

WORKING PAPER

DESIGN OF AN AIR-POLLUTION MONITORING NETWORK

W.G. Mueller

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INTERNATIONAL INSTITUTE FOR APPLIED SYSTEMS ANALYSIS
A-2361 Laxenburg, Austria

Foreword

In this paper, Mr. Mueller presents some interesting results on the optimal design of monitoring networks, based on SO₂ data from 19 monitoring stations in Upper Austria for the year 1985.

Werner Mueller is a graduate student in the Department of Statistics at the University of Vienna. Since the winter of 1986-87, Mr. Mueller has been working with Prof. V. Fedorov, first as a guest scholar at IIASA, and in the summer of 1988 as a YSSP.

I welcome this collaboration between IIASA and the University of Vienna. It is the kind of activity that should be strongly encouraged.

R.E. Munn
Head, Environment Project

DESIGN OF AN AIR-POLLUTION MONITORING NETWORK

An application of experimental design theory

W.G. Mueller

(I) INTRODUCTION

The paper consists of two main parts. The first contains an application of the results developed by Fedorov & Mueller (1987) (hereafter *FM*), to a comparatively simple experimental situation. The second part gives a description of the software concerning the algorithms proposed in *FM*. All the examples are related to the air-pollution monitoring network but it is clear that many other scientific areas could be similarly supported.

It is assumed that the reader is familiar with *FM*'s results and notations. The method described in section II of *FM* will be referred to as the ODE (optimal design of experiments) approach, while the method in section III of *FM* will be called the MR (multiple regression) method.

Two FORTRAN computer programs (see Fedorov et al. (1987)) originally created for the standard regression case were adapted for the regression model of the second kind. The first program is called JDOPT and relies on the first order iterative algorithm as described in *FM* p.5; see also Fedorov et al. (1987). The second is called JDOPTX and performs a version of an exchange type algorithm, which is described in Appendix A. Appendix B contains a user's guide for these programs.

(II) DESCRIPTION OF THE DATA (UPPER AUSTRIA AS A TEST EXAMPLE)

The data for the study have been collected at 19 monitoring sites from the current Upper-Austrian network and consist of half-hourly SO₂ concentrations at the various sites during the whole year 1985. The data were used with the friendly permission of the Austrian Central Institute for Meteorology and Geodynamics. The results are based on a data set with 59 cases

(days) out of 365, containing at least one observation for each of 19 stations. For every day, the arithmetic average was used :

$$y_{ij} = n_{ij}^{-1} \sum_{l=1}^{n_{ij}} y_{ijl}$$

where i is the number of a station, j is the day, l is the number of the half-hours and n_{ij} is the number of non-missing data values y_{ijl} .

Figure 1 shows the region and the current network in the official presentation (with enlarged Linz-area) and in the form which was used in the analysis (grid-representation).

The network was probably designed following empirical and cost considerations and it appears that all but three stations (Perg, Wurzeralm and Schöneben) are located near industrial centers.

For the sake of simplicity the topography was not included in the analysis but it should be kept in mind that the southern quarter of Upper Austria is covered by the Alps.

(III) EMPIRICAL COMPARISON OF THE TWO APPROACHES

To illuminate the results from *FM* and the software facilities the network optimization approach initiated by Der Megreditchian (1985) (MR-procedure) will be applied first. This approach is based upon the heuristic idea that subsequent removal of less informative stations will lead to an effective network with a comparatively small number of observation stations.

A theoretical analysis of the kind of optimality criterion minimized can be made, if one makes some assumptions on the process that generates the data. In *FM* it has been assumed that the data-field was generated by a regression of second kind model (sometimes referred to as 'regression model with random parameters'):

$$y_j = F^T \vartheta_j + \varepsilon_j \quad , \quad \vartheta_j = \vartheta_0 + \Delta \quad (1)$$

where:

- $y_j^T = (y_{1j}, \dots, y_{n_j})$ are observed values (for instance pollution data in air monitoring networks; $i=1, \dots, n_j$ represents the number of an observational station and $j=1, \dots, k$ stands for the date of the measurement),

- ϑ_0 (dimension m) is the 'true' parameter vector of the average process (it is the mean value of the 'actual' vector $\vartheta_j = \vartheta_0 + \Delta_j$, where Δ_j is assumed to be a random vector distributed with $E[\Delta_{ij}] = 0$ and a priori known $E[\Delta_j \Delta_j'] = D_0$,

- $\varepsilon_j^T = (\varepsilon_{1j}, \dots, \varepsilon_{n_j})$ ε is a random noise component with: $E[\varepsilon_{ij}] = 0$, $E[\varepsilon_{ij}, \varepsilon_{i'j'}] = \delta_{ii'} \delta_{jj'}$. These random values usually consists of observational errors and local disturbances.

The main difference between model (1) and the standard regression case is the fact that in model (1) parameters of the distribution do not remain constant over time but have stochastic fluctuations (ϑ_0 is the "average" parameter, ϑ_j represents the current situation). In other words, the structure of the response function is constant over the considered time interval but its parameters fluctuate.

One can see that if all D_0 -elements equal 0, the model is reduced to the standard regression situation. The random vector Δ simulates the "intrinsic" fluctuation of the system under consideration.

