Sensitivity Analysis

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Local Methods

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5.1 INTRODUCTION

Mathematical models are widely used in various disciplines, and most of these models are based on systems of algebraic and differential equations. A growth in the number of variables and parameters of mathematical models has been observed over recent years. The basic reason for this is that, in the course of refinement of physical insight, models become more sophisticated. In addition, since the capacity of computers has grown, models that are more complex can be handled more easily. A common problem is that, in large models, the role of various parameters is not obvious. Usually it is not clear which are the important parameters, what is the effect of changing parameters, what is the uncertainty of the model results, originating from the uncertainty of parameters, and so on.

Local sensitivities provide the slope of the calculated model output in the parameter space at a given set of values. In many applications, this is exactly the information needed. In other areas, such as uncertainty analysis, local sensitivity analysis is a computationally efficient technique that allows a rapid preliminary exploration of the model.

There have been a number of reviews of local methods: A comprehensive review of sensitivity analysis was given by Rabitz *et al.* (1983). This review dealt mainly with local methods, and concentrated on distributed-parameter systems. Applications, mainly in chemical kinetics and molecular dynamics, were presented there. The review of Turányi (1990a) described both global and local methods, and provided an almost complete list of applications in chemical kinetics up to 1989. The review by Radhakrishnan (1990) dealt with the numerical aspects of local sensitivity methods, with an emphasis on combustion chemical modeling. The review by Tomlin *et al.* (1997) discussed the applications of several mathematical methods, including sensitivity analysis, to combustion kinetics.

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Finally, we discuss some case studies that use SB. The ecological case study mentioned at the beginning of this section took 154 simulation runs to identify and estimate the 15 most important factors among the original 281 factors. Some of these 15 factors surprised the ecological experts, so SB may be a powerful statistical (black box) technique. Notice that on hindsight it turned out that there are no important interactions between factors, so only $154/2 = 77$ runs would have sufficed (no foldover).

Another case study is the building thermal deterministic simulation in De Wit (1997). In his simulation, SB gave the 16 most important inputs among the 82 factors, after only 50 runs. He checked these results by applying Morris' screening technique described in Section 4.4; the latter technique took 328 runs.

4.8 CONCLUSIONS

In the initial phase of a simulation, it is often necessary to find out which factors amongst the multitude of potential factors are really important. The goal is then to reduce the number of factors to be further explored in the next phase.

Some designs (called supersaturated designs) require fewer runs than factors! In this chapter, we have surveyed several types of design: one-at-a-time (OAT) designs (including Morris's design), the systematic fractional replicate design proposed by Cotter, the iterated fractional factorial design (IFFD), and Bettonvil's sequential bifurcation (SB). Each type has its own advantages and disadvantages.

OAT designs have as a major limitation the neglect of factor interactions. The advantage is that OAT does not make simplifying assumptions such as that only a few factors have important effects or that the input/output (I/O) function is monotonic. Moreover, the computational cost of OAT designs is linear in the number of factors. However, OAT methods provide unbiased estimators of the effects of each individual factor, provided that these effects are the same at different settings of the other factors; that is, the factors act additively, over the range of interest. Such an assumption, although advantageous to simplify the problem, can be rarely accepted. In fact, interactions are usually relevant, and need to be estimated by varying factors simultaneously. On the other hand, when the model is expensive to run, and there are many factors, Morris' method is both efficient and easy to implement. The Morris' method is available in the software package PREP-SPOP (SIMLAB) (see the software Appendix).

The systematic fractional replicate design of Cotter (1979) is computationally efficient and does not require any prior assumption about interactions or few important factors. However, the design lacks precision and cannot detect factors having effects that cancel each other out.

IFFD estimates the main effects, quadratic effects, and two-factor interactions of the most influential factors, with a number of runs that is small compared with the total number of factors. However, for good results, the model output should be determined by only a few highly influential factors. Andres' IFFD is available in the package SAMPLE2 (see the software Appendix).

Sequential bifurcation is simple, efficient, and effective (as several case studies have illustrated). Its major limitations are that the signs of main effects must be known, and that metamodels with only main effects and two-factor interactions must be adequate I/O approximations.

The screening designs described in this chapter are only a small subset of the total number available in the literature. We have presented only those designs that focus on the problem of the identification of the few important factors in a model.

5.2 FEATURES OF LOCAL SENSITIVITIES

Time-independent (stationary) systems can be characterized by the following system of algebraic equations:

$$0 = \mathbf{f}(\mathbf{y}, \mathbf{k}) \tag{5.1}$$

where $\mathbf{y}$ is the n-vector of variables and $\mathbf{k}$ is the m-vector of parameters. The solution of the implicit algebraic Equation (5.1) is denoted by $\mathbf{y}^s$. The solution changes when the values of parameters $\mathbf{k}$ are changed, and the new solution can be obtained from the following equation:

$$\mathbf{y}^s(\mathbf{k} + \Delta\mathbf{k}) = \mathbf{y}^s(\mathbf{k}) + \sum_{j=1}^{m} \frac{\partial y_i}{\partial k_j} \Delta k_j + \frac{1}{2} \sum_{l=1}^{m} \sum_{j=1}^{m} \frac{\partial^2 y_i}{\partial k_l \partial k_j} \Delta k_l \Delta k_j + \cdots \tag{5.2}$$

A chemical example of such a system is the concentration in a well-stirred (i.e. spatially homogeneous) stationary reactor.

Non-stationary systems can be described by differential or differential–algebraic systems of equations. Consider the following initial-value problem:

$$\frac{d\mathbf{y}}{dt} = f(\mathbf{y}, \mathbf{k}), \qquad \mathbf{y}(0) = \mathbf{y}^0. \tag{5.3}$$

Here again, $\mathbf{y}$ is the n-vector of variables and $\mathbf{k}$ is the m-vector of system parameters, and $\mathbf{y}^0$ is the array of initial values. Solution of the initial-value problem (5.1) provides the time evolution of the system variables.

The effect of parameter change on the solution can be expressed through a Taylor series expansion:

$$\mathbf{y}^s(t, \mathbf{k} + \Delta\mathbf{k}) = \mathbf{y}^s(t, \mathbf{k}) + \sum_{j=1}^{m} \frac{\partial y_i}{\partial k_j} \Delta k_j + \frac{1}{2} \sum_{l=1}^{m} \sum_{j=1}^{m} \frac{\partial^2 y_i}{\partial k_l \partial k_j} \Delta k_l \Delta k_j + \cdots \tag{5.4}$$

In both the time-dependent and time-independent cases, the partial derivatives $\partial y_i / \partial k_j$ are called first-order local sensitivities, $\partial^2 y_i / \partial k_l \partial k_j$ are called second-order local sensitivities, and so on. The first-order local sensitivities form the sensitivity matrix $\mathbf{S} = \{s_{ij}\} = \{\partial y_i / \partial k_j\}$.

Global sensitivity coefficients depend on the assumed probability density function of the parameters, and usually also on the method of calculation chosen. In contrast, local sensitivity coefficients are defined exactly by Equations (5.2) and (5.4). There are several numerical methods for the calculation of local sensitivities, but the calculated values should be identical within the numerical accuracy of the method used. Also, calculation of local sensitivities is much faster than that of global sensitivities. However, local sensitivities have some special limiting features that have to be kept in mind.

