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Terminology list for threshold modelling, identification and uncertainty evaluation

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Executive Summary

Modelling is a cross-cutting discipline used in all scientific fields. Unfortunately there is a tendency for different fields to develop their own vocabulary, which may lead to “reinventions” using different words. In this report the basic modelling terminology is discussed and defined, and a framework for the model building process is presented. Finally, methods for uncertainty assessment are also presented. The methods and terminology presented are summarised in a glossary.

The document also gives a mathematical definition of thresholds and thresholds models. It is anticipated that this definition will provide clarity towards when an observed phenomenon is a threshold or not.

The report should comprise a “terms of reference” for bridging the modelling communication gap within the Thresholds project.

1. Introduction

The scientific society within marine ecology is comprised by a multitude of scientists with very different backgrounds, such as mathematicians, statisticians, microbiologists, environmental engineers, ecologists, biologists, etc. These researchers have to communicate and collaborate across the linguistic, cultural and terminological barriers in order to mitigate pollution problems of coastal ecosystems (eutrophication and harmful substances). In Thresholds, the solution to these multifaceted problems can only be found by integrating several scientific disciplines. Therefore, it is crucial for the collaboration that a common reference of terminology is established and that potential communication gaps are bridged.

There are two main sources of scientific communication problems:

1. misuse of existing terminology
2. use of unclear terminology

The first main source is the most serious since it might potentially undermine the established terminology, while both sources lead to confusion. As a result, the message is often misunderstood by the recipient.

The terminology problem is closely related to the methodology problem - model building and application. It must be stressed that a universal model does not exist. Models have to be customised to the given application. Model building is a complicated task comprised of many steps and in each step there are many tools available. It is important to establish an overview of model types, model building, model application and the tools used in the processes.

The objective of this document is

- to clarify the use of modelling terms
- to define the threshold concept
- to iterate the model building process

A glossary of modelling terms is given at the end of the document.

2. Model characterisation

The first fundamental question to be answered is: “what is a model?”. Philosophically speaking a model is an abstraction of reality. This means, that a model could be a scale-down physical model (e.g. of an offshore construction), an analogous representation (e.g. using electrical devices for simulation) or a mathematical model (e.g. a set of equations describing the real system), but it will never be a true representation of reality. Here the focus is entirely on mathematical models and these shall be referred to as ‘models’.

2.1. Model structure

A model may be considered as a ‘machine’ transforming inputs (u) to outputs (y) by a set of relations (Casti, 1977; Chui and Chen, 1988). These relations can be formulated as algebraic equations, differential/difference equations and/or partial differential/difference equations.

If inputs u are transformed directly to outputs y , the model consists of transfer functions or alternatively, the structure of the model is *a transfer function*. This is illustrated in Figure 2.1.

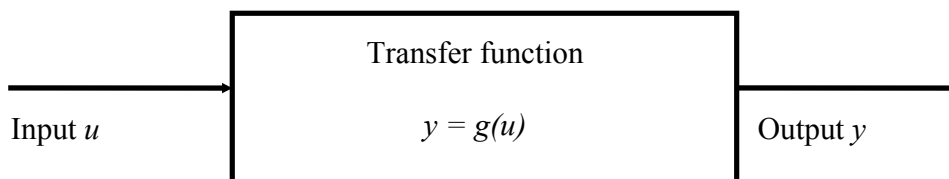


Figure 2.1 Transfer function model

Regression models are typical examples of transfer functions where empirical relationships between the output or response variable is modelled as function of inputs (typically pressures). However, such models do not necessarily consider the processes involved in transforming u to y .

The transfer function model structure may for some systems prove inadequate in representing the system, since the underlying mechanisms are not truly reflected in the model. For this reason, the *state-space model* approach was introduced in the early 1960s (Kalman, 1960).

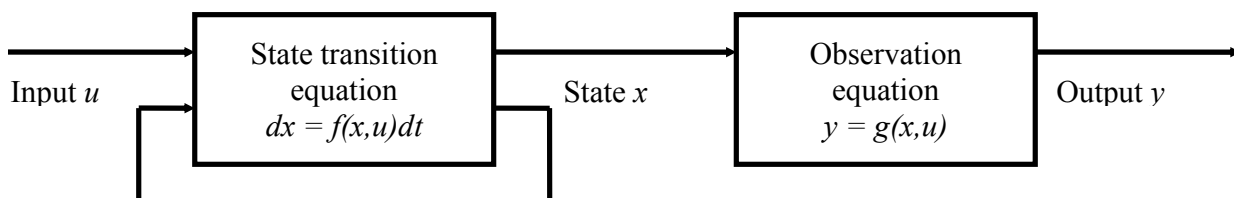


Figure 2.2 State-space model

The state-space model structure includes state variables (x) which act as mediators between the inputs and outputs (Figure 2.2). The state variables contain all information necessary to determine the state of the system. The state transition equations are in most cases formulated as differential equations, but difference equations are seen as well. Some of the state variables may not be observable (*unobserved components*).

The structure of a model is given by the equations comprising the model (see later structural identifiability).

2.2. Model constituents

There are three basic components in a model:

1. variables
2. constants
3. parameters

Inputs, outputs and states are all *variables* in the model and as such also referred to as input variables, output variables and state variables.

Model constituents which never change their value throughout all possible applications are termed as *constants*.

Model constituents that change their value according to the application are called *parameters*. The value of a parameter can be related to time, location or input variables which for the given application are constant. In some cases model parameters may gradually change their value with time (time-varying parameters), but not to an extent where they are considered dynamic variables (see below).

2.3. Model attributes

In the sections above, the building blocks of models have been described. However, there are an infinite number of ways these building blocks can be combined into a model. Therefore, it is necessary to add some adjectives or model attributes in order to characterise a model. Some model attributes have a clear and stringent definition which we shall refer to as *strong model attributes*, while some attributes are less stringent and thus termed *weak model attributes*.

2.3.1. Strong model attributes

Linear versus non-linear: These attributes relates to the structure of the model. Linear models are frequently used, because an analytical solution can be explicitly found. Non-linear models are all models that cannot be formulated as a linear model (e.g. in matrix notation). Non-linear models often require numerical methods to find the solution.

A model can also be linear with respect to the parameters but non-linear with respect to the variables (e.g. $Y = a + b \ln X$). Tong (1990) has also described a bi-linear model being a non-linear model which is linear in the parameters, when variables are held constant, and linear in the variables, when the time-varying parameter (see later) are held constant.

It should be noted that the distinction between a linear and a non-linear model is sharp from the mathematical point of view, but it might be more relevant from an application point-of-view to consider whether or not a biological system displays 'nonlinear phenomena'. The distinction arises from the fact that changes in input variables applied to linear models can give rise to nonlinear behaviour in the output variables, although the model from a mathematical point-of-view is linear. Similarly, some complicated nonlinear models can be transformed into linear ones by means of suitable changes. Finally, there are phenomena that can never be explained with linear models, independently of the number of changes that you do to their variables.

Linear models have well-defined mathematical properties making them attractive relative to non-linear models. Non-linear models may even be approximated by linear models within a limited range of validity, but the true range of this validity may only be truly examined from the non-linear model.

Dynamic versus static: In case the variables evolve over time the model is termed dynamic otherwise static. This differentiation is often seen in the model formulation where dynamic models include time t as variable and static models do not have a time component.

