PRACTICAL ASPECTS OF SENSITIVITY ANALYSIS FOR DYNAMIC MODELS

Dirk J.W. De Pauw and Peter A. Vanrolleghem, Biomath, Ghent University, Belgium
Corresponding author: Dirk J.W. De Pauw
Biomath - Ghent University
Coupure Links 653, 9000 Ghent, Belgium
Phone: +32 9 264 5935, Fax: +32 9 264 6220
email: dirk.depauw@biomath.rug.ac.be

Abstract. Sensitivity analysis can be used to quantify the magnitude of the dependency of model predictions on certain modelling assumptions, e.g. parameter values, initial conditions or inputs. The finite difference method, a local sensitivity analysis technique, is discussed in detail and situated among other methods. A lot of attention is paid to the practical issues concerning the implementation of this technique, more specifically the effect of non-linearities of the model and numerical problems. The influence of the perturbation factor on the sensitivity calculations is investigated and different criteria are proposed to assess the quality of the sensitivity functions. The influence of numerical integrator settings is also demonstrated.

1. Introduction

Sensitivity analysis studies the "sensitivity" of the outputs of a system to changes in the parameters, inputs or initial conditions which are often poorly known. Sensitivity analysis can be divided into two large categories: local and global sensitivity analysis. Local sensitivity analysis methods refer to small changes of parameters, while global methods refer to the effect of simultaneous, possibly orders-of-magnitude parameter changes. Both categories will be described in section two of this paper, with the focus on local sensitivity analysis techniques. One of these sensitivity analysis techniques, the finite difference method, will be discussed in detail in section four. The finite difference technique is often used to obtain a sensitivity measure, most of the time without considering the nonlinearity of the model or the round-off error introduced by the output calculations. These influences will be analysed and discussed in detail.

2. Sensitivity analysis

The general form of the systems that will be discussed is given by following equation.

$$\frac{dy}{dt} = f(y, \theta) \tag{1}$$

where y is an n-dimensional vector of state variables, θ is the p-dimensional vector of system parameters (which can include the initial conditions y^0 and input variables), and t is the independent variable.

The sensitivity of a state variable y to a parameter θ can be expressed as a sensitivity function (equation 2). A state variable y is called sensitive to θ if small changes in θ produce significant changes in y. On the other hand, a variable y is called insensitive to θ if changes in θ produce no changes in y.

$$S(t) = \frac{\partial y(t)}{\partial \theta} \tag{2}$$

This partial derivative can be analytically solved if the analytical solution of equation 1 is known. Unfortunately, this is rarely the case and numerical methods have to be used in order to approximate the sensitivity function (equation 2). Local sensitivity analysis techniques evaluate this partial derivative at one specific parameter value, also called the nominal parameter value. On the other hand global techniques evaluate this partial derivative in various points of the parametric domain. Both local and global analyses are useful in studying the behaviour of a system since each has advantages and disadvantages. For a detailed review of existing sensitivity techniques reference is made to the reviews of Turanyi [22] and Rabitz et al. [18]. The main focus of this paper will be the local sensitivity analysis techniques. Various techniques for local sensitivity analysis will be described here, which are (a) the finite difference

method, (b) the direct differential method, (c) the Green's function method, (d) the polynomial approximation method and (e) automatic differentiation.

The simplest way of calculating local sensitivities is to use the finite difference approximation. This technique is also called the brute force method or indirect method. It is very easy to implement because it requires no extra code beyond the original model solver. The partial derivative defined in equation 2 can be mathematically formulated by the equation given below (forward difference).

$$\frac{\partial y_i}{\partial \theta_j} = \lim_{\Delta\theta_j \to 0} \frac{y_i(t, \theta_j + \Delta\theta_j) - y_i(t, \theta_j)}{\Delta\theta_j} \tag{3}$$

This equation is only valid if we consider an infinitesimal variation (perturbation) of the parameters, inputs or initial conditions θ ($\Delta\theta_j \to 0$).