For all models of real systems, the values of the parameters are subject to some uncertainty. In most cases, such uncertainties can be very high, and sometimes when the parameters are changed within the range of uncertainty, a qualitatively different model is obtained. Unlike global sensitivities, local sensitivities are totally incapable of providing information on the effect of significant parameter changes. Local sensitivities are really local, and the information provided is related to a single point in the space of parameters. The point investigated is usually the point of best parametric estimate, also called the nominal value of parameters. Small variations in parameter values usually do not change

the local sensitivities dramatically, but a significantly different parameter set may result in a completely different sensitivity pattern.

Sensitivity analysis of time-dependent systems has another characteristic feature. In most cases, sensitivity analysis can be considered as probing the model using another set of parameters. However, sensitivity analysis can also be used for the analysis of a model via perturbation of the parameters. In the former case, the parameters are changed at simulation time zero, and therefore the initial time of sensitivity calculation is equal to the initial time of simulation. In the general case, however, the initial times of the model and of the sensitivities are different. Let the simulation be started at time 0, let the parameters be perturbed at time t_1, and let the effect of the perturbation be studied at time t_2. The perturbed solution $\mathbf{y}'$ can be approximated from the original solution $\mathbf{y}$ and sensitivity matrix $\mathbf{S}$:

$$\mathbf{y}'(t_2) \approx \mathbf{y}(t_1) + \mathbf{S}(t_2, t_1)\Delta\mathbf{k}_{t_1}. \tag{5.5}$$

This means that the sensitivity matrix $\mathbf{S}$ has double time dependence in the general case, and the time limits t_1 and t_2 provide a degree of freedom in the analysis of models.

5.3 NUMERICAL METHODS FOR THE CALCULATION OF LOCAL SENSITIVITIES

5.3.1 Finite-Difference Approximation

The simplest way to calculate local sensitivities is based on slightly changing one parameter at a time and rerunning the model. Using the *finite-difference approximation*, elements of the sensitivity matrix can be approximated by

$$\frac{\partial \mathbf{y}}{\partial k_j} \approx \frac{\mathbf{y}(k_j + \Delta k_j) - \mathbf{y}(k_j)}{\Delta k_j}, \qquad j = 1, \ldots, m. \tag{5.6}$$

This procedure is also called the *brute force method* or the *indirect method*. The main advantage of this method is that no modification to the original model or extensive extra coding is needed. However, the brute force method is slower and less accurate than more sophisticated methods.

Calculation of local sensitivities in this way requires $m + 1$ simulations of the original model. If central differences are used, $2m$ simulations are required. The accuracies of the sensitivities calculated depend on the parameter change Δk_j. In the case of nonlinear models, parameter changes that are too large (e.g. >5%) would damage the assumption of local linearity. If the parameter change is too small, the difference between the original and perturbed solutions is too small and the round-off error is too high. In most cases, a 1% perturbation is a good practical choice, but finding the best (or acceptable) value is a trial-and-error process.

5.3.2 Direct Method

Differentiation of Equation (5.3) with respect to k_j gives the following system of *sensitivity differential equations*:

$$\frac{d}{dt}\frac{\partial \mathbf{y}}{\partial k_j} = \mathbf{J}\frac{\partial \mathbf{y}}{\partial k_j} + \frac{\partial \mathbf{f}}{\partial k_j}, \tag{5.7}$$

or, in matrix form,

$$\dot{\mathbf{S}} = \mathbf{JS} + \mathbf{F}. \tag{5.8}$$

Here $\mathbf{J} = \{\partial f_i/\partial y_l\}$ is the derivative of the right-hand side of the differential equation with respect to the system variables (called the Jacobian matrix) and $\mathbf{F} = \{\partial f_i/\partial k_j\}$ is the derivative with respect to the parameters, sometimes called the parametric Jacobian. The initial condition of the differential equation (5.7) is a zero vector.

Direct methods are based on the solution of the ODE (5.7). Numerical solution of Equation (5.7) requires knowledge of the values of the matrices **J** and **F** at each step of the ODE solver. To evaluate these matrices, the actual values of the system variables have to be known, and therefore a simultaneous or preceding solution of the ODE (5.3) is needed. In the first realizations of the direct method, Equations (5.3) and (5.7) were solved independently but simultaneously, and the solution of Equation (5.3) was used for setting up Equation (5.7). All variants of this algorithm were relatively slow.

Dunker (1981, 1984) was the first to show that a special relation between Equation (5.3) and Equation (5.7) allows a numerical shortcut, and called this algorithm the *decoupled direct method* or *DDM*. Equations (5.3) and (5.7) have the same Jacobian, and therefore a stiff ODE solver selects the same step size and order of approximation for the solution of both equations. In Dunker's method, the ODE solver decomposes the Jacobian only once, and then takes a timestep solving Equation (5.3) and then solving Equation (5.7) with all parameters one after the other. Since the triangularization of the Jacobian is the most time-consuming part of a stiff ODE solution, using the decoupled direct method, sensitivities can be calculated with relatively little extra cost.

Several implementations of the DDM exist, and the DDM has proved to be the best general method for the numerical calculation of local sensitivities.

In the case of stationary systems, if the stationary point is asymptotically stable, the stationary sensitivity coefficients are limits in time of the dynamic ones, and their time derivatives tend to zero. Therefore, Equation (5.8) can be transformed to

$$\mathbf{S}^s = -\mathbf{J}^{-1}\mathbf{F}. \tag{5.9}$$

The matrix $\mathbf{S}^s$ is the *stationary sensitivity matrix* and the matrices **J** and **F** are evaluated at the variable values of the stationary point. Equation (5.9) can also be applied when the original model is defined as a system of algebraic equations (5.1).

5.3.3 The Green Function Method

Differentiating Equation (5.3) with respect to the initial values $\mathbf{y}^0$, the following equation is obtained:

$$\frac{d}{dt}\mathbf{K}(t, t_1) = \mathbf{J}(t)\mathbf{K}(t, t_1). \tag{5.10}$$

where t_1 and t are the time of perturbation and the time of observation, respectively, and **K** is the initial value sensitivity matrix, that is

$$\mathbf{K}(t, t_1) = \left\{\frac{\partial c_i(t)}{\partial c_j^0(t_1)}\right\}, \qquad \mathbf{K}(t_1, t_1) = \mathbf{I}, \qquad t \geqslant t_1.$$

Equation (5.7) is a linear inhomogeneous system of differential equations, and therefore it can be solved by first determining the homogeneous part (5.10) and then calculating the particular solution:

$$\mathbf{S}(t_1, t_2) = \int_{t_1}^{t_2} \mathbf{K}(t_2, s)\mathbf{F}(s)\, ds. \tag{5.11}$$

In this equation, $\mathbf{K}$ is known as the *Green function* or *kernel*, and the numerical method based on the solution of Equation (5.11) is called the *Green function method*.

The Green function method also has several variants. The most developed of these is called the analytically integrated Magnus version of the Green function method (GFM/AIM) (Kramer *et al.*, 1981). In this version, the matrix $\mathbf{K}$ is approximated by a matrix exponential:

$$\mathbf{K}(t + \Delta t, t) = \exp\left[\int_t^{t+\Delta t} \mathbf{J}(s)\, ds\right]. \tag{5.12}$$

The GFM/AIM method is several times faster than other versions of the Green function method.