Time-invariant versus time-variant: If the model parameters are constant in time the model is characterised as time-invariant, otherwise time-varying. In physics synonyms for these terms are non-autonomous and autonomous, respectively. The change in parameters may be gradual reflecting changes on a long-term scale or abrupt following a regime shift.

Distributed parameter model: Similar to the time-dependency a model can have a space-dependency, i.e. spatially extended models. Such models are formulated as partial differential equations involving derivatives with respect to both time and space. This is only relevant for models resolving spatial differences. The space-dependency is also frequently formulated using a coarse discretisation in the form of box models (see also discrete-space below).

Discrete-time versus continuous-time: These attributes relates to whether the time-dependency is formulated by difference or differential equations. Most computer programs for simulating dynamic processes use a discretisation of the differential equations.

Discrete-space versus continuous-space: Similar to the above the partial differential equations can be formulated as difference or differential equations with respect to the spatial distribution. Many computer programs for hydrodynamic modelling use a lattice (2D to 4D) discretisation for the partial differential equations.

Stochastic versus deterministic: The output of a deterministic model is a single value and the output of a stochastic model is a stochastic variable, i.e. by applying several times the stochastic model to the same inputs one gets different outputs, distributed according to a probability distribution that characterises the model output.

2.3.2. *Weak model attributes*

Simple versus complex: These attributes relates to the degree of simplicity or complexity in the model, which is a subjective measure of the number of equations, parameters and their relationship. Thus, these terms only have a meaning when another model is given for reference (e.g. this model is more

simple/complex than the reference model). For this reason the terms segregated and aggregated/lumped are commonly used when one model is derived from another.

Mechanistic versus phenomenological: These terms are used to describe the degree to which a model is based upon physical, chemical and biological laws. Mechanistic, physical, white-box and transparent are attributes used to stress that a model is based upon laws of physics, chemistry and biology (deductive). Phenomenological, black-box, empirical and heuristic are terms used to denote that the model is based on empiricism (data-driven or inductive). Between the two categories are hybrid models which have a structure based on partly physical, chemical and biological laws and partly empiricism. These models are also referred to as grey-box models or semi-physical models.

2.4. Thresholds and threshold models

Assume that there is an input-output relationship between a specific driver and an ecological state indicator variable. Let us consider three potential candidate thresholds:

1. A predetermined value (fixed arbitrarily or by some scientific criterion) on a smooth (continuous and differentiable) response curve such as total maximum daily load (TMDL) or critical value in a statistical test.
2. A value where a change of gradient (discontinuity in the derivatives) occurs. The response curve is continuous but not differentiable in the threshold point.
3. A value where a discontinuity occurs. The response curve is therefore neither continuous nor differentiable in the threshold point. If the threshold value is surpassed a jump or bifurcation (see below) in the system response occurs.

Although the first type of threshold could be relevant for managing ecosystems, it is not a functional threshold in a mathematical sense defining a shift between two model formulations. Thus, a threshold is mathematically defined as a value where a discontinuity in the function or its derivative occurs. Hence, a threshold is a fixed location or value where an abrupt change occurs (in the gradient or in the response curve itself), invalidating predictions based on mathematical relationships satisfying either side of the threshold only. For example, species diversity of an ecosystem may decline steadily with increasing habitat degradation to a certain point, and then fall sharply after a critical threshold of degradation is reached. Thresholds, where irreversible changes occur, are denoted points-of-no-return.

Threshold models are mathematical formulations that switch between different modes, depending on the values of variables or parameters relative to given thresholds. The switch between different modes may also be referred to as regime shifts and the models as regime models. Threshold models are inherently non-linear by virtue. To exemplify the difference between a threshold and a threshold model, consider the two curves in Figure 2.3. Both curves reflect changes around the indicated thresholds, but only the solid curve is based on a mathematical threshold mechanism whereas the dashed curve is a differentiable logistic model. It could be argued that although the locations of the thresholds are not well determined for the logistic model this model still mimics a smooth transition from a constant level to a steep gradient to a new constant level. However, if the objective of the analysis is to identify the location of a threshold then a threshold model is more appropriate than a model that does not have the threshold as a parameter in the model formulation.

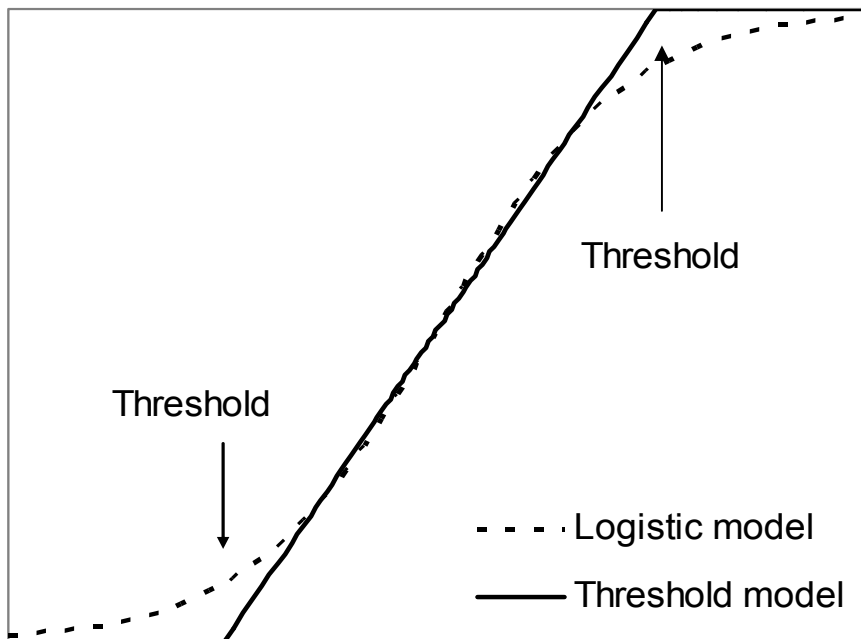


Figure 2.3 Comparison of a smooth response to a threshold model

Stable regimes are characterised by having an equilibrium state (attractors, i.e. limit points or limit cycles). The change between regimes is called a bifurcation. For nonlinear models several stable regimes can be observed for the same environmental conditions (inputs and parameters). This phenomenon gives rise to hysteresis, where sufficiently large perturbations may cause shifts between the stable regimes. The perturbations required to cause such shifts may change with environmental conditions as shown in Figure 2.4. The front and back “landscapes” have a single equilibrium, whereas the 3 middle “landscapes” have two stable regimes (bistability). The magnitude of perturbation required for a bifurcation depends on both the environmental conditions and the regime from which the bifurcation occurs.