Equation 3 shows that the application of the finite difference method requires the solution of the model (equation 1) using the nominal value of the parameters $y_i(t, \theta_j)$ and p solutions of the equations using perturbed parameters $y_i(t, \theta_j + \Delta\theta_j)$. It should be noted that only one parameter is perturbed at a time while all others are kept at their nominal value. The sensitivities obtained belong to the $(\theta + \Delta\theta/2)$ parameter set because equation 3 can also be seen as the average of the sensitivities of the model output y_i at θ_j and $\theta_j + \Delta\theta_j$. If the sensitivity coefficients are desired to belong to the nominal values θ_j, equation 3 should be modified into

$$\frac{\partial y_i}{\partial \theta_j} \approx \frac{y_i(t, \theta_j + \Delta\theta_j) - y_i(t, \theta_j - \Delta\theta_j)}{2\Delta\theta_j} \tag{4}$$

This central difference formula requires $2p$ solutions.

The finite difference technique was found to be too calculation intensive, especially in cases where sensitivities to many parameters were required. Therefore Atherton et al. [1] developed the direct method for sensitivity analysis. Differentiation of equation 1 with respect to θ_j yields the following set of sensitivity differential equations. The solution of these equations results in the sensivity functions.

$$\frac{d}{dt}\frac{\partial y}{\partial \theta_j} = \frac{\partial f}{\partial y}\frac{\partial y}{\partial \theta_j} + \frac{\partial f}{\partial \theta_j} \tag{5}$$

The term $\partial f/\partial y$ of equation 5 is recognised as the Jacobian J of the original system given by equation 1. Equations 1 and 5 are coupled through $\partial f/\partial y$ and $\partial f/\partial \theta$. This means that the solution of equation 5 requires the knowledge of the solution of equation 1 in all points where the ODE solver calculates the right-hand side of equation 5. Connections between these two sets of equations can be made in one of the following ways:

1. Solve equations 1 and 5 for every parameter θ simultaneously, which requires the solution of (p+1)n ODE's. The direct solution of this large system is inefficient. Although a solver has been built for these systems, based on the decomposed direct method [23], it is not used very often.

2. Solve the couple of equations 1 and 5, which requires the solution of 2n ODE's p times (for every parameter) [3]. This version is the simplest to code, but is the least economical and might cause numerical problems due to ill conditioned Jacobian matrices [4, 5, 14].

3. The solution of equations 1 and 5 can be decoupled. First, differential equations 1 are solved and the results are stored in a table. Then equations 5 are solved using the values stored in the table. If values are required at times without tabulated values, they are computed by interpollation [1, 4, 14, 15].
   An improved version of this decoupled method was introduced by Dunker [6, 7]. His method made use of the fact that the Jacobian matrix of equations 1 and 5 is the same and that it only has to be triangulated once every time step.

The difficulties of solving the large sets of differential equations led to the development of the Green's function method or variational method [13]. This method makes use of the fact that the sensitivities (equation 5) can be expressed in integral, rather than differential form.

$$\frac{\partial y(t)}{\partial \theta} = K(t, 0)\frac{\partial y(t)}{\partial \theta}(0) + \int_0^t K(t, \tau)\frac{\partial f(\tau)}{\partial \theta}d\tau \tag{6}$$

In this equation, $K(t, \tau)$ is an $n \times n$ Green's function matrix or kernel, given by:

$$\frac{d}{dt}K(t, \tau) - J(t)K(t, \tau) = 0, t > \tau \tag{7a}$$

$$K(\tau, \tau) = I \tag{7b}$$

There are a number of variations of the Green's function method and they differ from each other in the calculation of the matrix K. Probably the most used method is the GFM/AIM method (Analytically Integrated Magnus). This method approximates K by a matrix exponential [14]. It is beyond the scope of this paper to go into more details on these solving techniques.
In all Green's function methods, the numerical effort is proportional to the number of variables and not the number of parameters. So this method should be preferred when a large number of parameters is involved compared to the number of variables. When the number of variables is much larger than the number of parameters, direct differential methods should be used.

In 1983 another local sensitivity analysis technique was developed by Hwang [11, 12] called the polynomial approximation method. The basic idea behind this method is that the temporal behaviour of the solution of equation 1 is approximated by Lagrange interpolation polynomials. From these polynomials the sensitivity coefficients can easily be calculated. This method however was never applied to a real problem.

Recently a technique called automatic differentiation gained a lot of attention. Automatic differentiation techniques are based on the fact that every function, no matter how complicated, is executed on a computer as a sequence of elementary functions. By applying the chain rule repeatedly to the composition of these elementary operations, one can compute the derivative information exactly and in a completely mechanical fashion. This method produces a code that evaluates derivatives exactly (up to machine precision) with a minimum of human effort [10].

