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Working with Dynamic Crop Models
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Chapter 3

Uncertainty and sensitivity analysis for crop models

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1. Introduction

A crop model is the result of a long and complex construction process, involving data at multiple stages for understanding basic processes, elaborating model structure, estimating parameters and evaluating prediction quality. In various stages of a model's life, however, there is a need to study the model on its own, with an emphasis on its behaviour rather than on its coherence with a given data set. This is where uncertainty analysis sensitivity analysis and related methods become useful for the modeller or model user.

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Uncertainty analysis consists of evaluating quantitatively the uncertainty or variability in the model components (parameters, input variables, equations) for a given situation, and deducing an uncertainty distribution for each output variable rather than a misleading single value. An essential consequence is that it provides methods to assess, for instance, the probability of a response to exceed some threshold. This makes uncertainty analysis a key component of **risk analysis** (Vose, 1996).

The aim of **sensitivity analysis** is to determine how sensitive the output of a crop model is, with respect to the elements of the model which are subject to uncertainty or variability. This is useful as a guiding tool when the model is under development as well as to understand model behaviour when it is used for prediction or for decision support. For dynamic models, sensitivity analysis is closely related to the study of **error propagation**, i.e. the influence that the lack of precision on model input will have on the output.

Because uncertainty and sensitivity analysis usually relies on simulations, they are also closely related to the methods associated with **computer experiments**. A computer experiment is a set of simulation runs designed in order to explore efficiently the model responses when the input varies within given ranges (Sacks et al., 1989; Welch et al., 1992). The goals in computer experiments identified by Koehler and Owen (1996) include optimization of the model response, visualization of the model behaviour, approximation

by a simpler model or estimation of the average, variance or probability of the response to exceed some threshold.

Within a given model, model equations, parameters and input variables are all subject to variability or uncertainty. First, choices have to be made on the model structure and on the functional relationships between input variables and state and output variables. These choices may sometimes be quite subjective and it is not always clear what their consequences will be. Martinez et al. (2001) thus perform a sensitivity analysis to determine the effects of the number of soil layers on the output of a land surface–atmosphere model. For spatial models, there is frequently a need to evaluate how the scale chosen for input variables affects the precision of the model output (see e.g. Salvador et al., 2001).

Second, parameter values result from estimation procedures or sometimes from bibliographic reviews or expert opinion. Their precision is necessarily limited by the variability and possible lack of adequacy of the available data. Some parameters may also naturally vary from one situation to another. The uncertainty and natural variability of parameters are the central point of many sensitivity analyses. Bärlund and Tattari (2001), for example, study the influence of model parameters on the predictions of field-scale phosphorus losses, in order to get better insight into the management model ICECREAM. Ruget et al. (2002) perform sensitivity analysis on parameters of the crop simulation model STICS, in order to determine the main parameters that need to be estimated precisely. Local sensitivity methods, based on model derivatives with respect to parameters, are commonly used for checking identifiability of model parameters (Brun et al., 2001).

Third, additional and major sources of variability in a model output are, of course, the values of its input variables. Lack of precision when measuring or estimating input variables needs to be quantified when making predictions from a model or when using it for decision support. Aggarwal (1995) thus assesses the implications of uncertainties in crop, soil and weather inputs in the spring wheat WTGROWS crop model. Rahn et al. (2001) compare contrasted input scenarios for the HRI WELL-N model on crop fertilizer requirements through a sensitivity analysis. They identify the main factors which need to be measured precisely to provide robust recommendations on fertilization. Contrasted settings of the input variables are used for performing sensitivity or uncertainty analyses assuming different scenarios by Dubus and Brown (2002).

Model structure, model parameters and input variables represent three basic sources of model uncertainty. It is often advisable to study their influence on a model simultaneously (Saltelli et al., 2000) and alternative groupings of uncertainty sources may then be more adequate. Rossing et al. (1994), for example, distinguish sources that can be controlled by more intensive data collection (model parameter estimates), and uncontrollable sources when predictions are made (daily temperature, white noise). Ruget et al. (2002), on the other hand, decompose the sensitivity analyses according to STICS sub-modules on, e.g. energy conversion, rooting or nitrogen absorption. Jansen et al. (1994) advocate to divide uncertainty sources into groups of parameters or input variables which can be considered to be mutually independent.

As shown by the examples above, uncertainty and sensitivity analysis may have various objectives, such as:

- to check that the model output behaves as expected when the input varies;
- to identify which parameters have a small or a large influence on the output;

- to identify which parameters need to be estimated more accurately;
- to detect and quantify interaction effects between parameters, between input variates or between parameters and input variates;
- to determine possible simplification of the model;
- to identify input variables which need to be measured with maximum accuracy.

Some of these objectives have close links with other methods associated with modelling, like model construction, parameter estimation or model use for decision support.

The diversity of motivations for performing sensitivity analysis is associated with a large choice of methods and techniques. In this chapter, we present a selection of approaches representative of this diversity. This selection, however, will be far from exhaustive. We refer to the book edited by Saltelli et al. (2000) for a recent and comprehensive exposition of sensitivity analysis methods and applications, and to Saltelli et al. (2004) for a more practical presentation.

In this chapter, Section 2 is dedicated to preliminary notions on the basic components of an uncertainty and sensitivity analysis. Section 3 covers several methods of uncertainty analysis. Methods of sensitivity analysis are presented in Section 4 – local and one-at-a time sensitivity analysis methods, and more global methods (variance-based sensitivity analysis) which enable to study simultaneously the influence of several model components.

2. Ingredients of uncertainty and sensitivity analysis

2.1. The crop model

The structure and properties of the crop model may influence the choice of the uncertainty and sensitivity analysis. One reason is that the objectives depend on the crop model capabilities and complexity.

More specifically, as remarked by Koehler and Owen (1996), the number of inputs (variables or parameters), the number of outputs and the speed with which the model f can be calculated may vary enormously in applications, and these quantities will obviously play an important role in the objectives of a sensitivity analysis and on the adequacy of the various available methods. Among the methods presented in the sequel, some are adapted to small numbers of model simulations (e.g. local and one-at-a-time methods, methods based on experimental designs), while others require a large number of simulations (methods based on Monte-Carlo sampling, for instance).

A price has to be paid while using more economical methods, and this price depends on the main model properties – it may be necessary to select a number of factors smaller than desired, or most interactions between factors may have to be assumed as negligible, or the investigation may be unable to detect model departures from linearity or near-linearity. It follows that some methods are well-adapted only if the model is well-behaved in some sense, while other methods are more "model-independent" (Saltelli et al., 1999), i.e. more robust to complex model behaviours such as strong non-linearity, discontinuities, non-monotonicity or complex interactions between factors.

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2.2. Input factors

The model components whose influence on the output is to be investigated will be called the *input factors* of the sensitivity analysis. An input factor may be:

- either a set of alternative model structures or functional relationships within a sub-module of the model;
- or an uncertain or variable parameter θ_j;

A winter wheat dry matter model

A simple crop model will be used in this chapter to illustrate the different methods of uncertainty and sensitivity analysis. The model has a single state variable, the above-ground winter wheat dry matter, denoted by $U(t)$ with t the day number since sowing. This state variable is calculated on a daily basis as a function of cumulative degree-days $T(t)$ (above a baseline of 0°C) and of daily photosynthetically active radiation $\mathrm{PAR}(t)$. The model equation is:

$$U(t+1) = U(t) + E_{\mathrm{b}} E_{\mathrm{i\,max}} \left[1 - \mathrm{e}^{-K.\mathrm{LAI}(t)}\right] \mathrm{PAR}(t) + \varepsilon(t),$$

where E_{b} the radiation use efficiency, E_{imax} the maximal value of the ratio of intercepted to incident radiation, K the coefficient of extinction, $\mathrm{LAI}(t)$ is the leaf area index on day t, and $\varepsilon(t)$ is a random term representing the model error. In this chapter, we consider the deterministic part of the model only, so this model error will be assumed null in the simulations. $\mathrm{LAI}(t)$ is calculated as a function of cumulative degree-days $T(t)$, as follows (Baret, 1986):

$$\mathrm{LAI}(t) = L_{\max} \left\{ \frac{1}{1 + \mathrm{e}^{-A[T(t)-T_1]}} - \mathrm{e}^{B[T(t)-T_2]} \right\}.$$

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The dry matter at sowing ($t = 1$) is set equal to zero: $U(1) = 0$. In addition, the constraint $T_2 = \frac{1}{B} \log[1 + \exp(A \times T_1)]$ is applied, so that $\mathrm{LAI}(1) = 0$.
We will assume that the *dry matter at harvest* $U(t_{\mathrm{H}})$ is the main output variable of interest, and denote

$$\hat{Y} = U(t_{\mathrm{H}})$$

$$= \sum_{t=1}^{t_H - 1} E_{\mathrm{b}} E_{\mathrm{imax}} \left[1 - \mathrm{e}^{-K\mathrm{LAI}(t)}\right] \mathrm{PAR}(t)$$

While presenting sensitivity analysis, it is convenient to consider the model in the form

$$\hat{Y} = f(X; \theta).$$

In this expression, $X = (T(1), \ldots, T(t_H), \mathrm{PAR}(1), \ldots, \mathrm{PAR}(t_H))$ denotes the daily climate input variables, and $\theta = (E_{\mathrm{b}}, E_{\mathrm{i\,max}}, K, L_{\max}, A, B, T_1)$ denotes the vector of parameters, with $L_{\max}$ the maximal value of LAI, T_1 a temperature threshold and A and B two additional parameters.

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- or an input variable X_l;
- or a series of several related input variables X_l, e.g. annual series of daily climate variables in a given region.

The choice of the input factors depends on the objective of the sensitivity analysis. They must include, of course, the model components of direct interest in the study. But in many cases, the sensitivity of the model with respect to these components is likely to depend on additional components. For instance, the sensitivity of a crop model with respect to its main parameters is often highly dependent on the values of climate- or soil variables. Consequently, these variables must also be considered for inclusion in the list of input factors, unless, alternatively, separate sensitivity analyses are performed with different modalities of these variables.

Note that each input variable of the model may or may not be selected as an input factor of the sensitivity analysis. For instance, if a sensitivity analysis is performed for a given soil type, the input variables related to soil can be fixed. In this case, the soil input variables will not be included among the input factors of the sensitivity analysis. The term *input factor* is further reserved for factors of the sensitivity analysis.

Notation

The number of input factors will be denoted by s and the input factors will be denoted by $Z_1, \ldots, Z_s$, in order to distinguish them clearly from the *model input variables* X_l. An *input scenario* will be defined as a combination of levels $\mathbf{z} = (z_1, \ldots, z_s)$ of the sensitivity input factors. When several input scenarios need to be defined simultaneously, they will be denoted by $\mathbf{z}_k = (z_{k,1}, \ldots, z_{k,s})$, with subscript k identifying the scenarios.

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Whatever the choice of the factors, it is assumed that for each input scenario $\mathbf{z}$, the other crop model components f, $\mathbf{x}$ and θ are completely determined so that the output $f(\mathbf{x}, \theta)$ can be calculated. We will keep the same notation f to identify the model expressed as a function of input variables $f(\mathbf{x}, \theta)$ or as a function of an input scenario $f(\mathbf{z}) = f(z_1, \ldots, z_s)$.

A winter wheat dry matter model (continued)

In the winter wheat dry matter model, the seven parameters have associated uncertainty and so they represent seven input factors for the uncertainty and sensitivity analyses. The other source of uncertainty to be considered in this example is that related to the input variables of the model. Instead of considering each input variable $\mathrm{PAR}(t)$ and $T(t)$ at each time t as a separate sensitivity input factor, a set of fourteen annual series of climate measurements in the region of interest will constitute the eighth factor of the sensitivity analysis.
Thus, there are eight factors: the seven parameters E_{b}, E_{imax}, K, $L_{\max}$, A, B, T_1 and the climate factor C. An input scenario is a vector

$$\mathbf{z} = (z_{E_{\mathrm{b}}}, z_{E_{\mathrm{imax}}}, z_K, z_{L_{\max}}, z_A, z_B, z_{T_1}, z_C)$$

specifying a combination of values of the input parameters. As this example shows, a factor may be quantitative – the seven parameters – or categorical – the climate series.