Applying the direct method, the numerical effort increases linearly with the number of parameters. In the case of Green function methods, the numerical effort is proportional to the number of variables. In practice, however, the GFM is faster than the DDM only at a very high ratio of the number of parameters to the number of variables, and the numerical error is less easily controllable than in the case of the much simpler DDM algorithm.

5.3.4 Other Methods

Other methods have also been described in the literature, but they are much less widespread. It is frequently useful (Miller and Frenklach, 1983) to approximate the integrated solution of the original model by an array of simpler empirical equations as a function of parameters in a parameter region. Preparation of such an empirical model is very time-consuming, and cannot be justified by only the sensitivity calculations. However, if such an empirical function is available, differentiating it provides an estimate of the local sensitivities as a by-product.

According to the polynomial approximation method (Hwang, 1983), the solution of the sensitivity differential equations (5.7) is approximated by Lagrange interpolation polynomials. Although high computational speed and good numerical stability were demonstrated, this method was never applied to real problems.

5.4 DERIVED SENSITIVITIES

In the case of models defined by the differential equations (5.3), not only the actual values of variables are interesting but also their rates of change at a given time. The rates of change of variables are given by the left-hand side of Equation (5.3). Since

$$\frac{d}{dt}\left(\frac{\partial y_i}{\partial k_j}\right) = \frac{\partial (dy_i/dt)}{\partial k_j},$$

the sensitivities of the rates of change of variables can be calculated by Equation (5.7), knowing the local sensitivity coefficients.

The *rate sensitivity matrix* $\dot{\mathbf{S}}(t_1, t_2)$ also has double time dependence. If the two times coincide ($t_1 = t_2$), the instantaneous effect of parameter change is obtained. It is clear from Equation (5.8) that the matrix $\mathbf{F} = \{\partial f_i/\partial k_j\}$ can be considered as an instantaneous rate sensitivity matrix. Knowing the values of variables at a given time, $\mathbf{F}$ can be calculated analytically and therefore the solution of the sensitivity ODE (5.8) is not needed. It has been shown (Turányi *et al.*, 1989) that $\mathbf{F}$ can provide valuable information on the structures of models.

Mathematical models may provide qualitative information. Such information can be whether a model oscillates, if a given variable reaches a threshold value during the time interval inspected, and so on. Sensitivity analysis cannot be used for the study of such information. On the other hand, frequently the information desired is quantitative, but may not be among the primary outputs of the model, although it can be deduced from the time histories of variables. Such information might be the maximum value of a variable, the time needed for a variable to reach a threshold value, or, in the case of periodic solutions, the period time. Such quantitative information can be called a feature, and its sensitivity is named *feature sensitivity*.

The brute force method offers a direct way to calculate feature sensitivities (Frenklach, 1984). A particular feature is evaluated from the original and perturbed solutions, and the feature sensitivity is calculated using finite differences.

In many cases, the feature sensitivities can also be calculated from the local sensitivities of variables. As an example, assume that variable i has a maximum (or minimum) at time t^*. This implies that the time derivative of the variable is zero:

$$\dot{y}_i(\mathbf{k}, t)|_{t=t^*} = 0. \tag{5.13}$$

Differentiating Equation (5.13) with respect to the parameter k_j, the following equation is obtained (Rabitz *et al.*, 1983) for the calculation of the sensitivity of the location of the maximum:

$$\frac{\partial t^*}{\partial k_j} = -\frac{\dfrac{\partial^2 y_i(t^*)}{\partial t\, \partial k_j}}{\dfrac{\partial^2 y_i(t^*)}{\partial^2 t}}. \tag{5.14}$$

The numerator contains the appropriate rate sensitivity coefficient $\dot{s}_{ij}(0, t^*)$, while the denominator can be calculated from the Jacobian and the right-hand side of the original ODE:

$$\frac{\partial^2 \mathbf{y}}{\partial t^2} = \mathbf{J}\mathbf{f}(\mathbf{y}). \tag{5.15}$$

Another frequently applied feature sensitivity is the sensitivity of the period time of periodic (oscillating) models. Period time sensitivities can also be calculated (Edelson and Thomas, 1981) approximately from the local variable sensitivities:

$$\frac{\partial \tau}{\partial k_j} = \frac{\dfrac{\partial y_i(t_2)}{\partial k_j(t_1)} - \dfrac{\partial y_i(t_2 + \tau)}{\partial k_j(t_1)}}{\dfrac{dy_i(t_2)}{dt}}. \tag{5.16}$$

5.5 INTERPRETATION OF SENSITIVITY INFORMATION

5.5.1 Effect of Changing One Parameter on a Single Variable

The sensitivity coefficient $\partial y_i/\partial k_j$ is a linear estimate of the number of units change in the variable y_i as a result of a unit change in the parameter j. This also means that the sensitivity result depends on the physical units of variables and parameters, and is meaningful only when the units of the model are known. In the general case, the variables and the parameters each have different physical units, and therefore the sensitivity coefficients cannot be compared with each other.

To make the sensitivity results independent of the units of the model, usually normalized sensitivity coefficients are applied. The normalized local sensitivity matrix is denoted by $\bar{\mathbf{S}}$ and is defined as

$$\bar{\mathbf{S}} = \left\{ \frac{k_j}{y_i} \frac{\partial y_i}{\partial k_j} \right\}. \tag{5.17}$$

These coefficients represent a linear estimate of the percentage change in the variable y_i caused by a one percent change in the parameter k_j. The normalized sensitivity coefficients are independent of the original units of the model, and are comparable with each other.

A practical difficulty in handling sensitivity matrices comes from their size. A reasonably sized model may consist of 50 variables and 100 parameters. This results in a sensitivity matrix of 5000 elements. In addition, if the sensitivities are studied at 20 time points then 10^5 numbers have to be compared and analyzed. It is inevitable that some methods have to be used for summarizing the sensitivity information.

5.5.2 Effect of Changing one Parameter on Several Variables

In model optimization, the improvement of the fit is expressed by the change in a single number. This is achieved by introducing an objective function, which converts the multivariate output of the model to a single value. As an example, such an objective function can be:

$$e(t_1, t_2) = \sum_{i=1}^{n} w_i \left[\frac{y_i^*(t_1, t_2) - y_i(t_2)}{y_i(t_2)} \right]^2, \tag{5.18}$$

where $y_i(t_2)$ is the solution of the model at time t_2 at the nominal parameter set and $y_i^*(t_1, t_2)$ is the solution of the model at time t_2 using a parameter set perturbed at time t_1. The weights w_i allow the expression of the relative importance of the model variables according to the modeller. For some variables, this weight can be zero, showing that the variable has to be present in the model as an auxiliary variable, but its value is not interesting at all.

The sensitivity of the objective function above can be calculated from the local variable sensitivities:

$$\frac{\partial e}{\partial k_j}(t_1, t_2) = \sum_{i=1}^{n} w_i \left[\frac{1}{y_i} \frac{\partial y_i}{\partial k_j}(t_2, t_1) \right]^2. \tag{5.19}$$

Investigation of the sensitivity of objective functions significantly decreases the number of sensitivities to be inspected. However, for a fixed time of perturbation t_1, the sensitivities still have to be studied at several time points t_2 to get an impression of the change of sensitivities in time.