All above techniques except for the finite difference technique have one thing in common. They all require complex manipulations of the model equations. In many studies this is not practically feasible because the models are too complicated or the model equations are not directly accessible (e.g. because they are compiled in executable commercial code). This is the basic reason why the finite difference method, although inefficient, is still used very often. The practical issues concerning this sensitivity analysis technique will be discussed in section four.

3. Model under study

In order to illustrate some practical issues concerning the finite difference method, the COST Simulation Benchmark model will be used [2]. This wastewater treatment model was designed to provide an unbiased basis for comparison of control strategies without reference to a particular wastewater treatment facility. It was also succesfully used for comparing different simulation packages in the wastewater community.
The Simulation Benchmark has five biological tanks in series and a secondary settling tank. The biological tanks are modelled by the Activated Sludge Model No. 1 (ASM1) [8]. ASM1 has 13 components and 8 processes describing growth and decay of biomass, hydrolysis of organic compounds and ammonification. The secondary settler is modelled using the 1D settling model of Takacs [21]. The model was implemented in the modelling and simulation tool WEST [24] and consists of 150 (5x14+80) differential equations. The fourteenth equation in each tank is used to model the volume of that tank. The plant layout is shown in figure 1.
From this model, 5 variables and 8 parameters were selected for the illustrative sensitivity analysis study. Three effluent variables were selected: ammonia (S_{NH}), nitrate (S_{NO}) and readily biodegradable substrate (S_S). In reactor 3 of the system, two biomass components were also selected: active heterotrophic biomass ($X_{B,H}$) and active autotrophic biomass ($X_{B,A}$). Four biological parameters were selected: the maximum heterotrophic growth rate (μ_{mH}), maximum autotrophic growth rate (μ_{mA}), heterotrophic yield (Y_H) and autotrophic yield (Y_A). Besides these, four physical parameters of the clarifier model were also evaluated: the clarifier surface (A), the clarifier height (H), the maximum settling velocity (v_0) and the non-settleable fraction (f_{ns}). The sensitivity functions of each of these variables to each of

these parameter were calculated (for days 117-120), resulting in a total of 40 sensitivity functions.
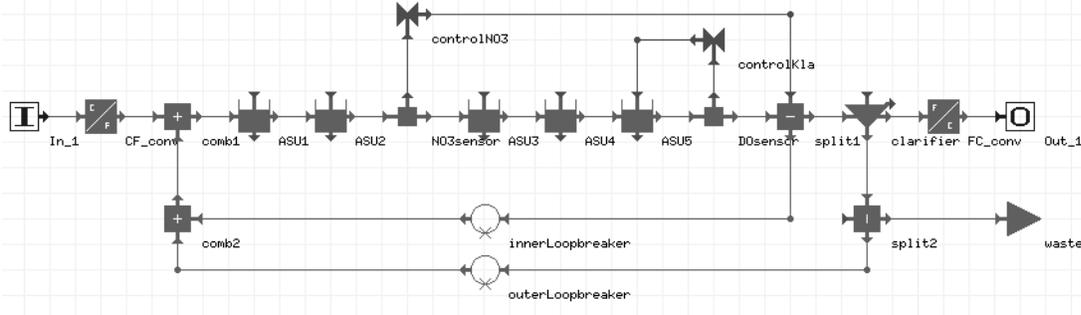

Figure 1: The plant layout of the Benchmark model.

4. Practical aspects of the finite difference method

Equation 3 forms the basis of the finite difference method, it was implemented as follows

$$\frac{\partial y}{\partial \theta_j} \approx \frac{y(t, \theta_j + \Delta \theta_j) - y(t, \theta_j)}{\Delta \theta_j} \tag{8}$$

where $\Delta \theta_j$ is the change of the parameter value. Practically $\Delta \theta_j$ was implemented as the nominal parameter value θ_j multiplied by a user defined perturbation factor ξ. The choice of this perturbation factor will determine the quality of the sensitivity function. Equation 8 is only equivalent to equation 3 if the perturbation factor approaches 0. From a theoretical point of view this is correct but numerically this can never be achieved because of the limited precision of the calculations. If the perturbation factor is taken too small it will result in numerical inaccuracies. On the other hand, $\xi \theta_j$ should not become too large because then the nonlinearity of the model will start to play an important role in the sensitivity calculations.