2.3. Uncertainty in input factors

For each input factor, the amount of uncertainty needs to be defined. The uncertainty in an input factor can be described in different ways. For a parameter, it is often given as the most likely value plus or minus a given percentage. Or it is specified through a continuous probability distribution over a range of possible values. The uncertainty about climate can either be summarized by series of climatic variable values measured during 10, 20 or 30 years, or be simulated by a climate generator (Richardson, 1981; Racsko et al., 1991).

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In this chapter, three main characteristics are considered for describing the uncertainty: nominal values, uncertainty domains and probability distributions.

The *nominal* value $z_{0,i}$ of an input factor Z_i represents the most standard setting of the corresponding model parameter or input variable in the conditions of the study. The *control scenario* $\mathbf{z}_0$ is defined as the input scenario with each input factor fixed at its nominal value. These notions are useful, in particular, for local sensitivity methods (see Section 4).

The *uncertainty range* represents the set of possible values for an input factor. Usually,

- for a parameter θ_j, it is an interval $[\theta_{\min(j)}, \theta_{\max(j)}]$ around the nominal value, representing the uncertainty range of the parameter values based on bibliography, expert opinion or experimental data;
- for a quantitative input variable X_l, it represents the range of variation $[x_{\min(l)}, x_{\max(l)}]$ under the conditions of the study; alternatively, it can be chosen to reflect the lack of precision when this variable is measured in a given field;
- for categorical factors, it is a set of modalities representative of the phenomenon under study; for climate series, typically, the domain of variation is a set of recently observed annual series in one or several sites.

Except for input factors with a negligible influence on model output, the influence of any given input factor will appear stronger if its uncertainty range is enlarged compared to other factors. Consequently, the uncertainty ranges must be tuned as finely as possible to the objectives and scales of the study.

Probability distributions must be specified for the methods of sensitivity analysis based on random sampling. The uniform distribution, which gives equal weight to each value within the uncertainty range, is commonly used in sensitivity analysis when the main objective is to understand model behaviour. In uncertainty analysis, more flexible probability distributions are usually needed to represent the input uncertainty (see Section 3). Practical methods to determine distributions from data or expert opinion are presented in Chapters 7 and 8 of Vose (1996).

Coding of input factors. It often simplifies presentation and calculation, when a common uncertainty range is used for all quantitative sensitivity factors. This may be done by coding the levels of the factors so that they vary between -1 and $+1$ or between 0 and 1. Coded values z_i^c of an input factor Z_i can easily be calculated from the uncoded values through the following relationship:

$$z_i^c = \frac{z_i - (z_{\min(i)} + z_{\max(i)})/2}{(z_{\max(i)} - z_{\min(i)})/2} \quad \text{for a } [-1, +1] \text{ range of variation,}$$

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or

$$z_i^c = \frac{z_i - z_{\min(i)}}{z_{\max(i)} - z_{\min(i)}} \quad \text{for a } [0, 1] \text{ range of variation.}$$

A winter wheat dry matter model (continued)

The chosen nominal values and uncertainty ranges are given in Table 1 for the parameters. These values come from past experiments, bibliography and expert knowledge. For the climate factor, a set of 14 annual series observed in the region of Grignon (France) was chosen. Note that for such a factor, there is no obvious nominal value.

Table 1. Uncertainty intervals for the parameters of the winter wheat dry matter models.

Parameter	Unit	Nominal value	Uncertainty range	
E_b	g/MJ	1.85	0.9	2.8
E_{imax}	–	0.94	0.9	0.99
K	–	0.7	0.6	0.8
L_{max}	–	7.5	3	12
T_1	C	900	700	1100
A	–	0.0065	0.003	0.01
B	–	0.00205	0.0011	0.003

To illustrate the coding of factors, let us consider the parameter E_b. The values z^c_{Eb} of E_b vary in the uncertainty range [0.9, 2.8]. By setting $z^c_{Eb} = (z_{Eb} - 1.85)/0.95$, we get coded values z^c_{Eb} which vary in $[-1, +1]$.

2.4. Methods of uncertainty and sensitivity analysis

An uncertainty analysis can be used to answer the question *What is the uncertainty in* $\hat{Y} = f(Z)$ *given the uncertainty in* Z*?* This type of analysis consists of four steps:

i. Definition of the distribution of the uncertain input factors.
ii. Generation of N scenarios of the input factors $\mathbf{z}_k = (z_{k,1}, \ldots, z_{k,s})$, $k = 1, \ldots, N$.
iii. Computation of the model output for each scenario, $f(\mathbf{z}_k)$, $k = 1, \ldots, N$.
iv. Analysis of the output distributions (computation of means, variances, quantiles ...).

These steps are discussed in details in Section 3.

Two types of sensitivity analysis are usually distinguished, *local* sensitivity analysis and *global* sensitivity analysis. Local SA focus on the local impact of the factors on the model outputs and is carried out by computing partial derivatives of the output variables with respect to the input factors. With this kind of methods, the factors are allowed to

vary within small intervals around nominal values. These intervals are not related to the uncertainty in the factor values.

Global sensitivity analysis can be used to answer the question *How important are the individual elements of Z with respect to the uncertainty in $\hat{Y} = f(Z)$?* Like uncertainty analysis, global SA consists in (i) defining the distributions of the input factors, (ii) generating scenarios of input factors and (iii) computing output variables for each scenario. But the fourth step is different and consists of calculating a sensitivity index for each element of Z. These indices are computed varying the factors over their whole uncertainty ranges. Methods of global sensitivity analysis are very useful because they allow the crop modeller to identify the factors that deserve an accurate measure or estimation. Most of Section 4 is devoted to these methods.

3. Uncertainty analysis

3.1. Probability distributions for input factors

The first step of an uncertainty analysis is to define the probability distributions for the input factors. When performing an uncertainty analysis, attention must be paid choosing in adequate probability distributions. The range of input values usually has more influence on the output than the distribution shapes, but some characteristics such as the degree of symmetry or skewness may also play a role.

There is a large choice of probability distributions available. In this section, we give a brief overview and refer to Vose (1996) for a more detailed presentation. The uniform distribution puts equal weight on each value in the uncertainty range. In most cases, however, the extreme values of the uncertainty ranges are less likely than the middle values. Among symmetric distributions, the well-known Gaussian distribution is often convenient since it requires only the specification of a mean value and a standard deviation. In uncertainty analysis, it is often replaced by the truncated Gaussian distribution or by symmetric beta distributions, which give upper- and lower bounds to the possible values.

Sometimes the distribution should be asymmetric, for example if the input parameter or variable is positive and likely to be near zero. Then log-normal, gamma or beta distributions offer a large range of possibilities.

Finally the triangular distributions (or more general piecewise-linear distributions) are often convenient for a simple representation of subjective beliefs, because they are defined entirely by their uncertainty range and their most-likely value. The distribution is zero outside the uncertainty range, it is maximum at the most-likely value, and it is linear between the extreme values of the range and the most-likely value.

3.2. Generation of input factor values

Once the probability distributions have been specified, representative samples have to be drawn from these distributions. This is done most often by Monte Carlo sampling. In Monte Carlo sampling, the samples are drawn independently, and each sample is generated by drawing independently the value of each sensitivity factor Z_i. Note that

many mathematical or statistical softwares include routines for quasi-random number generation, so that Monte Carlo samples are quite easy to generate. Provided the quasi-random generators are reliable, Monte Carlo sampling provides unbiased estimates of the expectation and variance of each output variable.

Latin hypercube, importance and LP_τ sampling (see Helton and Davis, 2000) are alternatives to Monte Carlo sampling. The basic principle of Latin hypercube sampling is briefly described here in the case of uniform distributions. First, the range of each factor is divided into P intervals of equal probability and one value is selected at random from each interval. Second, the P values obtained for the factor Z_1 are paired at random and without replacement with the P values obtained for the factor Z_2. The P pairs are then randomly combined without replacement with the P values obtained for the factor Z_3 and so on. The interest of Latin hypercube sampling is that it ensures the full coverage of the range of variation of each factor. A drawback of this method is that it gives biased estimates of the variance. According to Helton and Davis (2000), Latin hypercube sampling is useful when large samples are not computationally practicable and the estimation of very high quantiles is not required.

For illustration, we generated two samples of 10 values of a pair of independent and uniformly distributed random variables, $Z_1 \sim U(0, 1)$ and $Z_2 \sim U(0, 1)$. One sample was generated by Monte Carlo sampling (Fig. 1a) and the other one by Latin hypercube sampling (Fig. 1b). The results show that the values generated by Latin hypercube sampling cover the whole ranges of variation of the random variables. This is not necessarily the case when a Monte Carlo method is used as shown in Figure 1a.

It is necessary sometimes to consider correlations between some input parameters or variables. This requires generating samples from joint multivariate probability distributions. When the distributions are normal, the following method can be used. Assume that the vector $Z = (Z_1, \ldots, Z_s)^T$ is distributed as $Z \sim N(0, \Sigma)$, where Σ is a $(s \times s)$ variance–covariance matrix. Define U as an upper triangular matrix such as $\Sigma^{-1} = U^T U$ (Cholesky decomposition). The vector UZ is normally distributed with mean equal to zero and with a variance–covariance matrix equal to the identity matrix: $var(UZ) = UU^{-1}(U^T)^{-1}U^T = I$. A random value z of Z is obtained by generating a vector d including s values randomly generated from N(0, 1) and then by calculating $U^{-1}d$.

When the input factors are not normally distributed, the method proposed by Iman and Conover (1982) can be used to generate samples from joint multivariate probability distributions. Taking account of correlations is particularly important for series of climatic variables. As mentioned before, this case can be tackled by using past climatic series or climate generators.

3.3. Computation of the model output for each scenario

Once the sample of factor values, $\mathbf{z}_1, \ldots, \mathbf{z}_N$, have been generated, the corresponding model output values, $f(\mathbf{z}_1), \ldots, f(\mathbf{z}_N)$, must be computed. If the computation of the model output requires a lot of time, this step may be difficult to carry out. With some very complex models, the sample size N must be set equal to a small value due to the computation time. This problem is illustrated in Chapter 16. On the contrary, this step is straightforward for models that are less complex and computationally intensive as shown by Makowski et al. (2004) with the AZODYN model.

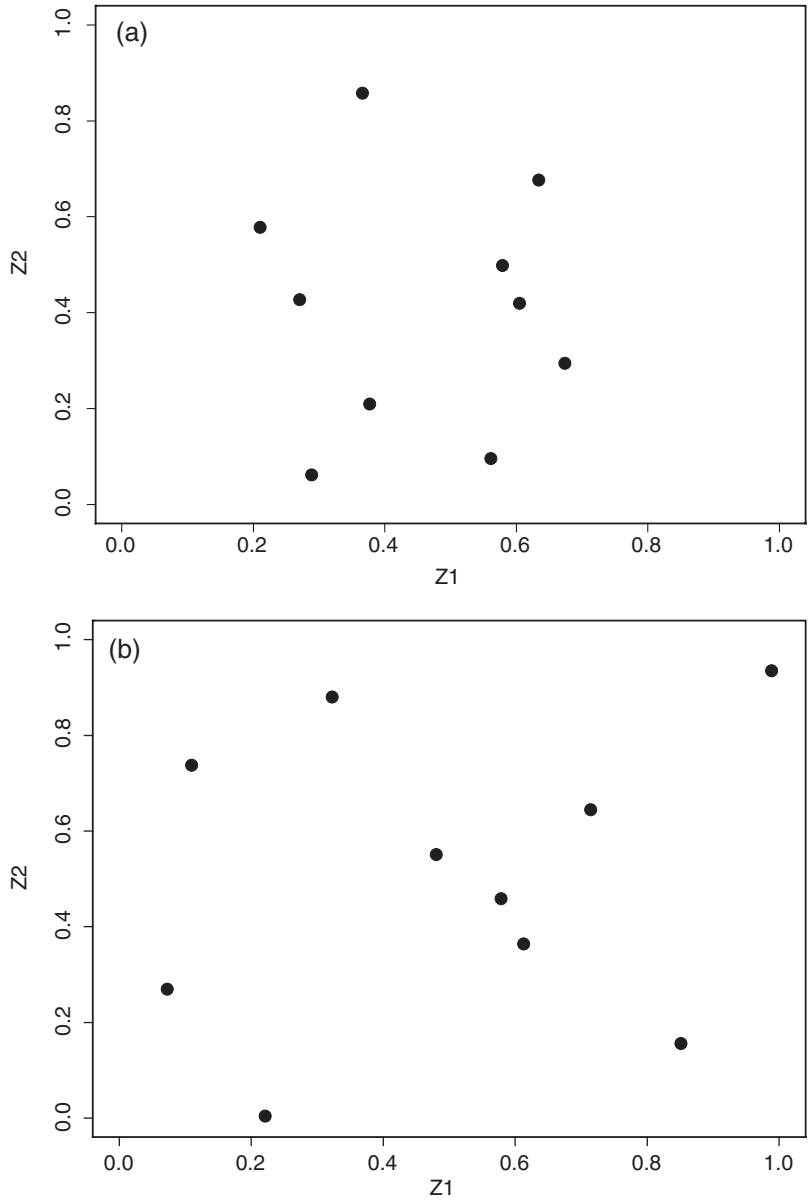

Figure 1. Samples of 10 values of two independent random variables. $Z_1 \sim U(0, 1)$ and $Z_2 \sim U(0, 1)$ obtained by Monte-Carlo sampling (a) and by latin hypercube sampling (b).

