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Applications of system identification and parameter estimation in water quality modelling

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Abstract. Applications of techniques of system identification and parameter estimation in water quality modelling are surveyed. This survey of the literature covers three areas: river water quality, lake water quality, and waste water treatment plant modelling. The applications cited are classified according to the type of algorithm used for calibration, the type of model, and the field data used. Two broad distinctions are made between: (1) off-line and recursive methods of parameter estimation; and (2) internally descriptive (state–space) and black box (input–output) model types. To assist the classification, a number of estimation algorithms are very briefly introduced. Although there are clearly different lines of development in each area of water quality modelling, it is possible to identify problems common to all three areas. The major problems discussed concern the availability of field data, levels of noise in the data, and model structure identification.

Applications d'identification systémique et d'estimation de paramètres dans la modélisation de la qualité de l'eau

Résumé. Des applications des techniques d'identification systémique et d'estimation de paramètres dans la modélisation de la qualité de l'eau sont passées en revue. Cette revue de la littérature couvre trois domaines: qualité des eaux courantes, qualité des eaux de lacs, et modélisation des unités de traitement des eaux usées. Les applications mentionnées sont classées selon le type d'algorithme utilisé, le type de modèle et les données expérimentales. Deux distinctions principales sont faites entre: (1) méthodes récursives et 'off-line' d'estimations des paramètres et (2) types de modèles à description interne (espace–d'états) et boîte noire (input–output). Afin d'aider la classification un certain nombre d'algorithmes d'estimation sont brièvement introduits. Bien qu'il y ait évidemment des lignes de développement différents pour chaque domaine de modélisation de la qualité de l'eau, il est possible d'identifier des problèmes communs à tous ces domaines. Les principaux problèmes discutés concernent la disponsibilité de données expérimentales, les niveaux de bruit dans les données, et l'identification de structure des modèles.

INTRODUCTION

Calibration of models for water quality in rivers, lakes, and waste water treatment processes is, in several important respects, different from the problem of calibrating, for example, rainfall–runoff and flood routing models. Records of water quality data are often restrictively short and inadequate for the purposes of time series analysis; the data are subject to particularly high levels of error; the system to be described is rarely of the multiple input–single output form (a form which permits substantial simplification of the analysis); and significant input perturbation of the system behaviour, such as the storm event, is often absent from the recorded data. Indeed, relationships between 'causes' and 'effects' are not always self-evident prior to the analysis of the field data. One may argue, therefore, that applying techniques of system identification and parameter estimation to problems of water quality modelling is not to be treated as a straightforward extension of the approaches typically used in the analysis of other forms of hydrological modelling.

This paper surveys the literature of water quality model calibration. Since the applications cited are classified according to the type of parameter estimation algorithm used, the following section introduces a minimum of explanation for a number of potentially applicable algorithms. The principal component of the survey, and the salient problems of current applications of parameter estimation algorithms in water quality modelling are dealt with in subsequent sections.

ESTIMATION ALGORITHMS

Many algorithms are available for parameter estimation, although the majority of these algorithms are not substantially different from the basic notion of a *least squares* estimator. Certainly, the fundamental role of least squares as the point of departure in developing more complex algorithms is undisputed (Draper and Smith, 1966; Eykhoff, 1974; Gelb, 1974; Young, 1974; Kashyap and Rao, 1976; Graupe, 1976).

Let us define, therefore, the following criterion function for model parameter estimation (or calibration):

$$J \triangleq \sum \epsilon^T(\hat{\alpha})\, \mathbf{W}\epsilon(\hat{\alpha}) \tag{1}$$

in which $\hat{\alpha}$ is a vector of model parameter estimates and ϵ is a vector of errors between model-based estimates of the system responses and field observations of those responses. $\mathbf{W}$ is a matrix of weighting coefficients, various choices for which define different estimation algorithms. When $\mathbf{W} = \mathbf{I}$, the identity matrix, minimization of (1) with respect to $\hat{\alpha}$ yields the least squares estimates. In most cases of practical interest, the least squares estimates will be biased because, in general, the noise (or random error) sequences assumed to be present in the observed field data do not conform to white noise sequences. Thus, it cannot be assumed that the least squares estimates will equal the supposedly 'true' values of the system parameters. One of the most widely used algorithms that avoids this problem is the method of *maximum likelihood* (see, for example, Åström and Bohlin, 1966; Box and Jenkins, 1970). Maximum likelihood estimation is equivalent to the substitution $\mathbf{W} = \mathbf{R}^{-1}$ in the criterion function (1), where $\mathbf{R}$ is either the covariance matrix of the output response measurement errors (Gelb, 1974) or the computed covariance matrix of the errors ϵ (Källström *et al.*, 1976). Assumptions about the statistical properties of the noise sequences (their mean and covariance) are necessary in order to make this substitution. If, in addition, it is assumed that each element of the noise sequence vector is independent of all other elements, then a somewhat simpler estimator results. Under this assumption, $\mathbf{W}$ is a diagonal matrix and the estimator is frequently referred to as *weighted least squares.*