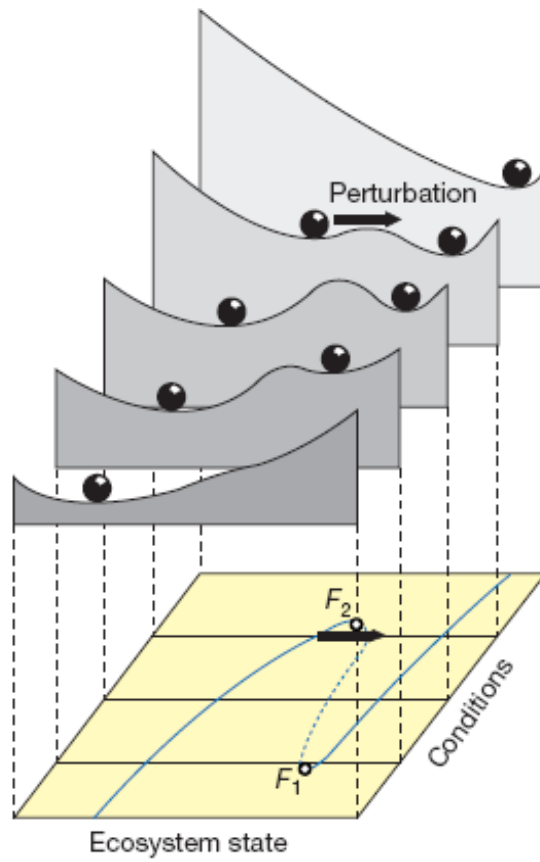


Figure 2.4 Illustration of hysteresis effect and stable regimes (from Scheffer et al. 2001)

3. Model building - methodology

Using the “story” of a model building exercise, a number of terms involved in this activity will be introduced within their appropriate context. At the same time a short review is given on the current state-of-the-art in modelling methodology. The diagram in the figure below summarises the aspects of model building which are described in detail below (Figure 3.1). Only when all the steps in the figure have been fulfilled successfully, the model can be applied for its intended purpose. These applications typically involve simulation that may be regarded as virtual experimentation with the virtual reality described by the model.

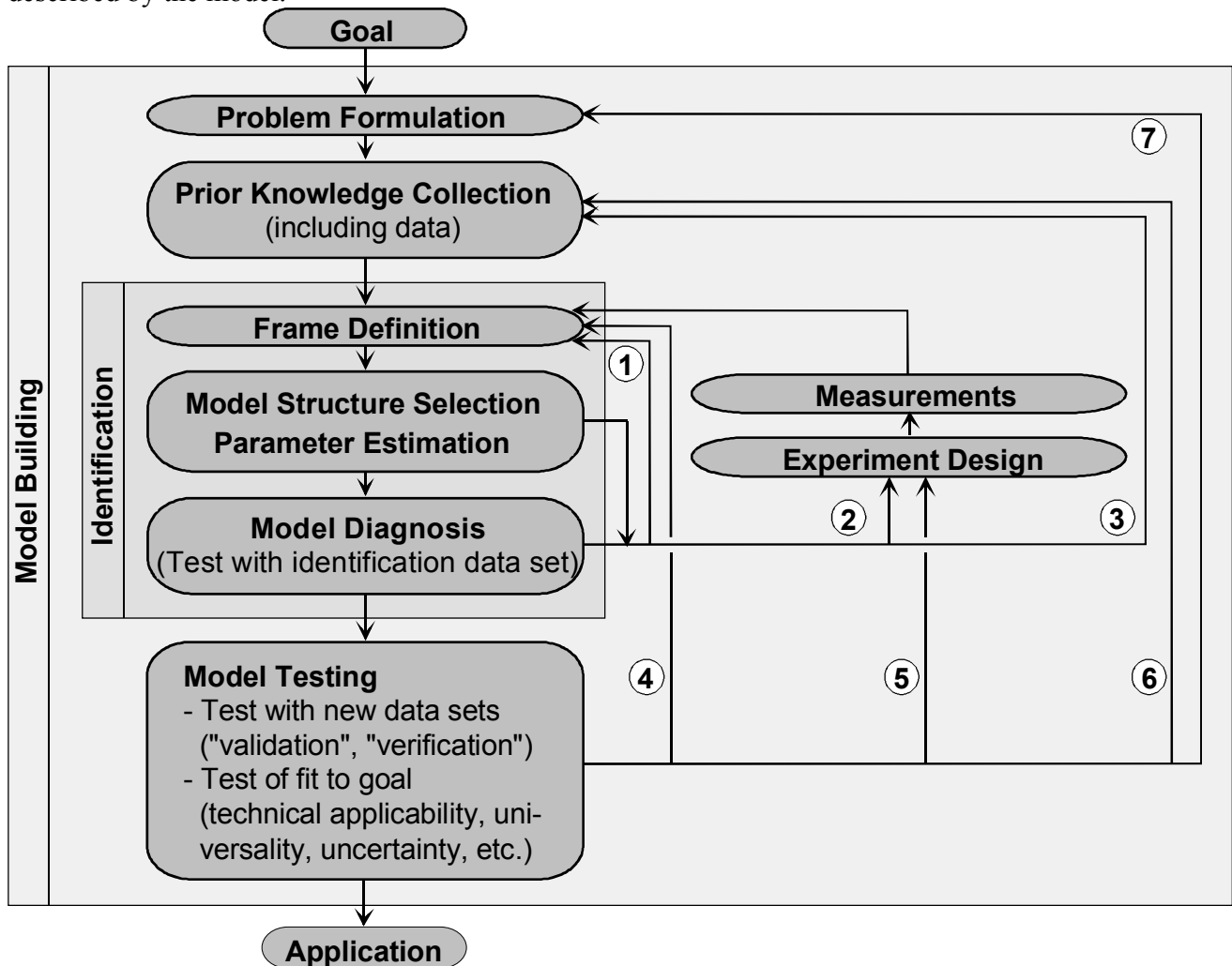


Figure 3.1 Illustration of the model building process

3.1. Problem formulation

An often forgotten task in a model building exercise is the clear formulation of the goal of the model that is to be constructed. While in most cases this task is rather intuitively performed by the modeller in case he is also the problem supplier, problem formulation or goal incorporation is much more difficult

in case these persons are not the same. In this case, an important effort must be spent to answer questions related for instance to accuracy of the results, degree of uncertainty in the provided answers, time scale of the solution, system boundaries, important variables, environmental conditions for which the model must give an answer, etc.

3.2. Prior knowledge collection

The next task is to collect the available, relevant a priori knowledge from literature and experts or from a model building environment that supports re-use of model-encapsulated knowledge. At this (early) stage of the exercise, some experiments may be conducted or some data collected during previous experiments may be retrieved and stored in the experimental database.

3.3. Frame definition

As soon as these two tasks have been performed once, a first iteration of the model building can start. The frame definition phase aims to delineate the conditions under which a model will be used (e.g. temperature), to choose the class of models that seems fit for the task (time series, state-space, distributed parameter, stochastic...), to specify the variables that seem important to find a solution to the formulated problem (inputs, outputs, states), the range of time constants that need to be covered by the model, etc.

3.4. Model structure selection

With this frame of work defined, candidate models may be constructed combining the collected a priori knowledge and the creativity of the model builder. The goal of classical model structure selection (model structure characterisation) is to select a unique model structure according to the principles of a quality of fit and parsimony (Harvey, 1989). However, it is also possible to select a set of models that are attributed different weights reflecting their probability of appropriateness (Draper, 1995; Reichert and Omlin, 1996).

Most model structure selection criteria require the parameter values θ to be estimated (see below) on the basis of $Ndata$ measurements and from that a measure of the residual errors (SSR).

However, structural selection criteria that only require basic data analysis also exist for particular applications (Vanrolleghem and Dochain, 1998). The advantage of these methods is that they don't require computationally intensive parameter estimations to be performed for the different candidate models.