3.4. Analysis of the output distribution

The last step of the analysis is to summarize the values of $f(\mathbf{z}_1), \ldots, f(\mathbf{z}_N)$. Different quantities can be easily calculated. For example, when $f(Z)$ is a single output variable, estimates of the expected value and variance of $f(Z)$ are given by $\bar{f} = \sum_{k=1}^{N} f(\mathbf{z}_k)/N$ and $1/(N-1)\sum_{j=1}^{N}\left[f(\mathbf{z}_j) - \bar{f}\right]^2$ respectively. It is also useful to estimate the quantiles associated to the distribution and the probabilities that $f(Z)$ is lower than some thresholds. Lacroix et al. (2005) used this method to study the risk of pollution of water by nitrate from crop model simulations. The probabilities are often plotted as a function of the threshold values and the resulting curve is called *cumulative probability distribution*.

The quantile q, defined by $P[f(Z) < q] = \alpha$, can be estimated as follows. The first step is to order the output values. The ordered values are noted $f(\mathbf{z}_{(1)}), \ldots, f(\mathbf{z}_{(i)}), \ldots, f(\mathbf{z}_{(N)})$. The second step is to determine the value i such as $(i-2)/(N-1) \leq \alpha < (i-1)/(N-1)$. The quantile is then defined by $\hat{q} = s \times f(\mathbf{z}_{(i-1)}) + (1-s) f(\mathbf{z}_{(i)})$ where $s = i - 1 + (1-N)\alpha$.

A histogram representation of the output variable values can also provide interesting information as shown in the following example.

A winter wheat dry matter model (continued)

The winter wheat dry matter model was used to compare uncertainty analyses with the uniform distribution and with a symmetric bell-shaped distribution. For sake of simplicity, we considered the Beta distribution with both shape parameters equal to 5, denoted by Beta(5,5). This distribution is symmetric and bounded between 0 and 1, and it puts more weight on the middle values of the [0, 1] interval (see Fig. 2). By applying the transformation $z = z_{\min(i)} + B \times (z_{\max(i)} - z_{\min(i)})$ where B follows a Beta(5,5) distribution, it yields a similar distribution over the uncertainty range of Z_i.

In the second stage of the uncertainty analyses, $N = 5000$ scenarios were generated, using the generators of quasi-random numbers implemented in the *R* software (www.r-project.org) for uniform or Beta distributions. For each scenario, the climatic year was chosen at random with equi-probability. The values of the seven parameters were generated one after another, assuming independence between factors.

In the third stage, the biomass at harvest was calculated with the model for each simulated scenario.

The fourth stage here included a histogram representation of the output and the calculation of basic statistics. The histograms of the model responses are shown in Figure 2. When input data was generated assuming a uniform distribution, combinations of parameter values very unlikely in practice appeared quite frequently, giving extreme output values. By contrast, the Beta(5,5) distribution made samples with extreme values of several factors very rare and the output distribution was much less flat. Some statistics on the simulated output distributions are given in Table 2.

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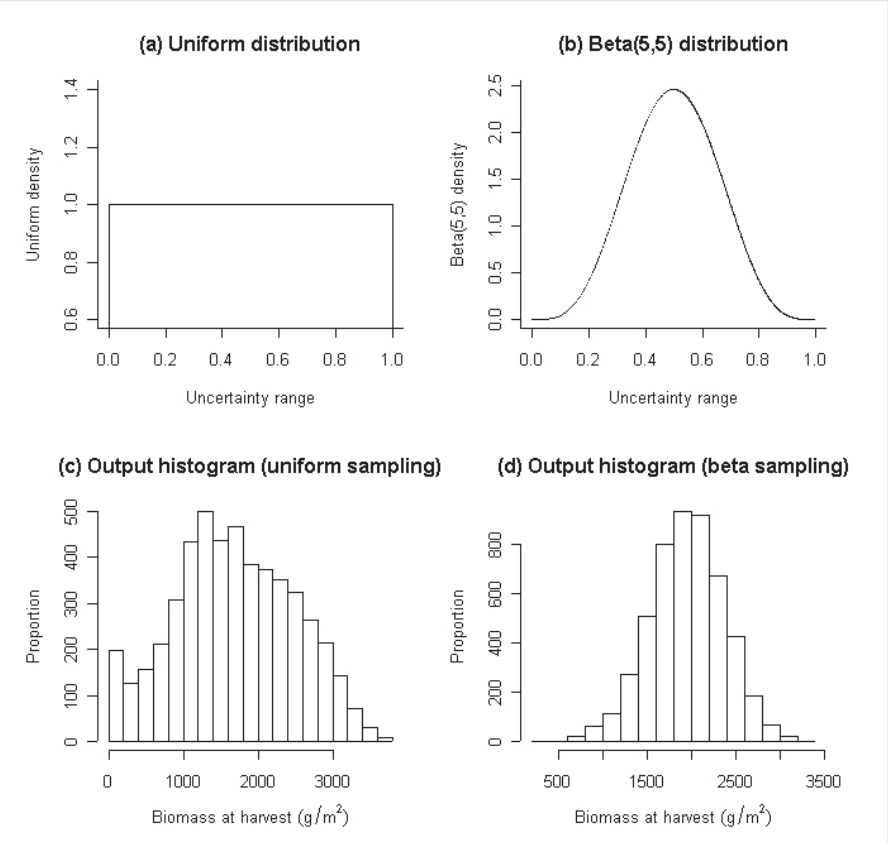

Figure 2. Density functions of the standard uniform (a) and Beta(5, 5) distributions (b). Histograms of the winter wheat model output (biomass at harvest) from samples of size 5000, generated assuming the uniform (c) or Beta(5, 5) (d) distributions.

Table 2. Some statistics on the biomass distributions (g/m^2) resulting from the uncertainty analyses.

Sampling	Minimum	1st Quartile	Median	3rd Quartile	Maximum
Uniform	0	1119	1636	2257	3785
Beta(5,5)	134	1665	1955	2233	3305
	Mean	Standard deviation			
Uniform	1669	785			
Beta(5,5)	1946	420			

4. Sensitivity analysis

4.1. Overview of the different methods

There are many different ways to define sensitivity of a model with respect to its inputs. This section presents the main approaches, without detailing precise criteria. The sensitivity with respect to a single input factor is first considered, then the sensitivities with respect to several factors.

4.1.1. One input factor

Figure 3 illustrates the basic approaches to measure sensitivity from the relationship between a single input factor Z and a model output $\hat{Y} = f(Z)$.

Local sensitivity analysis is based on the local derivatives of output $\hat{Y}$ with respect to Z, which indicate how fast the output increases or decreases *locally* around given values of Z. The derivatives can sometimes be calculated analytically, but they are usually calculated numerically for complex models. Problems may arise if the derivative of the model does not exist at some points. In addition, the derivatives may depend strongly on the Z-value. This problem is illustrated in Figure 3a where three derivatives are reported.

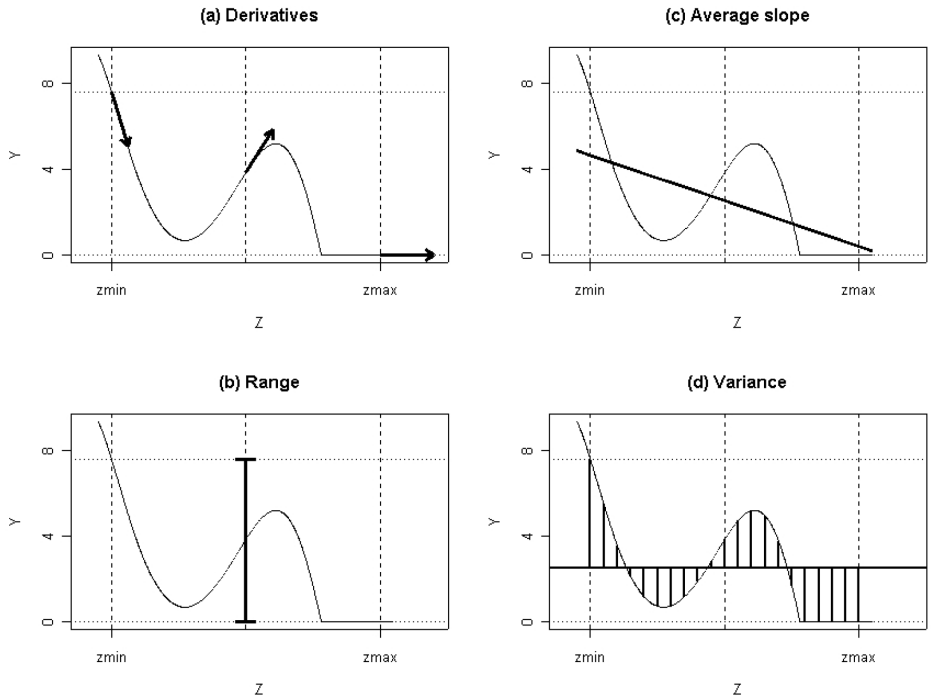

Figure 3. Bases for defining sensitivity criteria of model output $\hat{Y}$ with respect to input factor Z.

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The local (first-order) sensitivity coefficient $S_i^{\text{local}}(\mathbf{z}_k)$ is defined as the partial derivative of the output variable $\hat{Y}$ with respect to factor Z_i, calculated at the scenario $\mathbf{z}_k$:

$$S_i^{\text{local}}(\mathbf{z}_k) = \left.\frac{\partial f(Z)}{\partial Z_i}\right|_{\mathbf{z}_k}$$

This criterion is equivalent to the slope of the calculated model output in the parameter space. The $S_i^{\text{local}}(\mathbf{z}_k)$ criterion is an absolute measure of sensitivity, which depends on the scales or measurement units of $\hat{Y}$ or Z_i. A standardized version, called the relative sensitivity, is defined by:

$$S_i^{\text{local}}(\mathbf{z}_k) = \left.\frac{\partial f(Z)}{\partial Z_i}\right|_{\mathbf{z}_k} \times \frac{z_{k,i}}{f(\mathbf{z}_k)}$$

Local sensitivity analysis can be used to study the role of some parameters or input variables in the model. But this method is less useful than global sensitivity analysis when the purpose of the analysis is to study the effect of uncertainty of several factors on model outputs. A more detailed description of local sensitivity analysis is given by Turányi and Rabitz (2000).

A winter wheat dry matter model (continued)

For illustration, the local sensitivity coefficient for parameter E_{b} is defined by

$$S_{Eb}^{\text{local.r}}(\mathbf{z}) = \sum_{t=1}^{t_H-1} z_{E_{i\max}} \left[1 - e^{-z_K z_{\text{LAI}(t)}}\right] z_{\text{PAR}(t)}.$$

In *global sensitivity analysis* (Fig. 3b,c,d), on the other hand, the output variability is evaluated when the input factors vary in their whole uncertainty domains. This provides a more realistic view of the model behaviour when used in practice. There are several methods to perform global sensitivity analyses and the whole Section 4.2 is concerned with their description, while the book edited by Saltelli et al. (2000) is a comprehensive reference.