The next stage of information compression is the application of time-integrated sensitivities. The corresponding objective function is

$$e = \int_{t_1}^{t_2} \sum_{i=1}^{n} w_i \left[\frac{y_i^*(t_1, t_2) - y_i(t_2)}{y_i(t_2)} \right]^2 dt \tag{5.20}$$

The sensitivity of this objective function can be approximately calculated by

$$\frac{\partial e}{\partial k_j} = \sum_{h=2}^{l} \sum_{i=1}^{n} w_i \left[\frac{1}{y_i} \frac{\partial y_i}{\partial k_j}(t_h, t_1) \right]^2. \tag{5.21}$$

Sensitivities of objective functions, calculated from normalized sensitivities are called *overall sensitivities* (Vajda *et al.*, 1985). Selecting proper weights w_i, the overall sensitivities provide information on the importance of model parameters.

5.5.3 Effect of Simultaneously Changing Several Parameters on Several Variables

The overall sensitivities give information on the change of single parameters only. However, changing several parameters simultaneously can strengthen or weaken the effect of single parameter changes. First-order local sensitivities always correspond to 'changing one parameter at a time', and do not show the effect of simultaneous parameter changes. *Principal component analysis* (Vajda *et al.*, 1985; Vajda and Turányi, 1986) can, however, be used to estimate the effect of simultaneous parameter changes on several variables, based on local sensitivities only.

Use the time-integrated objective function (5.20) to assess the effect of parameter changes and replace the integral by a summation:

$$e(\boldsymbol{\alpha}) = \sum_{h=2}^{l} \sum_{i=1}^{n} \left[\frac{y_i^*(t_h) - y_i(t_h)}{y_i(t_h)} \right]^2. \tag{5.22}$$

Assuming that all parameters are positive, normalized parameters, $\boldsymbol{\alpha}$, defined as $\boldsymbol{\alpha} = \ln \mathbf{k}$, can be used. If some of the parameters are negative, a simple modification of the model can lead to all-positive parameters. For simplicity, let the weights now be either 1 or 0. Weight 0 deletes the corresponding row from the sensitivity matrix. The local change of the objective function above around the nominal values of parameters $\boldsymbol{\alpha}^0$ can be approximated by the local sensitivity matrix:

$$e(\boldsymbol{\alpha}) \approx (\Delta\boldsymbol{\alpha})^{\mathrm{T}} \tilde{\mathbf{S}}^{\mathrm{T}} \tilde{\mathbf{S}} (\Delta\boldsymbol{\alpha}), \tag{5.23}$$

where $\Delta\boldsymbol{\alpha} = \boldsymbol{\alpha} - \boldsymbol{\alpha}^0$, and the matrix $\tilde{\mathbf{S}}$ has been composed from a series of local sensitivity matrices, belonging to times $(t_1, t_2), \ldots, (t_1, t_h)$:

$$\tilde{\mathbf{S}} = \begin{bmatrix} \hat{\mathbf{S}}_2 \\ \hat{\mathbf{S}}_3 \\ \vdots \\ \hat{\mathbf{S}}_h \\ \vdots \\ \hat{\mathbf{S}}_l \end{bmatrix}. \tag{5.24}$$

Equation (5.23) is a quadratic approximation to the real shape of the objective function. Any cross-section of this approximate objective function is a hyperellipsoid, defined by the matrix $\tilde{\mathbf{S}}^T\tilde{\mathbf{S}}$. The orientation of the ellipsoid with respect to the parameter axes is defined by the eigenvectors of the matrix $\tilde{\mathbf{S}}^T\tilde{\mathbf{S}}$, while the relative lengths of the axes of the ellipsoid are revealed by the eigenvalues of this matrix.

If the axes of the ellipsoid are parallel to the axes of the parameter space, there is no synergistic effect among the parameters, and the relative lengths of the axes define the relative importance of parameters. However, if, say, the direction of the longest axis of the ellipsoid is at 45° on the plane of two of the parameter axes, this means that the effect on all variables by changing one parameter can be well corrected by also changing another parameter.

A similar interpretation can be given using the term *principal component*. A principal component is a new parameter, obtained via a linear combination of the original parameters. Let matrix $\mathbf{U}$ denote the matrix of normalized eigenvectors of $\tilde{\mathbf{S}}^T\tilde{\mathbf{S}}$. Principal components are defined as

$$\boldsymbol{\Psi} = \mathbf{U}^T\boldsymbol{\alpha}, \tag{5.25}$$

and, using principal components, the objective function (5.23) can be given in a simpler form:

$$e = \sum_{i=1}^{n} \lambda_i(\Delta\Psi_i)^2, \tag{5.26}$$

where $\Delta\boldsymbol{\Psi} = \mathbf{U}^T\Delta\boldsymbol{\alpha}$ and $\boldsymbol{\lambda}$ is the vector of eigenvalues. Equation (5.26) provides another explanation of why the eigenvectors of matrix $\tilde{\mathbf{S}}^T\tilde{\mathbf{S}}$ reveal the related parameters and why the corresponding eigenvalues show the relative weights of these parameter groups.

From a practical point of view, principal component analysis is an inexpensive post-processing technique that extracts otherwise-unavailable information from the local sensitivity matrices.

5.6 INITIAL SENSITIVITIES

The solution of the initial-value problem (5.3) depends on the values of the parameters, but also on the initial values of the variables. Calculation of the *initial-value sensitivity matrix* has been introduced as a first step in the calculation of local sensitivities, according to the Green function method. It has been shown in Section 5.3.3 that the initial-value sensitivity matrix $\mathbf{K}(t, t_1) = \{\partial c_i(t)/\partial c_j^0(t_1)\}$ can be obtained as the solution of the following initial-value problem (Equation (5.10)):

$$\frac{d}{dt}\mathbf{K}(t, t_1) = \mathbf{J}(t)\mathbf{K}(t, t_1).$$

The initial value of $\mathbf{K}$ is a unit matrix. The initial-value sensitivities can be considered as if a unit perturbation were applied to the initial values, one-by-one, and the fate of this perturbation were monitored.

Initial-value sensitivities are interesting because they are related to time scales of models. If the time scales are well separated, variables can be categorized as fast or slow. The slow variables respond very slowly to a perturbation, since the perturbation puts them on a trajectory almost parallel to their original one, and therefore the initial value sensitivity of

a slow variable (i.e. the diagonal element belonging to a slow variable) remains close to unity for a long time. Fast variables quickly return to their original trajectory after the perturbation, and therefore their initial-value sensitivities decay to zero quickly. If the initial-value sensitivity of a variable exceeds the unit value instead of remaining close to unity or decaying this indicates that a slight increase in the variable increases its production rate. Such behavior is called *autocatalysis* in chemical kinetics.

The point of the quasi-steady-state approximation (QSSA) is that the values of slow variables determine the values of fast variables (Turányi *et al.*, 1993). This means that it is enough to solve a system of differential equations for the slow variables, and the values of fast variables can be calculated from the values of the slow ones using algebraic equations. The critical step in the application of the quasi-steady-state approximation is appropriate division of variables into fast and slow ones. Initial-variable sensitivities can do the job, but there are other approximate techniques, which provide similar information in a computationally less expensive way.