Since the model selection criteria that require prior parameter estimation are more generally applicable, some details are given here on these methods. A more extensive overview is presented in Vanrolleghem and Dochain (1998). First, the so-called information criteria should be mentioned, such as AIC (Akaike, 1974), FPE (Ljung, 1987) and BIC (Schwartz, 1978). There are no defined threshold values for these criteria for which the model is considered suitable or not, but two different candidate models can be compared by means of these criteria giving preference to the model having the lowest criterion value

$$AIC = N \log \left(\frac{SSR}{Ndata} \right) + 2 \dim(\theta)$$

$$FPE = \frac{SSR}{Ndata} \left(1 + \frac{2 \dim(\theta)}{Ndata - \dim(\theta)} \right)$$

$$BIC = N \log\left(\frac{SSR}{Ndata}\right) + \dim(\theta) \log(Ndata)$$

Another criterion that has been developed and applied within ecology is the concept of predictive power (Håkanson 1997), which based on a number of model validations with regression of observed versus predicted gives a measure between 0 and ∞ . The criterion is an empirical measure not linked to any statistical assumptions calculated from the coefficients of determination, slopes and coefficients of variations derived from the model validation regressions. In order to penalise excess use of parameters in the model the adjusted R^2 can be employed as alternative to R^2 .

Methods that go back to statistics can also be used for model selection, e.g. the well-known F-test in which the residuals SSR of two models, a complex one (M_j) and a simple one (M_i) are compared:

$$F_w = \frac{\left(\frac{SSR(M_j) - SSR(M_i)}{\dim(\theta_j) - \dim(\theta_i)}\right)}{\frac{SSR(M_j)}{Ndata - \dim(\theta_j)}}$$

This calculated value is to be compared with tabulated values for a significance levels $\alpha F_{\alpha}(\dim(\theta_j) - \dim(\theta_i); Ndata - \dim(\theta_j))$. Notice that quite some similarities exist between the F-test and the above information based criteria and also with the likelihood ratio test (Söderström and Stoica, 1989)

Finally, very powerful techniques are available in which an analysis is made of the residuals between model predictions and measured data

$$\varepsilon(t_k) = Y(t_k) - Y(\theta, t_k)$$

In many applications, residuals are supposed to be randomly distributed and independent of each other. The so-called runs test evaluates the number of sign changes in the residual sequence and compares that to the expected number $N/2$ (e.g. Söderström and Stoica, 1989).

Another method for evaluating the properties of the residuals sequence is the autocorrelation test. An autocorrelation with *time lag* τ quantifies the dependency of a variable at any time t_k and the variable at time $(t_k - \tau)$:

$$r_{\varepsilon}(\tau) = \sum_{k=1}^{Ndata-\tau} \varepsilon(t_k - \tau) \cdot \varepsilon(t_k)$$

A suggested model selection criterion consists of comparing the value of the autocorrelation r_{ε} for each lag τ with the limit value $N(0,1)/\sqrt{Ndata}$ with $N(0,1)$ the standard normal distribution. For a significance level $\alpha=0.05$, for instance, this means that only 5 percent of the autocorrelations may be larger than $1.96/\sqrt{Ndata}$.

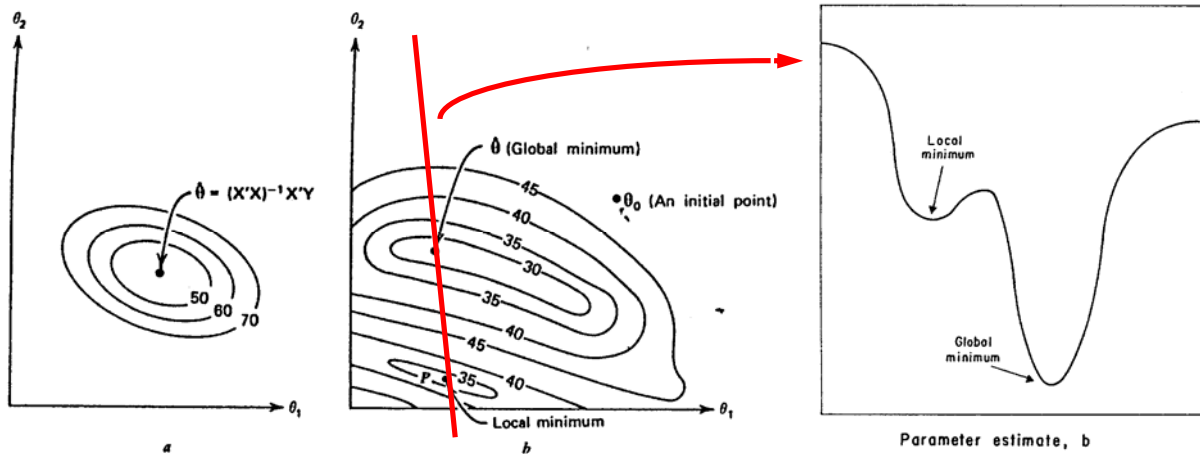


Figure 3.2 Parameter estimation viewed as an optimisation problem

3.5. Parameter estimation

Parameter estimation is based on the maximisation or minimisation of a goodness-of-fit criterion such as Least Squares, Weighted Least Squares, Maximum Likelihood, etc. when measured data is present. Below a quite general weighted least squares criterion is given in which multivariable (number of variables $Nvar$) datasets are available for $Nrespons$ experiments.

$$J(\theta) = \sum_{k=1}^{Nrespons} w_k \sum_{j=1}^{Nvar_k} w_{jk} \sum_{i=1}^{Ndata_{jk}} w_{ijk} (Y_{ijk}(t_{ijk}) - Y_{ijk}(\theta, t_{ijk}))^2$$

Optimisation of such criterion function aims to provide values for the parameters in the model and, in some cases, also values for the initial (and boundary) conditions of the state variables (in case a state space representation is adopted). Several powerful estimation (non-linear regression) algorithms are available. In case only one data point is used at a time to estimate parameter values, one uses the term recursive estimation and when the whole data set available is used at once to obtain the parameter values the term batch estimation is applied.

Estimation is a basic optimisation problem that is subject to a number of pitfalls, the most important being the presence of local minima in the criterion (or objective or cost) function. This is illustrated in Figure 3.2. On the left the topography (contour lines of criterion function values) of the criterion function is given for a linear optimisation problem. We see ellipses and can imagine that an optimisation algorithm will easily find the lowest value (imagine a ping pong ball rolling at once to the lowest point when starting from different initial locations (initial parameter guess)). In the middle of the figure the same topography is shown for a non-linear optimisation problem (as we are facing nearly always when dealing with wastewater treatment process models). On the right, a slice through the surface is made along the thick line of the centre figure. One observes multiple minima and one can imagine that the optimiser (the algorithm that directs the “ping pong ball” to the minimum) may have problems in finding the global minimum, i.e. finding the best parameter estimates. The algorithm may get stuck in a local minimum, yielding a non-optimal parameter set.

The success of the parameter estimation under such difficult (non-linear) conditions is highly dependent on the experimental dataset available. To find out how the chances are for finding reliable parameter values one can (and should) perform an identifiability analysis.

The identifiability analysis performed prior to the parameter estimation itself can provide answers to the key question whether, given a set of measured variables, unique parameter values can be obtained. Two types of answers can be given depending on the applied method. In case structural (also termed theoretical or a priori) identifiability (Godfrey and DiStefano, 1987; Norton, 1986) is evaluated the answer is either yes or no, respectively meaning that the parameters can be given unique values or not at all (Dochain et al., 1995). However, it is not ensured that the data always contain sufficient information to provide unique estimates (e.g. in the model $Y=aX_1+bX_2+c(X_1+X_2)$ only the parameter combinations $a+c$ and $b+c$ are structurally identifiable and not the three parameters a , b and c . If in a model $Y=aX_1+bX_2$ measurements for Y are available for given X_1 and X_2 , the model is structurally identifiable but it will be practically unidentifiable if the dataset contains only values of Y for $X_1=\alpha X_2$).