The global degree of association between Z and $\hat{Y}$ over the interval $[z_{\min}, z_{\max}]$ can first be measured through a model approximation. For instance, if the crop model is approximated by a linear relationship between Z and $\hat{Y}$ (Fig. 3c), sensitivity can be measured by the squared regression coefficient or by the linear correlation between Z and $\hat{Y}$. This approach is described in Section 4.2.3. It is a simple and often efficient way to measure sensitivity, provided the model approximation is adequate.

The approaches illustrated in Figures 3b and d are different since they do not rely on a model approximation, in principle at least. They are called model-independent in the sense of Saltelli et al. (1999), because they measure variation of $\hat{Y}$ independently of how this

variation is distributed along the Z-axis. The sensitivity criterion illustrated in Figure 3b is simply based on the range of the model output when Z runs within $[z_{\min}, z_{\max}]$ and it will be briefly discussed in Section 4.2.1 on one-at-a-time methods. In the approach illustrated in Figure 3d, sensitivity is measured by the variance of $\hat{Y}$ over $[z_{\min}, z_{\max}]$. This approach will be described in Sections 4.2.2, 4.2.4 and 4.2.5.

4.1.2. Several input factors

Figure 4 presents an *interaction plot* between two input factors Z_1 and Z_2: in this plot, the relationship between input Z_1 and output $\hat{Y}$ is represented for several distinct values of Z_2. The numerical values shown in Figure 4 are also presented in Table 3. If the effects of Z_1 and Z_2 on $\hat{Y}$ were additive, then the curves would be parallel. On the contrary, Figure 4 shows that there are strong interaction effects on $\hat{Y}$ between factors Z_1 and Z_2. The interaction plot shows clearly that, in case of an interaction between Z_1 and Z_2, the sensitivity of $\hat{Y}$ to Z_1 depends on the value of Z_2 and vice-versa. This situation occurs with most crop models, because crop models are not simply additive functions of parameters and input variables.

It is common practice to measure sensitivity for each input factor Z_i separately, with all other factors fixed at their single nominal values. However, this prevents interactions from being detected and quantified, whereas taking interactions into account is a key aspect of most global sensitivity methods. We discuss below the interest of several criteria with respect to their ability to take into account interactions between factors.

Consider for instance, the variance criterion $\text{var}(\hat{Y})$ illustrated in Figure 3d, and suppose now that there are several input factors. Let us denote by $\text{var}(\hat{Y}|Z_j = z_j, j \neq i)$ the

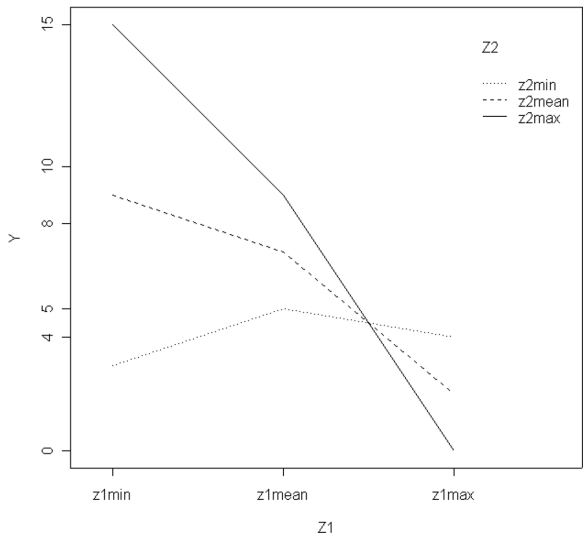

Figure 4. Two-factor interactions graphics: the output $\hat{Y}$ is represented as a function of the input factor Z_1, for three distinct values of Z_2.

Table 3. Output values $\hat{Y}$ for two interacting factors Z_1 and Z_2 and calculation of variance-based criteria for the first factor.

Z_1	Z_2	$\hat{Y}$	$E(\hat{Y}\,\vert Z_1)$	$\mathrm{var}(\hat{Y}\,\vert Z_1)$	$\mathrm{var}[E(\hat{Y}\,\vert Z_1)]$	$E[\mathrm{var}(\hat{Y}\,\vert Z_1)]$
1	1	3				
1	2	9	9	24		
1	3	15				
2	1	5				
2	2	7	7	8/3	$26/3 \approx 8.67$	$142/9 \approx 15.78$
2	3	9				
3	1	4				
3	2	2	2	8/3		
3	3	0				

variance of $\hat{Y}$ when z_i varies within its uncertainty domain and all other factors Z_j are fixed at given values z_j. Clearly, this variance gives information on the sensitivity of $\hat{Y}$ with respect to Z_i.

In a strict one-at-a-time approach, the criterion $\mathrm{var}(\hat{Y}|Z_j = z_j, j \neq i)$ is calculated at the nominal values $z_{0,j}$ only: it is equal to $\mathrm{var}(\hat{Y}|Z_j = z_{0,j}, j \neq i)$. If there are interactions between factors, however, then $\mathrm{var}(\hat{Y}|Z_j = z_j, j \neq i)$ depends on the z_j values and a more synthetic sensitivity criterion is preferable.

One possibility consists in using the variance of $\hat{Y}$ averaged over the z_js, rather than calculated at specific values $z_{0,j}$. Thus $\mathrm{var}(\hat{Y}|Z_j = z_{0,j}, j \neq i)$ is replaced by $\mathrm{var}[\mathrm{E}(\hat{Y}|Z_i = z_i)]$, where $\mathrm{E}(\hat{Y}|Z_i = z_i)$ denotes the expected (or average) model output when factor Z_i takes a given value z_i and the other factors vary within their uncertainty domains. The variance calculated in this way was called the *top marginal variance* by Jansen et al. (1994). It corresponds to the *main-effect* in an analysis of variance or to the *first-order* index in some sensitivity analysis methods. When this is applied to the example of Figure 4 (see Table 3), the first-order sensitivity to Z_1 is equal to $26/3 \approx 8.67$.

A second possibility consists in considering the expected value of $\mathrm{var}(\hat{Y}|Z_j = z_j, j \neq i)$ over all possible values of the z_js, for $j \neq i$, $\mathrm{E}[\mathrm{var}(\hat{Y}|Z_j = z_j, j \neq i)]$. The variance calculated in this way was called the *bottom marginal variance* by Jansen et al. (1994). By analogy to definitions given in Saltelli et al. (2001), we call such criteria *total* sensitivity criteria. When this is applied to the example of Figure 4 (see Table 3), the total sensitivity to Z_1 is equal to $142/9 \approx 15.78$.

AQ: Pl. list the reference

The total sensitivity of $\hat{Y}$ to Z_i can be interpreted as the expected remaining uncertainty in $\hat{Y}$ if all other input factors were determined exactly. In the example, the total sensitivities of both factors are larger than their main-effect sensitivities. This is a general property, and this difference between the total and main-effect sensitivities is entirely due to interactions between the factors.

Thus, total sensitivity gives a comprehensive measure of the influence of an input factor. This measure can be decomposed into main-effects and interactions, and this decomposition usually gives more insight on the model behaviour. As a conclusion, both types of criteria are useful and complementary. They will be illustrated, with the winter wheat model, in the sections on design of experiments and on sampling-based and variance-based methods.

4.2. Methods of global sensitivity analysis

4.2.1. One-at-a time methods

The most intuitive method to conduct a sensitivity analysis is to vary one factor at a time, while the other factors are fixed at their nominal values. The relationship between the values z_i of factor Z_i and the responses $f(z_{0,1} \dots z_{0,i-1}, z_i, z_{0,i+1}, \dots z_{0,s})$ determines a one-at-a-time response profile. Drawing response profiles is often useful, at least in preliminary stages. However, we have already argued that more global methods are preferable, because they take account of and quantify interactions between input factors.

In practice, each input factor Z_i takes k equispaced values from $z_{\min,i}$ to $z_{\max,i}$, with increments $\delta = (z_{\max,i} - z_{\min,i})/(k-1)$. The model responses $f(z_{0,1}, \dots z_{0,i-1} z_i, z_{0,i+1} \dots z_{0,s})$ are then calculated for the k discretized values z_i. Figure 5 represents the simulated scenarios when this procedure is applied to three input factors.

If the number of sensitivity factors is not too large, graphical representations are the best way to summarize the response profiles. Alternatively, summary quantities may be calculated for each factor's profile, and compared between factors. Bauer and Hamby (1991), for instance, proposed using the following index

$$I_i^{\mathrm{BH}} = \frac{\max_{z_i} f(z_{0,1} \dots z_{0,i-1}, z_i, z_{0,i+1} \dots z_{0,s}) - \min_{z_i} f(z_{0,1} \dots z_{0,i-1}, z_i, z_{0,i+1} \dots z_{0,s})}{\max_{z_i} f(z_{0,1} \dots z_{0,i-1}, z_i, z_{0,i+1} \dots z_{0,s})}$$

This index can be approximated by the difference between the maximum and minimum simulated values.

The number k of values per profile must be chosen carefully when the model is non-linear and particularly when it is non-monotonic. Provided k is odd, the number of model simulations to calculate all profiles is equal to $s(k-1)+1$. When k is small and the

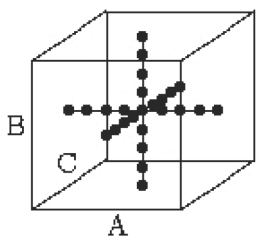

Figure 5. Sampled points when three factors are studied through one-at-a-time sensitivity profiles.

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model is non-linear, non-linear effects, as well as maxima or minima, may be undetected, which may lead to under-estimating sensitivity indices such as the index of Bauer and Hamby (1991). When k is large, the computing time may become too large if there are many input factors and the model is complex. In that case, it is more efficient to reserve computing time to more global methods of sensitivity analysis.

A winter wheat dry matter model (continued)

For the winter wheat dry matter model, no highly non-linear phenomena was expected, so that a small number of discretized values was considered sufficient. Besides, between-year variability was expected to have an influence on sensitivity. Consequently, one-at-a-time profiles were calculated with respect to each parameter and for each annual climate series.

The average profiles and their ranges over the climate series are represented in Figure 6. The results show that parameters E_b, A and B have a stronger influence on the simulated biomass value than the other parameters. They show that between-year variability depends on the values of the input factors. However, they give no information on the interactions between parameters.

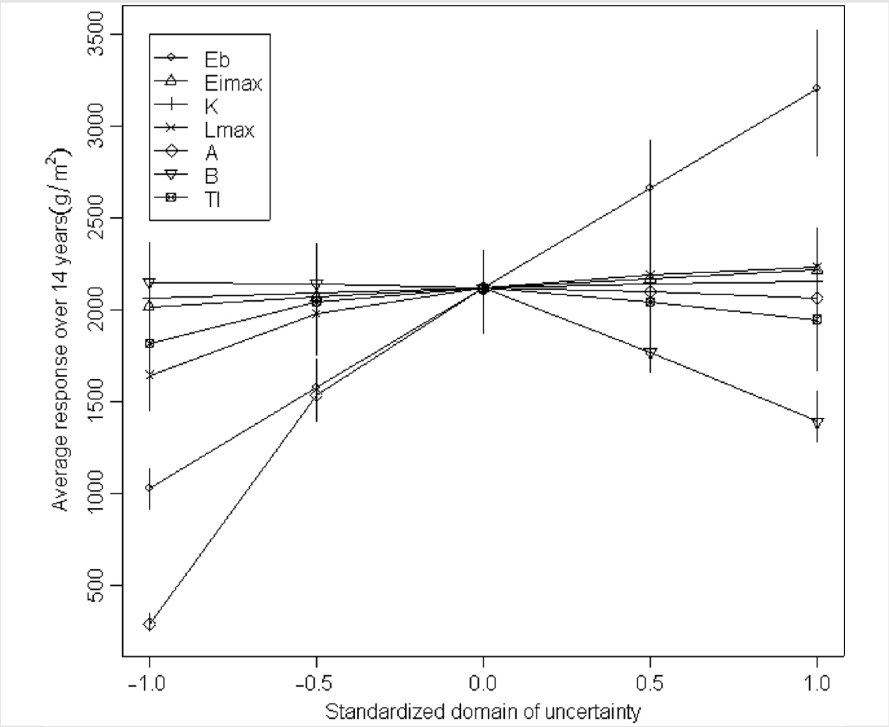

Figure 6. One-at-a-time profiles for the winter wheat dry matter at harvest simulated by the model over 14 climatic series. Points indicate the average simulated values over the climatic series and vertical bars indicate the ranges of variation.