Applying model (1) of the monitored process gives the following possibilities:

(a) to construct an observing network, which is optimal for estimate the average pollutant distribution (with parameters ϑ_0),
or

(b) to create a network for estimation of the current (say daily) situation (with ϑ_j).

It has already been shown in *FM* that the ODE-algorithm for case (b) and model (1) is theoretically equivalent to the MR-approach; therefore the MR-method can be used to construct optimal networks for the corresponding experimental situation.

In order to demonstrate this equivalence, *MR* was used to delete the 'worst' station subsequently which yielded the ranking related to the stations informativity; see figure 2. It is worthwhile to note that 5 of the 6 'best' stations are clustered in the area surrounding Linz (the capital and the main pollution source of Upper-Austria).

The ODE-approach was applied in a similar way. Because ODE is model oriented, some assumptions about the observed field had to be stated explicitly at the beginning. The second order polynomial response as a model for SO₂ distribution for the whole region has been chosen:

$$\eta(x, \vartheta) = \vartheta_1 + \vartheta_2 x_1 + \vartheta_3 x_1^2 + \vartheta_4 x_2 + \vartheta_5 x_2^2 + \vartheta_6 x_1 x_2. \quad (2)$$

Of course one has to be very cautious about this model, because it might not reflect the true situation, but due to its simplicity it will serve as a good reference for the compared approaches.

A regression analysis was performed for each date in order to estimate 59 $\hat{\vartheta}_j$'s, and subsequently the variance - covariance matrix \hat{D}_o , which characterizes the fluctuation of the response function (2) was obtained. In table 1 the simplest estimate :

$$\hat{D}_o = (k-1)^{-1} \sum_{j=1}^k (\hat{\vartheta}_j - \hat{\vartheta}_o) (\hat{\vartheta}_j - \hat{\vartheta}_o)^T$$

is presented.

<i>Table 1:</i>	3.82	0.83	-1.63	3.38	-5.66	-11.26
	0.83	1.33	-0.07	0.87	-1.41	-3.61
	-1.63	-0.07	5.57	-2.08	2.10	4.38
	3.38	0.87	-2.08	8.85	-8.76	-24.00
	-5.67	-1.42	2.10	-8.77	17.99	28.09
	-11.26	-3.61	4.38	-23.9	28.09	77.56

The use of the ODE-algorithm with \hat{D}_0 substituted for by D_0 yields figure 3, which to some extent shows the reverse image of figure 2. Here none of the 'best' stations appeared to be in the Linz-area. This result of course contradicts the theoretical conclusions from FM.

Table 2 shows means and the standard deviation for the original and the logarithmically transformed value (transformation before daily averaging). It can be seen that the 'best' points of MR-procedure appeared where the standard deviation was significantly high. More attentive consideration of MR reveals that this approach implicitly assumes that errors or noise are additive (i.e. $y_{ij} = y_{oj} + \varepsilon_{ij}$, where y_{oj} is the mean at point x_i and ε_{ij} is the noise). At the same time, it can be noted that the second column in table 2 is roughly proportional to the first one. This can mean that in the considered case, $y_i = \varepsilon_i \eta(x_i, \theta_0)$ (multiplicative error with $\varepsilon_i > 0$, $y_i > 0$). Taking the logarithm is a standard way to transform a multiplicative model to an additive one. The result of the transformation is presented in the last two columns of table 2.

Table 2: Means and Standard-deviations of SO₂ Measurements
(in E-3 mg/m³)

observation station	original		logarithmic	
	mean	std	mean	std
1 HAUSERHL	54.6	81.1	2.3	2.5
2 URFABHL	25.5	36.3	1.3	2.4
3 TRAUN	34.1	53.4	0.9	3.3
4 ASTEN	17.4	33.0	0.2	3.0
5 WELS	27.1	34.2	2.0	2.0
6 VOECKLAB	19.2	23.3	1.4	2.4
7 PERG	15.4	22.6	0.7	2.6
8 STEYR	26.2	33.5	1.8	2.3
9 BRAUNAU	12.8	20.2	0.4	2.7
10 ENNSCHEM	21.9	30.1	1.3	2.3
11 KLEINMUL	36.9	50.4	2.3	2.0

12	URSULINL	41.9	43.4	2.7	1.8
13	ORFZENTL	60.5	55.9	3.1	1.7
14	URFAH24L	23.5	19.9	2.6	1.2
15	BERUFSSL	49.0	61.8	2.7	2.1
16	STEYREGG	40.6	30.0	3.0	1.3
17	LENZING	47.6	51.3	2.7	1.6
18	WURZERA	14.0	18.9	1.3	2.1
19	SCHOENEB	5.9	9.6	-0.5	2.3

The stability of the standard deviation for the transformed data confirms the expediency of the chosen transformation from the statistical point of view.

Through this transformation, the model used in ODE-approach implicitly changed:

$$\eta(x, \vartheta) = \exp \{ \vartheta_1 + \vartheta_2 x_1 + \vartheta_3 x_1^2 + \vartheta_4 x_2 + \vartheta_5 x_2^2 + \vartheta_6 x_1 x_2 \} . \quad (3)$$

is now assumed to be the proper model for the SO₂ distribution.