As an example, figure 2 shows the concentration and sensitivity of the effluent nitrate (S_{NO}) to the maximum heterotrophic growth (μ_{mH}). The perturbation factor ξ was taken as 10^{-3}.
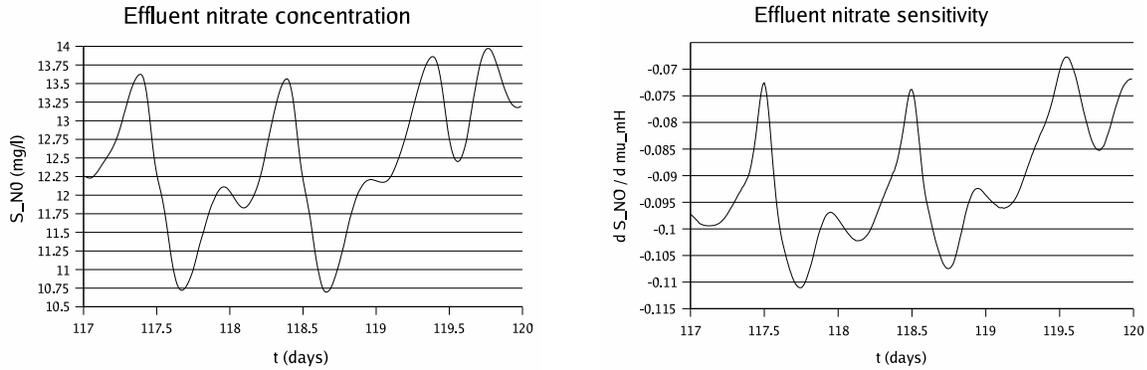

Figure 2: Concentration of the effluent nitrate (S_{NO}) (left) and the sensitivity of nitrate to the maximum heterotrophic growth rate (μ_{mH}) for a perturbation factor of (10^{-3}) (right).

The practical implementation of equation 8 has two major drawbacks. The resulting sensitivity function relates to the ($\theta_j + \xi \theta_j / 2$) parameter set and it does not provide any information on the quality of the sensitivity function. As already mentioned in section two, if sensitivities are required around the nominal values of the parameters then the central difference formula should be used (equation 4). Although this method requires $2p$ model evaluations, it also provides additional information concerning the quality of the sensitivity function. To implement the central difference method two sensitivity functions are calculated. The first sensitivity function is calculated by increasing the nominal parameter value by $\xi \theta_j$,

the second sensitivity function is calculated by decreasing the nominal parameter value by $\xi\theta_j$.

$$\frac{\partial y}{\partial \theta_j}_+ = \frac{y(t, \theta_j + \xi\theta_j) - y(t, \theta_j)}{\xi\theta_j} \tag{9a}$$

$$\frac{\partial y}{\partial \theta_j}_- = \frac{y(t, \theta - \xi\theta_j) - y(t, \theta_j)}{\xi\theta_j} \tag{9b}$$

To calculate the centralised sensitivity function the average of both sensitivity functions is taken. To make the numerical error and the error introduced by the nonlinearity of the model as small as possible the difference between these two sensitivity functions should be minimal. Several criteria can be used to quantify this difference.

1. Sum of squared errors (SSE).

$$\frac{\sum \left(\frac{\partial y}{\partial \theta}_+ - \frac{\partial y}{\partial \theta}_- \right)^2}{N} \tag{10}$$

   For this criterion, the squared error between both sensitivity functions is calculated and summed over all times where the sensitivity is required (N).

2. Sum of absolute errors (SAE).

$$\frac{\sum \left| \frac{\partial y}{\partial \theta}_+ - \frac{\partial y}{\partial \theta}_- \right|}{N} \tag{11}$$

   For this criterion, the absolute error between both sensitivity functions is calculated and summed over all times where the sensitivity is required (N).

3. Maximum relative error (MRE).

$$\left| \frac{\frac{\partial y}{\partial \theta}_+ - \frac{\partial y}{\partial \theta}_-}{\frac{\partial y}{\partial \theta}_+} \right|_{MAX} \tag{12}$$

   This criterion returns the maximum value of the relative difference between both sensitivity functions. One should be careful with this criterion because $\partial y/\partial \theta_+$ or $\partial y/\partial \theta_-$ may become 0. In this special case the criterion returns 0.

