μ is an undefined multiplier.

For the optimal value of $\underline{p}$ the first derivative of ϕ must be equal to zero:

$$\frac{d\phi}{d\underline{p}} = \underline{\theta} + 2D\underline{p} - \mu(\underline{b} + 2B\underline{p}) = \underline{0}$$

Consequently

$$(-\mu B + D)\underline{p} = (\mu\underline{b} - \underline{\theta})/2. \tag{23}$$

The second derivative is

$$\frac{d^2\phi}{dpdp^T} = (-\mu B + D)2. \tag{24}$$

The solution is a minimum if (24) is a positive definite matrix, i.e. $-\mu B + D > 0$ or

$$\mu B - D < 0. \tag{25}$$

Let $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m)$ be a matrix of eigenvalues of $D^{-1}B$ and $T-$ a matrix of its corresponding eigenvectors.It is well known that

$$T^T DT = I, \tag{26}$$

$$T^T BT = \Lambda. \tag{27}$$

Further on we use the substitution

$$\underline{p} = T\underline{\xi}. \tag{28}$$

Multiplying (23) by T^T we obtain

$$-T^T(\mu B - D)T\underline{\xi} = T^T(\mu\underline{b} - \underline{\theta})/2.$$

Taking into account (26) and (27) we can rewrite this equation as follows:

$$(\mu\Lambda - I)\underline{\xi} = -T^T(\mu\underline{b} - \underline{\theta})/2.$$

and

$$\underline{\xi} = -(\mu\Lambda - I)^{-1}T^T(\mu\underline{b} - \underline{\theta})/2. \tag{29}$$

From (28) and (29) we obtain

$$\underline{p} = -T(\mu\Lambda - I)^{-1}T^T(\mu\underline{b} - \underline{\theta})/2 = -1/2\sum_{i=1}^{m} t_i t_i^T(\mu\lambda_i - 1)^{-1}(\mu\underline{b} - \underline{\theta}), \tag{30}$$

where t_i are the eigenvectors of $D^{-1}B$.

The relationship (25) can be written as follows:

$$T^T(\mu B - D)T = \mu\Lambda - I < 0.$$

Consequently for any λ_i following inequality must be fulfilled:

$$\mu\lambda_i - 1 < 0, i = 1, 2, \ldots, m. \tag{31}$$

Denote by λ_{min} and λ_{max} the minimal and maximal eigenvalues of $D^{-1}B$. Then we obtain from (31)

$$\mu > \lambda_{min}^{-1} \text{ if } \lambda_{min} < \lambda_{max} < 0, \tag{32}$$

$$\mu < \lambda_{max}^{-1} \text{ if } 0 < \lambda_{min} < \lambda_{max}, \tag{33}$$

$$\lambda_{min} < \mu < \lambda_{max}^{-1} \text{ if } \lambda_{min} < 0 \text{ and } \lambda_{max} > 0. \tag{34}$$

Consequently the indefinite multiplier μ must be chosen so that to minimize $\hat{\sigma}^2$ under the conditions (32), (33), (34) and $\hat{y} = \tau$. For this purpose following algorithm can be used:

1. Compute λ_{min} and λ_{max} and their corresponding eigenvectors. Choose appropriate inequality from (32), (33) and (34).

2. Using q different values of μ: $\mu_1, \mu_2, \ldots, \mu_q$, which satisfy (32) , (33) or (34) one can obtain a set of q values of $\underline{p}_i$, $\hat{\sigma}_i^2$ or $\hat{\sigma}^2(\underline{p}_i)$, $\hat{y}_i$, $i = 1, 2, \ldots, q$ computing these variables by use of equations (30), (8), (9).

3. Graphs of $\hat{y}$ and the components of $\underline{p}_i$ as functions of $\hat{\sigma}_i^2$ can be drawn. Putting $\hat{y} = \tau$ in the first graphics one can find $\hat{\sigma}_{opt}^2$, which corresponds to τ. Then from the second graphics one can find the values of parameters $\underline{p}_{opt} = (p_{opt1}, p_{opt2} \ldots p_{optm})^T$.

3.4 Optimization in a spherical space of product parameters

Suppose that the region of the experiment is a sphere which is defined by the equation

$$\sum_{i=1}^{m} p_i^2 = R^2. \tag{35}$$

If the solution is within this region, it can be found by use of the algorithms described in (3.2) and (3.3). However if the solution is outside of the sphere (35) an additional condition must be imposed as follows:

$$\underline{p}^T\underline{p} = R^2 \tag{36}$$

Define following function:

$$\phi = \hat{\sigma}^2(\underline{p}) - \mu[\hat{y}(\underline{p}) - \tau] - \delta(\underline{p}^T\underline{p} - R^2) = \underline{p}^T\underline{\theta} + \underline{p}^T D\underline{p} + d_2 - \mu(\underline{p}^T\underline{b} + \underline{p}^T B\underline{p} + d_1 - \tau) - \delta(\underline{p}^T\underline{p} - R^2). \tag{37}$$

where μ and δ are undefined Lagrange multipliers.

The first derivative of ϕ is:

$$\frac{\partial\phi}{\partial p} = \underline{\theta} + 2D\underline{p} - (\mu\underline{b} + 2\mu B\underline{p}) - 2\delta\underline{p} = \underline{0}.$$

This equation can be also written as follows:

$$(D - \mu B - \delta I)\underline{p} = (\mu\underline{b} - \underline{\theta})/2. \tag{38}$$

Let $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m)$ be a matrix of the eigenvalues of $D - \mu B$ and T be a matrix of the corresponding eigenvector. Putting $\underline{p} = T\underline{\xi}$ in (38) and multiplying by T^T one can obtain

$$T^T(D - \mu B - \delta I)T\underline{\xi} = T^T(\mu\underline{b} - \underline{\theta})/2. \tag{39}$$

Taking into account that $T^T(D - \mu B - \delta I)T = \Lambda - \delta I$ one can write (39) in the form

$$\underline{\xi} = (\Lambda - \delta I)^{-1}T^T(\mu\underline{b} - \underline{\theta})/2. \tag{40}$$

Consequently

$$\underline{p} = T\underline{\xi} = T(\Lambda - \delta I)^{-1}T^T(\mu\underline{b} - \underline{\theta})/2 = 1/2\sum_{i=1}^{m} t_i t_i^T(\lambda_i - \delta)^{-1}(\mu\underline{b} - \underline{\theta}). \tag{41}$$

The second derivative of ϕ must be positive definite if the solution (41) corresponds to a minimum of $\hat{\sigma}^2$:

$$\frac{\partial^2\phi}{\partial\underline{p}\partial\underline{p}^T} = (-\mu B + D - \delta)2 > 0.$$

This can also be written as follows:

$$T^T(-\mu B + D - \delta)T = \Lambda - \delta I > 0.$$

Consequently the inequalities $\lambda_i - \delta > 0, i = 1, 2, \ldots, m$ have to be fulfilled, or $\delta < \lambda_{min}$, where λ_{min} is the minimal eigenvalue.

Following algorithm can be defined:

1. Arbitrary values $\mu = \mu_i$, $i = 1, 2, \ldots, r$ are chosen.
2. The minimal eigenvalue λ_{min} of $D - \mu B$ and corresponding T matrix are computed.
3. A set of q values of δ are chosen: $\delta_{i1}, \delta_{i2}, \ldots, \delta_{iq}$. Using (41) , (8) and (9) the values of $\underline{p}_{ij}$, $\hat{\sigma}^2_{ij}$ and $\hat{y}_{ij}$ are computed, where $i = 1, 2, \ldots, r$ and $j = 1, 2, \ldots, q$.
4. For any μ_i three graphs can be drawn: $\hat{y}$, $\hat{\sigma}^2$ and components of $\underline{p}$ as functions of R. The graphs are used these values $\underline{p}_{opt} = (p_{1opt}, p_{2opt} \ldots p_{mopt})^T$, which ensure $\hat{y} = \tau$ while $\underline{p}_{opt}$ is on a sphere with a radius equal to R. This value of $\underline{p}_{opt}$ corresponds to minimal variance under these conditions.

№	p_1	p_2	p_3	x_1	x_2	y
1	2	3	4	5	6	7
1	0	-1	1	1	0	14.43
2	1	1	-1	1	0	-0.48
3	0	1	1	1	-1	27.77
4	0	-1	-1	1	-1	-5.2
5	0	1	-1	-1	-1	11.61
6	-1	0	1	1	1	14.82
7	1	0	1	-1	1	-3.57
8	1	-1	0	0	-1	-1.68
9	1	0	1	1	-1	24.06
10	-1	0	1	-1	-1	7.06
11	-1	1	0	1	1	10.31
12	1	1	0	-1	1	-7.14
13	-1	-1	0	-1	1	11.17
14	1	1	0	1	0	13.8
15	-1	0	0	1	-1	-0.7
16	-1	1	0	-1	-1	13.48
17	-1	1	1	0	1	6.66
18	1	-1	1	0	1	13.33
19	1	1	1	0	-1	24.44
20	-1	-1	1	0	-1	3.03
21	-1	1	-1	0	-1	8.81
22	1	-1	1	1	0	21.67
23	-1	-1	-1	1	0	5.52
24	1	1	1	-1	0	4.43
25	-1	-1	1	-1	0	0.74
26	1	-1	-1	-1	0	-0.74
27	0	0	1	-1	1	-2.51
28	0	-1	0	-1	-1	5.17
29	0	1	-1	0	1	5.86

№	p_1	p_2	p_3	$\hat{y}$	$\hat{\sigma}$	$\bar{y}$	s
1	2	3	4	5	6	7	8
1	0	-1	1	7.29	3.09	7.21	3.10
2	1	1	-1	-3.11	2.07	-3.06	2.06
3	0	1	1	14.83	5.18	14.49	5.15
4	0	-1	-1	7.48	3.75	7.61	3.44
5	0	1	-1	3.27	1.45	3.36	1.71
6	-1	0	1	3.96	2.27	4.05	2.37
7	1	0	1	11.92	5.58	12.43	5.80
8	1	-1	0	.87	2.95	.97	2.67
9	1	0	1	11.92	5.58	11.81	5.70
10	-1	0	1	3.96	2.27	4.16	2.32
11	-1	1	0	5.08	1.69	5.13	1.86
12	1	1	0	4.77	4.26	4.67	4.35
13	-1	-1	0	5.65	2.65	5.70	2.74
14	1	1	0	4.77	4.26	4.79	4.29
15	-1	0	0	3.21	1.29	3.17	1.41
16	-1	1	0	5.08	1.69	5.17	1.92
17	-1	1	1	8.77	3.70	8.71	3.49
18	1	-1	1	9.19	4.74	8.97	4.76
19	1	1	1	18.96	6.82	19.26	6.79
20	-1	-1	1	3.46	1.79	3.42	1.79
21	-1	1	-1	7.72	2.55	7.67	2.66
22	1	-1	1	9.19	4.74	9.10	4.85
23	-1	-1	-1	14.16	5.03	14.37	4.87
24	1	1	1	18.96	6.82	19.00	6.80
25	-1	-1	1	3.46	1.79	3.53	1.92
26	1	-1	-1	-1.13	3.07	-1.06	2.35
27	0	0	1	8.91	3.86	8.81	3.75
28	0	-1	0	4.23	2.14	4.28	2.01
29	0	1	-1	3.27	1.45	3.25	1.51

Table 1: Experimental data, Table 2: Results of simulation

4 EXAMPLE

4.1 Estimation of $\hat{y}$ and $\hat{\sigma}^2$

Consider a simulated example. Let the true value of the performance characteristic is

$$\begin{aligned} y \;=\; & 2.5 - 1.2p_1 + 0.9p_2 + 2.6p_3 - 0.7p_1^2 + 1.3p_1p_2 + 5.3p_1p_3 + 2.1p_2^2 + 2.8p_2p_3 + 3.2p_3^2 + \\ & +2.8x_1 + 1.2x_2 + 0.6x_1^2 + 4.1x_1x_2 + 2.4x_2^2 + 4.3p_1x_1 + 0.2p_1x_2 + 1.5p_2x_1 - \\ & -3p_2x_2 + 6.2p_3x_1 - 2.1p_3x_3 + v. \end{aligned}$$

Data corresponding to a sequentially generated D-optimal design are given in Table (1). They were simulated with $E(v) = 0$ and $\sigma_v = 0.4$.

Column 7 shows the simulated values of the performance characteristic without errors in $\underline{p}$ and $\underline{x}$. Stepwise regression is used to compute regression model coefficients. The

predicted model is

$$\begin{aligned}\bar{y} \;=\; & 2.22 - 1.27p_1 + 0.83p_2 + 2.84p_3 - 0.97p_1^2 + 1.12p_1p_2 + 5.26p_1p_3 + 2.15p_2^2 + 2.94p_2p_3 + \\ & +3.16p_3^2 + 2.94x_1 + 1.38x_2 + 0.89x_1^2 + 4.24x_1x_2 + 2.49x_2^2 + 4.29p_1x_1 + 0.09p_1x_2 + \\ & +1.48p_2x_1 - 3.02p_2x_2 + 6.05p_3x_1 - 2.17p_3x_2\end{aligned}$$

The coefficients of this model are used for computation of the predicted value $\hat{y}$ and standard deviation $\hat{\sigma}$ with errors in parameters $\underline{p}$ and random noise factors x_1 and x_2. Formulae (8) and (9) are applied for this purpose. Following moments of noises were used:

$$E(\underline{e}) = \underline{0}, E(\underline{x}) = \underline{0}, \Sigma_e = \mathrm{diag}\,(0.1^2, 0.3^2, 0.2^2), \Sigma_x = \mathrm{diag}(1/9, 1/9).$$

The results are given in columns 5 and 6 of Table (2). Columns 7 and 8 show the values $\bar{y}$ and S of the performance characteristic and its standard deviation obtained by 100 repeated simulations in each design point. One can see that the coincidence between y and $\bar{y}$ as well as between $\hat{\sigma}$ and S is good enough.

4.2 Optimization by use of algorithm of Section 3.2

Assume first that the target value is $\tau = 1$. Using the estimates of regression coefficients we found that equation (19) can be written as follows:

$$-1.6038\xi_*^2 + 1.2401\xi_* + 2.2544 = 0.$$

The discriminant $\rho_2^2 - 4\rho_1\rho_3 = 16,00039 > 0$ and the solutions of this equation are $\xi_{*1} = 0,8642$ and $\xi_{*2} = 1,6336$. The minimal eigenvalue is $\lambda_* = 1,5683$ and the variance, computed by use of equation (21) is $\sigma_*^2 = 1.1711$. The optimal values of parameters are computed by use of equation (22). They are as follows: $p_{1*} = -1.4183$, $p_{2*} = -0.1814$, $p_{3*} = 0.6211$.

4.3 Use of Lagrangian multipliers

Change the target value to $\tau = 4$. Then the equation (19) becomes

$$-1.6083\xi_*^2 + 1.2401\xi_* - 0.7456 = 0.$$

Its discriminant is negative ($\rho_2^2 - 4\rho_1\rho_3 = -3.2456$) and the method of Section (3.2) can not be used. The minimal and maximal eigenvalues of $D^{-1}B$ are $\lambda_{min} = -7.1847$ and $\lambda_{max} = 1.0380$. Then using (35) one can see that μ must be in the interval $-0,1392 < \mu < 0,9633$. Several values of μ were given in this interval to obtain the plots on Fig. (2). For $\hat{y} = \tau = 4$ one can obtain the variance from Fig. (2), which is $\sigma_*^2 = 1.2051$. Then the values of p_1, p_2 and p_3 can be found from Fig. (2): $p_{1*} = -0.6482$, $p_{2*} = -0.5639$ and $p_{3*} = -0.2595$.