The new matrix \hat{D}_0 for model (3) is presented in table 3.

Table 3:

1.000	-0.146	-1.485	0.511	-0.691	-1.369
-0.146	0.267	-0.141	0.260	-0.096	-0.874
-1.485	-0.141	3.916	-1.586	1.710	4.085
0.511	0.260	-1.586	1.353	-1.055	-3.150
-0.691	-0.096	1.710	-1.055	1.281	2.591
-1.369	-0.874	4.085	-3.150	2.591	9.556

Algorithms MR and ODE were both recalculated for transformed data and now the results are almost identical (Figures 4 and 5) in accordance with theory (FM) . This fact confirms that the new model is appropriate.

It is clear that none of the present designs presents the final or complete solution of a real world problem. Too many restrictions were introduced, and too many simplifications have been applied . But this was done to avoid technical details which could cloud the main ideas.

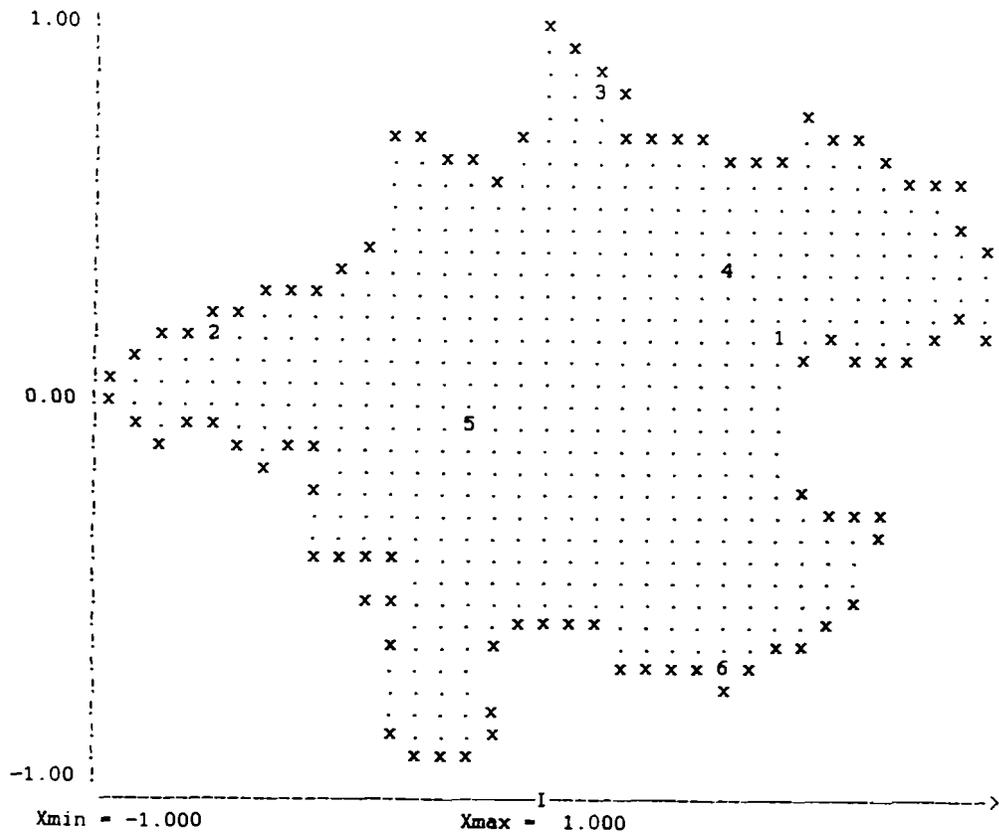


Figure 4: MR procedure results for logarithmic data

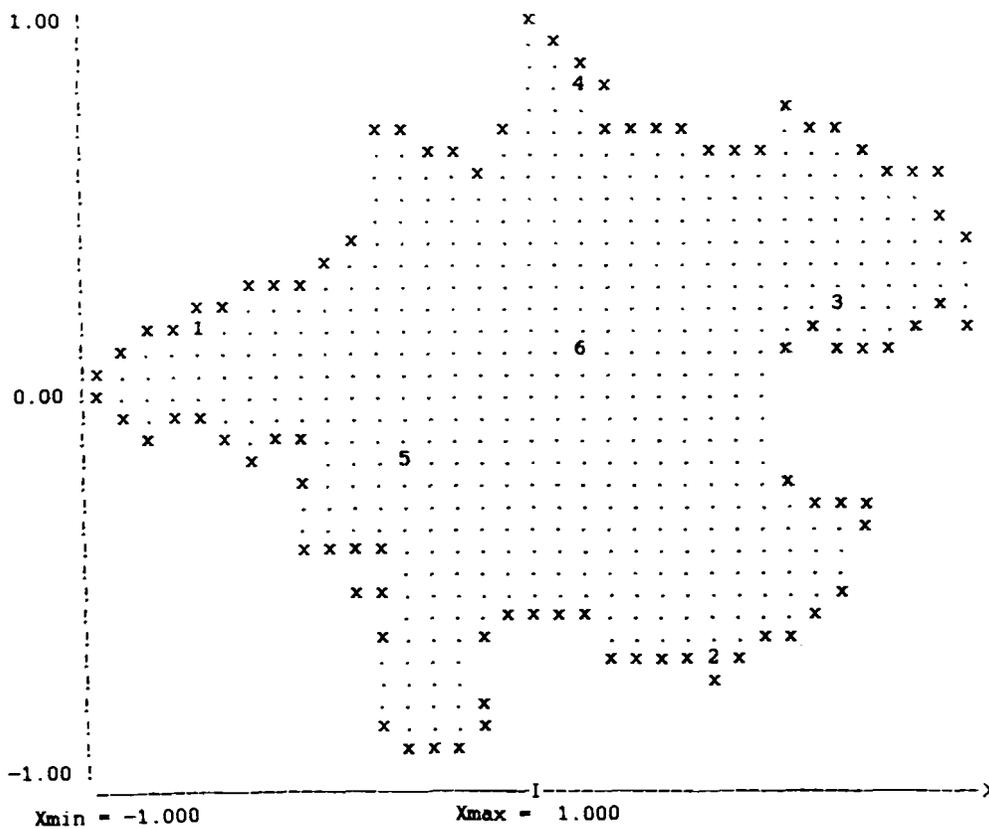


Figure 5: ODE procedure results for logarithmic data

(IV) COMMENTS

For practitioners the following questions are usually of interest:

- (1) How does the existing network perform against other possible ones in terms of optimality ?
- (2) How can the existing network be improved : via adding, removing or relocating stations ?
- (3) How are the existing stations ranked in terms of informativity ?
- (4) What is the optimal number of stations ?

At first glance the methods described above do not seem to be able to answer any of these practical questions. One could also claim that the simplicity of the methods would hide reality's complexity itself and therefore lead to inadequate solutions. This is partly true, but application of these methods in order to gain a rough view of the real world is in fact evident.

Considering practitioners needs, the detection of some 'hot' areas where observation stations should be located seems to be of most interest rather than exact locations of positions of observation stations: there are a lot of nonquantified factors that enter into station siting.

A possible objection to ODE-methods could also be, that if there exists no exact model of the observed process, the ODE-method will serve for none of the questions at all. But in fact this is not so. See figures 6-8.