During the solution of initial-value problem (5.10), the values of variables change, and therefore the elements of the matrix $\mathbf{J}$ are continuously changing. On fixing the elements of $\mathbf{J}$ at the starting time, Equation (5.10) becomes a homogeneous linear system of differential equations with constant parameters. The solution of such a system is

$$\mathbf{K}' = \exp[\mathbf{J}(t_1)t]. \tag{5.27}$$

It has been shown that the Jacobians of chemical kinetic differential equations can frequently be rearranged to approximately lower triangular form (Turányi *et al.*, 1993). It is possible that a similar observation holds for many models in other disciplines. Consequently, for most chemical kinetic systems, the eigenvalues of the Jacobian are close to the diagonal elements of the Jacobian, $\lambda_i \approx j_{ii}$, where j_{ii} is the ith diagonal element of the Jacobian. Since the lifetime can be defined as $\tau_i = -1/j_{ii}$, this relation supports the traditional observation that short-lifetime variables decay rapidly after perturbation and behave as fast variables. This also means that the time history of the diagonal of the initial-value sensitivity matrix can be approximated as

$$k_{ii}(t) \approx \exp(j_{ii}t). \tag{5.28}$$

A more sophisticated handling of timescales takes into account that eigenvectors of the Jacobian define variable groups. The time scale separation is better if variable groups, not single variables, are considered and therefore a more accurate quasi-steady-state approximation with fewer variables can be applied. The corresponding numerical techniques (Lam and Goussis, 1988; Maas and Pope, 1992) represent a further development of the classical QSSA.

So far, only the interpretation of the diagonal elements of the initial-value sensitivity matrix has been discussed. The off-diagonal elements of the matrix $\mathbf{K}$ also contain important dynamic information, but their interpretation depends on the actual physical model. In general, the off-diagonal elements show the displacement of the trajectory of all other variables, in response to perturbing a given variable slightly. As an example, a large off-diagonal element indicates strong coupling between a fast and a slow variable, introducing large error into the QSSA calculation (Turányi *et al.*, 1993).

The whole initial-value sensitivity matrix can also be approximated based on an eigenvector–eigenvalue analysis of $\mathbf{J}(t_1)$ (Maas and Pope, 1994). Let t_2 be the time of observation of the initial-value sensitivity calculation and let $\mathbf{V}$ and $\tilde{\mathbf{V}}$ denote the matrices of right- and left-eigenvectors of $\mathbf{J}(t_1)$, respectively. The matrices $\mathbf{V}_f$ and $\tilde{\mathbf{V}}_f$ are truncated arrays, obtained

by deleting the columns and rows, respectively, belonging to the eigenvalues of the Jacobian larger than $-1/(t_2 - t_1)$. This means that the matrices $\mathbf{V}_f$ and $\tilde{\mathbf{V}}_f$ have dimensions $n \times n_f$ and $n_f \times n$, respectively, and belong to the n_f fast eigenvectors of the Jacobian. The initial-value sensitivity matrix can now be approximated by

$$\mathbf{K}(t_1, t_2) \approx \mathbf{P} = \mathbf{I} - \mathbf{V}_f \tilde{\mathbf{V}}_f. \tag{5.29}$$

5.7 FUNCTIONAL SENSITIVITIES

Many physical models contain input functions $k_i = k_i(\boldsymbol{r}, t), i = 1, 2, \ldots$, that depend on spatial coordinates $\boldsymbol{r}$ and/or time t. All of the same general questions about parametric sensitivity carry over to this function case, where the system output y is a *functional* of the inputs. Thus, Equations (5.2) and (5.4) have functional analogs at any order. For example, to first order, we have

$$\delta y = \sum_i \int \frac{\delta y}{\delta k_i(\boldsymbol{r}, t)} \delta k_i(\boldsymbol{r}, t)\, d\boldsymbol{r}\, dt, \tag{5.30}$$

and the functional sensitivity density is given by $S_i(\boldsymbol{r}, t) = \delta y / \delta k_i(\boldsymbol{r}, t)$. Keeping in mind that the model output y can also have position and/or time dependence, it is evident that the functional sensitivities provide a detailed input–output map. The analogy with parametric sensitivities extends beyond those defined in Equation (5.30), to include the full family of derived sensitivities for various applications.

Input functions $k_i = k_i(\boldsymbol{r}, t), i = 1, 2, \ldots$, can arise in many physical circumstances, but the most common case occurs in atomic and molecular physics, where the input involves fundamental intermolecular interactions between the atoms and molecules, and the goal is to reveal how these input functions influence the observable chemical and physical properties. In turn, the sensitivity of these properties to the input functions provides a basis for attempting to extract these functions from suitable observed laboratory output data. The basis for such inversions is rooted in Equation (5.30), where δy is the deviation between the observed value and that of the current theoretical model, with $\delta k_i(\boldsymbol{r}, t)$ being the deviation of the input function from its true value. Such inverse problems are typically ill-posed, calling for suitable regularization, and a number of inversions along these lines have been carried out (Ho and Rabitz, 1993).

5.8 SCALING AND SELF-SIMILARITY RELATIONS

Substantial effort can be involved in calculating sensitivity coefficients. The recognition of any patterns of behavior amongst these coefficients would be of considerable significance, not only for simplifying the sensitivity information, but also for the fundamental insight gained about the intimate workings of the system. There is certainly no *a priori* reason to expect the existence of particular patterns or relationships amongst the numerous sensitivity coefficients in a system, since this would imply the presence of hidden dynamical couplings between the system dependent and independent variables. However, such relationships amongst sensitivity coefficients have been identified through patterns of similar behavior in a variety of sensitivity calculations arising from problems in chemical kinetics,

especially of a combustion nature (Rabitz and Smooke, 1988). Such connections have been referred to as scaling and self-similarity relations, and the possibility of their existence has potentially important implications for model analysis, as well as system simplification. To be specific, the discussion here will be confined to the treatment of one-dimensional steady problems described by reaction–diffusion equations, often arising, for example, in combustion problems.

In typical case studies, the system differential equations are strongly coupled, and, even more importantly, it is generally possible to identify a distinct and *dominant* member of the dependent variable set, denoted without loss of generality as y_1. The assumed role of y_1 is to provide the strong coupling linkage between all of the N differential equations or dependent variables. A typical example of this behavior in combustion might be the identification of y_1 as the temperature or the concentration of some particularly important chemical species. This dominance is asserted to imply total coordinate and parametric entrainment such that

$$y_n(x, \boldsymbol{\alpha}) \approx F_n(y_1(x, \boldsymbol{\alpha})), \tag{5.31}$$

where F_n is an appropriate non-determined function. Clearly, this relation is an approximation, and we take it as a working anstatz to explore its consequences. Simple differentiation of Equation (5.31) with respect to the system parameter α_j, as well as to x, will lead to

$$\frac{\partial y_n(x)}{\partial \alpha_j} \approx \frac{\partial y_1(x)}{\partial \alpha_j} \frac{\partial y_n}{\partial x} \left(\frac{\partial y_1}{\partial x} \right)^{-1}. \tag{5.32}$$

Equation (5.32) is referred to as a scaling relation in that the sensitivity of the nth dependent variable is prescribed in terms of the sensitivity of the first member and relevant slope information. Also, note that these relations are independent of the unknown function F_n.