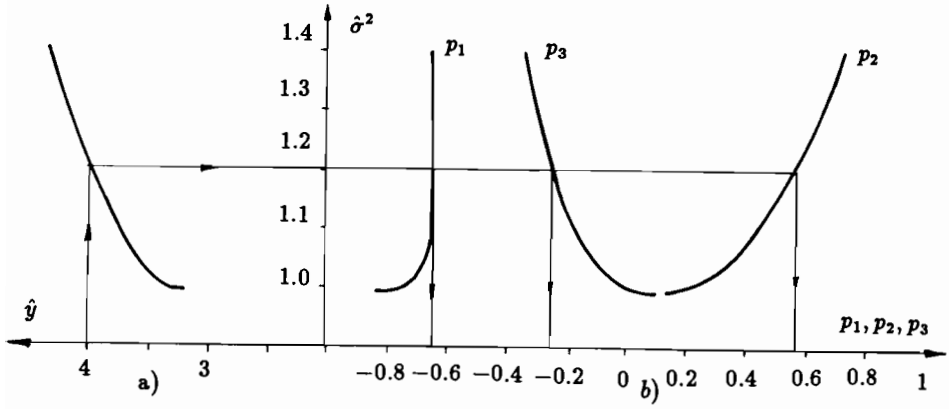


Figure 2: Plots of variance as a function of (a) mean value $\hat{y}$ and of (b) values of parameters p_1, p_2, p_3.

4.4 Optimization in a spherical region of interest

Assume that the target value is $\tau = 1$ and $\underline{p}^T\underline{p} < R^2 = 1$. The solution of Section (4.2) is inappropriate in this case, because for it $\underline{p}^T\underline{p} = 2.43 > 1$. That is why we apply the method of Section (3.4). For this purpose we gave three values of μ: $\mu = -0.2$, $\mu = -0.3$ and $\mu = -2$ and computed following minimal eigenvalues of $D - \mu B$:

$$\begin{aligned} \lambda_{min}(\mu = -0.2) &= -0.1149, \\ \lambda_{min}(\mu = -0.3) &= -0.3113, \\ \lambda_{min}(\mu = \ -2) &= -3.9963. \end{aligned}$$

Plots of R as function of $\underline{p}$, $\hat{y}$ and $\hat{\sigma}^2$ respectively are drawn for $\mu = -0.2$, $\mu = -0.3$ and $\mu = -2$. They are given on Figures (3), (4) and (5) respectively. For $\hat{y} = \tau = 1$ one can find the values of variance and corresponding parameters. One can see from Fig. (3) that the variance is smallest for $\mu = -0.2$, and $\hat{\sigma}^2 = 1.1711$. However this solution does not satisfy the condition that $R = 1$, because for it $R = 1.559$. The optimal solution can be found from Fig. (4) for $\mu = -0.3$. For $\hat{y} = 1$ and $R < 1$ one can find that the variance is $\hat{\sigma}^2 = 1.5917$. The optimal values of parameters are $p_{1*} = 0.2728$, $p_{2*} = 0.3435$ and $p_{3*} = -0.6749$.

For $\mu = -2$ the variance is $\hat{\sigma}^2 = 2.178$, which is larger than for $\mu = -0.3$ (Fig. (5)).

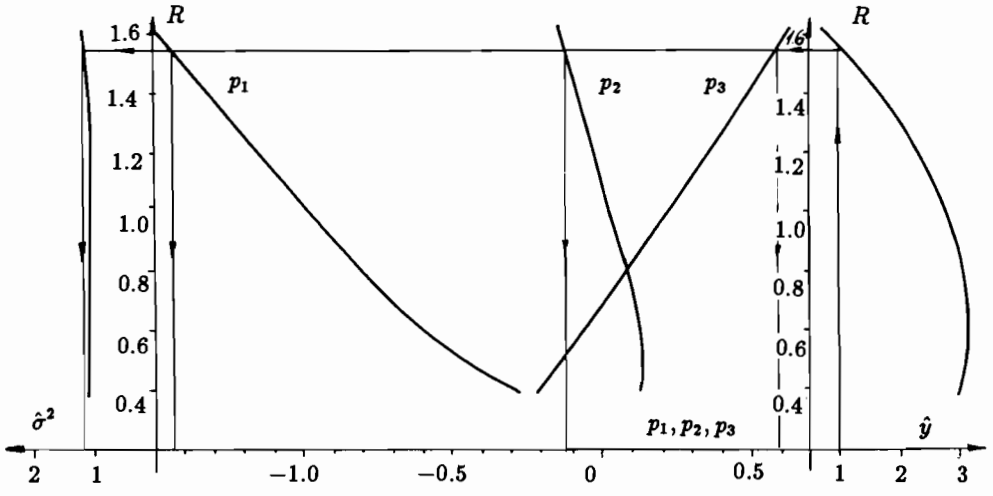


Figure 3: Plots of R as function of $\hat{y}$, $\hat{\sigma}^2$ and $\underline{p}$ for $\mu = -0.2$.

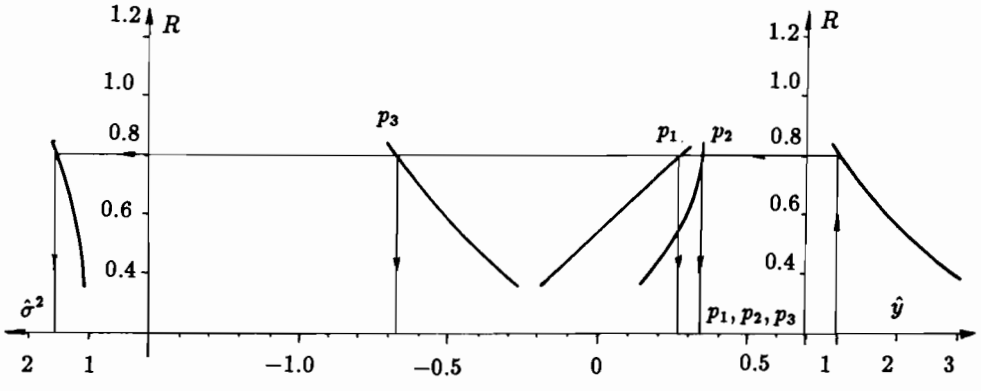


Figure 4: Plots of R as function of $\hat{y}$, $\hat{\sigma}^2$ and $\underline{p}$ for $\mu = -0.3$.

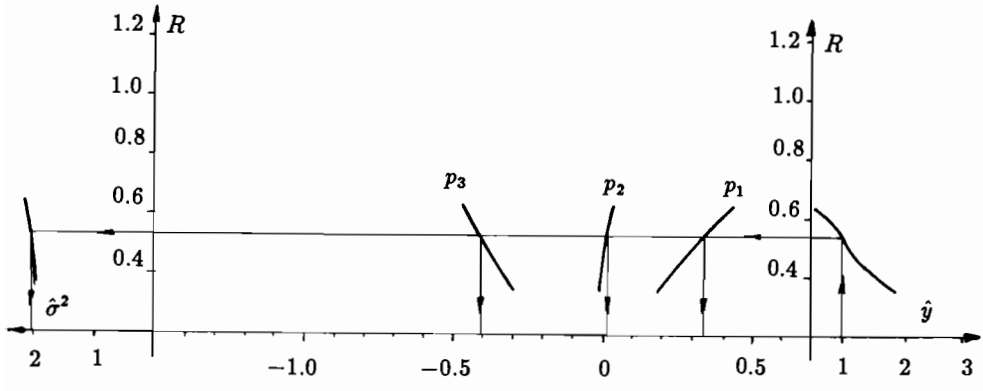


Figure 5: Plots of R as function of $\hat{y}$, $\hat{\sigma}^2$ and $\underline{p}$ for $\mu = -2$.

REFERENCES

Kackar, R.N. (1985). Off-Line Quality Control, Parameter Design and the Taguchi Method. Journal of Quality Technology, 17, 176- 188.

Myers, R.H. and Carter W.H.Jr. (1973). Response Surface Techniques for Duar Response Systems. Technometrics, 15, 301-317.

Taguchi G. (1984). Specification value and quality control 3. The International QC Forum, vol. II, No. 6, 10-27.

Taguchi G. (1986). Introduction to Quality Engineering. Asian Productivity Organization, Tokyo.

Vuchkov, I.N. and Boyadjieva, L.N. (1988). The robustness against tolerances of performance characteristics described by second order polynomials. In Y. Dodge, V.V. Fedorov and H.P. Wynn (Eds). Optimal Design and Analysis of Experiments. North Holland, Amsterdam, 293-309.

Appendix

Equation (4) can be rewritten in the form:

$$y(\underline{p}, \underline{x}) = \beta_o + \underline{\beta}^T \underline{p} + \underline{p}^T \mathcal{B} \underline{p} + \eta_e + \eta_x + \eta_{ex} + v \tag{42}$$

where

$$\begin{aligned} \eta_e &= \underline{\beta}^T \underline{e} + 2\underline{p}^T \mathcal{B} \underline{e} + \underline{e}^T \mathcal{B} \underline{e}, \\ \eta_x &= \underline{\alpha}^T \underline{x} + \underline{x}^T \mathcal{A} \underline{x} + \underline{p}^T \mathcal{T} \underline{x}, \\ \eta_{ex} &= \underline{e}^T \mathcal{T} \underline{x}. \end{aligned}$$

1. *Proof of equation (5)*

Taking expectations of (42) with respect to $\underline{e}$ and $\underline{x}$ and having in mind that $\underline{e}$ and $\underline{x}$ are independently distributed with $E(\underline{e}) = E(\underline{x}) = \underline{0}$, $E(v) = 0$, one can write

$$\tilde{y} = E[y(\underline{p})] = \beta_o + \underline{\beta}^T\underline{p} + \underline{p}^T\mathcal{B}\underline{p} + E(\underline{e}^T\mathcal{B}\underline{e}) + E(\underline{x}^T\mathcal{A}\underline{x}) + E(\underline{e}^T\mathcal{T}\underline{x}) \qquad (43)$$

Equation (5) follows from (43) because $E(\underline{e}^T\mathcal{B}\underline{e}) = \mathcal{B}E(\underline{e}\underline{e}^T) = \operatorname{tr}\mathcal{B}\Sigma_e$ and $E(\underline{x}^T\mathcal{A}\underline{x}) = \mathcal{A}E(\underline{x}\underline{x}^T) = \operatorname{tr}\mathcal{A}\Sigma_x$.

2. *Proof of equation (6)*

Taking into account (42) one can write

$$\begin{aligned}\sigma^2(\underline{p}) \;=\; & \operatorname{var}[y(\underline{p},\underline{x})] = var(\eta_e) + \operatorname{var}(\eta_x) + \operatorname{var}(\eta_{ex}) + \operatorname{var}(v) + 2[\operatorname{cov}(\eta_e,\eta_x) + \\ & + \operatorname{cov}(\eta_e,\eta_{ex}) + \operatorname{cov}(\eta_x,\eta_{ex})] + 2\operatorname{cov}[(\eta_e + \eta_x + \eta_{ex}), v]. \qquad (44)\end{aligned}$$

Compute the terms of (44) under following conditions:

- The elements of $\underline{e}$ are independent of each other. The same is true for the elements of $\underline{x}$.
- $\underline{e}$, $\underline{x}$ and v are independent of each other.
- $E(\underline{e}) = \underline{0}_m$, $E(\underline{x}) = \underline{0}_l$, $E_v = 0$, where $\underline{0}_m$ and $\underline{0}_l$ are vectors of m and l elements equal to zero.
- $E(\underline{e}\underline{e}^T) = \Sigma_e$, $E(\underline{x}\underline{x}^T) = \Sigma_x$.
- $\underline{e}$ and $\underline{x}$ are normally distributed and $E(e_i^3) = E(x_j^3) = 0$, $i = 1,2,\ldots,m$; $j = 1,2,\ldots,l$, while $E(e_i^4) = 3\sigma_i^4$ and $E(x_i^4) = 3\sigma^4(x_i)$.

2.1 $\operatorname{var}(\eta_e)$

$$\begin{aligned}\operatorname{var}(\eta_e) = \operatorname{var}(\underline{\beta}^T\underline{e} + 2\underline{p}^T\mathcal{B}\underline{e} + \underline{e}^T\mathcal{B}\underline{e}) = \operatorname{var}(\underline{\beta}^T\underline{e}) + 4\operatorname{var}(\underline{p}^T\mathcal{B}\underline{e}) + \operatorname{var}(\underline{e}^T\mathcal{B}\underline{e}) + \\ 2\operatorname{cov}(\underline{\beta}^T\underline{e}, 2\underline{p}^T\mathcal{B}\underline{e}) + \operatorname{cov}(\underline{\beta}^T\underline{e}, \underline{e}^T\mathcal{B}\underline{e}) + \operatorname{cov}(2\underline{p}^T\mathcal{B}\underline{e}, \underline{e}^T\mathcal{B}\underline{e}). \qquad (45)\end{aligned}$$

Consider any of terms of (45)

- $$\operatorname{var}(\underline{\beta}^T\underline{e}) = E[(\underline{\beta}^T\underline{e})^2] - [E(\underline{\beta}^T\underline{e})]^2 = E(\underline{\beta}^T\underline{e}\underline{e}^T\underline{\beta}) - \underline{0}_m = \underline{\beta}^T\Sigma_e\underline{\beta}. \qquad (46)$$

- $$4\operatorname{var}(\underline{p}^T\mathcal{B}\underline{e}) = 4E(\underline{p}^T\mathcal{B}\underline{e}\underline{e}^T\mathcal{B}\underline{p}) - 4[E(\underline{p}^T\mathcal{B}\underline{e})]^2 = 4\underline{p}^T\mathcal{B}\Sigma_e\mathcal{B}\underline{p}. \qquad (47)$$

- $$\operatorname{var}(\underline{e}^T\mathcal{B}\underline{e}) = \operatorname{var}(\sum_{i=1}^{m}\beta_{ii}e_i^2 + \sum_{i=1}^{m-1}\sum_{j=1}^{m}\beta_{ij}e_ie_j) = \sum_{i=1}^{m}\beta_{ii}^2\operatorname{var}(e_i^2) + \sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\beta_{ij}^2\operatorname{var}(e_ie_j) + \delta, \qquad (48)$$

where δ includes all possible covariances between the pairs of errors, for example $e\,e$ and $e\,e$ for $i,j,r,s = 1,2,\ldots,m$ and i, j not coinciding with r, s.

For the first two terms of (48) one can write

$$\mathrm{var}(e_i^2) = E(e_i^4) - (E(e_i^2))^2 = 2\sigma_i^4. \tag{49}$$

$$\mathrm{var}(e_i e_j) = E(e_i^2 e_j^2) - E[(e_i e_j)]^2 = E(e_i^2)E(e_j^2) - 0 = \sigma_i^2\sigma_j^2. \tag{50}$$

For computation of δ take into account that four combinations of indices are possible. For the first three combinations one can write

$$E(e_i e_j e_r e_s) = E(e_i^2 e_r e_s) = E(e_i^3 e_s) = 0.$$

For the fourth combination of indices following equation exists:

$$\mathrm{cov}(e_i e_j, e_r e_s) = E(e_i^2 e_r^2) - E(e_i^2)E(e_r^2) = \sigma_i^2\sigma_r^2 - \sigma_i^2\sigma_r^2 = 0.$$

Consequently $\delta = 0$. Putting (49) and (50) in (48) one can obtain

$$\mathrm{var}(\underline{e}^T \mathcal{B} \underline{e}) = 2\sum_{i=1}^{m} \beta_{ii}^2 \sigma_i^4 + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij}^2 \sigma_i^2 \sigma_j^2. \tag{51}$$

- $$\mathrm{cov}(\underline{\beta}^T \underline{e}, 2\underline{p}^T \mathcal{B} \underline{e}) = 2E(\underline{\beta}^T \underline{e}, \underline{p}^T \mathcal{B} \underline{e}) - 2E(\underline{\beta}^T \underline{e})E(\underline{p}^T \mathcal{B} \underline{e}) = 2\underline{\beta}^T E(\underline{e}\underline{e}^T)\mathcal{B}\underline{p} = 2\underline{\beta}^T \Sigma_e \mathcal{B} \underline{p}. \tag{52}$$

- $$\mathrm{cov}(\underline{\beta}^T \underline{e}, \underline{e}^T \mathcal{B} \underline{e}) = E(\underline{\beta}^T \underline{e}\underline{e}^T \mathcal{B} \underline{e}) - E(\underline{\beta}^T \underline{e}).E(\underline{e}^T \mathcal{B} \underline{e}) = E(\underline{\beta}^T \underline{e}\underline{e}^T \mathcal{B} \underline{e}) = 0. \tag{53}$$

  The term $E(\underline{\beta}^T \underline{e}\underline{e}^T \mathcal{B} \underline{e})$ is third order moment and is equal to zero for normally distributed errors.