Here it was assumed that a practitioner had no concrete idea about the process but only that it can be represented by polynomial of unknown order. Then ODE was performed three times, always assuming a different response function:

Figure 6 Linear response:

$$f(x_i) = \vartheta_1 + \vartheta_2 x_{i1} + \vartheta_3 x_{i2} + \varepsilon_i$$

Figure 7 Polynomial of second order:

$$f(x_i) = \vartheta_1 + \vartheta_2 x_{i1} + \vartheta_3 x_{i1}^2 + \vartheta_4 x_{i2} + \vartheta_5 x_{i2}^2 + \vartheta_6 x_{i1} x_{i2} + \varepsilon_i$$

Figure 8 Polynomial of third order:

$$f(x_i) = \vartheta_1 + \vartheta_2 x_{i1} + \vartheta_3 x_{i1}^2 + \vartheta_4 x_{i1}^3 + \vartheta_5 x_{i2} + \vartheta_6 x_{i2}^2 + \vartheta_7 x_{i2}^3 + \vartheta_8 x_{i1} x_{i2} + \vartheta_9 x_{i1}^2 x_{i2} + \vartheta_{10} x_{i1} x_{i2}^2 + \varepsilon_i$$

The results show a somehow stable pattern, in most of the observation points being at or near the boundary of the region.

It is clear that the number of stations has to be increased with increasing complexity of the response function.

Another approach to more general rules is to give a practitioner more freedom in choosing a location even when the monitored process is known.

As an example, the algorithm described in Appendix A of this paper was applied to optimize the Upper-Austrian network. With the help of this procedure, it is possible to identify 'hot areas' (not points as previously), where observing stations (Figure 9) should be located.

Finally it seems that the ODE-technique could help practitioners at different stages of the monitoring network design not least because of its relation to other so called model-free methods (which has been shown in *FM* and in the earlier sections of this paper). For instance it can provide:

- optimal design for comparison of different models
- optimal design for parameter estimation
- optimal design oriented for better prognoses
- optimal design for estimation of various average characteristics (in space and time)

In addition, the ODE technique permits explicit introduction of various optimality criteria (see for instance *FM*) and therefore could be used in a more efficient way than usual design-methods.