4. Ratio between sensitivities (RATIO).

$$\left| 1 - \frac{\frac{\partial y}{\partial \theta}_-}{\frac{\partial y}{\partial \theta}_+} \right|_{MAX} \tag{13}$$

   This criterion is based on the ratio of the sensitivity functions. The ideal case is when this ratio equals 1, because then both sensitivity functions are equal. The criterion returns the maximum deviation from this ideal situation. Like the MRE criterion one should be careful if $\partial y/\partial \theta_+$ becomes 0. In this special case the criterion returns 0.

Figure 3 illustrates the use of these criteria for the sensitivity of nitrate S_{NO} to μ_{mH} for perturbation factors (ξ) ranging from 10^{-1} to 10^{-7}. This figure clearly illustrates the nonlinearity effects of the model for perturbation factors higher than 10^{-3}. An example is given in figure 4 for a perturbation factor 10^{-2}. In this figure the sensitivity function for the optimal perturbation factor 10^{-3} is also shown. It is clear that the $\partial y/\partial \theta_-$ differs significantly from $\partial y/\partial \theta_+$. Figure 3 also illustrates the effect of numerical errors for perturbation factors lower than 10^{-3}. An example of this is given in figure 5 for a perturbation factor of 10^{-5}.

The optimal perturbation factor for the sensitivity of S_{NO} to μ_{mH} is 10^{-3} (figure 3). Let us now investigate whether this perturbation factor is the same for other variables and parameters. Table 1 gives an overview of the optimal perturbation factor ranges for all variables with respect to all parameters. This table clearly shows that optimal perturbation factors are parameter dependent, some parameters have an optimal perturbation factor of 10^{-2} others 10^{-4}. Applying a fixed perturbation factor to all
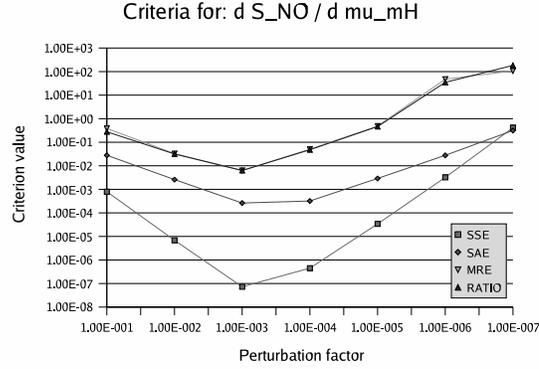
Figure 3: Different criteria calculated for the sensitivity of the effluent nitrate (S_{NO}) to the maximum heterotrophic growth rate (μ_{mH}) using a range of perturbation factors (10^{-1} to 10^{-7}).
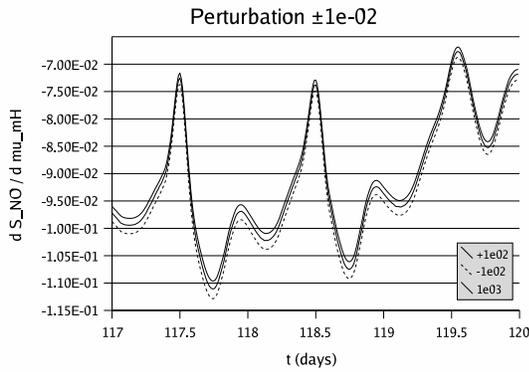

Figure 4: Effect of the nonlinearity of the model on the sensitivity function. Perturbation factor 10^{-2}.
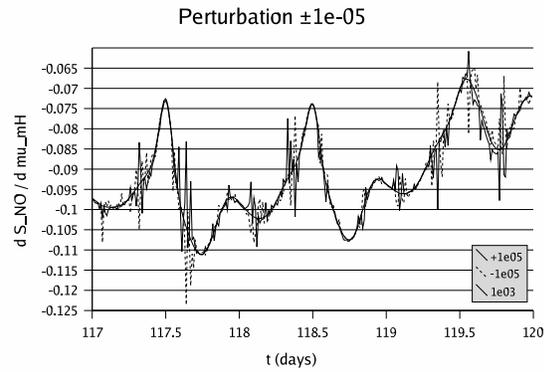
Figure 5: Effect of numerical error on the sensitivity function. Perturbation factor 10^{-5}.

parameters is not advisable. In literature, however, this is frequently done [9, 16, 19, 20]

We can also see that the optimal perturbation factor depends on the variable considered. For example, the optimal perturbation factors for μ_{mH} are within the range of 10^{-2} to 10^{-4} for the SSE criterion. This means that the sensitivity of different variables to the same parameter (μ_{mH}) resulted in different optimal perturbation factors for that parameter. However, taking the average of the indicated range as the perturbation factor results in acceptable sensitivity functions for all variables.