- $$\mathrm{cov}(2\underline{p}^T \mathcal{B} \underline{e}, \underline{e}^T \mathcal{B} \underline{e}) = 0. \tag{54}$$

  The proof of (54) is similar to that of (53). Substituting (46) - (54) in (45) one can obtain

$$\mathrm{var}(\eta_e) = (\underline{\beta} + 2\mathcal{B}\underline{p})^T \Sigma_e (\underline{\beta} + 2\mathcal{B}\underline{p}) + 2\sum_{i=1}^{m} \beta_{ii}^2 \sigma_i^4 + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \beta_{ij}^2 \sigma_i^2 \sigma_j^2. \tag{55}$$

2.2 $\mathrm{var}(\eta_x)$

$$\begin{aligned} \mathrm{var}(\eta_x) \;=\; & \mathrm{var}(\underline{\alpha}^T \underline{x} + \underline{x}^T \mathcal{A} \underline{x} + \underline{p}^T \mathcal{T} \underline{x}) = \mathrm{var}(\underline{\alpha}^T \underline{x}) + \mathrm{var}(\underline{x}^T \mathcal{A} \underline{x}) + \mathrm{var}(\underline{p}^T \mathcal{T} \underline{x}) + \\ & + 2\,\mathrm{cov}(\underline{\alpha}^T \underline{x}, \underline{x}^T \mathcal{A} \underline{x}) + 2\,\mathrm{cov}(\underline{\alpha}^T \underline{x}, \underline{p}^T \mathcal{T} \underline{x}) + + 2\,\mathrm{cov}(\underline{x}^T \mathcal{A} \underline{x}, \underline{p}^T \mathcal{T} \underline{x}). \end{aligned} \tag{56}$$

Consider the terms of (56):

- $$\mathrm{var}(\underline{\alpha}^T \underline{x}) = E(\underline{\alpha}^T \underline{x}\underline{x}^T \underline{\alpha}) - [E(\underline{\alpha}^T \underline{x})]^2 = \underline{\alpha}^T \Sigma_x \underline{\alpha}. \tag{57}$$

- $$\mathrm{var}(\underline{x}^T\mathcal{A}\underline{x}) = 2\sum_{i=1}^{l}\alpha_{ii}^2\sigma^4(x_i) + \sum_{i=1}^{l-1}\sum_{j=i+1}^{l}\alpha_{ij}^2\sigma^2(x_i)\sigma^2(x_j). \quad (58)$$

The proof of (58) is the same as for (51).

- $$\mathrm{var}(\underline{p}^T\mathcal{T}\underline{x}) = E(\underline{p}^T\mathcal{T}\underline{x}\underline{x}^T\mathcal{T}^T\underline{p}) - [E(\underline{p}^T\mathcal{T}\underline{x}]^2 = \underline{p}^T\mathcal{T}E(\underline{x}\underline{x}^T)\mathcal{T}\underline{p}^T = \underline{p}^T\mathcal{T}\Sigma_x\mathcal{T}^T\underline{p}. \quad (59)$$

- $$\mathrm{cov}(\underline{\alpha}^T\underline{x}, \underline{x}^T\mathcal{A}\underline{x}) = E(\underline{\alpha}^T\underline{x}\underline{x}^T\mathcal{A}\underline{x}) - E(\underline{\alpha}^T\underline{x})E(\underline{x}^T\mathcal{A}\underline{x}) = E(\underline{\alpha}^T\underline{x}\underline{x}^T\mathcal{A}\underline{x}) = 0, \quad (60)$$

because the third order terms of normally distributed vector $\underline{x}$ are equal to zero.

- $$\mathrm{cov}(\underline{\alpha}^T\underline{x}, \underline{p}^T\mathcal{T}\underline{x}) = E(\underline{\alpha}^T\underline{x}, \underline{p}^T\mathcal{T}\underline{x}) - E(\underline{\alpha}^T\underline{x})E(\underline{p}^T\mathcal{T}\underline{x}) = E(\underline{\alpha}^T\underline{x}\underline{x}^T\mathcal{T}^T\underline{p} = \underline{\alpha}^T\Sigma_x\mathcal{T}^T\underline{p}. \quad (61)$$

- $$\mathrm{cov}(\underline{x}^T\mathcal{A}\underline{x}, \underline{p}^T\mathcal{T}\underline{x}) = E(\underline{x}^T\mathcal{A}\underline{x}\underline{p}^T\mathcal{T}\underline{x}) - E(\underline{x}^T\mathcal{A}\underline{x})E(\underline{p}^T\mathcal{T}\underline{x}) = 0. \quad (62)$$

Substituting (57) - (62) in (56) one can obtain

$$\mathrm{var}(\eta_x) = (\underline{\alpha} + \mathcal{T}^T\underline{p})^T\Sigma_x(\underline{\alpha} + \mathcal{T}^T\underline{p}) + 2\sum_{i=1}^{l}\alpha_{ii}^2\sigma^4(x_i) + \sum_{i=1}^{l-1}\sum_{j=i+1}^{l}\alpha_{ij}^2\sigma^2(x_i)\sigma^2(x_j). \quad (63)$$

2.3 $\mathrm{var}(\eta_{ex})$

$$\mathrm{var}(\eta_{ex}) = E(\underline{e}^T\mathcal{T}\underline{x}\underline{x}^T\mathcal{T}^T\underline{e}) - [E(\underline{e}^T\mathcal{T}\underline{x})]^2 = E[\mathrm{tr}(\mathcal{T}\underline{x}\underline{x}^T\mathcal{T}^T\underline{e}\underline{e}^T)] = \mathrm{tr}\,\mathcal{T}\Sigma_x\mathcal{T}^T\Sigma_e. \quad (64)$$

2.4 $\mathrm{var}(v)$

$$\mathrm{var}(v) = \sigma_v^2 \quad (65)$$

2.5 $2\,\mathrm{cov}(\eta_e, \eta_x)$

$$\mathrm{cov}(\eta_e, \eta_x) = E_{ex}(\eta_e\eta_x) - E_{ex}(\eta_e)E_{ex}(\eta_x).$$

Taking into account that $\underline{x}$ and $\underline{e}$ are independent one can write this equation as follows:

$$\mathrm{cov}(\eta_e, \eta_x) = E_e(\eta_e)E_x(\eta_x) - E_e(\eta_e)E_x(\eta_x) = 0. \quad (66)$$

2.6 $2\,\mathrm{cov}(\eta_e, \eta_{ex})$

$$\mathrm{cov}(\eta_e, \eta_{ex}) = E(\eta_e\underline{e}^T\mathcal{T}\underline{x}) - E(\eta_e)E(\underline{e}^T\mathcal{T}\underline{x}) = E(\eta_e e^T\mathcal{T})E(x) = 0. \quad (67)$$

2.7 $2\,\mathrm{cov}(\eta_x, \eta_{ex})$

$$\mathrm{cov}(\eta_x, \eta_{ex}) = E(\eta_x \underline{e}^T \mathcal{T} \underline{x}) - E(\eta_x) E(\underline{e}^T \mathcal{T} \underline{x}) = E(\eta_x \underline{x}^T \mathcal{T}^T \underline{e}) = E(\eta_x x^T \mathcal{T}^T) E(\underline{e}) = 0. \tag{68}$$

2.8 $2\,\mathrm{cov}[(\eta_e + \eta_x + \eta_{ex}), v]$

$$2\,\mathrm{cov}(\eta_e, v) = 2E(\eta_e v) - E(\eta_e) E(v) = 0. \tag{69}$$

In a similar way one can see that

$$2\,\mathrm{cov}(\eta_x, v) = 2\,\mathrm{cov}(\eta_{ex}, v) = 0. \tag{70}$$

Substituting the obtained results in (44) one can obtain the result (6) .

STATISTICAL METHODS FOR QUALITY CONTROL
-BEYOND THE ANALYSIS OF VARIANCE-

Chihiro Hirotsu
Faculty of Engineering, University of Tokyo, Bunkyo-ku, Tokyo, Japan

1. INTRODUCTION

There are all sorts of statistical or nonstatistical data processing procedures, which should be properly used in various phases of experiments. Among them we discuss here some beyond analysis of variance (BANOVA) techniques which should be useful for explanatory or confirmatory experiments. In particular we propose

(1) some multiple comparisons procedures for modelling the generalized interaction effects, and

(2) a method for testing and/or modelling ordered parameters.

It should be noted that these two topics have many applications. The generalized interaction covers a very wide range of statistical inferences including the usual two-way interaction in the analysis of variance model, the association in a contingency table, the canonical correlation and the non-parametric regression analysis. The second takes a prior knowledge on parameters into statistical inferences, where the omnibus statistics such as F and χ^2 are inapropriate and one degree of freedom (1 df) statistics such as t and linear rank sum are too restricted.

2. PHASES OF EXPERIMENT

There are all sorts of data processing procedures including statistical data analysis, exploring data analysis (EDA), Taguchi's parameter design and so on. They are sometimes called to be opposing procedures. I should, however, stress that they are by no means in rivalry with but are complementary each other. They should respectively be useful in some of the four different phases of experiments.

(1) Exploring

This is the first phase of an experiment to find out some promising hypotheses. Various techniques of EDA are used, including cause and effect diagram, quality deployment and Box-whiskey plot. Analysis of variance and regression analysis can also be applied

but too much confidence should not be given to the results obtained by data dredging. They should be confirmed by the later phases of the experiment.

(2) Explanatory

A rigid statistical analysis is applied to prove the hypothesis under the well defined condition.

(3) Confirmatory

It is necessary to prove the accepted hypothesis by the phase 2 (laboratory) experiment to be also valid in the actual field. For the purpose Taguchi's idea of parameter design should be useful, where possible noises expected to occur in scaling up are taken into the experiment. The factor has been called a noise factor by Taguchi (1986) but we prefer to call it a variation factor distinguishing it from the pure measurement error which is brought about in a repetition. This is a sort of the interaction analysis between the controllable and the variation, or environmental, factors.

(4) Follow-up

Even if the earlier three phases are taken very carefully, the sample size is usually far from enough to foresee all the possibilities that may occur in actual field. So the follow-up analysis after marketing is an inevitable process and the obtained information should be immediately fed back to the first phase. In some sense this might be the first step of an experiment.

3. CLASSIFICATION OF FACTORS

In analyzing data the character of a factor plays an important role. We define here five factors and explain how they are incorporated in analyzing data.

(1) Controllable factor: Reproducible and can be specified by the experimenter. The purpose of the experiment will be to determine the optimal level of this factor.

(2) Indicative factor: Reproducible but uncontrollable by the experimenter. A typical example is the region in the adaptability experiment of the rice varieties.

(3) Concomitant factor: Reproducible but observable only after the experiment.

(4) Variation factor: Reproducible in the laboratory but not in the actual field of application. Individuals in a clinical trial give a typical example.

(5) Block factor: Nonreproducible factor introduced to reduce a systematic background variation.

The controllable, the indicative and the concomitant factors are considered to be of fixed effects. The variation factor may be treated as a fixed indicative factor within an experiment but works as if it were a random noise on extending the result to the actual field. The block factor can be treated either as fixed or random and may not either way cause serious effects excepting the recovery of interblock information since no interaction

is assumed in the relation with other factors in the experiment (see Hirotsu 1965, for example).

4. ANALYSIS OF INTERACTION EFFECTS

It seems that too less attention has been given to the analysis of interaction as compared with its importance. First the all-or-nothing procedure represented by F or χ^2 test is often not useful in an application since the degrees of freedom for interaction are usually large. The multiple comparisons procedure for interaction elements with 1 df is also often too conservative and not easy to interpret. Further, more importantly the characteristic of a factor seems not necessarily to have been well reflected upon the analysis.

In case of the controllable $\times$ controllable, the purpose of the experiment will be to determine the optimal combination of the levels of the two factors and some simple interaction models such as Mandel (1971) and Johnson & Graybill (1972) should be useful to point out it. If one factor is indicative the purpose will be to select the optimum level of the controllable factor for each level of the indicative factor. Then the procedure of grouping the homogeneous levels of the indicative factor is desirable so that a single level of the controllable factor can commonly be applicable to as many levels of the indicative factor as possible. If a variation factor is involved the purpose will be to find out an optimal level of the controllable factor which make the objective characteristics robust against the possible environmental variations. In all these situations the row-wise and/or column-wise multiple comparisons procedure for modelling interaction effects should be useful.

5. MODELING THE INTERACTION EFFECTS IN A TWO-WAY LAYOUT

Suppose that we are given two-way observations with replications and assume the model

$$y_{ijk} = \mu_{ij} + \varepsilon_{ijk} \qquad (i = 1, \cdots, a;\ j = 1, \cdots, b;\ k = 1, \cdots, r),$$

where the ε_{ijk} are independently distributed as $N(0, \sigma^2)$. The μ_{ij} may be modelled simply by $\mu_{ij} = \mu + \alpha_i + \beta_j$ if the hypothesis of no interaction is accepted. When it is rejected, however, we are faced with a more complicated model and it is desirable to have a simplified interaction model with a less degrees of freedom.

Reparameterize the μ_{ij} as

$$\boldsymbol{\mu} = \boldsymbol{\mu}_{+} + (P_a \otimes P_b)\gamma,$$

where $\boldsymbol{\mu}$ is the column vector of μ_{ij} 's arranged in dictionary order, $\boldsymbol{\mu}_+$ the additive part of $\boldsymbol{\mu}$ with $\bar{\mu}_{i\cdot} + \bar{\mu}_{\cdot j} - \bar{\mu}_{\cdot\cdot}$ as its $b(i-1)+j$th element and $\boldsymbol{\gamma} = (P_a' \otimes P_b')\boldsymbol{\mu}$ the interaction part. We use the usual dot and bar notation to denote the sum and the average over the suffix replaced by the dot, $\otimes$ denotes the Kronecker product and P_n' is an $(n-1)$ by n orthogonal matrix satisfying $P_n P_n' = I_n - n^{-1}\boldsymbol{j}_n\boldsymbol{j}_n'$, I being an identity matrix, $\boldsymbol{j}$ a vector of 1's.

The contribution of two particular rows, the mth and the nth, say, to $\boldsymbol{\gamma}$ is given by

$$\boldsymbol{L}(m;n) = (1/\sqrt{2})P_b'(\boldsymbol{\mu}_m - \boldsymbol{\mu}_n),$$

where $\boldsymbol{\mu}_i = (\mu_{i1}, \cdots, \mu_{ib})'$. This is called an interaction element between the two rows (Hirotsu 1973). If it is known to be zero, one can take into consideration only those contrasts which are orthogonal to it. Thus if by any means one can classify rows into homogeneous subgroups so that in each of them all interaction elements are zero, one can have a much simplified model. We can deal with the columns symmetrically.