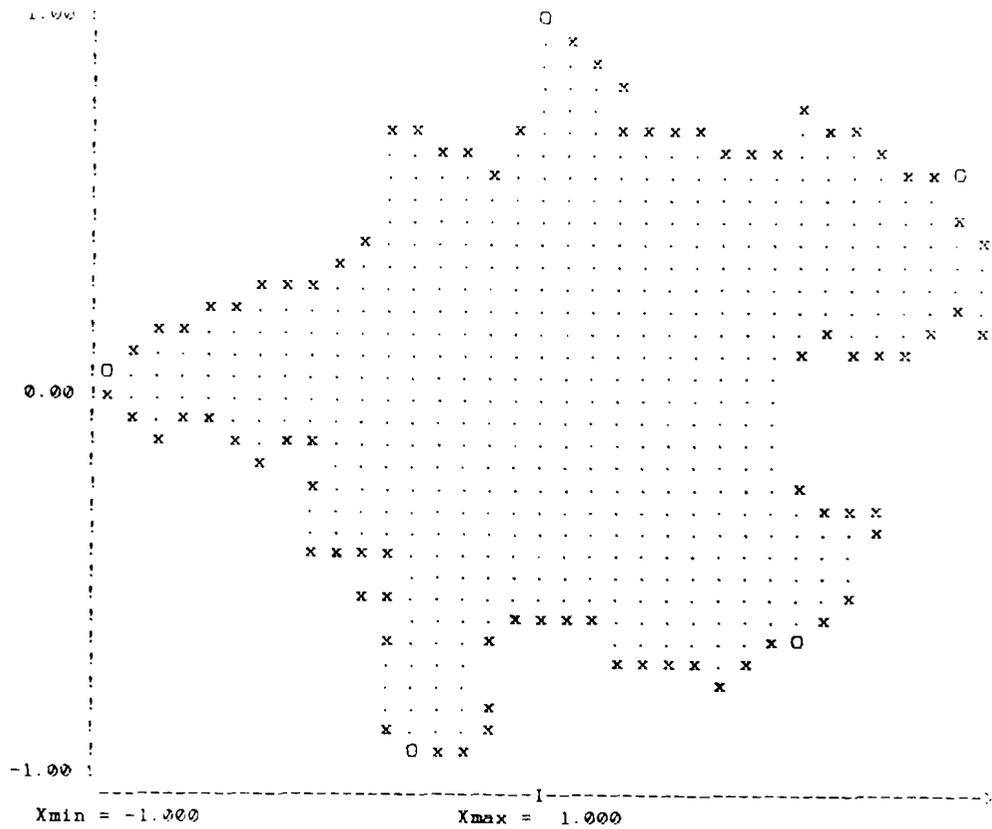


Figure 6: Optimal design for polynomial of first order (standard regression case)

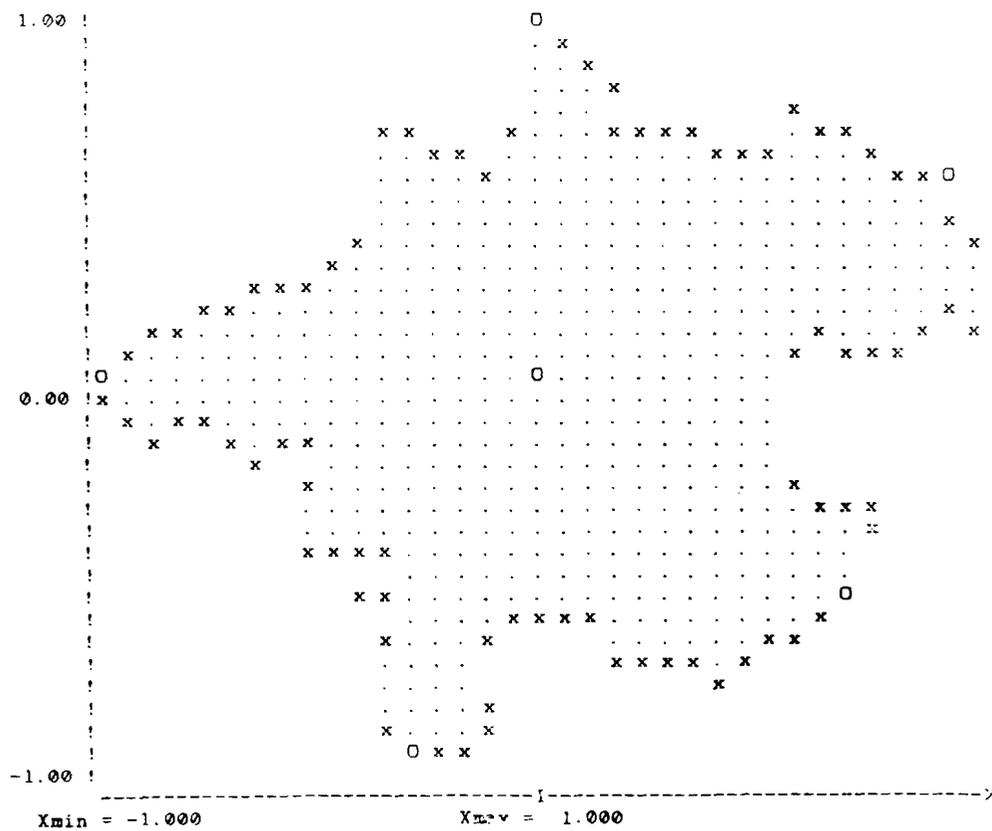


Figure 7: Optimal design for polynomial of second order (standard regression case)