From table 1, it can also be concluded that different criteria indicate roughly the same optimal perturbation factors. Still, for some parameters this is more pronounced than for others.

In order to find out whether the criteria can be used to predict if a sensitivity function is valid we have to

Table 1: Ranges of optimal perturbation factors for all variables to the given parameters

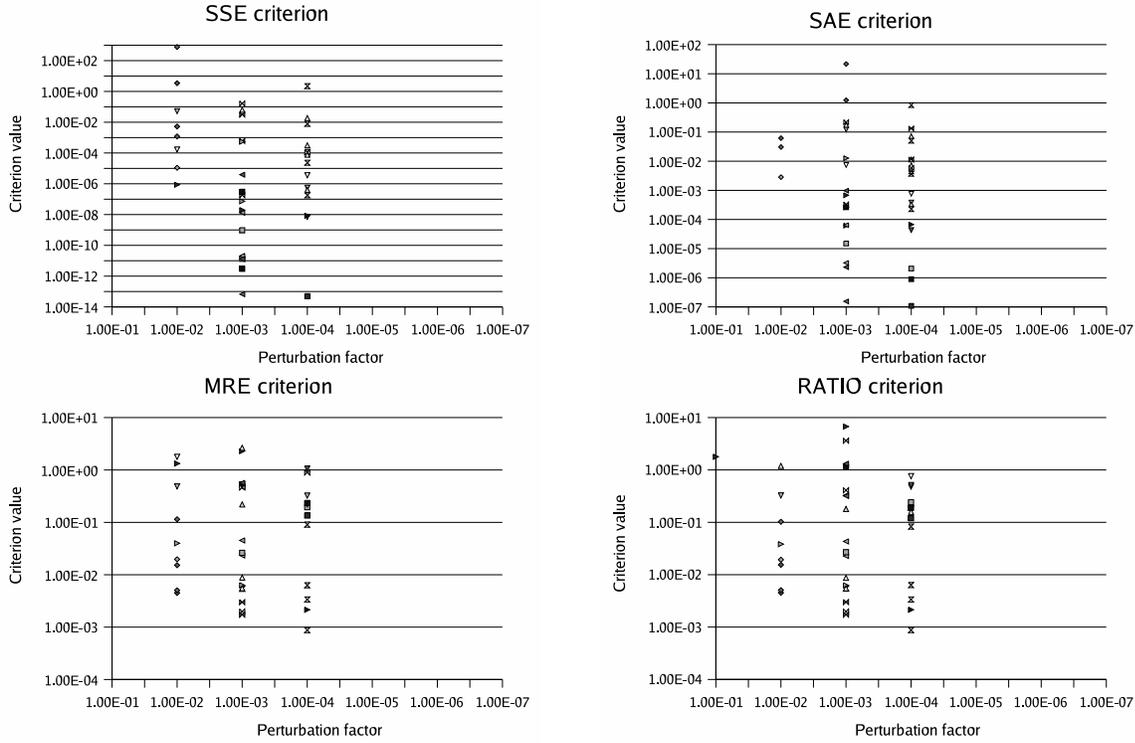|	SSE	SAE	MRE	RATIO
μ_{mH}	10^{-2} - 10^{-4}	10^{-3} - 10^{-4}	10^{-2} - 10^{-4}	10^{-1} - 10^{-4}
μ_{mA}	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}	10^{-2} - 10^{-4}
Y_H	10^{-4}	10^{-4}	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}
Y_A	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}
A	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}	10^{-3} - 10^{-4}
H	10^{-2} - 10^{-4}	10^{-3} - 10^{-4}	10^{-2} - 10^{-4}	10^{-2} - 10^{-4}
v_0	10^{-3}	10^{-3}	10^{-3}	10^{-3}
f_{ns}	10^{-2}	10^{-2} - 10^{-3}	10^{-2}	10^{-2}

Figure 6: Criteria values for the optimal perturbations factor for all 40 sensitivity functions.

take a closer look at the criterion values. Figure 6 shows the criterion values for the optimal perturbation factors for all 40 sensitivity functions, the values for each criterion are displayed on different graphs. From this figure we can again see that the optimal perturbation factors for different sensitivity functions are different and range from 10^{-1} to 10^{-4}.