Although the result in Equation (5.32) is based on the hypothesis in Equation (5.31) that $y_1(x, \boldsymbol{\alpha})$ is dominant, it is a simple matter to show that the scaling relations are in fact fully symmetrical with regard to all of the dependent variables. Consideration of Equation (5.32), along with the same equation for the n'th dependent variable immediately leads to the following result:

$$\frac{\partial y_n(x)}{\partial \alpha_j} \approx \frac{\partial y_{n'}(x)}{\partial \alpha_j} \frac{\partial y_n}{\partial x} \left(\frac{\partial y_{n'}}{\partial x} \right)^{-1} \tag{5.33}$$

for all n and n' strongly coupled dependent variables. This implies that Equation (5.31) may be used as reciprocal relations such that the special role provided by y_1 may be inverted and replaced by any member of the strongly coupled dependent variable set. In cases of non-monotonic coordinate dependence, this inversion has to be done on a piecewise basis. Similarly, singular points where $\partial y_l / \partial x = 0, l = 1, \ldots,$ indicate changes in the monotonicity of the dependent variables, and it is clear from Equation (5.32) that the scaling relations can exhibit singularities at these points (corrections to the scaling relations may be especially significant near these points).

The scaling relations have been shown to be remarkably accurate in a number of numerical calculations. The actual presence of scaling was only identified subsequent to finding evidence for the more powerful self-similarity conditions. The arguments leading to self-similarity involve a number of operations with the system dynamical equations and the use of the Green function analog of Equation (5.32). The net result is the identification of the

approximate similarity relationship

$$\frac{\partial y_n(x)}{\partial \alpha_j} \approx \frac{\partial y_n}{\partial x}\left(\frac{\partial y_1}{\partial x}\right)^{-1}\lambda(x)\sigma_j. \tag{5.34}$$

The term $\lambda(x)$ is a function and σ_j is a constant, with both being characteristic of the particular dynamic system. The self-similarity condition in Equation (5.34) has a surprisingly simple structure that states that, under its conditions of validity, all system sensitivities reduce to knowledge of a scalar function $\lambda(x)$, the dependent variable spatial slopes, and a vector of characteristic constants $\boldsymbol{\sigma}$. The vector $\boldsymbol{\sigma}$ has the same length as the parameter vector; however, its components are generally complicated functions of all the system parameters.

The simple form of Equation (5.34), upon substitution into Equation (5.31), leads to the prediction

$$\frac{\partial y_n(x)/\partial \alpha_j}{\partial y_n(x)/\partial \alpha_{j'}} \approx \sigma_j/\sigma_{j'}. \tag{5.35}$$

This equation states that the sensitivity of a given dependent variable, with respect to a sequence of parameters, may be approximately described by a self-similar set of curves in (coordinate) space, all related by constants in the vector $\boldsymbol{\sigma}$. The scaling behavior suggested by Equation (5.35) is often seen to be valid (Rabitz and Smooke, 1988) for at least a subset (i.e. the strongly coupled subset of dependent variables).

The essential assumption underlying the self-similarity and scaling results in Equations (5.32) and (5.35) is the basic entrainment conditions in Equation (5.31). A growing body of numerical results has justified these relations at least qualitatively, and even quantitatively in some cases. The consequences of scaling and self-similarity behavior go beyond mere simplification of the sensitivity coefficients. The existence of this behavior suggests that the physical system itself may be simplified.

The basic implication behind the existence of dominant variable dependence is that strongly coupled systems, in fact, may behave in a simpler fashion than was at first believed. It is curious that this behavior appears likely to be more valid in problems that are inherently nonlinear and normally thought of as having more complex behavior than arising in linear problems. In a sense, the strong mixing often found in nonlinear systems can lead to an unusual level of parametric simplicity under appropriate conditions.

5.9 APPLICATIONS OF LOCAL SENSITIVITIES

5.9.1 Uncertainty Analysis Based on Local Sensitivities

In some cases, many measurements are available for model parameters, and therefore the probability density functions or at least the variances of the parameters are known. The task of uncertainty analysis is to determine the probability density function (pdf) of the model output at a given time, if the pdfs of the parameters are known. A less ambitious task is the calculation of the variance of the model output, knowing the variance of parameters.

Capability for uncertainty analysis is one of the major features of global sensitivity analysis methods. However, a first estimate can also be made, based on local sensitivities (Atherton *et al.*, 1975).

Using the equations for the propagation of error, a linear estimate can be given for the variance of model output $\sigma^2(y_i)$:

$$\sigma_j^2(y_i) = \left(\frac{\partial y_i}{\partial k_j}\right)^2 \sigma^2(k_j). \tag{5.36}$$

$$\sigma^2(y_i) = \sum_j \sigma_j^2(y_i). \tag{5.37}$$

$\sigma^2(y_i)$ is the sum of the contributions of the uncertainties of each parameter k_j to model output y_i, denoted by $\sigma_j^2(y_i)$. The partial variances $S\%_{ij}$ give the percentage contribution of the uncertainty of parameter j to the total uncertainty of model output y_i:

$$S\%_{ij} = \frac{\sigma_j^2(y_i)}{\sigma^2(y_i)} 100. \tag{5.38}$$

Uncertainty analysis using local sensitivities is not a substitute for the better-based global methods, like FAST, but may provide an order-of-magnitude estimation.

One of the applications of uncertainty analysis is the determination of strategies for the improvement of a model. The most uncertain parameters should be studied in more detail for the most effective improvement of model reliability.

5.9.2 Global Parametric Mapping

The predictions of local sensitivity analysis are best in the neighborhood of the reference operating point in parameter space. Nevertheless, there is interest in extracting as much information from the analysis as possible, particularly regarding parameter behavior over larger domains. Short of employing techniques attempting to fully explore this issue, local gradient analysis has some special contributions to make. First, if a sufficient number of derivatives are available in Equations (5.2) or (5.4) then the results may often be extended by Padé approximates. In addition, power-law or other types of scaling relations may also be postulated to exist over the parameter space.

Feature sensitivity analysis (Kramer *et al.*, 1984) provides a systematic means of nonlinearly probing a region of parameter space. As an explicit illustration of this procedure, consider $y(\mathbf{r}, t, \alpha)$ as the objective of interest, where the parameter dependence is explicitly indicated. By an examination of the $\mathbf{r}$ and t dependence of this observation, it is assumed that meaningful characteristic features may be identified and an explicit functional form $\tilde{y}(\mathbf{r}, t, \beta)$ chosen that contains the feature parameters $\beta_1, \beta_2, \ldots$. By implication, the two forms of the observation are equivalent:

$$y(\mathbf{r}, t, \alpha) \cong \tilde{y}(\mathbf{r}, t, \beta(\alpha)). \tag{5.39}$$

Equation (5.39) implies a relationship between β and α. In practice, we shall only know a solution of the model equations and the sensitivities at a reference point α^0 in parameter space. This information will not be sufficient to determine the functional relation $\beta = \beta(\alpha)$; however, we may determine $\beta^0 = \beta(\alpha^0)$ at the system reference point and the corresponding sensitivity coefficients $(\partial\beta_i/\partial\alpha_j)_{\alpha^0}$. In order to achieve this goal, the feature parameters in Equation (5.39) must be adjusted consistently with that relation. One technique is to employ minimization of the least-squares functional

$$R = \int\int d\mathbf{r}\, dt [y(\mathbf{r}, t, \alpha) - \tilde{y}(\mathbf{r}, t, \beta)]^2. \tag{5.40}$$

Minimization of R with respect to the feature parameters will yield the equation

$$\frac{\partial R}{\partial \beta_i} = \int\int d\mathbf{r}\, dt\, [y(\mathbf{r}, t, \alpha) - \tilde{y}(\mathbf{r}, t, \beta)] \frac{\partial \tilde{y}}{\partial \beta_i}(\mathbf{r}, t, \beta) = 0. \tag{5.41}$$

The derivative in the integrand of Equation (5.41) may be explicitly evaluated by recalling that $\tilde{y}$ has a known functional form with respect to its variables. Equation (5.41) implies the existence of the relationship $\beta = \beta(\alpha^0)$, but again it must be recalled that $y(\mathbf{r}, t, \alpha^0)$ is assumed known only at the parameter reference point. Therefore, differentiation of Equation (5.41) with respect to one of the input parameters will yield an equation that may be solved for the desired feature sensitivity coefficients $(\partial \beta_i / \partial \alpha_j)_{\alpha^0}$. In carrying out this last differentiation, it is evident that the system sensitivity coefficients $\partial y_i(\mathbf{r}, t, \alpha)/\partial \alpha_j$ (or, if appropriate, their functional analog) will enter. The implementation of this overall procedure of feature sensitivity analysis is quite straightforward, and, in practice, it is only limited by one's ingenuity in choosing simple but flexible functional forms $\tilde{y}(\mathbf{r}, t, \beta)$.