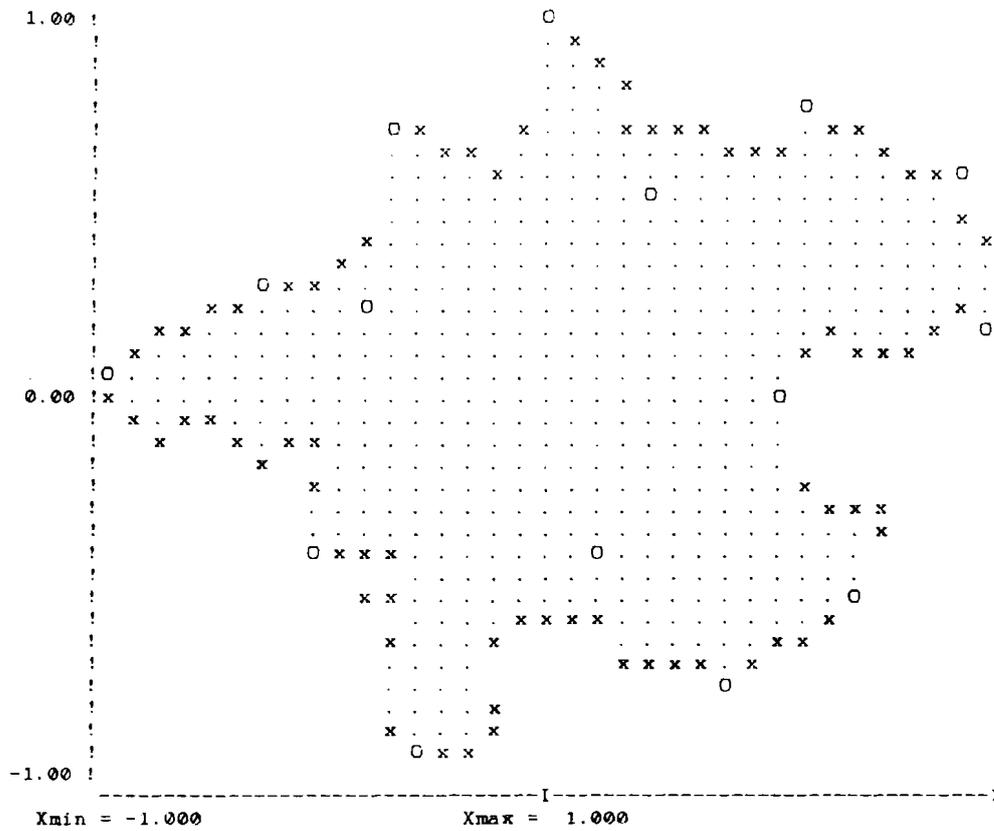


Figure 8: Optimal design for polynomial of third order (standard regression case)

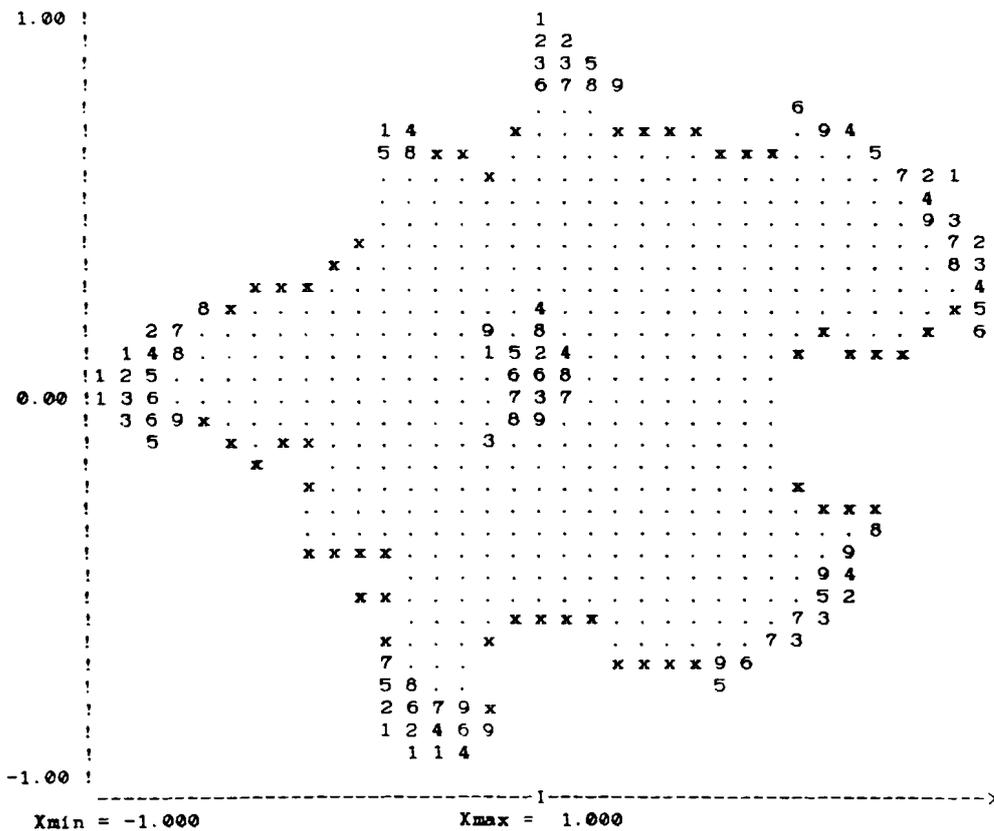


Figure 9: 'HOT' AREAS identified by EXCHANGE TYPE ALGORITHM

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(A) GRID ORIENTED EXCHANGE TYPE ALGORITHM