In its most restricted application, one-at-a-time sensitivity analysis is applied at the nominal values of the sensitivity factors only. In that case, it gives information on the model only in a small neighbourhood of the nominal values. However, more global sensitivity analyses may be obtained by calculating one-at-a-time local sensitivity criteria for a lot of different input scenarios. This idea is exploited by Morris (1991). Morris defines the elementary effect of the ith factor for a given scenario $\mathbf{z}_0 = (z_{0,1}, \ldots, z_{0,s})$ as

$$d_i(\mathbf{z}_0) = \frac{f(z_{0,1} \ldots z_{0,i-1}, z_{0,i} + \Delta, z_{0,i+1} \ldots z_{0,s}) - f(z_{0,1} \ldots z_{0,i-1}, z_{0,i}, z_{0,i+1} \ldots z_{0,s})}{\Delta}$$

where $z_{0,i} + \Delta$ is a perturbed value of $z_{0,i}$. The principle of Morris' method is to sample a series of scenarios $\mathbf{z}_0 = (z_{0,1}, \ldots, z_{0,s})$ in the s-dimensional space defined by the values $[z_{\min(i)}, z_{\min(i)} + \delta, z_{\min(i)} + 2\delta, \ldots, z_{\max(i)}]$, $i = 1, \ldots, s$ and to calculate $d_i(\mathbf{z}_0)$ for each sampled value. The resulting distribution of the elementary effects of the ith factor is then characterized by its mean and variance. A high mean indicates a factor with an important influence on the output. A high variance indicates either a factor interacting with another factor or a factor whose effect is non-linear.

4.2.2. Factorial design and analysis of variance

The sensitivity analysis of a crop model is similar to an experiment where nature is being replaced by the simulated crop model. It follows that the classical theory of experimental design provides very useful tools for sensitivity analysis. In particular, factorial designs make it possible to evaluate simultaneously the influence of many factors, with possibly a very limited number of runs. An additional practical advantage is that the methods of analysis are available in general statistical packages.

Despite the analogy between natural experiments and sensitivity analyses, some differences must be pointed out. First, there is nothing like measurement error in simulated experiments, at least when the model is deterministic. As a consequence, there is no residual variance and it is unnecessary to replicate the same scenarios and introduce blocking, whereas replication and blocking are the key components of designed experiments. The second difference is that the number of runs may quite often be much larger in simulation studies than in real experiments.

Many books are dedicated to the design of experiments. A very good reference on factorial designs and response surface methods is Box and Draper (1987).

4.2.2.1. Complete factorial designs

With s input factors and m modalities per factor, there are m^s distinct input scenarios. The (unreplicated) complete m^s factorial design consists of running simulations for each of these scenarios exactly once.

The common point between the complete factorial design and the one-at-a-time profiles is that each factor is studied at a restricted number of levels. However, the major difference is that the emphasis in factorial designs is on making all factors vary simultaneously. This implies that the global "input space" of the model is much better investigated, as can be seen by comparing Figure 7 with Figure 5.

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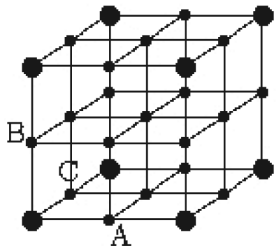

Figure 7. Sampled points when three factors are studied through a complete factorial design with two modalities per factor (large dots) or three modalities per factor (small and large dots).

Table 4. Number of runs for complete m^s factorial designs.

s	$m = 2$	$m = 3$	$m = 4$	$m = 5$
5	32	243	1024	3125
10	1024	59049	1048576	9765625
20	$1.05e + 06$	$3.49e + 09$	$1.10e + 12$	$9.54e + 13$

A less favourable consequence is that the complete factorial design requires many runs when the number of factors under study is large, as Table 4 shows. For this reason, the 2^s and 3^s factorial designs are the most frequently used complete factorial designs when the number of factors is large. These designs are very useful to quantify interactions between factors.

Factorial decomposition of the model response The analysis of variance (ANOVA) is based on the decomposition of the response variability between contributions from each factor and from interactions between factors. This decomposition is related to the statistical theory of the linear model.

Consider a model with two input factors Z_1 and Z_2, and let $\hat{Y}_{ab} = f(a, b)$ denote the model response when $z_1 = a$ and $z_2 = b$. In a complete m^2 factorial design, there are m possible values for a and m possible values for b and so there are m^2 distinct $\hat{Y}_{ab}$ values. Let $\hat{Y}_{\bullet\bullet}$ denote their general mean, $\hat{Y}_{a\bullet}$ denote the mean when $z_1 = a$, and $\hat{Y}_{\bullet b}$ the mean when $z_2 = b$. Then, when restricted to the m^2 design scenarios, the model can be decomposed into

$$\hat{Y}_{ab} = \mu + \alpha_a + \beta_b + \gamma_{ab}, \tag{1}$$

AQ: pl. clarify whether dot is used here to mean main effect.

where μ is the general mean, $\alpha_a = \hat{Y}_{a\bullet} - \mu$ is called the main effect of factor Z_1 when $z_1 = a$, $\beta_b = \hat{Y}_{\bullet b} - \mu$ is the main effect of factor Z_2 when $z_2 = b$, and $\gamma_{ab} = \hat{Y}_{ab} - (\mu + \alpha_a + \beta_b)$ is the interaction between Z_1 and Z_2 when $z_1 = a$ and $z_2 = b$. The factorial effects satisfy the properties $\sum_a \alpha_a = 0$, $\sum_b \beta_b = 0$, and $\sum_a \gamma_{ab} = \sum_b \gamma_{ab} = 0$. The number of free ANOVA parameters (α_a, β_b, γ_{ab}) associated with each factorial term is called its "degrees of freedom" number. There are $(m - 1)$ degrees of freedom for the main effects of Z_1 and Z_2 and $(m - 1)^2$ degrees of freedom for their interaction.

The response variability can be decomposed into factorial terms as follows:

$$\underbrace{\sum_{ab}(\hat{Y}_{ab}-\mu)^2}_{\mathrm{SS}_T} = \underbrace{m\sum_{a}\alpha_a^2}_{\mathrm{SS}_1} + \underbrace{m\sum_{b}\beta_b^2}_{\mathrm{SS}_2} + \underbrace{\sum_{a,b}\gamma_{ab}^2}_{\mathrm{SS}_{12}}, \tag{2}$$

where SS_T measures the total variability in the model responses, SS_1 is the sum of squares associated with the main effect of Z_1, SS_2 is the sum of squares associated with the main effect of Z_2, and SS_{12} is the sum of squares associated with the interaction between Z_1 and Z_2.

With s factors at m levels, the complete ANOVA decomposition is a sum of $(2^s - 1)$ factorial terms:

$$SS_T = \sum_{\mathrm{i}} SS_i + \sum_{i<j} SS_{ij} + \cdots + SS_{1\ldots s}, \tag{3}$$

including main effects (SS_i) and interactions between up to s factors ($SS_{1\ldots s}$). The number of degrees of freedom for an interaction between q factors is equal to $(m-1)^q$. Note that for a 2^s factorial design, all factorial terms have just one degree of freedom.

ANOVA results and sensitivity indices For the sensitivity analysis of a deterministic model, the main interest lies in comparing the contributions of the factorial terms to the total variability, while formal testing of hypotheses has no real meaning since there is no residual variability. It follows that the most useful information lies in the sums of squares. By dividing the sums of squares by the total variability, the following "ANOVA" sensitivity indices can be easily calculated:

- main effects sensitivity indices $S_1 = \frac{SS_1}{SS_T}$, $S_2 = \frac{SS_2}{SS_T}$;
- interaction sensitivity indices $S_{12} = \frac{SS_{12}}{SS_T}$;
- total sensitivity indices such as $TS_1 = \frac{SS_1+SS_{12}}{SS_T}$ or $TS_2 = \frac{SS_2+SS_{12}}{SS_T}$, which summarize all factorial terms related to a particular factor.

A winter wheat dry matter model (continued)

For the eight sensitivity factors of the "winter wheat dry matter model" example, a 2^8 complete factorial design would require the number of climatic series to be limited to two. We applied instead a $2^7 \times 14$ complete factorial design, where the 14 climatic series were crossed with the 2^7 scenarios based on the minimum and maximum values of the parameter uncertainty ranges. There were thus a total of $1792 = 2^7 \times 14$ simulations of the crop model. The analysis of variance on the simulation results can be performed assuming the complete factorial model, including interactions between up to eight factors. In practice, simpler models are often sufficient to capture the most interesting sensitivity features.

For illustration, the results presented in Table 5 were calculated assuming a model with 8 main effects (7 parameters + climate) and interactions between two factors only. The sums of squares in Table 5 are given by many statistical software packages, but not the sensitivity column which was calculated by dividing the sum-of-squares column by the total variability SS_T of the data. In this analysis, the quantities associated with the residuals correspond to all terms which were not included in the model, that is here, interactions between three or more factors. The coefficient of determination R^2 of a model is, by definition, the percentage of the total variability explained by the model. Here, it is equal to 0.94, indicating that only 6% of the variability in the simulated model output is accounted for by interactions between more than three factors.

Sensitivities are represented graphically in Figures 8 (factorial indices) and 9 (total indices). For these figures, the complete factorial model was used, but the differences with the model with main effects and two-factor interactions were small. The most influential factors are the parameters E_b, A and B, which confirms results of the one-at-a-time profiles (Figure 6). The figures also show that the influence of interactions is high, which could not be detected by the one-at-a-time profiles.

Table 5. Analysis of variance table of the complete factorial design applied to the winter wheat dry matter model; the table was calculated for the model including main effects and two-factor interactions. Sensitivities smaller than 0.01 are not displayed.

	SS	Sensitivity index
E_b	777 593 320	0.33
E_{imax}	6686 674	
K	3662 758	
L_{max}	80 732 881	0.03
A	520 104 586	0.22
B	309 742 948	0.13
TI	551 495	
YEAR	7330 246	
E_b:E_{imax}	1763 250	
E_b:K	965 855	
E_b:L_{max}	21 288 948	
E_b:A	137 149 566	0.06
E_b:B	81 678 016	0.04
E_b:TI	145 427	
E_b:*YEAR*	1932 958	
E_{imax}:K	8306	
E_{imax}:L_{max}	183 068	
E_{imax}:A	1179 375	
E_{imax}:B	702 365	
E_{imax}:TI	1251	
E_{imax}:*YEAR*	16 622	
K:L_{max}	823 631	
K:A	82 704	
K:B	635 271	

continued

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Table 5.—Cont'd.