An *instrumental variable* estimator (Kendall and Stuart, 1961; Johnston, 1963; Young, 1976) also avoids the problem of biased estimates. The method seeks to generate a sequence of variables with specific statistical properties – the instrumental variables – that may be substituted into an essentially least-squares-like algorithm. For certain forms of the instrumental variable estimator (Young, 1974), the instrumental variables are virtually equivalent to state estimates. There are, therefore, strong similarities between this estimator and the *extended Kalman filter* (Jazwinski, 1970), an algorithm that treats the problem of parameter estimation as a problem of combined state–parameter estimation. In that sense the method of *quasi-linearization* is similar to the extended Kalman filter since it too sets up the parameter estimation problem by interpreting the model parameters as additional system state variables (Bellman and Kalaba, 1965; Lee, 1968).

Many of the above and closely related algorithms can be implemented as either *off-line* or *recursive* schemes of parameter estimation. The basic difference between the two schemes is that an off-line scheme assumes that a single, fixed set of estimates $\hat{\alpha}$ may be substituted for computation of the response errors (ϵ) for all N field observations sampled from time $t_1 \to t_N$. With a recursive scheme it is possible to compute estimates $\hat{\alpha}(t_k)$ for each kth instant of time, and therefore it is possible to estimate time-varying parameter values.

TABLE 1. Summary of recent applications of parameter estimation algorithms in water quality modelling

Author(s)	Field data	Algorithm	Type of model*
Stream water quality modelling			
Koivo and Phillips (1971)	—	Stochastic approximation (least squares); *R*	Time and space; BOD, DO; analytical solution to first-order partial differential equation
Koivo and Phillips (1972)	—	Least squares; *O*	Space; BOD, DO; steady-state analytical solution to first-order partial differential equation
Koivo and Phillips (1976)	—	Linear Kalman filter; *R*	Time and space; BOD, DO; difference equations
Koivo and Koivo (1978)	—	Least squares (state estimation only); *R*	Time and space; BOD, DO; first-order partial differential equation
Lee and Hwang (1971)	—	Quasi-linearization (least squares); *O*	Space; BOD, DO; ordinary differential equation
Shastry *et al.* (1973)	Sacramento River (1962)	Weighted least squares; maximum likelihood; *O*	Space; BOD, DO; ordinary differential equation
Huck and Farquhar (1974)	St Clair River (1971)	Maximum likelihood; *O*	Single point spatial location, time-variations; DO, chloride; black box time-series model
Beck (1975)	River Cam (1972)	Maximum likelihood; *O*	Time; BOD, DO; ordinary differential equation; also black box time-series model
Beck and Young (1976)	River Cam (1972)	Extended Kalman filter; *R*	Time; BOD, DO; ordinary differential equation
Whitehead and Young (1975)	Bedford Ouse River (1973)	Multivariable instrumental variable-approximate maximum likelihood (MIVAML); *R*	Time; BOD, DO; difference equations
Young and Whitehead (1977)	River Cam (1972); Bedford Ouse River (1973)	MIVAML; *R*	Time; BOD, DO; difference equations
Lettenmaier and Burges (1976)	—	Extended Kalman filter; *R*	Space; BOD, DO; ordinary differential equations
Ernie and Ruchti (1977)	Aare River	Differential approximation method; *O*	Single point spatial location; time-variations; DO; difference equations
Ivakhnenko *et al.* (1977)	River Cam (1972)	Group method of data handling (GMDH); *O*	Single point spatial location; time variations; BOD, DO; difference equations
Stehfest (1978)	Rhine River (1971)	Quasi-linearization (least squares); *O*	Space; BOD, DO; ordinary differential equations
Stehfest (1978)	Rhine River (1971)	Quasi-linearization (least squares); *O*	Space; easily degradable organic matter, slowly degradable organic matter, bacterial mass, protozoan mass; DO; ordinary differential equations
Bowles & Grenney (1978a)	Jordan River, Utah	Extended Kalman filter; *R*	Space; BOD, DO, NH_3–N, NO_3–N, algal–N, organic–N; ordinary differential equations