If the operability region X can be approximated by some grid with elements Δ_s at s -th step, then we can construct the following algorithm (compare with (19) and (20) from *FM*):

- [1] There is $\xi_{ns} = (x_{1s}, \dots, x_{ns})$, where the x_{is} are some points (say the vertices) of the grid elements Δ_s . Point

$$x_s^+ = \arg \max_{x \in X_{\Delta_s}} \varphi(x, \xi_{ns}), \quad X_{\Delta_s} = X_{\Delta_s} \setminus \text{supp } \xi_{ns}$$

has to be found and the new design

$$\xi_{(n+1)s} = (x_{1s}, \dots, x_{ns}, x_s^+)$$

has to be taken into consideration.

- [2] Point

$$x_s^- = \arg \min_{x \in \text{supp } \xi_{(n+1)s}} \varphi(x, \xi_{(n+1)s})$$

has to be deleted from design $\xi_{(n+1)s}$.

The procedure can be started with either forward [1] or backward [2] steps. In the second case, the length of excursion has to be smaller than $s-m$, where m is the number of parameters to be estimated.

It has to be mentioned that for convergence of this algorithm, it is of importance, that $\Delta_s \rightarrow 0$, but for practical needs it will be sufficient to use sufficiently small $\Delta_s = \Delta$ with a very small grid (this has been done in program WDOPTX).

For more detailed information about this procedure, see *Fedorov (1986)*.

(B) USER'S GUIDE

Both programs perform optimization over a region, which is described in the file 'reg.dat' (constructed by the special program MAP). Initial design ξ_1 and matrix \hat{D}_0 are stored in 'des.dat'.

Program MAP is intended for mapping a controllable region X. The current version of the program handles one- and two-dimensional regions but generalization to higher dimensions should not be difficult.

The region X is defined on a uniform grid with given densities for each variable. Such a presentation of X is explained by the fact that usually a user deals with irregular regions, which cannot be described analytically (non-convex, with subregions where the location of observing stations is impossible, for example lakes, densely populated areas, etc.). Two output files are created by the program:

'reg.dat' contains the data in its original scale
'scale.dat' contains the normalized data ($-1 \leq x_i^{(nor)} \leq +1$)

The main program utilizes three files:

'out.dat' is for output information (see example)
'reg.dat' contains the designs grid (see above)
'des.dat' contains the initial information

The last of the three is constructed as follows:

$$\begin{array}{ccc} n & & \\ x1_1 & (x2_1) & p_1 \\ . & (.) & . \\ x1_n & (x2_n) & p_n \\ \\ \hat{D}_{011} & \dots & \hat{D}_{01m} \\ \vdots & \dots & \vdots \\ \hat{D}_{0m1} & \dots & \hat{D}_{0mm} \end{array}$$

where n stands for the initial number of points, $x1_i$ and $x2_i$ for

the coordinates of points i , p_i for its initial weight and $\hat{D}_{oi,j}$ stands for the corresponding element to prior known matrix \hat{D}_o .

All auxiliary subroutines (matrix inversion, calculation of the initial determinant, minimization of a function $\varphi(x, \xi)$ etc.) for programs JDOPT and JDOPTX are saved in the files 'subd.for' and 'subdex.for' respectively.

INSTRUCTIONS FOR PROGRAM MAP - MAPPING OF A CONTROLLABLE REGION

----- ! SCREEN ! -----	----- ! COMMENTS ! -----
------------------------------	--------------------------------

- | | |
|---|---|
| 1. SPACE DIMENSION - ? (L) | L is a number of controllable variables |
| 2. X1<min>, X1<max> - ?
(X1min, X1max) | X1min, X1max are the minimal and maxima values of the first coordinate |
| 3. GRID FOR X1 ? (NX1) | Interval (X1<min>, X1<max>)
is divided into NX1 parts,
rx defines an initial grid for X1:
rx = (X1<max> - X1<min>)/NX1 |

Messages 4 - 7 appear if L = 2 .

- | | |
|---|--|
| 4. X2<min>, X2<max> - ?
(X2min, X2max) | X2min, X2max - minimal and maximal values of the second coordinate |
| 5. GRID FOR X2 ? (NX2) | Interval (X2<min>, X2<max>)
is divided into NX2 parts,
ry defines an initial grid for X2:
ry = (X2<max> - X2<min>)/NY |

3. NUMBER OF ESTIMATED PARAMETERS - ? (M) M - number of parameters (M must correspond to subroutine RESP , where a response function is calculated)

4. NUMBER OF POINTS IN INITIAL DESIGN - (NO) NO - number of supporting points in an initial design, input from file des.dat

Message 5 appears if L=2

5. GRAPHICAL PRESENTATION OF INITIAL DESIGN: yes - 1, no - 0 (IDO) IDO = 1 - subroutine GRAPH is executed for initial design

Message 6 appears if initial covariance matrix is singular.