The resulting model may be expressed in terms of nonzero elements of $\boldsymbol{\gamma}$. The contribution of two subgroups of rows $G_1 = (1, \cdots, p_1)$ and $G_2 = (p_1+1, \cdots, p_1+p_2)$ to $\boldsymbol{\gamma}$ is, for example, defined by

$$L(G_1;G_2) = \{p_1p_2(p_1+p_2)\}^{-\frac{1}{2}}\{(p_2, \cdots, p_2, -p_1, \cdots, -p_1, 0, \cdots, 0) \otimes P_b'\}\boldsymbol{\mu}.$$

A more convenient expression of the model is, however,

$$\mu_{ij} = \bar{\mu}_{i\cdot} + \bar{\mu}_{\cdot j} - \bar{\mu}_{\cdot\cdot} + (\alpha\beta)_{ij} \tag{5.1}$$

with $(\alpha\beta)_{i\cdot} = 0$, $(\alpha\beta)_{\cdot j} = 0$ and $(\alpha\beta)_{ij} = (\alpha\beta)_{i'j'}$ if $i, i' \in G_u$ and $j, j' \in J_v$, where G_u, $u = 1, \cdots, A$, and J_v, $v = 1, \cdots, B$, denote the homogeneous subgroups of rows and columns, respectively. The model (5.1) may be called the block interaction model.

6. ROW- AND COLUMN-WISE MULTIPLE COMPARISONS FOR INTERACTION

To obtain such a classification we propose simultaneous tests of the hypotheses

$$H(G_1;G_2) : \boldsymbol{L}(G_1;G_2) = \boldsymbol{O}$$

for any subgroups $G_1, G_2 \in (1, \cdots, a)$ based on the squared distances between G_1 and G_2

$$S(G_1;G_2) = \|\hat{\boldsymbol{L}}(G_1;G_2)\|^2,$$

where the $\hat{\boldsymbol{L}}(G_1;G_2)$ are obtained from the $\boldsymbol{L}(G_1;G_2)$ with $\boldsymbol{\mu}$ replaced by $\bar{\boldsymbol{y}}$, the vector of cell means. This may be called the row-wise multiple comparisons procedure.

For every choice of G_1 and G_2 the statistic $S(G_1; G_2)$ is bounded above by the maximum of $r\|(\boldsymbol{a}' \otimes P_b')\bar{\boldsymbol{y}}\|^2$ with respect to $\boldsymbol{a}$ subject to the condition that $\|\boldsymbol{a}\| = 1$, $\boldsymbol{a}'\boldsymbol{j} = 0$, which is, under the null hypothesis of interaction, distributed as the maximum roof of the Wishart matrix $W(\sigma^2 I_{\nu_1}, \nu_2)$ where $\nu_1 = \min(a-1, b-1)$ and $\nu_2 = \max(a-1, b-1)$ (see Hirotsu 1983a, for details).

To cancel out the unknown σ^2, we divide the $S(G_1; G_2)$ by the unbiased variance

$$\hat{\sigma}^2 = \nu^{-1}\Sigma\Sigma\Sigma(y_{ijk} - \bar{y}_{ij\cdot})^2$$

with the df $\nu = n - ab$, then $S(G_1; G_2)/\hat{\sigma}^2$ is bounded above by

$$\lambda_1(\nu_1, \nu_2)/(\chi^2_\nu/\nu) \tag{6.1}$$

where $\lambda_1(\nu_1, \nu_2)$ is the maximum root of $W(I_{\nu_1}, \nu_2)$ and the $\chi^2{}_\nu$ is the chi-squared variable independent of the λ_1.

We explain the row-wise multiple comparisons procedure by an example.

Example 1. The data summarized in Table 1 are taken from Davies (1954).

TABLE 1 Averaged corrosion resistance of aluminum alloys ($r = 4$).

	Alloys								
Sites	1	2	3	4	5	6	7	8	9
1	5.50	5.50	5.25	5.00	6.50	5.00	2.25	6.00	7.00
2	8.00	8.00	7.25	7.50	6.00	5.00	5.50	5.75	6.50
3	3.25	3.75	5.00	3.25	4.50	3.00	1.00	5.50	6.25
4	4.25	4.00	6.00	4.75	6.00	4.50	3.75	7.00	6.00
1,3,4	4.33	4.42	5.42	4.33	5.67	4.17	2.33	6.17	6.42
2	8.00	8.00	7.25	7.50	6.00	5.00	5.50	5.75	6.50

The data relate to the testing of nine Aluminum alloys for their resistance to corrosion in a chemical plant atmosphere. Four typical sites in the factory were chosen, and at each of them a plate made from each alloy was exposed for a year. The plates were then submitted to four observers, who assessed their condition visually and awarded marks to each from 0 to 10 according to the degree of resistance to attack. Thus the data were originally of a $9 \times 4 \times 4$ experiment. We can, however, treat them as a two-way table like Table 1 averaged over the observers since there is no evidence of interaction of observers with sites and alloys. According to Davies the unbiased estimate of the variance to assess the interaction involved in Table 1 is $\hat{\sigma}^2 = 0.90$ with the df 105.

The purpose of the experiment is to choose an appropriate alloy for each of four sites which are considered to be an indicative factor. Then it is preferable if an alloy is suitable for as many sites as possible since it would be inconvenient to have to use

different alloys in different sites in a factory. So this is the problem of the row-wise multiple comparisons for interaction.

The squared distances between rows divided by $\hat{\sigma}^2$ are $S(1;2)/\hat{\sigma}^2 = 42.62$, $S(1;3)/\hat{\sigma}^2 = 9.48$, $S(1;4)/\hat{\sigma}^2 = 19.66$, $S(2;3)/\hat{\sigma}^2 = 58.61$, $S(2;4)/\hat{\sigma}^2 = 55.12$, and $S(3;4)/\hat{\sigma}^2 = 12.99$, which should be evaluated by the distribution of (6.1). In this case, however, the df for $\hat{\sigma}^2$ is large enough so that we can approximate the distribution by that of $\lambda_1(3,8)$ and obtain critical values 22.62 ($\alpha = 0.05$) and 27.52 ($\alpha = 0.01$). Thus the site 2 is proved to behave very differently from the other sites and there is no evidence of inhomogeneity among sites 1,3 and 4. The squared distance between the two groups $G_1 = (1,3,4)$, and $G_2 = (2)$ is found to be $S(G_1;G_2)/\hat{\sigma}^2 = 71.16$, which is very highly significant elucidating 71.7% of the total sum of squares for interaction.

The mean responses of alloys averaged over the sites in each subgroup are shown in the lower half of Table 1. From it we can derive a tentative conclusion that for sites represented by 1, 3 and 4 the alloy 9 or 8 would be suitable and the alloy 1 or 2 for those sites for which the site 2 is the representative.

7. PROCEDURE FOR A TWO-WAY LAYOUT WITH EXACTLY ONE OBSERVATION PER CELL

When $r = 1$ we do not have the unbiased variance $\hat{\sigma}^2$ derived from the within cell sum of squares. We therefore divide the between groups sum of squares by the total sum of squares for interaction

$$T = \sum\sum(y_{ij} - \bar{y}_{i\cdot} - \bar{y}_{\cdot j} + \bar{y}_{\cdot\cdot})^2.$$

Then for every choice of subgroups G_1 and G_2, $S(G_1;G_2)/T$ is bounded above by the ratio of the largest root $\lambda_1(\nu_1,\nu_2)$ of the Wishart matrix to its trace. The null distribution of the ratio is given in Johnson & Graybill (1972) by which we can evaluate $S(G_1;G_2)/T$.

In this situation it is very important to have an estimate of σ^2. It is obtained if the block interaction model (5.1) fits the data well.

First the least squares estimator of the model and its variance are obtained for general case as

$$\hat{\mu}_{ij} = \bar{y}_{i\cdot\cdot} + \bar{y}_{\cdot j\cdot} - \bar{y}_{\cdots} + [\sum_{i\in G_u}\sum_{j\in J_v}\bar{y}_{ij\cdot}/\{n(G_u)n(J_v)\} - \sum_{i\in G_u}\bar{y}_{i\cdot\cdot}/n(G_u) - \sum_{j\in J_v}\bar{y}_{\cdot j\cdot}/n(J_v) + \bar{y}_{\cdots}],$$

$$V(\hat{\mu}_{ij}) = [(a+b-1)/ab + \{a-n(G_u)\}\{b-n(J_v)\}/\{abn(G_u)n(J_v)\}](\sigma^2/r),$$

where $n(G_u)$ and $n(J_v)$ denote the number of rows and columns contained in the sets G_u and J_v, respectively. Then in case $r = 1$, an estimator of σ^2 is given by

$$\hat{\sigma}^2 = \sum_i \sum_j (y_{ij} - \hat{\mu}_{ij})^2 / f = \{T - \|\hat{\gamma}\|^2\}/f,$$

where $f = (a-1)(b-1) - (A-1)(B-1)$ with $(A-1)(B-1)$ being the number of orthogonal interaction contrasts remaining in the model.

An example of 7×3 two-way table without replication is given in Hirotsu (1983a), where the 3×2 block interaction model is successfully fitted to the data. Another example given in Hirotsu (1976) is a two-way layout examining the adaptability of 18 varieties of rice (the controllable factor) to 44 combinations of regions and years (the indicative factor). The procedure succeeded in classifying varieties into four types, Formosan type, Indian type, Japanese and Korean type and the special variety called Hybrid. Regions were also classified properly into six groups, Korea and the northern part of Japan, southern part of Japan, tropical regions, Nepal, Egypt and Mexico.

8. GENERALIZED INTERACTION

The previous notion is extended to the analysis of the generalized interaction. The analysis of generalized interaction covers a very wide range of statistical inference.

As an example consider the rank data from one-way layout, $y_{ij} = \mu_i + \varepsilon_{ij}$. They are summarized as in Table 2 and the treatment differences are reflected upon the pattern of 0,1 occurrences. If the μ_i is large then for the treatment 1's occur more often in the right side than left. So this is the problem of interaction analysis with ordered column categories.

TABLE 2 Rank data.

	Rank												
Treatment	1	2	3					⋯		$n-2$	$n-1$	n	Total
1	0	0	0	0	1	0	0	⋯	0	0	1	1	n_1
2	1	0	1	0	0	1	0	⋯	1	0	0	0	n_2
3	0	1	0	1	0	0	1	⋯	0	1	0	0	n_3
Total	1	1	1	1	1	1	1	⋯	1	1	1	1	n

It should be noted that linear rank tests with 1 df such as Wilcoxon-Mann-Whitney, Fisher-Yates, Savage, and so on are by no means powerful enough for a wide range of alternative models if they are criterion robust. So we recommend to apply the statistics with more than 1 df such as the cumulative chi-squared statistic.

Table 3 taken from Bradley, Katti & Coons (1962) gives another example of a similar kind.

TABLE 3 Taste testing data.

	Rating					
Foods	1.Terrible	2	3	4	5.Excellent	Total R_i
1	9	5	9	13	4	40
2	7	3	10	20	4	44
3	14	13	6	7	0	40
4	11	15	3	5	8	42
5	0	2	10	30	2	44
Total C_j	41	38	38	75	18	210

For these ordered categorical data, the ordinal regression models such as proportional odds model are usually applied, see McCullagh & Nelder (1989), for example. There can also be applied the block interaction model derived from the row- and column-wise multiple comparisons based on the cumulative chi-squared statistic.

9.TESTING AND MODELLING ORDERED PARAMETERS

Two examples given in the previous section prove also the necessity of testing and modelling the ordered parameters. If the underlying distributions have monotone likelihood ratio in those examples then the one- and the two-sided alternatives $H_1 : \mu_1 < \mu_2$ and $H_2 : \mu_1 \neq \mu_2$ correspond to the ordered alternatives (9.1) and (9.2), respectively, where the p_{ij} denote the occurrence probability of the ith treatment in the jth column.

$$K_1 : \quad \frac{p_{11}}{p_{21}} \geq \frac{p_{12}}{p_{22}} \geq \cdots \geq \frac{p_{1n}}{p_{2n}}, \tag{9.1}$$

$$K_2 : \quad \frac{p_{11}}{p_{21}} \geq \frac{p_{12}}{p_{22}} \geq \cdots \geq \frac{p_{1n}}{p_{2n}} \quad \text{or} \quad \frac{p_{11}}{p_{21}} \leq \frac{p_{12}}{p_{22}} \leq \cdots \leq \frac{p_{1n}}{p_{2n}} \tag{9.2}$$

The data in Table 4 were taken for comparing the efficacy of two sleeping drugs. After the dosage the brain wave of each subject was observed every second for eight hours and the total hours spent in each of the four levels of the depth of sleep were recorded. Then the efficacy of a drug was evaluated by the relative length of hours spent in the deeper level against the lighter level. So the superiority of drug A_2 over A_1 is suggested by the decreasing trend of the mean differences along with the levels of B. The main effects have no information on the efficacy of the drug and this again demonstrates the necessity of testing ordered alternative for interaction like

$$K_2: \quad \mu_{2j} - \mu_{1j} - (\mu_{2j+1} - \mu_{1j+1}) \geq 0 \quad (j = 1,2,3), \quad \text{or}$$
$$\mu_{2j} - \mu_{1j} - (\mu_{2j+1} - \mu_{1j+1}) \leq 0 \quad (j = 1,2,3). \tag{9.3}$$

TABLE 4 Total hours spent in stage B_j of depth of sleep.

	Drug A_1						Drug A_2				
Subject	B_1	B_2	B_3	B_4	$\bar{y}_{1\cdot k}$	Subject	B_1	B_2	B_3	B_4	$\bar{y}_{2\cdot k}$
C_1	3.2	1.6	0.8	2.4	2.0	C_1	2.8	4.4	0.4	0.4	2.0
C_2	2.0	1.6	3.2	1.2	2.0	C_2	3.2	3.2	0.8	0.8	2.0
C_3	2.4	3.2	1.2	1.2	2.0	C_3	1.6	6.0	0.4	0.0	2.0
C_4	1.6	2.0	2.8	1.6	2.0	C_4	2.8	1.2	3.6	0.4	2.0
C_5	1.2	2.4	2.4	2.0	2.0	C_5	2.4	2.8	2.4	0.4	2.0
C_6	0.8	2.8	1.6	2.8	2.0	C_6	2.8	2.4	1.2	1.6	2.0
$\bar{y}_{1j\cdot}$	1.9	2.3	2.0	1.9		$\bar{y}_{2j\cdot}$	2.6	3.3	1.5	0.6	

Degrees of depth of sleep : B_1, B_2, B_3, B_4
Mean differences $\bar{y}_{1j\cdot} - \bar{y}_{2j\cdot}$: −0.7, −1.0, 0.5, 1.3.

The detailed analysis of Table 4 is given in Hirotsu (1978).

10. CUMULATIVE CHI-SQUARED STATISTIC

Two major approaches for testing the equality of the ordered parameters are the likelihood ratio test represented by Bartholomew (1959) and Kudo (1963) and the score test represented by Abelson & Tukey (1963) and shaafsma (1966). The former is, however, sometimes too complicated to apply to such a two-sided alternative like (9.2) or (9.3) for two-way data. Although the latter is easily applicable to many situations, it does not necessarily keep high powers against the wide range of the ordered alternatives. In those circumstances the cumulative chi-squared statistic (CCS) defined below will give a good compromise.

First consider the one-way analysis of variance model

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \in \text{NID}(0, \sigma^2) \quad (i = 1, \cdots, k;\ j = 1, \cdots, r),$$

Then the essentially complete class for testing $H_0: \mu_1 = \cdots = \mu_k$ against the ordered alternative $K_1: \mu_1 \geq \mu_2 \geq \cdots \geq \mu_k$, with at least one inequality strict, is given by all the tests that are increasing in every element of $(D_k' D_k)^{-1} D_k' \bar{y}$ (Takeuchi

1979, Hirotsu 1982), where $\bar{\boldsymbol{y}}$ is the vector of averages $\bar{y}_{i\cdot}$ arranged in dictionary order and

$$D_k' = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -1 \end{bmatrix}_{k-1\times k}.$$

Then the CCS defined by

$$\chi^{*2} = r\|P_k^{*\prime} y\|^2, \tag{10.1}$$

$$P_k^{*\prime} = \mathrm{diag}(\rho_i^{-\frac{1}{2}})(D_k' D_k)^{-1} D_k' = \mathrm{diag}(\rho_i^{-\frac{1}{2}}/k) \begin{bmatrix} k-1 & -1 & \cdots & -1 \\ k-2 & k-2 & \cdots & -2 \\ & \cdots & & \\ 1 & 1 & \cdots & -(k-1) \end{bmatrix}$$

$$\rho_i = i(k-i)/k \quad \text{(normalizing constant)}$$

is proved to be useful for the two-sided version of the ordered alternative $K_2 : \mu_1 \geq \mu_2 \geq \cdots \geq \mu_k$ or $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_k$ (Hirotsu 1979b). Note that the two sided version is useful for two-way data with natural ordering only in columns (say), where the problem is essentially two-sided since then the rows are permutable.