TABLE 1 *continued*

Author(s)	Field data	Algorithm	Type of model*
Moore and Jones (1978)	River Cam (1972)	Coupled Bayesian–Kalman filter; *R*	Time; BOD, DO; ordinary differential equations
Rinaldi *et al.* (1979)	Bormida River	Least squares; *O*	Space; BOD, DO; analytical solution to first-order ordinary differential equations
Tamura (1979)	—	Linear Kalman filter (and others); *R*	Time and space; BOD, DO; difference equations
Thé (1978)	River Rhine	Linear Kalman filter; *R*	Time and space; conductivity; second-order partial differential equation (finite difference approximation solution)
Lake water quality modelling			
Di Cola *et al.* (1976)	Leopold's Park Pond, Brussels (1973–1975)	Least squares; *O* (solved as an optimal control problem)	Time: autotrophs, herbivores, carnivores; ordinary differential equations
Gnauck *et al.* (1976)	Saidenbach Reservoir, GDR (1966–1970); Klicava Reservoir, CSSR (1963–1972)	Least squares; *R*	Time; DO, chlorophyll-*a*, particulate organic matter; regression relationship
Jolánkai and Szöllősi-Nagy (1978)	Lake Balaton, Hungary (1971–1977)	Maximum likelihood; *R*	Time; soluble reactive phosphorus, chlorophyll-*a*, exchangeable phosphorus in sediment; ordinary differential equations
Lewis and Nir (1978)	Greifensee, Switzerland (1973)	Weighted least squares; *O*	Time; soluble reactive phosphorus, particulate phosphorus; ordinary differential equations
Halfon *et al.* (1979)	Small lake ecosystem	Least squares (also frequency domain analysis); *O*	Time; soluble phosphorus, particulate phosphorus, a low molecular weight form of phosphorus, colloidal phosphorus; ordinary differential equations
Benson (1979)	Lake Placid, British Columbia, Canada	Least squares; *O*	Time; phytoplankton biomass; ordinary differential equation
Di Toro and van Straten (1979)	Lake Ontario (1972)	Weighted least squares; *O*	Time; 16 state variables divided between epilimnion and hypolimnion layers; ordinary differential equations
Waste water treatment plant modelling			
Svrcek *et al.* (1974)	—	Extended Kalman filter; *R*	Time; cell and substrate concentrations (general continuous culture process); ordinary differential equations
Olsson and Hansson (1976)	Kaeppala Works, Stockholm	Maximum likelihood; *O*	Time; DO (activated sludge unit); black box time-series model
Crowther *et al.* (1976)	Philipshill Works, Scotland	Maximum likelihood; *O*	Time; BOD, suspended solids (primary sedimentation tanks); black box time-series model

TABLE 1 *continued*

Author(s)	Field data	Algorithm	Type of model*
Beck (1976)	Norwich Works, England	Instrumental variable; *R*	Time; gas production rate (anaerobic digestion unit); black box time-series model
Berthouex *et al.* (1978)	Madison Works, Wisconsin, USA	Maximum likelihood; *O*	Time; BOD (activated sludge unit); black box time-series model
Adayemi *et al.* (1979)	Jones Island Works, Milwaukee, Wisconsin, USA	Maximum likelihood; *O*	Time; total soluble phosphorus (phosphorus precipitation unit); black box time-series model
Beck (1979b)	Norwich Works, England	Extended Kalman filter; *R*	Time: NH_3–N, NO_3–N, *Nitrosomonas, Nitrobacter* (activated sludge unit); ordinary differential equations
Marsili-Libelli (1979)	Pilot plant, Florence, Italy	Least squares (with cubic splines smoothing); *O*	Time; BOD, bacterial concentration (activated sludge unit); ordinary differential equations

R denotes a recursive estimation algorithm.
O denotes an off-line estimation algorithm.
* Includes definition of independent and dependent variables.

SURVEY OF APPLICATIONS

Table 1 gives a broad survey of the literature on applications of parameter estimation to water quality modelling in streams, lakes, and waste water treatment plants. Classification according to the type of model used is chosen partly because it is instructive to judge the size of the model being calibrated, and partly because the choice of model (internally descriptive, or black box) defines, to some extent, the nature of an appropriate estimation algorithm. Unless otherwise indicated, as either a 'regression' or 'black box' model, all the models referenced in Table 1 are internally descriptive models. By 'internally descriptive' it is meant that the model is derived from existing theory and that it attempts to describe those internal chemical, biological, and physical mechanisms which are thought to govern system behaviour.

A few remarks are necessary in order to qualify the contents of Table 1. For example, the paper by Ivakhnenko *et al.* (1977) is primarily concerned with the problems of model discrimination and model structure identification (see below) as opposed to the problem of parameter estimation (which the GMDH algorithm treats by least squares estimation). Other references, Shastry *et al.* (1973), Beck and Young (1976), Beck (1976), Jolánkai and Szöllősi-Nagy (1978), and Halfon *et al.* (1979) are similarly oriented towards the analysis of identifying model structure.