	SS	Sensitivity index
K:TI	395	
K:*YEAR*	6643	
L_{max}:A	60 448	
L_{max}:B	17 116 469	
L_{max}:TI	35 467	
L_{max}:*YEAR*	145 584	
A:B	193 147 537	0.08
A:TI	28 101 635	0.01
A:*YEAR*	2586 798	
B:TI	1425 195	
B:*YEAR*	1178 019	
TI:*YEAR*	2471 694	
Residuals	128 829 265	

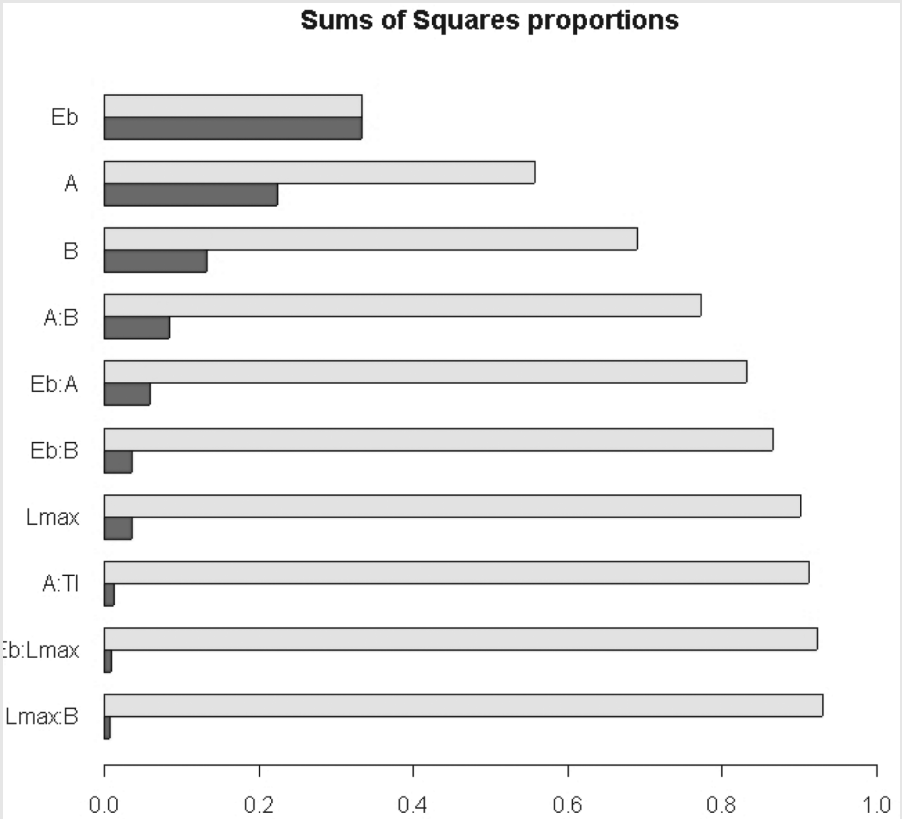

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Figure 8. The eight largest factorial sensitivity indices based on the $2^s \times 14$ factorial design and its analysis of variance with a complete factorial model, for the winter wheat crop model; the lower bars show cumulative indices.

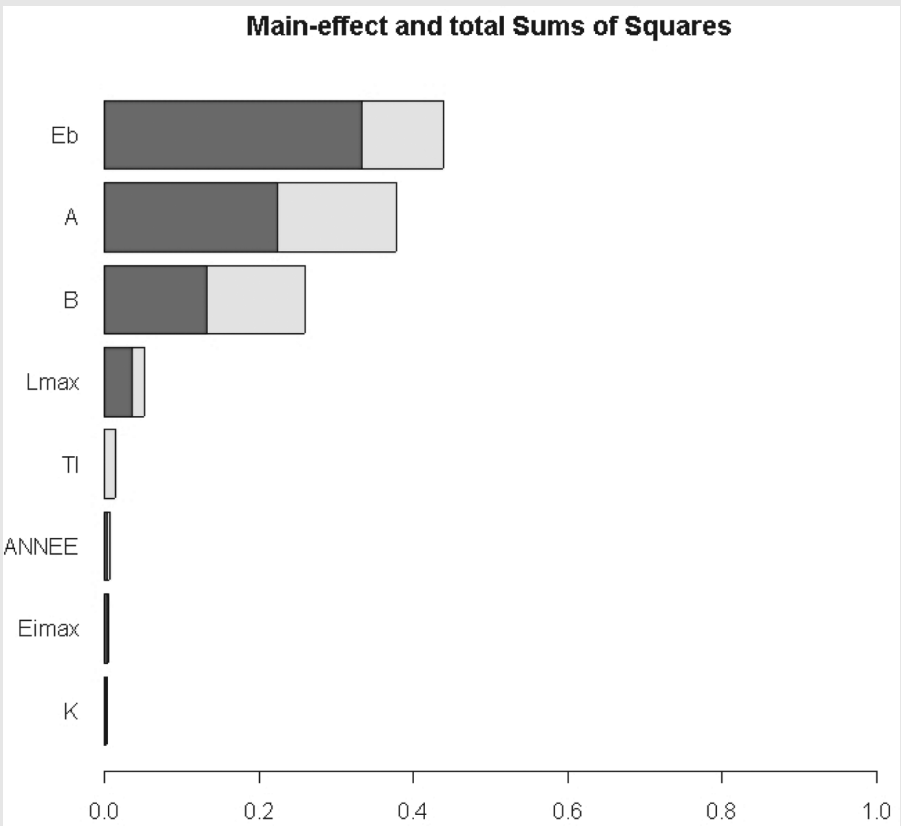

Figure 9. Main-effect (first part of the bars) and total (full bars) sensitivity indices based on the $2^s \times 14$ factorial design and its analysis of variance, for the winter wheat model.

4.2.2.2. Fractional factorial designs

When there is a large number of factors, the factorial main effects and low-order interactions can usually be estimated quite accurately by running only a fraction of the complete factorial design. When applied to sensitivity analysis, fractional factorial designs are very useful for screening a large number of factors and for detecting the most influential ones, with a relatively small number of runs. This requires, however, the assumption that higher-order interactions are negligible. It also requires that the fraction be carefully chosen. This can be done through algebraic methods of construction (see Box and Draper, 1987; Kobilinsky, 1997).

Consider, for example, the fractional design for seven factors at two modalities ± 1 given in Table 6. This is a complete factorial design for factors A, B and C, which are called the basic factors of the fraction. The modalities of the basic factors have been used to calculate those of four additional factors D, E, F and G.

Consider first the design restricted to factors A, B, C and G. This is a half-fraction of the 2^4 complete factorial design, with eight runs instead of 16. Because this is an

Table 6. Complete 2^3 factorial design and fractional design defined by $ABC = 1$.

A	B	C	$D = AB$	$E = AC$	$F = BC$	$G = ABC$	Y
-1	-1	-1	$+1$	$+1$	$+1$	-1	Y_1
-1	-1	$+1$	$+1$	-1	-1	$+1$	Y_2
-1	$+1$	-1	-1	$+1$	-1	$+1$	Y_3
-1	$+1$	$+1$	-1	-1	$+1$	-1	Y_4
$+1$	-1	-1	-1	-1	$+1$	$+1$	Y_5
$+1$	-1	$+1$	-1	$+1$	-1	-1	Y_6
$+1$	$+1$	-1	$+1$	-1	-1	-1	Y_7
$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	Y_8

incomplete factorial design, not all factorial terms can be estimated. However, there are quite simple rules to determine which terms can be estimated. Thus, the relationship $G = ABC$ which was used for defining G implies that the main-effect of G is confounded with the A:B:C interaction. The two effects cannot be estimated separately, but if A:B:C is assumed to be negligible, then the main-effect of G can be estimated. By multiplying both sides of the $G = ABC$ equality with factor letters and by adopting the convention that $A^2 = B^2 = C^2 = G^2 = 1$, other confounding rules can be obtained. For example, multiplying by A yields $AG = A^2BC$ which gives $AG = BC$ after simplification. This implies that the interactions A:G and B:C are confounded. More generally, there is one confounding relationship associated with each factorial effect between the basic factors. Here, the confounding relationships are:

$$
\begin{aligned}
1 &= ABCG \\
A &= BCG \\
B &= ACG \\
C &= ABG \\
AB &= CG \\
AC &= BG \\
BC &= AG \\
ABC &= G,
\end{aligned}
$$

where 1 indicates the general mean. The resolution of a fractional design is, by definition, the minimum order among the interactions confounded with the general mean. Here, there is only one fourth-order interaction confounded with the mean, so the fraction has resolution IV (by convention, the resolution is often written with roman numbers). With a fraction of resolution IV, the general mean is confounded with the four-factor interaction, main effects are confounded with three-factor interactions, and two-factor interactions are

mutually confounded. Assuming that three- and four-factor interactions are negligible, all main effects can be estimated.

Consider now the design with the seven factors A to G. This is a $1/(2^4)$ fraction of the complete factorial design, with 8 runs instead of 128! Now, instead of being confounded by pairs, factorial effects are confounded by groups of size 16. For example, the confounding relationships involving the general mean are

$$1 = ABD = ACE = BCF = ABCG = BCDE = ACDF = CDG = ABEF$$
$$= BEG = AFG = DEF = ADEG = BDFG = CEFG = ABCDEFG$$

and the confounding relationships involving the main effect of A are

$$A = BD = CE = ABCF = BCG = ABCDE = CDF = ACDG = BEF$$
$$= ABEG = FG = ADEF = DEG = ABDFG = ACEFG = BCDEFG.$$

This is a resolution III fractional design, and with such a design, the main effects are confounded with interactions between two and more factors. Thus the main effects can be estimated provided all interactions are considered negligible.

Both examples given above can be generalized to more factors and more modalities per factors. With 2^n simulations, it is possible to study up to $2^n - 1$ factors in a resolution III fraction, and up to 2^{n-1} factors in a resolution IV design. Of course, higher resolutions should be preferred when possible. The main difficulty is to find the most appropriate confounding relationships when defining new factors from the basic ones. Tables are given in Kobilinsky (1997). The PROC FACTEX procedure of the SAS QC module can generate fractional designs automatically.

4.2.2.3. Other experimental designs

In a 2^s complete or fractional factorial design, all information on each quantitative factor Z_i is based on the model behaviour at only two levels per factor. This is optimal when, for any setting of the other factors, the model is a linear or near-linear function of z_i. It often remains efficient when the model is monotonous. However, 2^s designs do not allow one to detect and quantify non-linear relationships between a sensitivity factor and the output.

In that case, it is necessary to consider designs with more levels per factor. One may use 3^s, 4^s complete or fractional designs, which ensure that quadratic effects may be detected as well as linear effects. Flexible fractional designs exist also for these designs, in fact for all m^s designs where m is a prime number or a power of a prime.

The response surface methodology (see Box and Draper, 1987) offers an alternative approach to study the influence of quantitative factors on a response function. It is based on an approximation of the crop model by a polynomial function of degree one or two of the input factors, and on convenient designs to estimate their parameters. This approach has been applied to the STICS crop model (Ruget et al., 2002) and we refer to this article for a detailed presentation in the context of crop models.

4.2.3. Intensive sampling and correlation criteria

In the sensitivity analysis methods presented in Section 4.2.2, the sampled modalities of the input factors are precisely defined by the factorial design. Another approach consists in randomly generating factor values by Monte Carlo sampling. The principle is to randomly generate N scenarios of the input factors $\mathbf{z}_k = (z_{k,1}, \ldots, z_{k,i}, \ldots, z_{k,s})$ $k = 1, \ldots, N$, and to compute the model output for each scenario, $f(\mathbf{z}_k)$ $k = 1, \ldots, N$, in a similar way to what is done for an uncertainty analysis. The statistical methods related to regression (see e.g. Venables and Ripley, 1999) are then used to represent and to measure the sensitivity of the output variables with respect to the input factors. These methods are presented below.

Correlation coefficients can be used to quantify the relationships between input factors and output variables. Let $s^2_{\hat{Y}} = \frac{1}{N}\sum_{k=1}^{N}[f(\mathbf{z}_k) - \bar{f}]^2$ and $s^2_{Z_i} = \frac{1}{N}\sum_{k=1}^{N}(z_{k,i} - \bar{z}_i)^2$ denote the empirical variances of $\hat{Y} = f(Z)$ and Z_i in the simulations, and let $\hat{\text{cov}}(\hat{Y}, Z_i) = \frac{1}{N}\sum_{k=1}^{N}[f(\mathbf{z}_k) - \bar{f}][z_{k,i} - \bar{z}_i]$ denote their covariance. Then the PEAR (Pearson Product Moment Correlation Coefficient) coefficient between Z_i and $\hat{Y}$ is defined by

$$r_{Z_i,\hat{Y}} = \frac{\hat{cov}(\hat{Y}, Z_i)}{s_{\hat{Y}}\, s_{Z_i}}.$$

It varies between -1 and $+1$ and it measures the degree of linear association between the variations of Z_i and those of $\hat{Y}$. Some non-linear associations may remain undetected and underestimated by the PEAR coefficient. An alternative is the Spearman correlation coefficient, which is calculated on the ranks of Z_i and Y. The Spearman correlation coefficient is more adequate in case of strongly non-linear, but still monotonous, relationships.