The CCS of (10.1) is well characterized by the expansion

$$\chi^{*2}/\sigma^2 = \sum_{i=1}^{k-1} \frac{k}{i(i+1)} \chi^2_{(i)},$$

where the $\chi^2_{(i)}$ denote the chi-squared components with 1 df for the Tshebycheff's ith order orthogonal polynomials. This suggests that the CCS is useful not only for testing ordered alternatives but also for testing goodness of fit of a model against some systematic departure, mainly but not exclusively linear. The two-step procedure, first detecting some systematic departure without being affected by short term deviations and then detecting the short term deviations by the follow-up analysis of residuals will give a good strategy for statistical modelling (Hirotsu 1986, 1990).

The CCS is generalized to testing the homogeneity of the parameters $H_0 : \beta_1 = \cdots = \beta_k \quad (= \beta_0)$ against $K_2 : \beta_1 \geq \cdots \geq \beta_k$ or $\beta_1 \leq \cdots \leq \beta_k$ in a general model with the likelihood $L(\boldsymbol{\beta}, \boldsymbol{\tau})$, where $\boldsymbol{\tau}$ is the vector of nuisance parameters. Define the efficient score vector evaluated at H_0 as

$$\boldsymbol{v}(\hat{\beta}_0, \hat{\boldsymbol{\tau}}) = \partial \log L(\boldsymbol{\beta}, \boldsymbol{\tau})/\partial(\boldsymbol{\beta}, \boldsymbol{\tau})|_{\boldsymbol{\beta}=\hat{\beta}_0 \boldsymbol{j}, \boldsymbol{\tau}=\hat{\boldsymbol{\tau}}},$$

where $\hat{\beta}_0$ and $\hat{\boldsymbol{\tau}}$ denote the maximum likelihood estimators. Then the CCS is defined by

$$\chi^{*2} = \|\mathrm{diag}(\rho_i^{*-1})(D_k' D_k)^{-1} D_k' \boldsymbol{v}(\hat{\beta}_0, \hat{\boldsymbol{\tau}})\|^2, \tag{10.2}$$

where the ρ_i^* are the normalizing constants (Hirotsu 1982).

Applying the general formula (10.2) to testing K_2 (9.3) for the two-way $(a \times b)$ analysis of variance model we obtain

$$\chi^{*2} = r\|(P_a' \otimes P_b^{*\prime})\bar{\boldsymbol{y}}\|^2.$$

Similarly for testing the two-sided alternative like K_2 (9.2) for two-way contingency table we obtain

$$\chi^{*2} = \|(R' \otimes C^{*\prime})\boldsymbol{y}\|^2,$$

where $\boldsymbol{y}$ is the vector of the observed cell frequencies and R' and $C^{*\prime}$ are defined analogously to P_a' and $P_b^{*\prime}$ each row of which are orthogonal to $\boldsymbol{r} = (\sqrt{R_1}, \cdots, \sqrt{R_a})'$ and $\boldsymbol{c} = (\sqrt{C_1}, \cdots \sqrt{C_b})'$, respectively, where the R_i and C_j are row and column totals (refer to Hirotsu 1982, for details).

The mull distribution of the χ^{*2} is well approximated by the distribution of the constant times the chi-squared variable $d\chi_\nu^2$, adjusted for the first two moments (refer to Hirotsu 1979a, for details).

11. ROW-WISE AND/OR COLUMN-WISE MULTIPLE COMPARISONS FOR TWO-WAY DATA WITH ORDERED COLUMN CATEGORIES

The method of §6 is extended to modelling the two-way data with natural ordering only in columns. It should be noted that in this case the procedures for rows and columns cannot be symmetrical.

For the analysis of variance model the squared distance between two rows is defined by

$$S^* = r\|\{(0, \ldots, 0, 1/\sqrt{2}, 0, \ldots, 0, -1/\sqrt{2}, 0, \ldots, 0) \otimes P_b^{*\prime}\}\bar{\boldsymbol{y}}\|^2$$

and is naturally extended to the squared distance $S^*(G_1; G_2)$ between two subgroups of rows. Similarly for the contingency table we define

$$S^*(i; i') = \|(1/R_i + 1/R_{i'})^{-1/2}\{0, \ldots, 0, R_i^{-1/2}, 0, \ldots, 0, -R_{i'}^{-1/2}, 0, \ldots, 0) \otimes C^{*\prime}\}\boldsymbol{y}\|^2$$

and also $S^*(G_1; G_2)$ as given in Hirotsu (1983b). Then for every choice of subgroups G_1 and G_2 the maximums are bounded above by

$$\max_{\|\boldsymbol{a}\|=1, \boldsymbol{a}'\boldsymbol{j}=0} r\|(\boldsymbol{a}' \otimes P_b^{*\prime})\bar{\boldsymbol{y}}\|^2 \quad \text{for the ANOVA model,} \quad \text{and}$$

$$\max_{\|\boldsymbol{a}\|=1, \boldsymbol{a}'\boldsymbol{r}=0} \|(\boldsymbol{a}' \otimes C^{*\prime})\boldsymbol{y}\|^2 \quad \text{for the contingency table,}$$

respectively. It is proved that when $a \geq b$ and under the null hypothesis of interaction the maximums are distributed as the maximum root of $W(P_b^{*\prime}P_b^*, a-1)$ and $W(C^{*\prime}C^*, a-1)$ (asymptotically), respectively (see Hirotsu 1983b).

Taking the natural ordering into the consideration it should be reasonable to restrict the statistics for comparing colmuns to

$$\chi_j^{*2} = r\|(P_a' \otimes \boldsymbol{p}_j^{*\prime})\bar{\boldsymbol{y}}\|^2 \quad \text{for the ANOVA model,} \quad \text{and}$$
$$\chi_j^{*2} = \|(R' \otimes \boldsymbol{c}_j^{*\prime})\boldsymbol{y}\|^2 \quad \text{for the contingency table,}$$

where $\boldsymbol{p}_j^{*\prime}$ and $\boldsymbol{c}_j^{*\prime}$ are the jth row of $P_b^{*\prime}$ and $C^{*\prime}$, $j = 1, \ldots, b-1$, respectively. The joint null distribution of χ_j^{*2} and $\chi_{j'}^{*2}$ is proved to be the bivariate chi-squared distribution with the correlation $\boldsymbol{p}_j^{*\prime}\boldsymbol{p}_j^*$ or $\boldsymbol{c}_j^{*\prime}\boldsymbol{c}_j^*$ (Hirotsu 1983b). It has been exploited to evaluate the significance level of the maximum of χ_j^{*2} by the Bonferroni inequality, which gives the exact result for $b = 3$ in the ANOVA model. Very recently we obtain an exact formula for a general case (paper under preparation).

12. TWO-STEP PROCEDURE FOR MODELLING THE ORDINAL DATA

The multiple comparisons procedure of the previous section is applied for modelling the data of Table 3. The data have been analyzed by several authors. Snell (1964) among others, fitted logistic distributions with a common scale parameter to get the goodness of fit chi-squared 50.3 with the df 12. McCullagh (1980) allowed the logistic distributions to have different scale parameters and reduced the chi-squared value to 21.3 with the df 8. Although his estimates of the location and scale parameters seem to well explain the data, the chi-squared value is still relatively large for its degrees of freedom.

Now the between rows sums of squares are obtained as in Table 5, where the rows are rearranged so that the larger the elements according as the more they are apart from the diagonal.

TABLE 5 Square distances between rows.

Foods:	3	4	1	2	5
3	0	12.27	18.61	36.62**	78.17**
4		0	9.74	23.07*	60.47**
1			0	3.18	23.59**
2				0	10.17
5					0

The critical values from the maximum root of the Wishart matrix are approximately 22.01 ($\alpha = 0.05$) and 30.81 ($\alpha = 0.01$). They suggest the homogeneous subgroups

$G_1 = (3,4)$, $G_2 = (1,2)$ and $G_3 = (5)$. The between groups sums of squares are $S^*(G_1;G_2) = 60.67$, $S^*(G_1;G_3) = 87.40$, $S^*(G_2;G_3) = 87.40$, and

$$S^*(G_1;G_2,G_3) + S^*(G_2;G_3) = S^*(G_1,G_2;G_3) + S^*(G_1;G_2) = 95.53$$

amounts to approximately 86 % of the total cumulative chi-squared statistic 110.78 obtained by (10.2).

As for columns we get the maximum

$$\chi_2^{*2} = \|(R' \otimes c_2^{*\prime})\boldsymbol{y}\|^2 = 50.56$$

by the partition $J_1 = (1,2)$ and $J_2 = (3,4,5)$, at the significance level 0.00015. Thus we obtain the block interaction model

$$p_{ij} = p_{i\cdot}p_{\cdot j}\lambda_{\mu\nu}, \quad (i \in G_u, u = 1,2,3, i = 1,\ldots,5; j \in J_v, v = 1,2, j = 1,\ldots,5). \quad (12.1)$$

The standardized block interaction effects are given in Table 6, from which we conclude that Food 5 is rated high, 3 and 4 are low, and 1 and 2 are intermediate.

TABLE 6 Estimating block interaction pattern.

	Subgroups of rating	
Subgroupes of foods	(1,2)	(3,4,5)
(1,2)	-2.21	2.21
(3,4)	6.47	-6.47
(5)	-5.09	5.09

The fitted value by the model (12.1) are given in Table 7.

TABLE 7 Fitted value to the data of Table 3.

	Rating				
Foods	1	2	3	4	5
1	5.931	5.497	8.288	16.358	3.926
2	6.524	6.047	9.117	17.994	4.318
3	13.418	12.436	4.104	8.099	1.944
4	14.089	13.058	4.309	8.504	2.041
5	1.038	0.962	12.183	24.046	5.771

The goodness of fit chi-squared statistic is, however, 24.9 and is still somewhat large for its df 14, suggesting the need to analyze the residuals. The standardized residuals from the fitted model (12.1) are given in Table 8. There are three eminent values, 4.64

from cell (4,5) and 2.25 and –2.05 from cells (5,4) and (5,5). The observation 8 from cell (4,5) seems too large since Food 4 is rated low by the global analysis. On the other hand the observation 2 from cell (5,5) seems too small since Food 5 is rated high by the global analysis. The residual analysis detects these phenomena very well.

TABLE 8 Standardized residuals from the fitted block interaction model.

	Rating				
Foods	1	2	3	4	5
1	1.62	–0.27	0.32	–1.28	0.04
2	0.24	–1.60	0.38	0.75	–0.19
3	0.25	0.24	1.10	–0.51	–1.54
4	–1.29	0.83	–0.74	–1.61	4.64
5	–1.49	1.49	–0.90	2.25	–2.05

13.CONCLUDING REMARKS

The BANOVA techniques discussed here are widely applicable to various kinds of statistical problems. In particular the two-step procedure, first analyzing the systematic effects by the cumulative chi-squared statistic and then analyzing the residuals to detect the short term deviations seems to give a good strategy for modelling ordered parameters.

REFERENCES

Abelson, P.R. and Tukey, J.W. (1963). Efficient utilization of nonnumerical information in quantitative analysis: general theory and the case of simple order. Ann. Math. Statist., 34, 1347-1369.

Bartholomew, D.J. (1959). A test of homogeneity for ordered alternatives. Biometrika, 46, 35-48.

Bradley, R.A., Katti, S.K. and Coons, I.J. (1962). Optimal scaling for ordered categories. Biometrics, 29, 205-220.

Davies, O.L. (1954). The design and analysis of industrial experiments. Olyver and Boyd, London.

Hirotsu, C. (1965). Research for a set of minimal sufficient statistics and Yate's combined estimator for BIBD and GDPBIBD. Reports of Statistical Application Research, JUSE, 12, 115-126.

Hirotsu, C. (1973). Multiple comparisons in a two-way layout. Reports of Statistical Application Research, JUSE, 20, 1-10, 1973.

Hirotsu, C. (1976). Analysis of variance (in Japanese). Kyoikushuppan, Tokyo.

Hirotsu, C. (1978). Ordered alternatives for interaction effects. Biometrika, 65, 561-570.

Hirotsu, C. (1979a). An F-approximation and its application. Biometrika, 66, 577-584.

Hirotsu, C. (1979b). The cumulative chi-squares method and a Studentized maximal contrast method for testing an ordered alternative in a one-way analysis of variance model. Reports of Statistical Application Research, JUSE, 26, 12-21.

Hirotsu, C. (1982). Use of cumulative efficient scores for testing ordered alternatives in discrete models. Biometrika, 69, 567-577.

Hirotsu, C. (1983a). An approach to defining the pattern of interaction effects in a two-way layout. Ann. Inst. Statist. Math., A 35, 77-90.

Hirotsu, C. (1983b). Defining the pattern of association in two-way contingency tables. Biometrika, 70, 579-89.

Hirotsu, C. (1986). Cumulative chi-squared statistic as a tool for testing goodness of fit. Biometrika, 73, 165-173.

Hirotsu, C. (1990). Discussion to "A critical look at accumulation analysis by Hamada & Wu". Technometrics, 32, 133-136.

Johnson, D.E. and Graybill, F.A. (1972). An analysis of a two-way model with interaction and no replication. J. Amer. Statist. Ass., 67, 388-394.

Kudo, A. (1963). A multivariate analogue of the one-sided test. Biometrika, 50, 403-418.

McCullagh, P. (1980). Regression models for ordinal data. J. R. Statist. Soc., B 42, 109-142.

McCullagh, P. and Nelder, J. A. (1989). Generalized linear model (2nd ed.). Chapman and Hall, London.

Mandel, J. (1969). The partitioning of interactions in analysis of variance. J. Res. Nat. Bur. Stand., B 73, 309-328.

Schaafsma, W. (1966). Hypothesis testing problem with the alternative restricted by a number of inequalities (Doctoral dissertation, Univ. Groningen). Noodhoff, Groningen.

Snell, E.J. (1964). Scaling procedure for ordered categorical data. Biometrics, 20, 592-607.

Taguchi, G.(1986). The way to quality engineering (in Japanese). Quality, J. Jap. Soc. Quality Control, 16, 127-136.

Takeuchi, K. (1979). Test and estimation problem under restricted null and alternative hypotheses (in Japanese). J. Economics, 45, 2-10.

MODEL BUILDING AND PARAMETER ESTIMATION OF PROCESSES WITH SIGNAL-DEPENDENT PARAMETERS

K.Velev, I. Vuchkov, V. Tsochev

Department of Automation
Higher Institute of Chemical Technology
1156 Sofia, Bulgaria

1. INTRODUCTION

A lot of dynamic processes work under significant changes in the operational conditions due to different causes - set-point changes, load changes, different raw materials, etc. In such cases the liearization conditions are violated and linear models with constant parameters commonly used in applications describe the process behaviour quite inaccurately.

Best results in terms of the accuracy of model building can be obtained by using analytical approach. Its application requires deep knowlege of the mechanism of the investigated processes. However, it is often difficult or even impossible to obtain the necessary phenomenological relations because of the considerable complexity of the process and lack of knowledge of its basic mechanism. Then the only possible approach is to use approximations.

When the variations of the proces variables are large, an appropriate description can be obtained using functional series representation of nonlinear systems. The most commonly used are the Volterra series (Hung and Stark, 1977). Despite their generality in describing smooth nonlinearities, they are connected with a large number of parameters to be estimated and they are not too expressive for the practice.