Once it is established (or assumed in case the theoretical identifiability analysis is not (or cannot be) performed) that a set of (combinations of) parameters is identifiable, the question rises with what accuracy that estimation can be performed. The optimisation algorithm will have difficulties in finding the best value in case that the criterion function J is hardly changing for very different values of parameter values.

Methods for the practical (also termed as numerical or posteriori) identifiability study are available and allow to evaluate the information content of the dataset intended for parameter estimation.

The basis of the methods for practical identifiability analysis is also underlying methods for optimal experimental design that can provide a solution to an encountered practical identifiability problem. This design procedure uses the model for which reliable parameter estimates are to be found to calculate experimental conditions such that sufficient information is contained in the data.

One should note that a structural identifiability problem encountered cannot be solved without altering the candidate model or frame definition (e.g. include other variables in the system description). Model reduction can lead to models that become less “data-hungry” and hence their identifiability properties may improve.

3.6. Model diagnosis

Once the parameters are estimated it remains to investigate whether the identified model violates the assumptions made in the frame definition. For instance, statistical tests of systematic deviations between model results and measurements (residuals) and their distribution are frequently used (see above).

3.7. Model testing

Fitness of a model can be evaluated by comparing its performance with data obtained under different conditions than the ones prevailing at the time of the data collection performed for model identification. This process of putting the model in jeopardy (Boyle and Berthouex, 1974) or, in other words, straining the model to its limits, may reveal model inadequacies that may be sufficient to conclude that the model is no longer “fit” for the purpose it was intended for. Hence, the whole model building process

may have to start all over. Sometimes this may even lead to a reformulation of the problem as the modelling exercise has provided considerable insight in the system under study and its behaviour.

This process of putting the model into jeopardy by confronting it with new data is most often called validation, but serious arguments are put forward against this term. As a model only describes part of the reality (the one defined in the frame) in a simplified manner, it is obvious that a model never can describe reality completely. Therefore, there will always exist experimental conditions for which the model is not valid. Hence, validation of a model is utopian! A completely other approach is to term this process of jeopardising the model a model falsification step (Caswell, 1976; Reckhow and Chapra, 1983), which if answered negatively, provides more confidence in the selected model. However, the term falsification appears too negative and one has therefore looked for other terminology that is less pronounced (quantitative) as validation but still gives a qualitative insight in the level of confidence one has in a selected identified model. The terms put forth for this are corroboration and confirmation (Popper, 1980). Finally, the term verification is frequently interchanged with validation, but the use of the term validation is advocated here.

To quantify the validity of a model recurrence is again made quite often to the residual analysis methods mentioned above.

4. Model uncertainty

Uncertainty is an inherent property of modelling. It is not realistic to expect that a model performs perfectly. Modelling along with uncertainty analysis provides us detailed information about why the model is performing poorly. For example:

- The data quality is not good enough to be useful
- The model structure is wrong, thus the model should not be applied in the first place
- The information is not sufficient for calibrating all parameters

It follows from the points above that the uncertainty encapsulated in any model is a combination of (Beck, 1987):

- Uncertainty in the input variables
- Uncertainty in the model structure
- Uncertainty in the model parameters

and in the case of model simulation, there is uncertainty in the initial boundary conditions.

By analysing the model output error, we

1. acknowledge the fact that model output is bounded with an error that must be quantitatively assessed (i.e. uncertainty bounds) in order to be taken into account in decision making.
2. gain information and insight that guide us to avoid pitfalls in the process of system modelling, thus achieving successful model performance.
3. obtain a ranked list for resource allocation plan for reducing models uncertainty (i.e. improving the model performance).

4.1. Uncertainty propagation

This subsection deals with the propagation of errors through a model. As described above, model results are imprecise due to uncertainty in input variables, model structure and parameters. For simulation studies initial values of state variables in a state-space formulation are also contributing to the output uncertainty. Thus, this subsection is concerned with estimating the magnitude of the output uncertainty given the magnitude and distribution of the errors imposed to the model. The most common application of uncertainty propagation is to investigate the contribution of parameter uncertainty to the output. However, the techniques can be applied as well to address the propagation of uncertainty in input variables, initial conditions and structural error.

In assessing the uncertainty propagation to the output there are generally two approaches:

- linearisation techniques
- Monte Carlo simulation

The *linearisation* approach includes two types of uncertainty propagation: first-order analysis and statistical linearisation. The *Monte Carlo* approach involves ordinary Monte Carlo runs and a refinement to this called the Least Squares Linearisation.

4.1.1. Linearisation techniques

Consider the linear model where the variances of the input variables are known and those of the parameters are small (parameter values assumed fixed).

$$Y = a \cdot X_1 + b \cdot X_2$$

If X_1 and X_2 are stochastic variables with uncertainty $\sigma^2_{X_1}$ and $\sigma^2_{X_2}$ the variance of the output Y would be according to the probability laws:

$$\sigma^2_Y = a^2 \cdot \sigma^2_{X_1} + b^2 \cdot \sigma^2_{X_2} + 2 \cdot a \cdot b \cdot \rho \cdot \sigma_{X_1} \cdot \sigma_{X_2}$$

where ρ is the crosscorrelation of the errors relating to X_1 and X_2 . Thus, for a linear model the propagation of uncertainty can be derived analytically.

Unfortunately, most ecosystem models are non-linear. One way of addressing this uncertainty propagation in a non-linear model is to use a *first order Taylor expansion* of the model to linearise around a given point.

It is crucial to the Taylor expansion approach that the approximation is good and the remainder in the approximation is negligible. The approach is only valid for small deviations (errors) from the expansion point - investigating the propagation of larger errors through the equation will fail due to the non-linearity (i.e. the remainder of the approximation is no longer negligible).

The *statistical linearisation* is similar to the Taylor expansion with the exception that weights instead of derivatives are found based on an optimisation of the squared error. For most models this integration is solved numerically. The difference between the first order linearisation and the statistical linearisation is illustrated in Figure 4.1.

First order linearisation uses the derivative in examination point m_x , while statistical linearisation uses a regression line which minimises the squared errors. The mean value of the output as well as the uncertainty differs between the two methods. Statistical linearisation is giving the most correct results, but it is also requiring more computation time.

4.1.2. Monte Carlo simulation techniques

Uncertainty propagation can also be examined assuming the uncertainty components to be given by a joint distribution. The stochastic equations are interpreted as an infinite set of deterministic equations, when simulated yields the output distribution. After a sufficient large number of simulations, the empirical distribution function of the output can be determined. Thus, Monte Carlo simulation is a numerical integration technique for deriving the output distribution.