With the PEAR or Spearman coefficients, no account is taken of the possible effects of input factors other than Z_i. In contrast, the partial correlation coefficient (PCC) aims at measuring the association between Z_i and $\hat{Y}$ after eliminating possible effects due to other input factors Z_j, $j \neq i$. The PCC coefficient is similar to the PEAR correlation coefficient, but it is calculated with $f(\mathbf{z}_k)$ and $z_{k,i}$ replaced by the residuals of the following two regression models

$$f(\mathbf{z}_k) = b_0 + \sum_{j\neq i} b_j z_{k,j} + \varepsilon_k, \quad z_{k,i} = c_0 + \sum_{j\neq i} c_j z_{k,j} + \varepsilon'_k,$$

where b_js and c_js are regression coefficients to be estimated.

Regression models give a general framework for studying the influence of all input factors simultaneously. By approximating the crop model under study, they make it possible to evaluate the influence of each input factor. Consider for instance the regression model with first-order effects only:

$$f(\mathbf{z}_k) = b_0 + \sum_{i=1}^{s} b_i z_{k,i} + \varepsilon''_{ik}, \tag{4}$$

where b_i are the regression coefficients to be estimated and ε''_{ik} is the approximation error term. The regression coefficients are estimated by least-squares. The quality

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of the adjustment is synthesized typically by calculating the model coefficient of determination R^2, that is, the percentage of output variability explained by the model.

The estimated regression coefficients $\hat{b}_i$ can be considered as sensitivity measures associated with the factors Z_i, provided they are standardized with respect to the variability in $\hat{Y}$ and in Z_i. The standardized regression coefficients (SRC) are defined as the quantities $\hat{b}_i(s_{Z_i}/s_{\hat{Y}})$.

Many more principles and techniques of regression are useful for sensitivity or uncertainty analysis, but it is out of the scope of this chapter to present them all. However, a few remarks can be made:

- the regression model in Eq. (4) can be extended in order to incorporate interactions between input variables, qualitative as well as quantitative factors, quadratic as well as linear effects. This is useful in particular if the regression coefficient of determination is small;
- when the number of terms in the model is large, model selection techniques (stepwise regression for instance) may become a precious aid to interpretation, since they can eliminate factors with negligible influence;
- the regression techniques presented here are good essentially at capturing linear effects between the Z_is and the Ys. Alternative methods should be considered when non-linear relationships are suspected;
- polynomial regression is one of the basic approaches in response surface methodology. It can be used on randomly selected simulations as described here, but also on simulations based on factorial or response surface design (Ruget et al., 2002).

A winter wheat dry matter model (continued)

$N = 5000$ scenarios were generated, using the generators of quasi-random numbers implemented in the *R* software (www.r-project.org) for Uniform and Beta distributions. Figure 10 shows scatterplots of the model simulations. A scatterplot is a representation of the points $\left[z_{k,i}, f(\mathbf{z}_k)\right]$, where $z_{k,i}$ is the value of Z_i in the k-th simulation and $f(\mathbf{z}_k)$ is the simulated response. In order to get a better visualisation, only 500 points have been represented in the plots of Figure 10. Non-parametric smoothing lines, based on local regressions, have been added to the plots in order to better visualize the relationship between $f(\mathbf{z}_k)$ and $z_{k,i}$. Figure 10 reveals a negative correlation between biomass at harvest and parameter B, and a positive correlation between the model output and parameters E_b and A.

PEAR and SRC coefficients for the parameters of the winter wheat dry matter model are given in Table 7. They have been calculated with the linear model function of the statistical package R, from the 5000 simulations. The results are very similar to those obtained with analysis of variance, with E_b, A and B the most influential parameters. The difference between the SRC and PEAR coefficients is small because the data set is large (5000 samples) and so the input factors are nearly orthogonal (the maximum empirical correlation between input factors is 0.037). There is a larger difference between the input sampling distributions, with a stronger sensitivity to E_b when the beta distribution is used.

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The coefficient of determination of the model with only first-order effects (uniform case) is $R^2 = 0.78$. This shows that interactions account for more than 20% of the output variability.

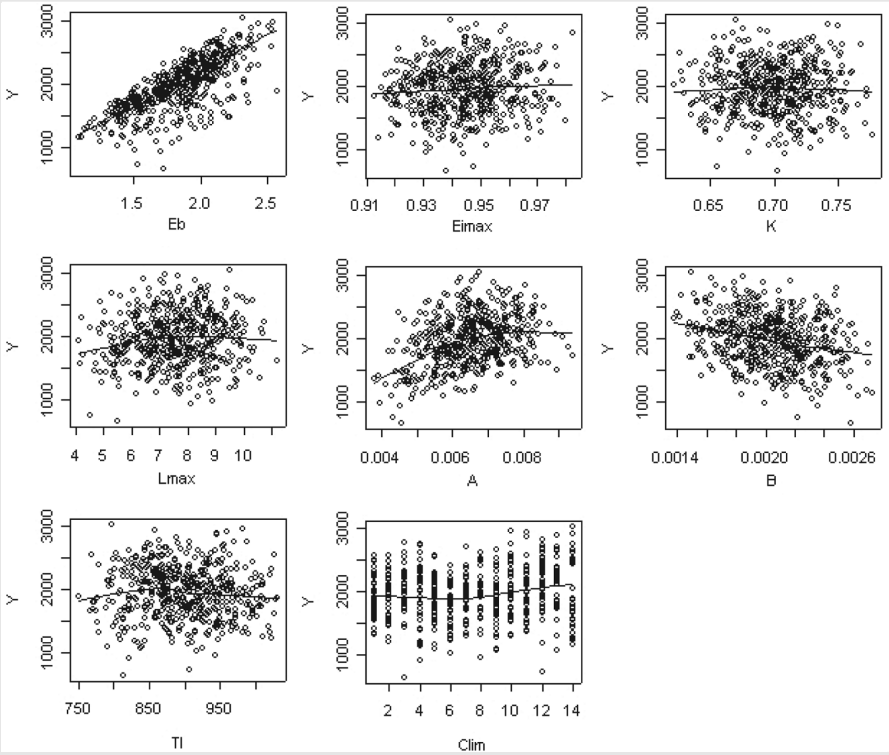

Figure 10. Scatter plots between the simulated values of biomass at harvest (g/m^2) and each input factor over its range of uncertainty, based on 500 simulations.

Table 7. PEAR and SRC coefficients for the winter wheat dry matter model, estimated from 5000 Monte Carlo samples.

Parameter	Uniform sampling		Beta sampling	
	PEAR	SRC	PEAR	SRC
E_b	0.62	0.63	0.71	0.73
E_{imax}	0.10	0.06	0.04	0.06
K	0.04	0.03	0.04	0.03
L_{max}	0.15	0.17	0.15	0.16
A	0.47	0.49	0.36	0.39
B	−0.33	−0.34	−0.30	−0.32
TI	0.04	0.03	0.04	0.04

4.2.4. Intensive sampling and variance-based sensitivity analysis

4.2.4.1. Variance-based measures of sensitivity
In the approaches based on experimental design followed by analysis of variance or on Monte Carlo sampling followed by regression, sensitivity analysis is based on an approximation of the crop model by a simpler linear model. In the variance-based methods described in this section, the principle is to decompose the output variability $D = \mathrm{Var}(\hat{Y})$ globally, without an intermediate simplified model.

Sobol decomposition of the model The methods are based on model and variance decompositions that are very similar to those encountered in analysis of variance. To emphasize the similarities and differences, we adopt a presentation which parallels that in Section 4.2.2.

Consider two quantitative input factors Z_1 and Z_2, and let $\hat{Y}_{ab}$ denote the model response when $z_1 = a$ and $z_2 = b$. The Sobol decomposition of the crop model f (Sobol, 1993) is given by

$$\hat{Y}_{ab} = \mu + f_1(a) + f_2(b) + f_{12}(a, b). \tag{5}$$

This decomposition is quite similar to the decomposition in Eq. (1), but, in contrast to Section 4.2.2, a and b are now assumed to vary continuously within the uncertainty interval [0, 1]. It follows that the general mean of the crop model f is now defined by

$$\mu = \int_0^1 \int_0^1 f(z_1, z_2) dz_1 dz_2.$$

The main effect of factor Z_1 is defined by the function

$$f_1(a) = \int_0^1 f(a, z_2) dz_2 - \mu$$

of a. Similarly, the main effect of B is defined by

$$f_2(b) = \int_0^1 f(z_1, b) dz_1 - \mu.$$

Finally, the interaction between Z_1 and Z_2 is defined by

$$f_{12}(a, b) = f(a, b) - f_1(a) - f_2(b) + \mu.$$

The factorial effects thus defined satisfy orthogonality properties which make the decomposition unique and give it a lot of nice properties. In particular, these properties

yield an orthogonal decomposition of the response variability into factorial terms:

$$\underbrace{\int_0^1 \int_0^1 (\hat{Y}_{z_1 z_2} - \mu)^2 dz_1 dz_2}_{\mathrm{Var}(\hat{Y})} = \underbrace{\int_0^1 f_1(a)^2 da}_{D_1} + \underbrace{\int_0^1 f_2(b)^2 db}_{D_2} + \underbrace{\int_0^1 \int_0^1 f_{12}(a,b)^2 dadb}_{D_{12}}, \quad (6)$$

where D_1 is the variability associated with the main effect of Z_1, D_2 is the variability associated with the main effect of Z_2 and D_{12} is the variability associated with the interaction between Z_1 and Z_2.

With s quantitative factors, the decomposition of the variance $\mathrm{Var}(\hat{Y})$ generalizes to:

$$\mathrm{var}(\hat{Y}) = \sum_{i=1}^{s} D_i + \sum_{i<j} D_{ij} + \cdots + D_{1\ldots s}. \quad (7)$$

In the decomposition Eq. (7), D_i corresponds to the main or first-order effect of Z_i denoted by $\mathrm{var}[\mathrm{E}(\hat{Y}|Z_i = z_i)]$ in Section 4.2.2. The terms $D_{ij}, \ldots, D_{1\ldots s}$ of Eq. (7) correspond to the interactions between the input factors. This is very similar to the analysis of variance. However, $\mathrm{var}(\hat{Y})$ now represents the variability of $\hat{Y}$ with respect to the overall uncertainty in the input factors, and not only over a limited number of experimental design points. This makes it more adequate for taking account of irregular and non-linear effects.

In probabilistic terms, D_i is the variance of the conditional expectation $\mathrm{E}(\hat{Y}\,|Z_i = z_i\,)$. If $\hat{Y}$ is sensitive to Z_i, $\mathrm{E}(\hat{Y}\,|Z_i = z_i\,)$ is likely to vary a lot when z_i changes and so D_i is likely to be large. This is why D_i is also called an "importance measure" in the vocabulary of sensitivity analysis.

Sensitivity indices Sensitivity indices are derived from the decomposition Eq. (7) by dividing the importance measures by $\mathrm{var}(\hat{Y})$:

$$S_i = D_i/\mathrm{var}(\hat{Y})$$

$$S_{ij} = D_{ij}/\mathrm{var}(\hat{Y})$$

$$\ldots$$

Consequently, the sensitivity indices satisfy

$$S_1 + \cdots + S_s + S_{1,2} + \cdots + S_{1,2,\ldots s} = 1$$

and can be interpreted as the proportions of $\mathrm{var}(\hat{Y})$ explained by the various factorial terms.

As explained in Section 4.1.2, two main types of sensitivity indices can be defined for each factor Z_i. The first-order sensitivity index S_i is useful for measuring the average influence of factor Z_i on the model output, but it takes no account of the interaction

effects involving Z_i. The second useful index is the total sensitivity index of Z_i, equal to the sum of all factorial indices involving Z_i:

$$TS_i = S_i + \sum_{j \neq i} S_{ij} + \cdots + S_{1\ldots s}.$$

Note that TS_i is also equal to $1 - S_{-i}$, where S_{-i} denotes the sum of all indices where Z_i is not involved.