Block-oriented nonlinear dynamic models can bring about some simplification of the model presentation, the most popular being the Hammerstein and the Wiener ones. A good survey of different possibilities of these models is made by Haber and Keviczky (1976). The advantages of the block-oriented models are their simplicity (fewer parameters to be estimated and more obvious structure) and the possibility to obtain exact description of some special nonlinearities. Unlike the Volterra series models, however, they are not always applicable and require a suitable structure of the model and a specification of the order of the nonlinearities, for which preliminary information must be available.

Another possibility of modelling such processes is provided by the approximation of the nonlinear dependence by a linear model, the parameters of which vary according to the changes of the operational conditions. Diekmann and Unbehauen (1985) suggest the use of a discrete set of linear models with constant parameters corresponding to different operational conditions. A recursive procedure for the estimation of the set of parameter vectors is developped applying least-squares and instrumental variables methods. The approach is relatively simple, but can only be applied if the operational conditions are well defined and their number is not too large.

Haber and Keviczky (1985) propose the use of quasilinear difference models with constant parameters when the gain or the time-constant of the system depend lineary or hyperbolically upon some measurable variable. Further development of this approach is provided by Vuchkov et al. (1985, 1986). They propose the use of linear difference models with parameters depending on the variation of some measurable external signals which specify the working conditions. The parameter changes are approximated by a linear combination of functions of the measurable signals and a generalized quasilinear model with constant parameters follows. The parameter estimates are obtained by a nonlinear estimation procedure minimizing the output error.

The estimation of the parameters of the generalized difference model can be accomplished also by method minimizing the equation error, for example linear least-squares, instrumental variables and correlation analysis as proposed by Velev (1986) and Velev and Vuchkov (1986).

Another approach to the modelling of the above mentioned class of processes consists in the use of continuous models represented by convolution integrals with weighting function (kernel) depending on the operational conditions. Parametrization of the kernel is obtained using expansion in orthogonal functions series (Velev, 1988).

The present paper is an overview of the main results of the authors concerning model building and parameter estimation of processes with operational conditions dependent dynamics.

2. PROBLEM FORMULATION AND MAIN MODELS

Consider a process with one input $u(t)$ and one output $\eta(t)$, the dynamic properties of which depend on the vector of external variables x specifying the operational conditions. In general the operator

$$\eta = A\ /u,x/$$

elucidating the relationship between $x(t)$, $u(t)$ and $\eta(t)$ is nonlinear. If we assume, however, that the changes of $x(t)$ are stepwise and seldom in comparison with the process dynamics and the input $u(t)$ varies in narrow limits around some working point, the output $\eta(t)$ can be described by a linear model with parameters depending on vector x.

Two main classes of models are proposed. The first one is the class of linear difference models with signal-dependent parameters:

$$A_x(q).\ \eta(x,t) = B_x(q).\ u(t), \qquad (1)$$

where

$$A_x(q) = 1 - a_1(x)q - \ldots - a_{na}(x)q^{na},$$

$$B_x(q) = b_1(x)q + \ldots + b_{nb}(x)q^{nb}$$

are polymomials the coefficients of which depend on the vector x value, q is the backward shift operator: $qy(t) = y(t-1)$ and t is time variable which takes integer values. For simplicity we shall assume further on $na = nb = n$.

The output of the process in disturbed by a stationary noise $\varepsilon(t)$ with zero mean and uncorrelated with the input $u(t)$, so that the available output data are:

$$y(x,t) = \eta(x,t) + \varepsilon(t)$$

From (1) and (2) we obtain the following two type of models:

$$y(x,t) = \frac{B_x(q)}{A_x(q)}\, u(t) + \varepsilon(t), \tag{3}$$

where $\varepsilon(t)$ is the output error, and

$$A_x(q)\, y(x,t) = B_x(q)\, u(t) + e(t), \tag{4}$$

where $e(t)$ is the equation error, or residual.

Assume that the dynamic properties of the process depend continuously on the external variables $x_1, x_2, \ldots, x_p$. Then the parameters $a_i(x)$ and $b_i(x)$ in (1) can be approximated by a polynomial:

$$a_i(x) = \sum_{j=1}^{m} c_{ij}\, f_j(x), \quad i = 1,2,\ldots,n, \tag{5}$$

$$b_i(x) = \sum_{j=1}^{m} d_{ij} f_j(x), \quad i = 1,2,\ldots,n, \tag{6}$$

where $f_j(x)$ are product of the degrees of $x_1, x_2, \ldots, x_p$.

Equations (3), (5) and (6) form the generalized output error difference model and (4), (5) and (6) - the generalized equation error difference model.

The second class of models can be expressed by the convolution integral:

$$\eta(x,t) = \int_0^{\infty} g(x,\tau)\, u(t-\tau)\, d\tau, \tag{7}$$

where $g(x,\tau)$ is the weighting function of the process which depends on the vector x value. If the process is stable, its weighting function is absolutely, hence square integrable in the interval (o,∞):

$$\int_0^{\infty} g^2(x,t)dt < \infty \quad \forall x.$$

Consequently the weighting function can be expanded into Lagguerre series of orthonormal functions:

$$g(x,t) = \sum_{i=1}^{\infty} a_i(x) L_i(t), \tag{8}$$

where

$$L_i(t) = e^{-\alpha t/2} \sum_{j=o}^{i} \frac{i!(-\alpha t)^j}{(i-j)!(j!)^2} \tag{9}$$

The coefficient α in (9) is a scale factor and in terms of mean squares its appropriate choice will provide for the best approximation of $g(x,t)$ by means of finite number of terms n of the series (8). Our investigations shows that the accuracy of approximation is not too sensitive to the choice of α and

$$\alpha = (0{,}1\ T_s)^{-1},$$

where T_s is the setteling time of the process, can be a good choice. Usually not more than 4-6 terms in (8) are needed.

Taking also into consideration (7), (2) and (8), the process model can be written in the form:

$$y(x,t) = \int_o^{\infty} \sum_{i=o}^{n} a_i(x)\, L_i(\tau)\, u(t-\tau)d\tau + e(t) =$$

$$= \sum_{i=o}^{n} a_i(x)\, z_i(t) + e(t), \tag{10}$$

where by

$$z_i(t) = \int_0^\infty L_i(\tau)\, u(t-\tau)d\tau \qquad (11)$$

the output of linear filters are denoted and the weighting function $L_i(\tau)$ are the orthonormal Laguerre functions. In (10) e(t) represents the noise and the approximation error.

The polynomial expansion

$$a_i(x) = \sum_{j=1}^{m} b_{ij}\, f_j(x) \qquad (12)$$

can be used again, so that substituting (12) in (10) the following generalized integral model is obtained:

$$y(x,t) = \sum_{i=1}^{n}\sum_{j=1}^{m} b_{ij}\, f_j(x)\, z_i(t) + e(t) \qquad (13)$$

3. PARAMETER ESTIMATION OF THE GENERALIZED OUTPUT ERROR DIFFERENCE MODEL

Let us consider the output error model (3). Given the estimates $B_x(q)$ and $A_x(q)$ the predicted output can be presented as

$$y(x,t) = \frac{B_x(q)}{A_x(q)}\, u(t) \qquad (14)$$

or in more detailed form:

$$y(x,t) = \sum_{i=1}^{n} a_i(x)\, y(x,t-i) + \sum_{i=1}^{n} b_i(x)\, u(t-i) \qquad (15)$$

Replacing (5) and (6) in (15) we obtain the following generalized output error difference model:

$$y(x,t) = \sum_{i=1}^{n}\sum_{j=1}^{m} c_{ij} f_j(x)\, y(x,t-i) + \sum_{i=1}^{n}\sum_{j=1}^{m} d_{ij} f_j(x) u(t-i) \qquad (16)$$

that can be used to predict the output behaviour of the process for some initial conditions and given input u(t) and vector x. The total number of unknown parameters in (16) is 2 nm. They can be estimated by minimizing the following functional:

$$J(c,d) = \sum_{k=1}^{M}\sum_{t=1}^{N_k} e^2(x^{(k)},t), \qquad (17)$$

where

$$\begin{aligned} e(x^{(k)},t) &= y(x^{(k)},t) - y(x^{(k)},t) = \\ &= y(x^{(k)},t) - \sum_{i=1}^{n}\sum_{j=1}^{m} c_{ij} f_j(x^{(k)})\, y(x^{(k)},t-i) - \\ &- \sum_{i=1}^{n}\sum_{j=1}^{m} d_{ij} f_j(x^{(k)})\, u(t-i) \end{aligned} \qquad (18)$$

is the output error. In (11) M denotes the number of different operational conditions while N_k denotes the number of samples for each realization.

A numerial procedure has to be used for minimization of (17) because the output error (18) is nonlinear in parameters

(via model (16)). This is a difficult computional problem due to the large number of parameters L = 2.nm and the complexity of the surface (17).

It is much easier to solve the estimation problem in two stages. In the first stage an appropriate procedure for the estimation of the parameters $a_i(x^{(k)})$ and $b_i(x^{(k)})$ in 15 is applied. For example, Gauss-Newton or Marquardt's iterative procedures (see Himmelblau (1970)) can be used. In the second stage the parameters c_{ij} and d_{ij} in (5) and (6) are estimated. As a result M nonlinear estimation problems of 2n parameters and a linear estimation problem of 2 nm parameters are solved. A considerable reduction of computational efforts can be obtained due to the fact that n is usually small ($n \leq 3$), while m is large (for some problems $M \geq 10$).

The algorithm of the parameter estimation procedure can be summarised as follows:

i) Take the data $u^{(k)}(t)$ and $y(x^{(k)},t)$, k = 1,2, ..., M; t = 1,2, ..., N_k and form the corresponding data matrices.

ii) Choose the order n of model (15) by using some test for order determination (see, for example, the matrix rank determination test in Golub et al. (1976)).

iii) Estimate the parameters $a_i^{(k)}$ and $b_i^{(k)}$ in (15) for $x = x^{(k)}$, k = 1,2, ..., M, using Marquardt's method. Estimate also the covariance matrices $V^{(k)}$ of the estimates which are obtained at the last iteration of the Marquardt's procedure.

iv) Plot the predicted by model (15) curves $y(x^{(k)},t)$ together with the experimental ones $y(x^{(k)},t)$ and decide if the order of model (15) is properly chosen. If not, go back to ii).

v) Choose the kind and number m of functions $f_j(x)$ in the relationships (5) and (6).

vi) Estimate the parameters c_{ij} and d_{ij}, i = 1,2, ..., n; j = 1,2, ..., m, using muluiple linear regession procedure with covariance matrix formed by the matrices $V^{(k)}$ obtained in iii).

vii) Verify the accuracy of the generalized model (16) plotting the predicted $y(x^{(k)},t)$ and the experimental $y(x^{(k)},t)$ curves and decide if the model approximates the process behaviour under different operational conditions in a satisfactory way. If not, go back to v).

4. PARAMETER ESTIMATION OF THE GENERALIZED EQUATION ERROR DIFFERENCE MODEL

A very essential computational improvement can be obtained if the estimation of the parameters c_{ij} and d_{ij} in (5) and (6) is fulfilled on the basis of the equation error model (4). The generalized model can be written in the form:

$$y(x,t) = \sum_{i=1}^{n}\sum_{j=1}^{m} c_{ij} f_j(x) y(x,t-i) + \sum_{i=1}^{n}\sum_{j=1}^{m} d_{ij} f_j(x) u(t-i) + e(t), \qquad (19)$$

where e(t) is the equation error due to the noise and to modelling errors. The unknown parameters c_{ij} and d_{ij} enter lineary in (19). To estimate them ordinary least-squares can be applied given the experimental data x(t), u(t) and y(x,t).

For this purpose the following overdetermined system of linear equation is formed:

$$y = \Phi\theta + e, \tag{20}$$

where

$$\Phi = [\varphi(n+1),\ \varphi(n+2),\ \ldots\ \varphi(N)]^T,$$

$$\varphi^T(t) = [f_{1t}y(t-1)\ldots\ f_{mt}y(t-1)\ \ldots\ f_{1t}y(t-n)\ldots f_{mt}y(t-n)\ f_{1t}u(t-1)\ldots\ f_{mt}u(t-1)\ \ldots\ f_{1t}u(t-n)\ldots f_{mt}u(t-n)]$$

$$f_{it} = f_i(x(t)),$$

$$\theta^T = [c_{11}\ldots c_{1m}\ \ldots\ c_{n1}\ldots c_{nm}\ \ d_{11}\ldots d_{1m}\ \ldots\ d_{n1}\ldots d_{nm}].$$

$$y^T = [y(n+1),\ y(n+2),\ \ldots,\ y(N)].$$

The least-squares estimate, minimizing the equation error, is

$$\theta_{LS} = \operatorname{argmin} e^Te = (\Phi^T\Phi)^{-1}\ \Phi^Ty \tag{21}$$

Unfortunately the equation error e(t) are correlated with the regressors y(x,t-i) so we obtain biased estimates of the parameters of model (19).

This drawback can be avoided if some modifications of the method are used. One of them is the instrumental variable method. An instrumental vector

$$\psi^T(t) = [f_{1t}v(t-1)\ldots\ f_{mt}v(t-1)\ \ldots\ f_{1t}v(t-n)\ldots f_{mt}v(t-n)\ f_{1t}u(t-1)\ldots\ f_{mt}u(t-1)\ \ldots\ f_{1t}u(t-n)\ldots f_{mt}u(t-n)]$$

is formed with the same structure as vector $\varphi(t)$ and the only difference is in the substitution of the output y(t) by the output of a linear stable filter:

$$v(t) = \frac{R(q)}{P(q)}\ u(t) = \frac{r_1q + \ldots + r_lq^l}{1-p_1q- \ldots -p_lq^l}\ u(t) \tag{22}$$

One very simle way to form the instrumental variables is to take delayed values of the input:

$$v(t) = q^lu(t), \tag{23}$$

where $l > n$.

The following expression can be used as an estimate of vector θ:

$$\theta_{IV} = (\Psi^T\Phi)^{-1}\ \Psi^Ty, \tag{24}$$

where

$$\Psi^T = [\psi(n+1),\ \psi(n+2),\ldots,\ \psi(N)]$$

Consistency conditions for the estimate (24) are given in Velev (1986).