6. SINGULAR COVARIANCE MATRIX

7. NUMBER OF FIXED POINTS IN INITIAL DESIGN (MFI) The first MFI points in initial design are fixed

8. CONSTANT FOR GAIN SEQUENCE (ALFA) - ALFA is evaluated by the program

9. NUMBER OF ITERATIONS - ? (MITER) MITER - maximal number of iterations

10. LENGTH OF EXCURSION - ? <forward and backward> (NFOR) NFOR - number of steps for forward and backward procedures (Attention : MITER = 2*NFOR*K, K - integer !!!

11. INITIAL PROCEDURE: forward - 1, backward - 2 (IPRO) The algorithm starts with: - forward procedure if IPRO = 1, - backward procedure if IPRO = 2.

12. STEPWISE INFORMATION : IINF = 1 - intermediate information
 yes - 1, no - 0 is saved in the file 'OUT.DAT'
 (IINF) and shown on the monitor (current
 design, value of the determinant
 etc)

Message 13 appears if L = 2 .

13. GRAPHICAL PRESENTATION OF DESIGN: IGR = 1 - subroutine GRAPH is
 yes - 1, no - 0 executed for final design
 (IGR)

14. SCALING OF DESIGN: yes - 1, ISC = 1 - scaling of final design
 no - 0 (ISC) is carried out

Messages 15 - 17 appear if ISC = 1.

15. X1<min>, X1<max> - ? X1min, X1max - minimal and maximal
 (X1min, X1max) values of the 1-st coordinate

Message 16 appears if L = 2 .

16. X2<min>, X2<max> - ? X2min, X2max - minimal and maximal
 (X2min, X2max) values of the 2-nd coordinate

17. GRAPH IN REAL SCALE: IGRS = 1 - subroutine GRAPH is
 yes - 1, no - 0 (IGRS) executed for final design
 in real scale.

INSTRUCTIONS FOR SUBROUTINE GRAPH -

GRAPHICAL PRESENTATION OF THE DESIGN

! SCREEN !

! COMMENTS !

1. Number of divisions for X1 ? (MX) The graph has MX positions for the first coordinate and
2. Number of divisions for X2 ? (MY) MY positions for the second coordinate

INSTRUCTIONS FOR PROGRAM JDOPT -

FIRST ORDER OPTIMIZATION ALGORITHM FOR D - CRITERION
IN THE REGRESSION OF SECOND KIND CASE

! SCREEN !

! COMMENTS !

1. SPACE DIMENSION - ? (L) L is a number of controllable variables
2. CONSTANT FOR CONVERGENCE CRITERION - ? (EPS) EPS - a constant for testing convergence of the algorithm
3. NUMBER OF ESTIMATED PARAMETERS - ? (M) M - number of parameters (M must correspond to subroutine RESP , where a response function is calculated)
4. NUMBER OF POINTS IN INITIAL DESIGN - (NO) NO - number of supporting points in an initial design, input from file des.dat

Message 5 appears if L=2

5. GRAPHICAL PRESENTATION OF INITIAL DESIGN: yes - 1, no - 0 (ID0) ID0 = 1 - subroutine GRAPH is executed for initial design

Message 6 appears if initial covariance matrix is singular.

6. SINGULAR COVARIANCE MATRIX

7. SELECTION OF GAIN SEQUENCE: IALF = 1 - gain sequence is constant
1 - $\text{alfa}(s) = \text{const}$ IALF = 2 - gain sequence is $1/s$
2 - $\text{alfa}(s) = 1/s$

Message 8 appears if IALF = 1

8. CONSTANT FOR GAIN SEQUENCE - ALFA is the chosen constant
(ALFA)
9. NUMBER OF ITERATIONS - ? MITER - maximal number of iterations
(MITER)
10. CONSTANT FOR MERGING OF SUPPORTING POINTS (CMER) CMER is an internal constant
11. FORWARD LENGTH OF EXCURSION NFOR - number of steps for forward
(NFOR) procedure
12. BACKWARD LENGTH OF EXCURSION NBAC - number of steps for backward
(NBAC) procedure
13. INITIAL PROCEDURE: The algorithm starts with:
forward - 1, backward - 2 - forward procedure if IPRO = 1,
(IPRO) - backward procedure if IPRO = 2.
14. STEPWISE INFORMATION : IINF = 1 - intermediate information
yes - 1, no - 0 is saved in the file 'OUT.DAT'
(IINF) and shown on the monitor (current
design, value of the determinant
etc)

Message 15 appears if L = 2 .

15. GRAPHICAL PRESENTATION OF DESIGN: yes - 1, no - 0 IGR = 1 - subroutine GRAPH is
(IGR) executed for final design
16. SCALING OF DESIGN: yes - 1, no - 0 (ISC) ISC = 1 - scaling of final design
is carried out

Messages 17 - 19 appear if ISC = 1.

17. X1<min>, X1<max> - ? X1min, X1max - minimal and maximal
 (X1min, X1max) values of the 1-st coordinate

Message 19 appears if L = 2 .

18. X2<min>, X2<max> - ? X2min, X2max - minimal and maximal
 (X2min, X2max) values of the 2-nd coordinate

19. GRAPH IN REAL SCALE: IGRS = 1 - subroutine GRAPH is
 yes - 1, no - 0 (IGRS) executed for final design
 in real scale.