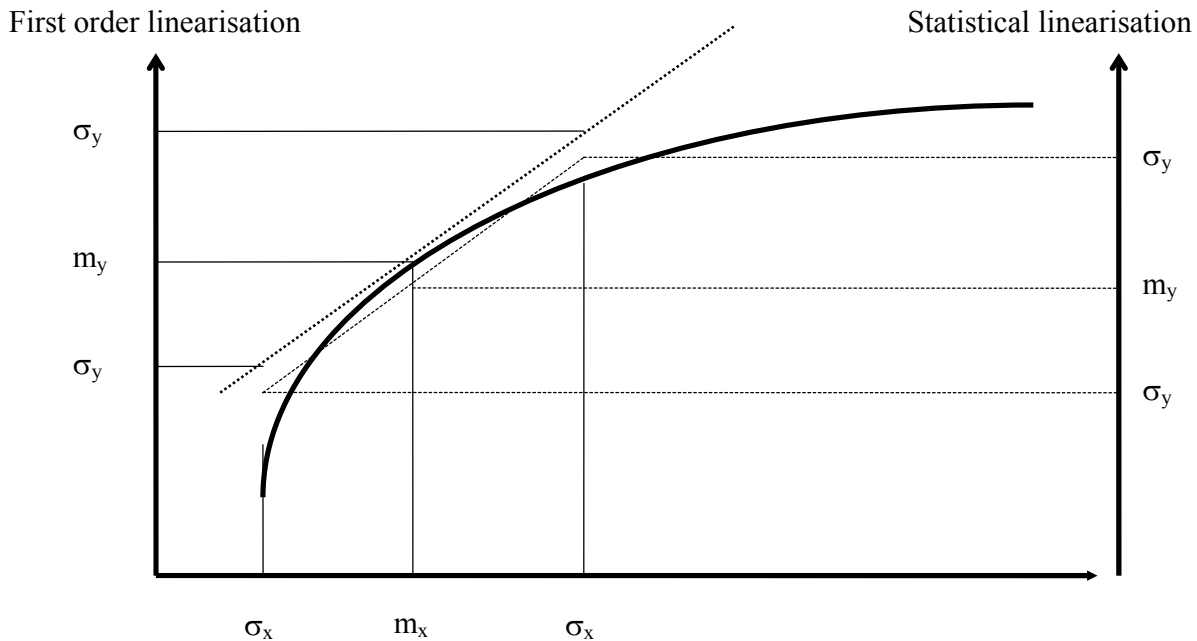


Figure 4.1 Error propagation from input to output quantified by two different techniques

There are two major concerns of using Monte Carlo simulation:

1. a joint distribution function for the uncertainty components is required.
2. a large number of simulation runs is required

Consider the uncertainty analysis of the nitrification rate with respect to the four parameters (Y_A , μ_A , K_{NH} and K_O). Assume that these parameters are uniformly and independently distributed in the following intervals:

$$\begin{array}{ll} Y_A \in [0.20;0.30] & K_{NH} \in [0.50;1.00] \\ \mu_A \in [0.40;0.60] & K_O \in [0.3;0.7] \end{array}$$

Given a constant biomass $X_{BA}=100 \text{ g COD/m}^3$, ammonia concentration $S_{NH}=1.0 \text{ g N/m}^3$ and oxygen concentration $S_O=1.0 \text{ g O}_2/\text{m}^3$, the rate distribution is found by Monte Carlo simulation (Figure 4.2).

It is clear to see that it requires at least 500 Monte Carlo simulations to get an idea of the distribution, but the true shape only appear after approximately 10000 runs. Monte Carlo Simulation has the flaw that the individual contributions of each independent variable cannot be determined, i.e. all uncertainty contributions are lumped into the output distribution.

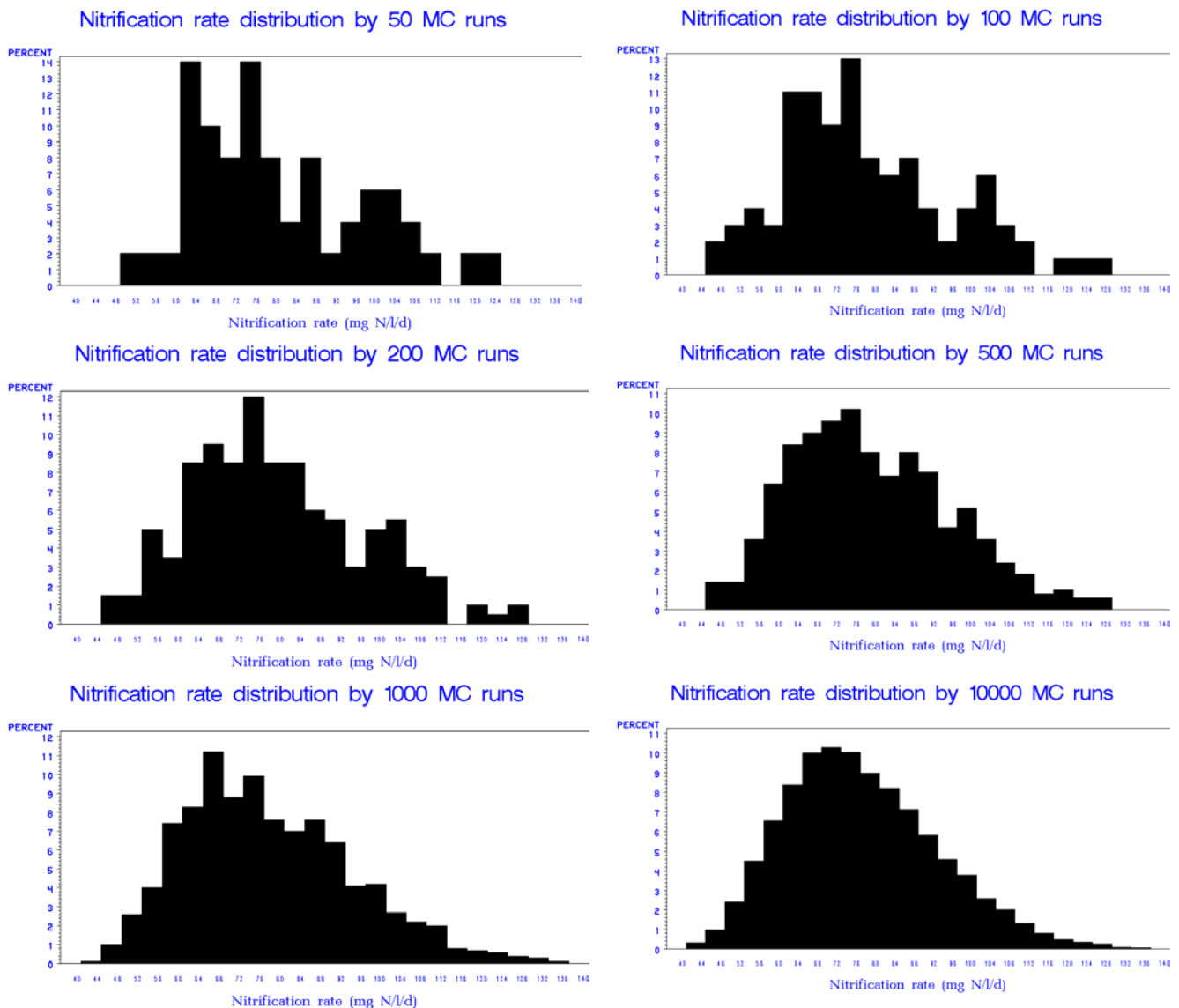


Figure 4.2 Monte Carlo simulation to obtain the distribution of nitrification rate from known uncertainties of the parameters.