The technique of feature sensitivity analysis embodied by the relation in Equation (5.39) has an immediate spin-off application to global parameter mapping. Equation (5.39), for the present purposes, may be recast into the following form:

$$y(\mathbf{r}, t, \alpha + \Delta\alpha) \equiv \tilde{y}(\mathbf{r}, t, \beta(\alpha + \Delta\alpha)). \tag{5.42}$$

This equivalence cannot be directly applied, since we do not have full knowledge about the relation between β and α. However, the feature sensitivity analysis based on Equation (5.39) leads to knowledge of β and the sensitivities of β about the nominal operating point. Therefore, we may consider the expansion

$$\beta(\alpha + \Delta\alpha) \approx \beta(\alpha) + \frac{\partial \beta}{\partial \alpha} \Delta\alpha. \tag{5.43}$$

Substitution of Equation (5.43) into Equation (5.42) will yield a *nonlinear* scaling expression with respect to the parameters $\Delta\alpha$. This feature parameter scaling approach is both computationally practical as well as likely to give acceptable results over an extended neighborhood around the system operating point. A clear example of this situation arises in the singular perturbation problem of parameter dependence in oscillating flames. In those cases where the parameters influence the system frequency (Kramer *et al.*, 1984), a local sensitivity analysis will produce secular growth. In contrast, a feature analysis on the system frequency should be stable.

5.9.3 Parameter Estimation

Some parameter estimation methods, such as the simplex method, do not use local sensitivities. However, in most cases, calculation of the slope of the objective function in the space of parameters is a part of the parameter estimation algorithm. Strangely, while much work was devoted to finding better algorithms for the calculation of local sensitivities, this knowledge was not recycled to the parameter estimation programs. Most parameter estimation programs, even nowadays, use the brute force method for calculation of the slope of the objective function. The inaccurate calculation of the slope usually does not spoil the final result of parameter estimation, but may slow the procedure. Application of the decoupled direct method (Section 5.3.2) and the conversion of variable sensitivities to the sensitivity of the objective function (Equation (5.21)) should be used to improve the numerical efficiency of most programs for the estimation of parameters of ordinary differential equations.

All parameter estimation procedures fail if an ill-conditioned problem is encountered. An ill-conditioned problem means that the data do not carry enough information to provide an estimate of all parameters fitted. Usually the only sign of this is that the parameter estimation algorithm fails to converge. Local sensitivities and principal component analysis (Turányi, 1990a) may help to avoid this problem in the following way.

In the case of parameter estimation, the normalized sensitivity matrix, to be investigated, is defined as

$$\tilde{\mathbf{R}} = \frac{\mathbf{k}}{\mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{k}}, \tag{5.44}$$

where $\mathbf{h}(\mathbf{y})$ is the instrumental function, which converts the calculated variables to the calculated observable quantities (e.g. signals of the experimental apparatus). The matrix $\tilde{\mathbf{P}}$ corresponds to the matrix $\tilde{\mathbf{S}}^{\mathrm{T}}\tilde{\mathbf{S}}$ of Equation (5.23):

$$\tilde{\mathbf{P}} = \sum_{l=1}^{L} \tilde{\mathbf{R}}^{\mathrm{T}}(t_l)\mathbf{W}_l(t_l)\tilde{\mathbf{R}}(t_l) \tag{5.45}$$

The matrix $\mathbf{W}$ is the weight matrix. In general, it is the inverse of the covariance matrix. If the covariances are not known or assumed to be zero, $\mathbf{W}$ is diagonal, where the diagonal elements are the inverses of the variances. In the unweighted case, $\mathbf{W}$ is the identity matrix.

Eigenvector–eigenvalue analysis of the matrix $\tilde{\mathbf{P}}$ reveals which parameters can be determined from a given experiment. Parameters that are not related to large eigenvector elements of large eigenvalues cannot be determined. Parameters that are not coupled to other parameters and are linked to large eigenvalues can be fitted easily. A typical situation is when several parameters are strongly coupled, for example when only the ratio of two parameters has an influence on the objective function. In this case, the corresponding eigenvector has the form $(\sqrt{2}, \sqrt{2}, 0, 0, \ldots, 0)$. If both parameters are fitted simultaneously, the result is a deep-valley-like objective function, and the fitting procedure fails. To avoid this problem, one of the parameters should be fixed at a nominal value, and only the other parameter has to be fitted. However, the result of fitting is always the ratio of the two parameters and not the individual values of parameters. Individual values can be obtained from independent experiments or other sources.

The matrix $\tilde{\mathbf{P}}$ has been calculated as the first guess of the parameter values. During the parameter estimation procedure, improved estimates of the parameters become available. A substantially different parameter set may provide a qualitatively different picture, and therefore the analysis should be repeated at every stage of the parameter estimation. Carrying out a principal component analysis at the beginning and during the parameter estimation helps to avoid many problems, and should always be encouraged.

5.9.4 Experimental Design

Experimental design is a branch of mathematical statistics where the aim is to find experimental conditions that provide the most information for the determination of some parameters in a model. Most experimental design algorithms are applicable only for linear models. The above procedure, based on eigenvector–eigenvalue analysis of the matrix $\tilde{\mathbf{P}}$, can be used also for experimental design in the case of any nonlinear model. By selecting the method of measurement (the function h), and the times of measurement t_l, the information content of the experiment for the determination of a given parameter can be optimized. Note, however, that this optimization is based on an *a priori* assumption of the parameters

and of the model structure. The experimental design, experiment, and parameter estimation cycle has to be repeated several times until a satisfactory result is obtained.

5.9.5 Stability Analysis

A common concern is the stability of dynamical systems to disturbances, either in the operating parameters or the state of the system during its evolution. An analysis of the system Green function in Equation (5.10) addresses both of these issues. This is evident, since $K_{ij}(t, t_1) = \partial C_i(t)/\partial C_j^0(t_1)$. The Green function dictates the response to all parameter disturbances, as is evident in Equation (5.11). Since Equation (5.10) for the Green function is a linear differential equation driven by the Jacobian, its eigenvalue analysis can reveal the stability of the dynamics. Any eigenvalues with positive real parts indicate growth behavior with respect to time, and, hence, instability with regard to disturbances. These eigenvalues may also be expressed in terms of Lyapunov stability numbers. A complete analysis would also include the general case where the Jacobian is time-dependent. Cases of this type have been explored (Hedges and Rabitz, 1985) for explosive chemical kinetics, limit-cycle oscillations, and classical dynamics.