If the input u(t) is stationary and the process is stable, i.e. the zeroes of A(q) are outside the unity circle, the least-squares can be combined with correlation analysis. As the output of the process is nonstationary because of the changes in process dynamics due to the external variables variation, some constraints on the experimental conditions have to be imposed. We shall consider further the case when vector x does not vary in a random manner but according to some experimental design. Then the estimation of the unknown parameters in model (19) can

be fulfilled according to the following algorithm:

i) Design an experiment with M m different values of vector x : $x^{(1)}, x^{(2)}, \ldots, x^{(M)}$.

ii) Measure the time series $u^{(k)}(t)$ and $y^{(k)}(t)$, $t=1,2,\ldots,N$ for each vector $x^{(k)}$, $k = 1,2, \ldots, M$.

iii) Calculate the correlation function estimates $R_u^{(k)}(\tau)$ and $R_{uy}^{(k)}(\tau)$, $\tau = l+1, \ldots, L$; $l \leq 0$, $L-l > 3.n$.

iv) Form the matrix

$$R = \begin{bmatrix} f_1^{(1)}R_{uy}^{(1)}(l+n)\ldots f_m^{(1)}R_{uy}^{(1)}(l+n) & \ldots & f_1^{(1)}R_{uy}^{(1)}(l+1)\ldots f_m^{(1)}R_{uy}^{(1)}(l+1) \\ \ldots\ldots & & \ldots\ldots \\ f_m^{(1)}R_{uy}^{(1)}(L-1) \ldots f_m^{(1)}R_{uy}^{(1)}(L-1) & \ldots & f_1^{(1)}R_{uy}^{(1)}(L-n)\ldots f_m^{(1)}R_{uy}^{(1)}(L-n) \\ \ldots\ldots & & \ldots\ldots \\ f_1^{(M)}R_{uy}^{(M)}(l+n) \ldots f_m^{(M)}R_{uy}^{(M)}(l+n) & \ldots & f_1^{(M)}R_{uy}^{(M)}(l+1)\ldots f_m^{(M)}R_{uy}^{(M)}(l+1) \\ \ldots\ldots & & \ldots\ldots \\ f_1^{(M)}R_{uy}^{(M)}(L-1) \ldots f_m^{(M)}R_{uy}^{(M)}(L-1) & \ldots & f_1^{(M)}R_{uy}^{(M)}(L-n)\ldots f_m^{(M)}R_{uy}^{(M)}(L-n) \end{bmatrix}$$

$$\begin{bmatrix} f_1^{(1)}R_u^{(1)}(l+n) \ldots f_m^{(1)}R_u(l+n) & \ldots & f_1^{(1)}R_u^{(1)}(l+1)\ldots f_m^{(1)}R_u^{(1)}(l+1) \\ \ldots\ldots & & \ldots\ldots \\ f_1^{(1)}R_u^{(1)}(L-1) \ldots f_m^{(1)}R_u^{(1)}(L-1) & \ldots & f_1^{(1)}R_u^{(1)}(L-n)\ldots f_m^{(1)}R_u^{(1)}(L-n) \\ \ldots\ldots & & \ldots\ldots \\ f_1^{(M)}R_u^{(M)}(l+n)\ldots f_m^{(M)}R_u^{(M)}(l+1) & \ldots & f_1^{(M)}R_u^{(M)}(l+1)\ldots f_m^{(M)}R_u^{(M)}(l+1) \\ \ldots\ldots & & \ldots\ldots \\ f_1^{(M)}R_u^{(M)}(L-1)\ldots f_m^{(M)}R_u^{(M)}(L-1) & \ldots & f_1^{(M)}R_u^{(M)}(L-n)\ldots f_m^{(M)}R_u^{(M)}(L-n) \end{bmatrix},$$

where $f_j^{(i)} = f_j(x^{(i)})$ and

$$r^T = \left[R_{uy}^{(1)}(l+n+1)\ldots R_{uy}^{(1)}(L) \ \ldots \ R_{uy}^{(M)}(l+n+1)\ldots R_{uy}^{(M)}(L)\right].$$

v) The estimate of the unknown parameters vector is obtained by the well known formula

$$\theta_{cls} = (R^TR)^{-1}R^Tr. \qquad (25)$$

The assymptotic properties of the estimate (25) are shown in Velev and Vuchkov (1986).

A very short comparison between the output and equation error methods of parameter estimation shows that the equation error method is superior for its computational simplicity and the lack of convergence problems (as a batch procedure).

However, the use of least-squares is constrained to the noise free case. The correlation analysis with least-squares gives better results in the noisy case but can be applied only for stable processes with stationary random input. The instrumental variable method is the less restricted equation error one but its efficiency is very low especially when the number of data sets is not much higher than the number of parameters.

5. PARAMETER ESTIMATION OF THE GENERALIZED CONVOLUTION INTEGRAL MODEL

The parameter estimation of model (13) is similar to the previous cases. The two-stage estimation procedure is used again.

In the first stage the parameters in (8) are estimated, i.e. the parameters.

$$a^{(k)} = \arg\min I_1^{(k)}, \quad k = 1,2, \ldots, M, \tag{26}$$

are determined, where

$$I_1^{(k)} = \sum_{l=1}^{N_k} \left[y^{(k)}(t_l) - \sum_{i=0}^{n} a_i^{(k)} z_i(t_l) \right]^2 . \tag{27}$$

In the second stage the parameters b_{ij}, forming a matrix B, of the generalized model (13) are estimated:

$$B = \arg\min I_2,$$

where

$$I_2 = \sum_{k=1}^{M} \left[a^{(k)} - Bf(x^{(k)}) \right]^T H^{(k)} \left[a^{(k)} - Bf(x^{(k)}) \right] . \tag{28}$$

The structure of $H^{(k)}$ depends on the noise characteristics and the shape of the input signal.

The algorithm of the parameter estimation procedure is given below:

i) For M different operational conditions take the data $u^{(k)}(t_l)$ and $y(x^{(k)}, t_l)$, $k = 1,2,\ldots,M$; $l=1,2,\ldots,N_k$.

ii) Form the matrices

$$Z^{(k)} = \begin{bmatrix} z_o^{(k)}(t_1) & z_1^{(k)}(t_1) & \ldots & z_n^{(k)}(t_1) \\ z_o^{(k)}(t_2) & z_1^{(k)}(t_2) & \ldots & z_n^{(k)}(t_2) \\ \ldots & \ldots & \ldots & \ldots \\ z_o^{(k)}(t_{N_k}) & z_1^{(k)}(t_{N_k}) & \ldots & z_n^{(k)}(t_{N_k}) \end{bmatrix} ,$$

where $z_i^{(k)}(t)$ are computed according (11), and the vectors

$$y^{(k)} = \left[y^{(k)}(t_1) \quad y^{(k)}(t_2) \ \ldots \ y^{(k)}(t_{N_k}) \right]^T$$

iii) By minimization of criterion (26) obtain the following least-squares estimate of the parameters of model (10):

$$a^{(k)} = \left[(Z^{(k)})^T Z^{(k)} \right]^{-1} (Z^{(k)})^T y^{(k)} . \tag{29}$$

iv) Form the matrices

$$H^{(k)} = (Z^{(k)})^T Z^{(k)}$$

v) Obtain the estimates of the parameters b_{ij} in the generalized model (13) using the generalized least-squares method:

$$b = (F^T H F)^{-1} F^T H a, \tag{30}$$

where

$$b = \left[b_o^T \quad b_1^T \ \dots \ b_n^T \right]^T , \quad b_i = \left[b_{io} \quad b_{i1} \ \dots \ b_{im} \right]^T ,$$

$$a = \left[(a^{(1)})^T \ (a^{(2)})^T \ \dots \ (a^{(M)})^T \right]^T ,$$

$$F = \left[(F^{(1)})^T \ (F^{(2)})^T \ \dots \ (F^{(M)})^T \right]^T ,$$

$$F^{(k)} = \begin{bmatrix} (f^{(k)}) & 0 & \dots & 0 \\ 0 & (f^{(k)}) & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & (f^{(k)})^T \end{bmatrix}$$

$$H = \begin{bmatrix} H^{(1)} & 0 & \dots & 0 \\ 0 & H^{(2)} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & H^{(M)} \end{bmatrix}$$

vi) Check up the adequacy of the model

$$a = Bf(x) + e$$

by using the X^2-test, proposed by Vuchkov et al.(1985)

$$X^2 = (a - Fb)^T H (a - Fb)$$

with degrees of freedom $v = (n+1)(M-m-1)$.

6. CONCLUSIONS

An approach for model bulding and parameter estimation of a class of nonlinear processes with signal-dependent dynamics was described in this paper. Two main types of models were proposed: parametric models in the form of difference equations and nonparametric models in the form of convolution integral. The changes in process dynamics due to variations in the operational conditions were described by the dependency of the parameters of the difference equation (the weighting function of the convolution integral) on the operational conditions determined by the values of several external signals. In order to parametrize the second type of models, the weighting function was expanded in Laguerre orthonormal functional series with parameters depending on theexternal signals. In both cases generalized models with constant parameters follow. A two-stage estimation procedure was proposed. In the first stage the parameters of a linear-in-variables models corresponding to different operational conditions were estimated and then they were approximated by polynomials of the external signals.

Comparing the two types of models and their estimation procedures the following conclusions can be made. Difference equation type of models is usually more parsimonial in the number of parameters to be estimated. It is also more convenient for both optimization and control applications. The drawbacks of

these models consist in the necessity of model order determination which is not a trivial task, the nonlinear estimation procedure when using the most general output error method and the possibility to obtain unstable generalized models due to subsequent approximations in the cases when for some operational conditions the roots of the characteristics equation a close to the unity circle.

The convolution integral type of models with expansion of the weighting function in Laguerre functional series gives always stable models. In both stages the estimation procedure is linear which is a very essential computational advantage. The number of estimated parameters, however, is usualy larger because of the use of relatively high number of terms in the functional series expansion in order to get a satisfactory approximation for different operational conditions.

REFERENCES

Diekmann, K. and Unbehauen, H. (1985). On-line parameter estimation in a class of nonlinear system via modified least-squares and instrumental variable algorithm. Proc. 7 th IFAC/IFORS Symp.Ident. and System Param. Estimation, York, UK.

Golub, G., Klema, V. and Stewart, G., (1976). Rank degeneracy and least-squares problems. Rep.Stan-CS-76-559, Stanford University, USA.

Haber, R. and Keviczky, L. (1976). Identification of nonlinear dynamic systems - a survey. Proc. 4 th IFAC Symp. Ident. and System Param.Estimation, Tbilissi, USSR.

Haber, R. and Keviczky, L. (1985). Identification of 'linear' systems having signal-dependent parameters. Int.J.Systems Sci., v.16, 869-884.

Himmelblau, D. (1970). Process analysis by statistical methods. Wiley, New York.

Velev, K. (1986). Identification of nonlinear systems by quasi-linear difference models. Prep.IASTED/AFCET Symp.Ident.and Pat.Rec., Toulouse, France.

Velev, K. (1988). Identification of nonlinear systems by signal-dependent nonparametric linear models using orthogonal functions, Proc. 8th IFAC/IFORS Symp.Ident.and Syst.Param. Est., Beijing, China.

Velev K. and Vuchkov, I.(1986). Identification and control of parametrically dependent stochastic processes. Prep.Second IFAC Symp.Stoch.Control, Vilinius, USSR.

Vuchkov I., Velev, K. and Tsochev, V. (1985). Identification of paramet. dependent processes with applications to chemical technology. Proc.7th IFAC/IFORS Symp.Ident. and Syst. Param. Est., York, UK.

Vuchkov, I., Velev K. and Tsochev, V.(1986). Parameter estimation and design of experimental for parametrically dependent processes, Prep. IMACS/IFAC Symp.Modelling and Simul.for Control of Lumped and Distributed Parameter Systems, Villeneuve, France.

ASYMPTOTIC CHARACTERISTICS OF THE LIKELIHOOD RATIO TEST FOR DETECTING RECTANGULAR CHANGE IN MEAN OF GAUSSIAN RANDOM VARIABLES

Anatoly A. Zhigljavsky
Mathematical Department, Leningrad University,
Bibliotechnaya sq., 2, Leningrad 198904, USSR

The nonsequential detection problem of a rectangular change in mean of independent Gaussian random variables is considered for the case when values of all parameters are known. An invariance theorem is proved which states that asymptotically the power function of the likelihood ratio test may be approximated by a family of boundary crossing probabilities for the Gaussian random process with triangular covariance function. Explicit formulae for these probabilities are presented. The Bahadur efficiency of the likelihood ratio test is also established.

Let $x_1,\dots,x_N$ be Gaussian independent random variables, $Ex_i=\mu_i$, and $\mathrm{var}(x_i)=\sigma^2$. The detection problem is to test the hypothesis

$$H_0:\ \mu_i=0 \text{ for all } i=1,\dots,N \tag{1}$$

versus the alternative

$$H_1:\ \text{there exists } \tau,\ 0<\tau<N-T \text{ such that}$$

$$\mu_i=\begin{cases} 0 & \text{for } i=1,\dots,\tau \text{ and } i=\tau+T+1,\dots,N \\ A>0 & \text{for } i=\tau+1,\dots,\tau+T \end{cases} \tag{2}$$

The problem of testing the hypothesis (1) versus (2) has been considered in a number of works, see in particular Bhattacharya and Brockwell (1976), Hogan and Siegmund (1986), Siegmund (1986,1988). This is a classical problem in the stochastic radiotechnics as a problem of signal detection occuring at an unknown moment in time. It also occurs in medicine, quality control, and some other engineering problems.

Unlike the above mentioned works we consider the case when the values of parameters T,A,σ^2 are known but may depent on N. We also suppose that $T=T_N$, $T_N/N \longrightarrow r$ where r is some known positive number. This particular problem has some specific properties which do not hold for more general setups. It was thourougly studied in Zhigljavsky and Kraskovsky (1988). Below we mention some results from this work but the main subject matter of the present work is to establish the Bahadur efficiency of the likelihood ratio test. In doing this we shall follow the approach which was developed in Haccou, Meelis, and van de Geer (1988).

The loglikelihood ratio for testing H_0 versus H_1 under the supposition $\tau=k$ can be written in the form

$$\log \Lambda_{H_1/H_0}(k) = \log(L(X|H_1,\tau=k)/L(X|H_0)) = A\sigma^{-2}\sum_{i=k+1}^{k+T} x_i - A^2T\sigma^{-2}$$

where $X=(x_1,\ldots,x_N)$ is the sample. Thus, the likelihood ratio test can be written in the form: reject H_0 if $U_N>H$ and accept H_0 otherwise where H is some threshold and

$$U_N = \max_{0<k<N-T} \sum_{i=k+1}^{k+T} x_i \qquad (3)$$

is the test statistics.

Let

$$\alpha_N(H)=\Pr\{U_N>H|H_0\}$$

be the first kind error probability of the likelihood ratio test and

$$\beta_N(H,k)=\Pr\{U_N\le H|H_1,\tau=k\}$$

be the second kind error probability of the test under the condition that the first change of the level occurs at time k. We approximate these probabilities by the corresponding passage probabilities of the continuous time stationary Gaussian process with triangular covariance function, namely, of the process s(t) given on [0,1] for which

$$Es(t)=0, \quad Es(t)s(v)=\max\{0,1-|t-v|\} \qquad (4)$$

Theorem 1. If $N\longrightarrow\infty$, $T=T_N\longrightarrow\infty$, $T/N\longrightarrow r>0$, $H=H_N\longrightarrow\infty$, $H\sigma^{-1}T^{-1/2}\longrightarrow h>0$ then

$$\alpha_N(H) \longrightarrow \alpha(h,1/r-1) \qquad (5)$$

where

$$\alpha(h,a) = \Pr\{ s(t) > h \text{ for some } t,\ 0\le t\le a \}$$

Proof. Introduce the statistics

$$U(N,k)=\sigma^{-1}N^{-1/2}\sum_{i=k+1}^{k+T_N} x_i$$

and note that

$$\alpha_N(H\sigma^{-1}N^{-1/2}) \longrightarrow \Pr\{\max_{0\le k\le 1-T/N} U(N,k)>h\} \quad \text{as } N\longrightarrow\infty$$

and that

$$U(N,k)= S(N,k+T_N) - S(N,k), \qquad k=1,\ldots,N-T_N$$

where

$$S(N,k)=\sigma^{-1}N^{-1/2}\sum_{i=1}^{k} x_i$$

Consider the random process

$$\xi_N(t)=S(N,k) \quad \text{for } (k-1)/N<t\le k/N, \quad k=1,\ldots,N$$

According to Billingsley (1986) there exist a sequence of random processes $\nu_N(t)$ on [0,1] that have the same finite-dimensional distributions as ξ_N and weakly converge to the standard Brownian motion process W(t), i.e.

$$\Pr\{\sup_{0\le t\le 1}|\nu_N(t)-W(t)|\ge\varepsilon\} \longrightarrow 0 \quad \text{as} \quad N\longrightarrow\infty \qquad (6)$$

for any $\varepsilon>0$.