Lei & Schilling (1996) have developed a method called least squares linearization which is a combination of the statistical linearization technique and the Monte Carlo approach. A number of Monte Carlo simulations are performed in order to obtain data by which the weights w_i and b in the statistical linearization can be obtained by multivariate regression. This method has the advantage like statistical linearization that the individual uncertainty contributions can be traced to the output and like the Monte Carlo approach it is computationally simple.

4.2. Uncertainty analysis

The previous section investigated the propagation of uncertainty through the model. It was implicitly assumed that the magnitude and distribution of the error components are well-known. This is often not the case. Uncertainty bounds for analysing the uncertainty propagation are frequently determined by

experience or adequate bounds. Thus, as a result the output uncertainty highly depends on the apriori assumptions. The intervals where a parameter value is likely to be found are normally determined based on literature references of calibrating the model to measured data. On the other hand, structural errors are often neglected and as a consequence, the use of a wrong model structure will lead to increased parameter uncertainty. The uncertainty attributed to input data and initial boundary conditions are likewise neglected.

As described previously, for models that are practically identifiable, the structural and parametric uncertainties can be determined. However, this often requires a simpler model structure than desired or fixation of given parameters. Thus, in order to obtain practical identifiability

- the model should be fairly simple
- the data set for identification should be information rich (persistently excited)

4.2.1. Statistical estimation

A regression analysis would yield parameter estimates and uncertainties for the estimates as well as a residual uncertainty. For most models the residual variation is quickly looked over, but it can be regarded as a combination of uncertainty in input data (both for the dependent and independent variables) and structural uncertainty.

Moreover, dynamical models formulated in a state-space form can be used to estimate the magnitude of several uncertainties components by application of a Kalman-filter (Kalman, 1960). In case the model is not linear, the problem can be addressed using the extended Kalman filter which uses a first-order Taylor approximation for the non-linearities (see e.g. Harvey, 1989).

If the model is practically identifiable, the covariance matrix of the parameters can be found either implicitly ($\sigma^2(X'\Sigma^{-1}X)^{-1}$ for generalised linear models) or explicitly from numerical optimisation (the inverse of the Hessian matrix in the optimisation point). Analyses of residuals and covariance matrix of the parameters may conclude that the model structure is wrong, and consequently a more adequate model has to be found. As an example, strong correlation in the parameter estimates (ill conditioned covariance matrix close to singularity) indicate a wrong model structure or bounds between model parameters.

4.2.2. The GLUE approach

Beven & Binley (1992) have developed a technique called Generalised Likelihood Uncertainty Estimation (GLUE), which is a tool for calibration and uncertainty estimation. The basis of the GLUE approach is that any model with any parameter set combination that predicts output variables reasonably well must be considered equally likely. It is based upon making a large number of runs of a given model with different sets of parameter values, chosen randomly from specified distributions. In general, this technique can be applied to different model structures, thus enabling the assessment of structural errors. Each set of parameter for a given model structure is assigned a goodness-of-fit value of being the 'true' system simulator.

The GLUE approach is divided into the following steps:

1. Defining a goodness-of-fit function for output data. The choice of function can be crucial to the results of the procedure. Further, a criterion based on the goodness-of-fit function for accepting or rejecting a model must be determined.

2. Defining initial ranges or distributions of parameter values to be considered for a particular model structure.
3. the parameter space is sampled to obtain realisations or simulations of the model. It is most common to use Monte Carlo simulation with uniform parameter distributions.

Going through the steps above yields empirical joint distributions for model parameters (Figure 4.3). Again, this approach can be extrapolated to involve many different model structures.

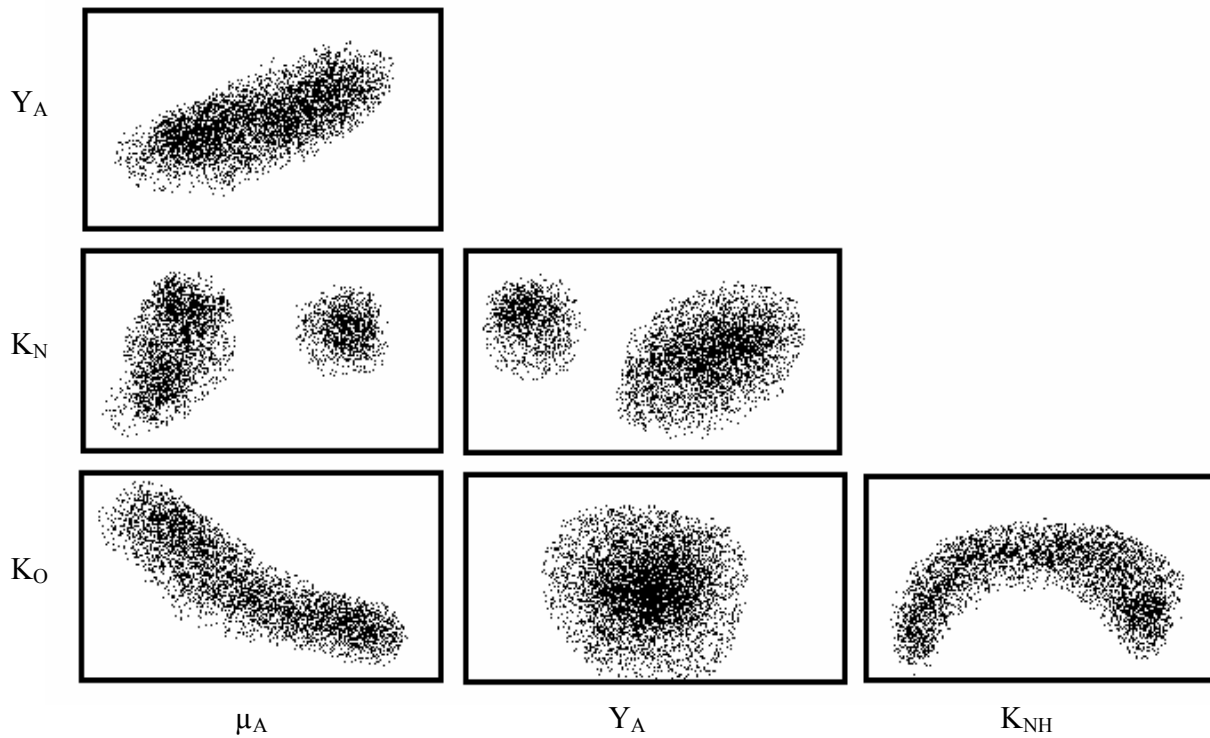


Figure 4.3 Illustration of the GLUE approach

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6. GLOSSARY

6.1. Model constituents

constant	model constituent, whose value is constant throughout all possible applications of the model
forcing function	function used as model input
input/output model	model that describes system behaviour as being a function of only present input and past inputs and outputs
model	abstraction of reality
model structure	the relations between inputs, outputs and eventually states formulated as equations
observation equation	equation in state-space model that relates the state variables to the outputs (sometimes also denoted as output equation)
parameter	model constituent, whose value needs to be determined for each specific application of the model
state	present situation of the system as described by the model
state variable	model constituent in state-space models, acting as mediator between inputs and outputs and used for a descriptive representation of the system
state-space model	model that includes a descriptive representation of the system by means of an additional set of state variables
state-transition equation	function that relates the future state of the system to the present state and inputs
transfer function	same as input/output function
variables	inputs, outputs and eventually state variables in model equations