5.9.6 Investigation of Models

Local sensitivity analysis can be considered as a perturbation study of models. In the case of time-dependent models, the change of a parameter value influences first the values of those variables that contain that parameter in their rate expression. This effect spreads further to other variables. By inspecting this spread, much new information can be gathered on the structure and behavior of the model. As has been shown in Section 5.2, the local sensitivity matrix $\mathbf{S}(t_1, t_2)$ depend on both the time of perturbation, t_1, and the time of observation of the effect, t_2. Selection of these times provides a wide range of opportunities (Hwang, 1988) for the study of models.

5.9.7 Reduction of Models

Reduction of models means that the same phenomenon is described by a smaller, simpler model, derived from the larger model. The derived model can be entirely different from the original one, e.g. when a dynamical system is modeled by a system of difference equations instead of a system of differential equations (see e.g. Turányi, 1994). Another way of reduction is variable lumping (see e.g. Tomlin *et al.*, 1994), when the array of variables is replaced by a smaller set of variables and the new and old set of variables are related to each other by linear or nonlinear functions. Also, effective model reduction can be based on the time scale separation of models (see e.g. Maas and Pope, 1992; Turányi *et al.*, 1993; Tomlin *et al.*, 1997).

In this section, a more restrictive meaning of model reduction is used. The reduced model is obtained from the original model by setting some of its parameters to zero. This might mean that some of the variables are also cut out from the model.

Detection of redundant variables should be the first step in model reduction. In the case of most models, the user is interested in only some of the variables and their effect on the model output. These variables can be called *important variables*. In most models, there are also auxiliary variables. They should be there for making the model work, but their actual value is not interesting for the modeler. Such variables are termed here *necessary variables*. Also, in most models, there are *redundant variables* as well, which can be deleted without any change of the model output.

Two methods have been proposed (Turányi, 1990b) for the detection of redundant variables in reaction kinetic models. The first method is based on the preparation and simulation of a series of reduced models. If all parameters related to a given variable are set to zero and the calculated model output for the important variables is practically identical to that of the original model, then this variable and the corresponding parameters can be eliminated from the model. However, in many cases, the elimination of a smaller number of parameters provides a more accurate reduced model. An algorithm was given to find the minimal number of parameters to be eliminated in this step, but it exploits the special structure of the kinetic differential equations, and therefore cannot be applied to any model.

The second method is based on the investigation of the Jacobian, and is more general, although it provides a suggestion only, which has to be checked by the preparation of the appropriate reduced model. The Jacobian $\mathbf{J} = \{\partial f_i/\partial y_j\}$ can also be considered as a sensitivity matrix. It indicates the sensitivity of the calculated variable rates to perturbing the values of variables. According to the ideas described in Sections 5.5.1 and 5.5.2, further processing of this matrix makes the information more readily available. Application of the normalized Jacobian $\tilde{\mathbf{J}} = \{(y_i/f_i)\,\partial f_i/\partial y_j\}$ makes the information independent of the units of variables, and the corresponding overall sensitivity shows the effect of variable perturbation on a group of N variables:

$$B_i = \sum_{j=1}^{N} \left(\frac{y_i}{f_j} \frac{\partial f_j}{\partial y_i} \right)^2 . \tag{5.46}$$

B_i shows the instantaneous or direct effect of changing variable i on the values of N other variables. Variable i influences the rate of variable j directly, if variable i is present in the rate term of variable j on the right-hand side of the ODE. Of course, an indirect effect is also possible, when variable i influences the rate of variable k, while k controls the rate of j. The Jacobian shows the direct effects only.

Redundant variables can be detected by using the following algorithm: Consider first the N important variables only, and calculate B_i, which expresses the strengths of direct effect of each variable on the important variables. The variables most closely connected directly to the important variables are added to the group of N variables to be investigated, and the procedure is repeated. The algorithm usually converges in a few steps, and the group now contains the important variables and all variables that have a strong influence on their rate, directly or indirectly. The variables left out are the redundant variables.

This algorithm is local in time, and therefore has to be repeated at several time points. Also, it is based on a local linear approximation, and therefore its findings have to be confirmed by trial calculation of appropriate reduced models. Having eliminated the redundant variables from the model, it contains important and necessary variables only. The next step is the identification of redundant parameters.

It is generally assumed, wrongly, that if the sensitivity of a parameter is small for all important variables, then this parameter can be eliminated from the model. However, the local sensitivities show only the effect of small changes of parameters (which may be called 'parameter tuning'). The order of importance of parameters deduced from the sensitivity of important variables can be called *tuning importance*. Considering a group of important variables, the order of tuning importance can be deduced from the overall sensitivity values (5.21).

Setting a parameter to zero is a drastic effect, and such a change may alter significantly the calculated value of an important variable even if the corresponding local sensitivity is small. The reason is the indirect effect again: setting a parameter to zero may significantly

influence the value of a necessary variable, and this effect extends to the important variable. However, strong influence on a necessary variable can usually be detected at the nominal point of parameters, and such a parameter has high sensitivity for some of the necessary variables. A rule of thumb is that a parameter can be eliminated (i.e. can be set to zero) in a model, if the sensitivity of all important and necessary variables of the corresponding parameter is small at any time during the interval considered (Hwang, 1982). It is important to scan the whole time interval, because if a parameter is influential only at the beginning and its value does not effect the location of the stationary point, then the calculated sensitivity goes to zero as time advances. Overall sensitivities, as defined in Equation (5.21), provide a good guess for *reduction importance*, if the summation has been extended to all important and necessary variables. Using principal component analysis, parameters of high reduction importance all appear with large eigenvector elements of large eigenvalues, if again all important and necessary variables are considered.

An alternative method for model reduction is based on the study of the normalized rate sensitivity matrix $\tilde{\mathbf{F}} = \{(k_i/f_i)\,\partial f_i/\partial k_j\}$. This matrix shows the instantaneous effect of changing a parameter on the rate of variables. Principal component analysis of $\tilde{\mathbf{F}}$, considering the important and necessary variables, reveals all parameters that can be eliminated from the model without significant changes in the values of important parameters (Turányi *et al.*, 1989). Since $\tilde{\mathbf{F}}$ can be calculated easily in an algebraic way, this technique is fast and simple. However, studying the effect of parameters on the rates instead of the model output is a less direct approach, and the reduced model that is found has to be validated by comparing its solution with that of the full model.

5.10 CONCLUSIONS

All modelling work includes the following steps: collection of information on the parameters and on the model structure, setting up the model, and validation of the model against experimental or observation data. The next step should be an analysis of the model, which includes the assessment of the importance of parameters and reduction of the model by eliminating the redundant parts.

Global sensitivity analysis methods have been designed to study the model in a wide range of parameters. However, in the case of large models, calculation of global sensitivities is computationally prohibitive, but local sensitivities can provide useful information on the behavior of the model near the nominal values of parameters.

A general purpose program package, called KINAL (Turányi, 1990c) is available for manipulating and processing the local sensitivity matrix in many ways discussed in this chapter. KINAL and a specific program, called KINALC, for the analysis of combustion and gas kinetic problems are available through the World Wide Web. The functionality of KINAL and KINALC are briefly described in the software Appendix.

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