The literature quoted for stream and lake water quality modelling shows a predominant bias towards the use of internally descriptive models, whereas the papers addressing waste water treatment plant models tend to exhibit the opposite bias towards the use of black box time series models. This reflects, in the latter case, a somewhat 'retarded' development of model calibration exercises in waste water treatment plant modelling. For stream water quality modelling Table 1 in fact reflects a rather selective survey of the literature. There have been several applications of frequency response, correlation analysis, and time series analysis techniques in stream quality modelling (Thomann, 1967, 1973; Fuller and Tsokos, 1971; Edwards and Thornes, 1973; Schurr and Ruchti, 1975; Mehta *et al.* 1975). Further applications of time series analysis in waste water treatment plant modelling can be found in Berthouex *et al.* (1975, 1976).

SALIENT PROBLEMS

It is apparent from the previous section (and Table 1) that model calibration has developed differently in the three chosen areas of water quality modelling. This is partly a consequence of different objectives for the use of models. However, similarities of the problems experienced in each area are more pronounced than their differences. Thus three general problems are discussed: (1) availability of field data; (2) noise levels in the data; and (3) degree of *a priori* knowledge.

Availability of field data

An essential difference between, for example, the calibration of rainfall–runoff and flood routing models and the calibration of water quality models is that data for the latter have usually been sampled not only at inadequately low frequencies but also for insufficient continuous periods of time. It is a characteristic feature of lake and biological waste water treatment systems that they exhibit relatively fast and relatively slow components of dynamic behaviour, both of which are important for obtaining a model of the system. A lake ecological model calibrated against short term records, under the inevitable assumption that longer-term dynamic properties are essentially at steady-state, would clearly be inappropriate for making forecasts of long term behaviour patterns. Two recent developments, one of an analytical nature and one related to instrumentation hardware, may significantly alter the situation regarding availability of data. First, Spear and Hornberger (1978), in their analysis of a lake eutrophication problem, propose that even patchy, inadequate field data and qualitative observations permit a meaningful calibration exercise; logical constraints on acceptable model performance, rather than a squared error function such as equation (1), provide the criterion for calibration. Second, improvements in specific-ion electrodes and the installation of telemetry networks for water quality monitoring will radically alter the quantity and kind of field data available for analysis.

Noise levels in the data

This problem is probably most emphasized in data collected from routine operations at waste water treatment plants. The lack of well identified 'deterministic' input disturbances, such as the storm event, leads to field data with apparently low signal : noise ratios. Consequently, it is difficult to estimate accurate input–output relationships and thus time series models will tend preferentially to identify autoregressive properties of the output observations sequence. There is, therefore, very little natural experimental basis for system identification. Moreover, extreme events in ecological systems, for instance, the sudden phytoplankton bloom, occur because a specific but relatively commonplace combination of environmental conditions force the state of the system into a region in which a nonlinear mode of behaviour is excited. Such significant variation of the responses is rarely related to extreme input disturbances.

Degree of *a priori* knowledge

A typical feature of water quality modelling is that the analyst is often uncertain of the basic cause–effect relationships in the system under investigation. And even when he knows these relationships it is not always clear what form they should take. Model structure identification is the problem of resolving such issues by reference to experimental field data (Beck, 1978, 1979a). More precisely, model structure identification may be defined as the problem of identifying the way in which the input disturbances are related to the state variables, how the states are related among themselves, and how in turn the measured output responses are related to the state variables. Solution of this problem naturally precedes accurate estimation of the model parameter values, although the solution may itself depend upon the application of an estimation algorithm. If one accepts that the issue of model structure identification is of major importance – and the literature does not suggest a widespread recognition thereof – then it is reasonable to argue that calibration of water quality models should concentrate on establishing that which is essentially 'deterministic' about the *observed* system behaviour. It is, in fact, premature to focus attention on detailed assumptions about the distributions and correlation properties of the random components of the system's behaviour.

CONCLUSIONS

The calibration of water quality models is still at a primitive stage of development. These conclusions summarize the status of applying parameter estimation techniques to the three areas of lake water quality, waste water treatment plant, and river quality modelling:

(1) A desire to characterize all the detailed features of a lake ecological system has led to the development of particularly complex internally descriptive models of such systems. These models have little likelihood of being rigorously calibrated against field data; indeed, their level of theoretical complexity seems disproportionately high when compared with the severely restricted range of available field data.

(2) In contrast, the objectives of quantifying and controlling the variability of waste water treatment plant behaviour have led typically to the calibration of low-order black box models for these systems. Such models, however, yield little insight into the dominant (microbiological) mechanisms that govern the dynamics of waste removal processes.

(3) For stream quality modelling there has been a more balanced progress in both black box and internally descriptive approaches to model construction and its associated calibration problems. With present techniques and data it would be possible to calibrate a dynamic lumped-parameter model that accounts for the basic properties of day-to-day variations in DO–BOD interaction, phytoplankton growth, and nitrification in rivers.

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