6.2. Model attributes

aggregated	model that contains state variables that represent functional classes of different constituents (e.g. organisms) or that simplifies the spatial configuration of a system by lumping it together (cf. segregated)
autonomous	equal to time-varying
bifurcation	the change between regimes
bistability	the presence of two stable regimes (cf. stable regime)
black-box	model that describes the observed behaviour of the corresponding system without being based on the mechanisms of this system (cf. white-box)
box model	equal to discrete space
complex	a relative attribute that values whether the model contains more state variables, parameters, forcing functions, etc or an attribute that qualifies that (irrespective of the number of variables) there exist chaotic solutions of the model equations (cf. simple)
continuous space	the model resolves the spatial domain of the system continuously (cf. discrete space)
continuous time	the model resolves the time axis continuously; the time evolution is usually described by differential equations (cf. discrete time)

conceptual	a model that contains a description of the ideas/hypothesis on system behaviour without giving a mathematical formulation
deterministic	the time evolution of the model solution is uniquely determined by the initial state (for state-space models) and the time evolution of inputs (cf. stochastic)
discrete space	the model approximates the spatial domain of the system by a number of mixed compartments (cf. continuous space)
discrete time	the model divides the time axis into periods of finite length and the output or the state of the model in the next period is given as an algebraic equation depending on the old inputs of states (cf. continuous time)
distributed parameter	model with more than one independent variable; i.e. model behaviour is governed by partial differential equations in time and space
dynamic	the model describes the time evolution of a system; a solution of the model may anyway be in steady-state (cf. static, steady-state)
empirical	the model equations are not based on generally accepted laws but are just of a descriptive nature (cf. phenomenological, mechanistic)
grey-box	the model consists of sub-models that partly are based on mechanistic, partly on phenomenological descriptions (cf. black-box, white-box)
heuristic	model not based on rigorous development but on rules of thumb, feeling, qualitative reasoning
hysteresis	the presence of more than one stable regime, occurring in such a way that a change to one of them occurs when increasing an input, but a change back to the original regime when decreasing the input does not occur at the same value
limit cycle	a stable regime in which variables oscillate periodically (cf. limit point, stable regime)
limit point	a single state of equilibrium (cf. stable regime)
linear	model equations are linear in input variables (for input-output models) or in state variables (for state-space models)
lumped	equal to aggregated
mechanistic	model with the goal of describing the mechanisms that lead to the observed behaviour (cf. phenomenological)
non-linear	model equations that are non-linear in input variables (for input-output models) or in state variables (for state-space models)
phenomenological	describing the observed phenomena without representing the mechanisms governing the behaviour (cf. mechanistic)
physical	model that is based on a description with physical, chemical or biological laws, sometimes also used for small scale reproductions of a system made in physical materials
point-of-no-return	a threshold value where irreversible change occurs (cf. threshold)
reduced order	model of reduced complexity obtained by direct deduction (e.g. by aggregation/lumping) from a more complex basic model
reductionist	hierarchical description of a system by resolving it in sub-systems that again are resolved in sub-systems until a description level is reached at which a satisfying description is possible without empirical assumptions (in the ideal case down to a description based entirely on natural laws)
regime	conditions that dictate the model formulation (cf. threshold model, regime model)
regime model	the same as threshold model (cf. threshold model)

segregated	model that separates variables in more functional classes (cf. aggregated)
semi-physical	equal to grey-box
simple	relative attribute that describes that the model equations contain only few state variables, parameters, forcing functions, etc. and the solutions show simple behaviour (periodic or quasi-periodic; cf. complex)
spatially extended	equal to distributed parameter
stable regime	regime (a limit point or limit cycle) that is recovered by the system after a perturbation has been applied on it, at least if the perturbation is small
static	the model only describes the steady-state solution of a system (cf. dynamic)
steady-state	a state of a system which does not change in time, e.g. steady-state solution of a dynamic models (cf. dynamic)
stochastic	the time evolution of the model contains random elements (cf. deterministic)
time-invariant	the way the model processes input to output does not change with time
threshold	a location or value where an abrupt change occurs
threshold model	a mathematical formulation that switches between different regimes depending on the value of a variable or parameter (cf. regime)
transparent	equal to white-box
white-box	model that describes a system by one or several sub-models (white boxes) that describe the observed behaviour of the corresponding sub-system by describing the relevant mechanisms of this sub-system (cf. black box)

6.3. Terms of model building

calibration	the same as parameter estimation but not necessarily by using statistical methods
corroboration	the same as validation; the term introduced by Popper (1980) makes it clearer that the correctness of the model cannot be proved and that each successful test only increases the belief that the model is correct (cf. confirmation, falsification, validation, verification)
falsification	demonstrating the invalidity of a model by showing that the model results deviate significantly from the measurements; confirmation, corroboration, validation and verification are failed trials of falsification (cf. confirmation, falsification, validation, verification)
frame definition	selection of which components of a system are to be described and specification of classes of models to be included in the model structure selection process and specification of the experimental conditions for use of the model (experimental frame)
identifiability analysis (structural, practical)	evaluation of the uniqueness of the model parameter estimates from measured data. Structural (theoretical, a priori) identifiability analysis assesses the uniqueness of parameter estimates from ideal data for a given experimental frame, practical (a posteriori) identifiability analysis assesses the accuracy with which parameters can be estimated with a given data set. In the latter case identifiability is not an objective property, but it depends on the required accuracy
model building	the process of finding an adequate model of a system by (iteratively) processing the following model building steps: Problem formulation, prior knowledge collection, system identification and model testing
model reduction	simplification of an existing model in order to improve its identifiability without losing the description of the most important phenomena.

model (structure) selection	selecting out of a given set of model structures the structure that makes an optimal (as simple as possible but as complicated as required for the intended purpose) description of measured data possible
optimal experimental design	using a (preliminary) model of a system in order to plan an experiment that maximises the possible gain in information
parameter estimation (batch, recursive)	process of finding parameter values that lead to an optimal agreement of model results with measured data by using statistical methods. Time series of data can be used as a whole (batch estimation) or data points from within a moving data window can be used. In the latter case the parameters become time-dependent and the algorithm can be implemented to modify the previous estimate by considering the omitted and the new data points (recursive estimation)
predictive power	an empirical measure for model goodness-of-fit derived from model validation regressions of observed versus predicted
regression (linear, non-linear)	the same as parameter estimation, however usually used for the special case of algebraically given linear or non-linear model equations and using the (weighted) least squares technique goodness-of-fit criterion
simulation (interactive, Monte Carlo)	calculating the solution of a model for given values of the parameters, inputs and initial values (usually numerically). Interactive simulations are processed on a computer which allows the user to interact with the program (stop, change parameter values, etc.). Monte Carlo simulation is a method to propagate probability distributions of parameters, inputs and initial values to probability distributions of model results by performing a lot of simulations with parameter values sampled randomly from the probability distribution of parameters, inputs and initial values. More generally, any simulation of a stochastic model can also be called a Monte Carlo simulation
system identification	finding a model to solve a given problem by (iteratively) processing the following steps: Frame definition, model structure selection, parameter estimation, model diagnosis
structure characterisation	the same as model (structure) selection
uncertainty analysis	estimating the uncertainty of model predictions and analysing the sources of uncertainty
validation	test of a model with a data set not used for identification; note that such tests only increase the belief in the correctness of the model, it is not possible to prove that the model is correct (cf. confirmation, corroboration, falsification, validation)
verification	the same as validation (cf. confirmation, corroboration, falsification, validation)