The values for the SSE criterion range from 10^{-14} to 10^{+3}. This is caused by the values of the sensitivity functions themselves. Sensitivity functions which are small in value result in small SSE values, while sensitivities which are large result in large SSE values. The same conclusion can be drawn for the SAE criterion. For the MRE and RATIO criteria we observe a much narrower range, from 10^{-3} to 10^{+1}. This is because these criteria are based on relative differences between the sensitivity functions. Both MRE and RATIO criteria can be used as an indicator of the quality of the sensitivity function calculations. Sensitivity function calculations resulting in a value below 10^{-1} can be considered correct. Sensitivity function calculations resulting in a value above 10^{-1} should be considered wrong although some correct sensitivity function calculations can result in MRE or RATIO criteria with such values.

All model evaluations used to calculate the sensitivity functions were performed using a Runge Kutta 4 Adaptive Stepsize Control integrator (RK4ASC) [17]. The adaptive stepsize option allows the integrator to decrease or increase the stepsize during the integration in order to maintain a user defined accuracy between two successive integration steps. The influence of this integrator accuracy on the calculated sensitivity functions and optimal perturbation factors was investigated as well. Figure 7 shows the optimal perturbation factor for the sensitivity of nitrate (S_{NO}) to the heterotrophic yield (Y_H) for different integrator settings. The left figure is the result of calculations with an integrator accuracy of 10^{-9} and the right with an accuracy of 10^{-6}. An accuracy of 10^{-9} has been used to produce all results shown before.

From both figures we can conclude that the accuracy has an influence on the optimal perturbation factor, 10^{-4} for an accuracy of 10^{-9} and 10^{-3} for an accuracy of 10^{-6}. The accuracy also has an influence on the criterion values. All criterion values are lower for the 10^{-9} accuracy and thus result in better sensitivity functions. It should be noted that higher integrator accuracies result in longer calculation times. For other parameters and variables this influence has also been demonstrated.
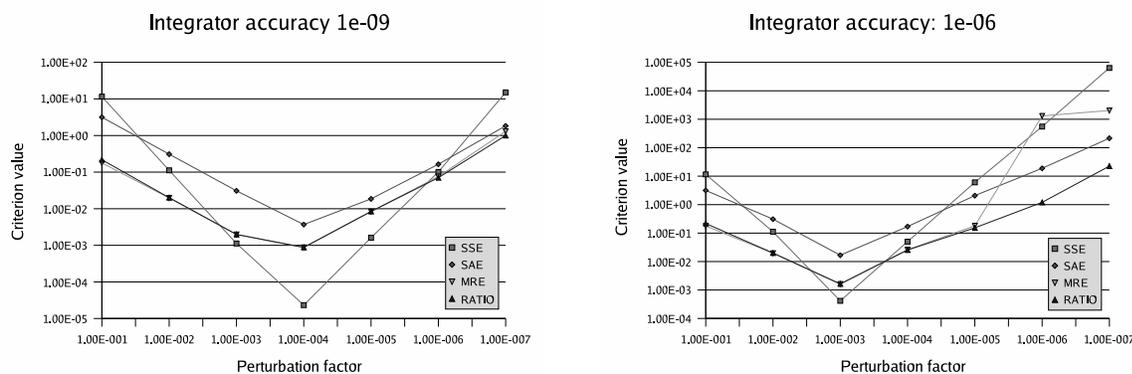
Figure 7: Optimal perturbation factor for the sensitivity of nitrate (S_{NO}) to the heterotrophic yield (Y_H) for different integrator accuracies: 10^{-9} (left) and 10^{-6} (right)

5. Conclusion

In this paper the finite difference sensitivity analysis technique was discussed in detail. Practically this technique was implemented using the central difference method. This method produces sensitivity functions around the nominal parameter values θ and at the same time it allows to assess the quality of the sensitivity function calculations. Different criteria were used as a measure for this quality.

The perturbation factor used in the finite difference method was found to be parameter dependent and to a lesser extent variable dependent. Among the proposed criteria the MRE and RATIO criterion were found useful to assess the quality of sensitivity function calculations. It was also found that the integrator accuracy has a large influence on the calculated sensitivity functions and the optimal perturbation factors.

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