We shall now prove that the process

$$W(t+r) - W(t), \quad 0\le t\le 1-r,$$

is the limit process for the sequence of processes

$$\{\nu_N(t+T_N/N) - \nu_N(t)\}.$$

Estimate the probability analogous to the left-hand side of (6):

$$\Pr\{\sup_{0\le t\le 1-T_N/N}|(\nu_N(t+T_N/N) - \nu_N(t))-(W(t+r) - W(t))|\ge\varepsilon\}\le$$

$$\Pr\{\sup_{0\le t\le 1-T_N/N}|(\nu_N(t+T_N/N) - W(t+T_N/N)|\ge\varepsilon/3\}+$$

$$+\Pr\{\sup_{0\le t\le 1-T_N/N}|\nu_N(t) - W(t)|\ge\varepsilon/3\}+$$

$$+\Pr\{\sup_{0\le t\le 1-T_N/N}|W(t+T_N/N) - W(t+r)|\ge\varepsilon/3\}$$

The first and second terms tend to zero due to (6), and the third is asymptotically negligible since W(t) has continuous trajectories a.s. Thus, we obtain

$$=\Pr\{\max_{0\le k\le 1-T/N} U(N,k)>h\} \longrightarrow \Pr\{\sup_{0\le t\le 1-r}|W(t+r) - W(t)|>h\}$$

as $N\longrightarrow\infty$. Changing the time of the limit process by u=t/r we obtain $s(t)=W(u+1)-W(u)$, $0\le u\le 1/r-1$. This implies the aseertion of the theorem.

Explicit formulas for the passage probabilities $\alpha(h,a)$ for the process $s(t)$, $0\le t\le a=1/r-1\le 1$, in the case of constant

boundary h were firstly obtained by Slepian (1961). In particular, for the case a=1 this passage probability is equal to

$$\alpha(h,1)=1-\Phi^2(h)+(2\pi)^{-1/2}h\Phi(h)\exp\{-h^2/2\}+(2\pi)^{-1}\exp\{-h^2\}$$

where

$$\Phi(h) = (2\pi)^{-1/2}\int_{-\infty}^{h} \exp\{-t^2/2\}dt.$$

The case a>1 is more complicated. Explicit formulas for passage probabilities in this case were derived by Shepp (1971). They are very complicated and instead of them we shall use the asymptotic equality

$$\alpha(h,a)=(1+o(1))ah(2\pi)^{-1/2}\exp\{-h^2/2\}, \qquad h\longrightarrow\infty \qquad (7)$$

which was proved in Revesz (1980) and holds for every a>0.

Formulas for the second kind error probabilities of the likelihood ratio test are not needed for investigating efficiency of the test and so we only mention the way of their derivation. (A thorough their investigation was done by Zhigljavsky and Kraskovsky (1988).)

Set

$$\beta(h,v,a,\gamma) = \Pr\{ s(t) < h-\gamma\max\{0,1-|t-v|\} \text{ for all } t,\ 0\le t\le a\}$$

$$\beta(h,a,\gamma) = \sup_{0\le v\le a} \beta(h,v,a,\gamma)$$

Analogously to Theorem 1 we can prove that if $N\longrightarrow\infty$, $T\longrightarrow\infty$, $T/N\longrightarrow r$, $k\longrightarrow\infty$, $k/N\longrightarrow v$, $H\sigma^{-1}T^{-1/2}\longrightarrow h$, $AT^{-1/2}/\sigma\longrightarrow\gamma$ then

$$\beta_N(H,k) \longrightarrow \beta(h,v,a,\gamma).$$

In these formulas γ is the signal/noise ratio and v is the first change-point moment for the limit model.

Thus, the problem of computation of the second kind error probability for the likelihood ratio test is also approximated by a boundary crossing probability computation problem for the stationary process s(t). Unlike the preceding case we have broken line boundary here which makes our problem more difficult. Explicit formulas for $\beta(h,v,a,\gamma)$ in the case $a\le 1$ were obtained in Zhigljavsky and Kraskovsky (1988). They are too complicated and we present only one of them, namely

$$\beta(h,1,\gamma)=\beta(h,0,1,\gamma)=\beta(h,1,1,\gamma)=$$

$$=\Phi(h)\Phi(h-\gamma)-(2\pi)^{-1/2}\gamma^{-1}[\Phi(h)\exp\{-(h-\gamma)^2/2\}-\Phi(h-\gamma)\exp\{-h^2/2\}]$$

Consider now the problem of Bahadur efficiency of the likelihood ratio test for testing (1) versus (2). Let us derive first the weak slopes c(r) determined from the asymptotic relation

$$P_{H_1} - \lim_{N->\infty} N^{-1}L_N = - \frac{1}{2} c(r) \qquad (8)$$

where the limit is considered under the supposition that H_1 is true and $L_N=\alpha_N(U_N)$ is the random value known as the level attained by the test statistic.

Theorem 2. The weak Bahadur slope of the likelihood ratio test statistic for testing (1) versus (2) equals

$$c(r)=rA^2/\sigma^2 \qquad (9)$$

Proof. Divide the problem of evaluating c(r) into two more simple problems and compute the limits

$$P_{H_1} - \lim_{N->\infty} N^{-1}U_N = b(r) \qquad (10)$$

and

$$\lim_{N->\infty} N^{-1}\log \alpha_N(Nt) = g(t) \qquad (11)$$

According to Bahadur (1967), if the limits (10) and (11) exist and g(t) is continuous at points t=b(r) then

$$c(r)=2g(b(r)) \qquad (12)$$

First prove that the limit (10) exists and equals

$$b(r)=rA \qquad (13)$$

Let $\varepsilon>0$ be arbitrary. It is easy to see that the inequality

$$P_{H_1}\{N^{-1}\max_{0\le k\le 1-T/N}\sum_{i=k+1}^{k+T_N} x_i < rA - \varepsilon\} \le$$
$$\le P_{H_1}\{N^{-1}\sum_{i=\tau+1}^{\tau+T_N} x_i < rA - \varepsilon\} \qquad (14)$$

where $\tau=\tau_N$ is the true first change-point.

By the strong law of large numbers

$$N^{-1}\sum_{i=\tau+1}^{\tau+T_N} x_i \longrightarrow rA \quad \text{a.s.}$$

as N—>∞. Thus, the right-hand side of (14) converges to zero as N—>∞.The same is true for the left-hand side of (14).

Next, using the formula of complete probability, we have

$$P_{H_1}\{N^{-1}U_N > rA + \varepsilon\} =$$

$$P_{H_1}\{N^{-1}\max_{0\le k\le 1-T/N}\sum_{i=k+1}^{k+T_N} x_i > rA + \varepsilon\} =$$

$$=\sum_{k=0}^{N-T_N} q_k\, P_{H_1}\{N^{-1}\sum_{i=k+1}^{k+T_N} x_i > rA + \varepsilon\} \qquad (15)$$

where

$$q_k = P_{H_1}\{\max_{0\le l\le 1-T/N}\sum_{i=l+1}^{l+T_N} x_i = \sum_{i=k+1}^{k+T_N} x_i\} \ge 0, \quad \sum_{k=0}^{N-T_N} q_k = 1.$$

The maximal probability in the right-hand side of (15) is

$$P_{H_1}\{N^{-1}\sum_{i=\tau+1}^{\tau+T_N} x_i < rA + \varepsilon\}$$

which tends to zero as $N \longrightarrow \infty$ due to the Chebyshev inequality. Since the right-hand side of (14) is upper estimated by (15) it tends to zero as well. This completes the proof of (13) and existence of the limit in (10).

To compute the limit in (11) we use the asymptotic equalities (5) and (7) which give

$$g(t) = -\lim_{N\to\infty} N^{-1}\log\{(r^{-1}-1)(2\pi T_N\sigma^2)^{-1/2}N\exp\{-N^2t^2/(2\sigma^2T_N)\}\} =$$

$$= t^2/(2r\sigma^2)$$

This function is positive and continuous. Thus, we can apply (12) which gives (9). This completes the proof.

Consider the problem of the Bahadur efficiency of the likelihood ratio test statistic. It is well known in the case of independent identically distributed observations that the Bahadur slope of a statistic can not exceed the Kullback-Leibler information of observations multiplied by 2 and if the equality holds then the statistic is Bahadur efficient. In the present case observations are not identically distributed under the validity of H_1 and so we shall use some generalization of this technique.

Theorem 3. The likelihood ratio test for testing the hypothesis (1) versus (2) is Bahadur efficient in the class of test statistics for which either limits (10) and (11) exist and function (11) is continuous or Bahadur slope is infinite.

Proof. Let $\log \Lambda_{H_1/H_0}$ be the loglikelihood ratio,

$$c_N(t)=\{\omega:\ N^{-1}\log \Lambda_{H_1/H_0}\le t\},$$

and

$$K = \inf \{t:\ \lim_{N\to\infty} P_{H_1}(c_N(t)) = 1 \}. \qquad (16)$$

So defined value K is the generalization of the Kullback-Leibler information.

Theorem 2.1 of Bahadur, Zabell, and Gupta (1980) asserts that if $\{A_N\}$ is a sequence of events such that A_N depends only on $\{x_1,\dots,x_N\}$ and

$$\liminf_{N\to\infty} \Pr\{A_N|H_1\} > 0 \qquad (17)$$

then

$$\liminf_{N\to\infty} N^{-1} \Pr\{A_N|H_0\} \ge K. \qquad (18)$$

Analogously with the proof of Theorem 2 we obtain

$$K= rA^2/(2\sigma^2).$$

Now let V_N be an arbitrary test statistic which depends on $\{x_1,\dots,x_N\}$ and for which limits (10) and (11) exist and assume

$$A_N=\{\omega:\ V_N \ge N(q-\varepsilon)\}$$

where q is defined as the limit

$$P_{H_1} - \lim_{N\to\infty} N^{-1} V_N$$

The validity of (17) follows from the definition of A_N and so (18) holds with the limit $-g_V(q-\varepsilon)$ in the left-hand side of (18) where g_V is the limit (11) for the sequence of statistics $\{V_N\}$. Since (18) holds for any $\varepsilon>0$ and g_V is continuous we have

$$c_V\le 2K \qquad (19)$$

where c_V is the weak Bahadur slope of the sequence of the test statistics $\{V_N\}$. The assertion of the theorem follows from the fact that there is equality in (19) for the seguence of the likelihood ratio statistics.

The author is acknowledged to Dr. E.Razumovskaya for fruitful discussions and interest to this work. It is worthwile to mention also that recent work of Prof. David Siegmund in the field changed the author's view on the subject and had a stimulating effect.

REFERENCES

Bahadur, R.R. (1967) Rates of convergence of estimates and test statistics. Ann. Mathem. Statistics, 38, 303-325.

Bahadur, R.R., Zabell, S.L., and Gupta, J.C. (1980) Large deviations, tests, and estimates. In I.M. Chakravarti (Ed.) Asymptotic Theory of Statistical Tests and Estimation. Academic Press, N.Y.,33-64.

Bhattacharya, P.K., and Brockwell, P.J. (1976) The minimum of an additive process with applications to signal estimation and storage theory. Z. Wahrschein. verw. Geb., 37, 51-75.

Billingsley, P. (1986) Probability and Measure. Wiley, N.Y.

Haccou, P., Meelis, E., and van de Geer, S. (1988) The likelihood ratio test for the change point problem for exponentially distributed random variables. Stochastic Processes and their Applications, 27, 121-139.

Hogan, M.L., and Siegmund, D. (1986) Large deviations for the maxima of some random fields. Advances in Applied Mathematics, 7, 2-22.

Revesz, P. (1980) A note to the Chung-Erdös-Sirao theorem. In I.M.Chakravarti (Ed.) Asymptotioc Theory of Statistical Tests and Estimation. Academic Press, N.Y., 147-158.

Shepp, L.A. (1971) First passage time for a particular Gaussian process. Ann. Mathem. Statistics, 42, 946-952.

Siegmund, D. (1986) Boundary crossing probabilities and statistical applications. Ann. Statistics, 14, 361-404.

Siegmund, D. (1988) Approximate tail probabilities for the maxima of some random fields. Ann. Probability, 16, 487-501.

Slepian, D. (1961) First passage time for a particular Gaussian process. Ann. Mathem. Statistics, 32, 610-612.

Zhigljavsky, A.A., and Kraskovsky, A.E. (1988) Detection of Abrupt Changes of Random Processes in Radiotechnics Problems. Leningrad University Press.

LIST OF CONTRIBUTORS

- A.M. Alahmadi, Department of Statistics, University of Glasgow, Faculty of Science, Glasgow G12 8QW, United Kingdom
- A.C. Atkinson, Department of Statistical and Mathematical Sciences, London School of Economics, London WC2A 2AE, United Kingdom
- L.N. Boyadjieva, Laboratory of Organization and Automation of Experimental Research, Higher Institute of Chemical Technology, 1156 Sofia, Bulgaria
- A.N. Donev, Dept. of Automation, Higher Institute of Chemical Technology, 1156 Sofia, Bulgaria
- B. Droge, Department of Mathematics, Humboldt University, P.O. Box 1297, D-O-1086 Berlin, Germany
- V.V. Fedorov, CLSEM, Academy of Sciences of the USSR, Krasikova 32, 117 418 Moscow, USSR
- S. Hadžikvuković, Velika Vlahovica 2, University of Novi Sad, 21000 Novi Sad, Yugoslavia
- C. Hirotsu, Dept. of Mathematical Engineering and Instrumentation Physics, Faculty of Engineering, University of Tokyo, Bunkyo-ku, Tokyo, Japan
- B.P. Kovachev, Laboratory of Computational Stochastics, Institute of Mathematics, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria
- H. Läuter, Karl Weierstrass Institute for Mathematics, Academy of Sciences of the German Democratic Republic, Mohrenstrasse 39, D-O-1086 Berlin, Germany
- N.E. Manolov, Dept. of Automation, Higher Institute of Chemical Technology, 1156 Sofia, Bulgaria
- W.G. Müller, Department of Statistics, University of Economics Vienna, Augasse 2-6, A-1090 Vienna, Austria
- E. Nikolić-Djorić, Velika Vlahovica 2, University of Novi Sad, 21000 Novi Sad, Yugoslavia
- A. Pázman, Mathématical Institute of the Slovak Academy of Sciences, Štefánikova 49, CS-81473 Bratislava, Czechoslovakia
- B.M. Pötscher, Department of Statistics, University of Vienna, Universitätsstraße 5/9, A-1010 Vienna, Austria
- L. Pronzato, Laboratoire des Signaux et Systèmes, CNRS/ESE, Plateau du Moulon, F-91192 Gif sur Yvette cedex, France
- R. Schwabe, Freie Universität Berlin, Fachbereich Mathematik, 1. Mathematisches Institut, Arnimallee 2-6, D-W-1000 Berlin 33, Germany

- B. Torsney, Department of Statistics, University of Glasgow, Faculty of Science, Glasgow G12 8QW, United Kingdom
- V. Tsochev, Laboratory of Organization and Automation of Experimental Research, Higher Institute of Chemical Technology, 1156 Sofia, Bulgaria
- J.Á. Víšek, Institute of Information Theory and Automation, Czechoslovak Academy of Sciences, 182 08 Prague 8, Pod vodarenskou vezi 4, CSFR
- K. Velev, Laboratory of Organization and Automation of Experimental Research, Higher Institute of Chemical Technology, 1156 Sofia, Bulgaria
- I.N. Vuchkov, Laboratory of Organization and Automation of Experimental Research, Higher Institute of Chemical Technology, 1156 Sofia, Bulgaria
- E. Walter, Laboratoire des Signaux et Systèmes, CNRS/ESE, Plateau du Moulon, F-91192 Gif sur Yvette cedex, France
- H. Yonchev, Dept. of Automation, Higher Institute of Chemical Technology, 1156 Sofia, Bulgaria
- A.A. Zhigljavsky, Mathematical Deptartment of Leningrad State University, Bibliotechnaya Square 2, 198904 Leningrad, U.S.S.R.

Printing: Druckhaus Beltz, Hemsbach
Binding: Buchbinderei Schäffer, Grünstadt

Contributions to Statistics

The series "Contributions to Statistics" contains publications in statistics and related fields. These publications are primarily monographs and multiple author works containing new research results, but conference and congress reports are also considered.

Apart from the contribution to scientific progress presented, it is a notable characteristic of the series that actual publishing time is very short thus permitting authors and editors to present their results without delay.

Manuscripts could be sent directly to Physica-Verlag:

Physica-Verlag GmbH & Co.
Tiergartenstraße 17
6900 Heidelberg, FRG

ISBN 3-7908-0624-2
ISBN 0-387-91422-6