4.2.4.2. Estimation based on Monte Carlo sampling

In order to estimate the first-order sensitivity index S_i, the basic idea is to evaluate the model response at N randomly sampled pairs of scenarios $sc_{A,k}$ and $sc_{B,k}$ defined by

$$\begin{aligned} sc_{A,k} &= (z_{k,1}, \ldots, z_{k,i-1}, z_{k,i}, z_{k,i+1}, \ldots, z_{k,s}) \\ & \qquad\qquad\qquad\qquad\qquad\qquad , \quad k = 1, \ldots, N \\ sc_{B,k} &= (z'_{k,1}, \ldots, z'_{k,i-1}, z_{k,i}, z'_{k,i+1}, \ldots, z'_{k,s}) \end{aligned}$$

with the same level $z_{k,i}$ of Z_i and all other levels sampled independently. Let D denote $\mathrm{var}(\hat{Y})$, then

$$\hat{f}_0 = \frac{1}{2N} \sum_{k=1}^{N} [f(sc_{A,k}) + f(sc_{B,k})]$$

$$\hat{D} = \frac{1}{2N} \sum_{k=1}^{N} [f(sc_{A,k})^2 + f(sc_{B,k})^2] - \hat{f}_0^2$$

$$\hat{D}_i = \frac{1}{N} \sum_{k=1}^{N} f(sc_{A,k}).f(sc_{B,k}) - \hat{f}_0^2$$

are unbiased estimators of, respectively, the average value of $\hat{Y}$, its total variance, and the main-effect of Z_i. An obvious estimator of S_i is then $\hat{S}_i = \hat{D}_i / \hat{D}$.

The procedure just described requires $2N$ model simulations for the estimation of each first-order index. When the first-order indices of all s factors must be calculated, the following procedure is more efficient computationally than performing s independent sets of $2N$ simulations:

- generate N input scenarios by Monte Carlo sampling, and store them in a $N \times s$ matrix M; the rows in M will form the $sc_{A,k}$ scenarios for all factors;
- generate N more input scenarios by Monte Carlo sampling, and store them in a $N \times s$ matrix M'; the rows in M' will be used to form the $sc_{B,k}$ scenarios;
- calculate the responses $f(sc_{A,k})$ for each scenario in M;
- for each factor Z_i calculate the responses $f(sc_{B,k})$ where $sc_{B,k}$ is determined by row k of M' for all factors different from Z_i and by row k of M for factor Z_i;
- apply the formulae given above for the calculation of $\hat{S}_i$.

This algorithm requires $N(s+1)$ model simulations for the calculation of the first-order sensitivity indices of s factors. An even more efficient sampling scheme, the winding stairs, was proposed by Jansen (1994). It is not described here for the sake of brevity.

A winter wheat dry matter model (continued)

Figure 11 displays results of a sampling-based sensitivity analysis. A Monte Carlo sample of size 1000 was used to generate a winding stairs set of simulations. Because there were eight factors (seven parameters + climate) in the model and we chose a basis of 1000 Monte Carlo samples, the number of model simulations needed to estimate first-order and total indices was equal to 9×1000. In order to show the variability of the estimates due to sampling,

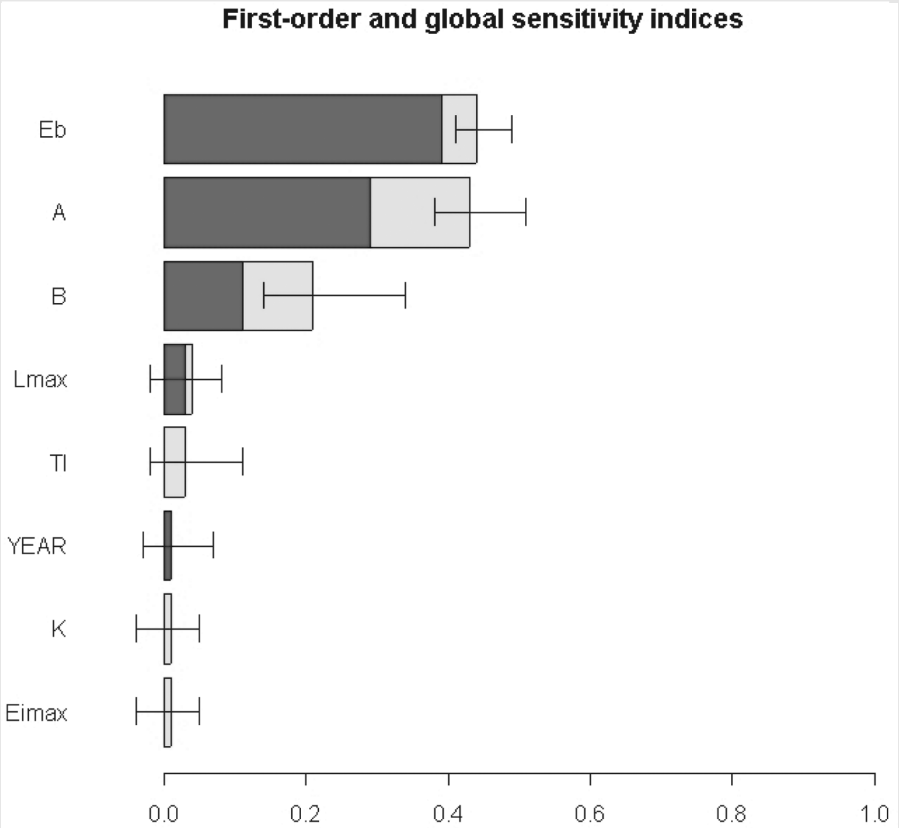

Figure 11. First-order and total Sobol sensitivity indices estimated from Latin hypercube sampling combined with winding stairs; there were 20 runs with 9×1000 model simulations for each run; the first part of the bars corresponds to the average (over the 20 runs) estimate of the first-order index, the full bars indicate average estimates of total indices, while the lines indicate extreme estimates of total indices.

this procedure was repeated 20 times, and the ranges of the estimates over the 20 series of simulations are displayed.

The results are different but quite consistent with those obtained with a designed experiments. This is not very surprising because the model behaves quite linearly and so the more intensive sampling-based method does not bring much more information on the model behaviour.

The sampling-based methods give unbiased estimates of the sensitivity indices, but the estimates can be quite variable and even take negative values, as Figure 11 shows. Homma and Saltelli (1996) propose a corrective term to improve this problem. Nevertheless, it remains important to evaluate the precision of the sensitivity indices by repeating the procedure a few times as we did.

The same principle can be generalized to the estimation of second-order or higher effects and to the estimation of total sensitivity indices. For estimating the interaction sensitivity S_{ij}, for instance, the model responses have to be calculated for pairs of scenarios $sc_{A,k}$ and $sc_{B,k}$ with the same levels of Z_i and Z_j. For estimating total sensitivity, the model responses have to be calculated for pairs of scenarios $sc_{A,k}$ and $sc_{B,k}$ with the same levels of all factors except Z_i. This allows the sensitivity index S_{-i} to be estimated, and TS_i is then estimated by $\hat{T}S_i = 1 - \hat{S}_{-i}$.

4.2.5. FAST method for sampling and estimating variance-based criteria

The Fourier amplitude sensitivity test (FAST) is another method for estimating variance-based measures of sensitivity. It is inspired by the Fourier decomposition of a time series in signal theory and was developed initially for analysing the sensitivity of chemical reaction systems to rate coefficients (Cukier et al., 1973, 1975; Schaibly and Shuler, 1978). Recently, its use has been generalized to many domains of applications and new developments have been proposed. The presentation below is limited to the main principles. More details can be found in Chan et al. (2000).

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4.2.5.1. FAST sampling

In the FAST method, all input factors are assumed to be quantitative and coded so that their domain of variation is $[0, 1]$. Then the possible scenarios belong to the multidimensional input space $[0, 1]^s$. With Monte Carlo sampling, the simulated scenarios are selected at random within $[0, 1]^s$. With the FAST method, they are selected systematically (or almost systematically) along a search trajectory which is specifically designed to explore efficiently the input space. This is illustrated, in the simple case of two factors, in Figure 12. Figure 12a shows a set of $N = 100$ scenarios sampled according to the FAST principles. These scenarios were generated by regular sampling along the curve visible in Figure 12b.

In the design of a FAST sampling scheme, an integer ω_i is associated with each input factor Z_i. This integer is called the frequency of Z_i and its choice will be explained below. The levels of the input factors Z_i for the simulated scenarios $\mathbf{z}_k (k = 1, \ldots, N)$,

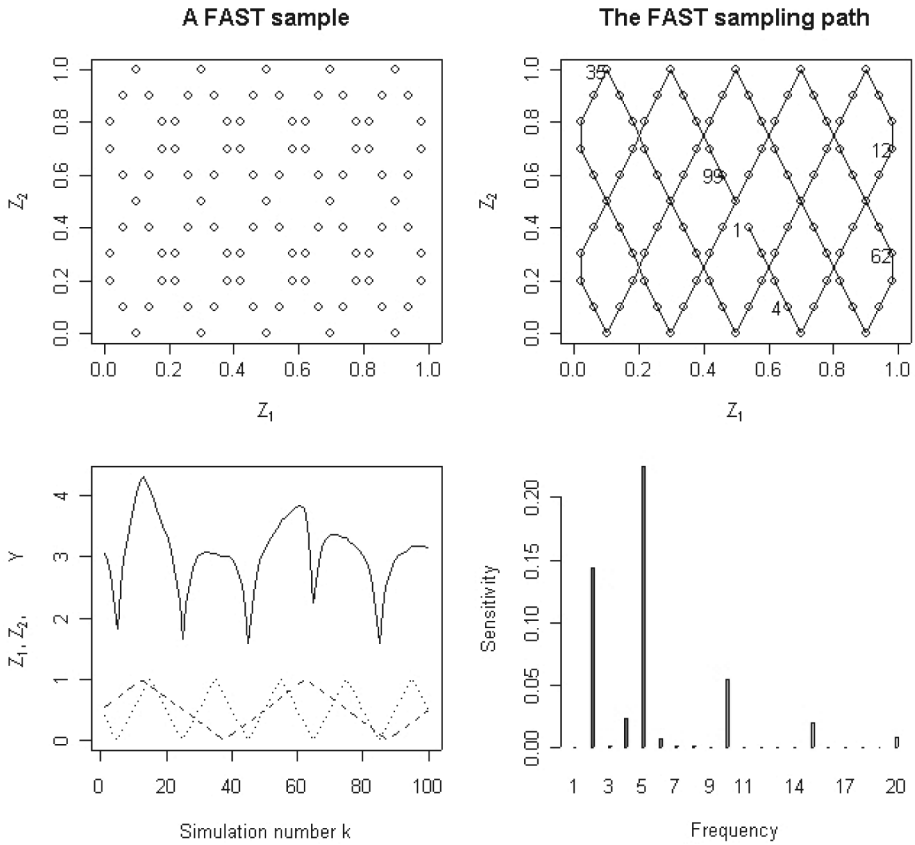

Figure 12. Illustration of FAST principles for two input factors Z_1 and Z_2. (a) Samples of (Z_1 ,Z_2) values with $\omega_1 = 2$, $\omega_2 = 5$, $\phi_1 = \phi_2 = 0$ and N=100. (b) FAST sampling path indicating the order of the generated scenarios (the numbers 1, 4 ... indicate the first, fourth ... generated scenarios). (c) Values of Z_1, Z_2, and of a response $\hat{Y}$ for N scenarios in ascending order of simulation. (d) Sensitivity indices obtained for several frequencies.

are given by

$$z_{k,i} = G(\sin(\omega_i u_k + \phi_i)),$$

where the scalars

$$u_k = -\pi + \frac{2k-1}{N}\pi$$

form a regularly-spaced sample of the interval $(-\pi, +\pi)$ and can be interpreted as coordinates on the search curve; $G(u)$ is a transformation function from $[-1, 1]$ to $[0, 1]$; and the

ϕ_is are optional random phase-shift parameter taking values in $[0, 2\pi)$. The transformation function

$$G(u) = \frac{1}{2} + \frac{1}{\pi}\arcsin(u),$$

proposed by Saltelli et al. (1999), ensures that the levels of each factor are uniformly, or almost uniformly, sampled.

In Figure 12, $\omega_1 = 2$, $\omega_2 = 5$ and $\phi_1 = \phi_2 = 0$. As can be verified in Figure 12b, each ω_i corresponds to the frequency with which the curve comes back to its starting value for the levels of factor Z_i. Figure 12b shows that the sampling path goes through each value of Z_1 exactly twice (in a given direction). Similarly, the sampling path goes through each value of Z_2 exactly five times.

4.2.5.2. Principles of FAST sensitivity estimation

The principle of FAST is that, if the response $\hat{Y}$ is sensitive to a given factor Z_i, then $\hat{Y}$ and Z_i should vary simultaneously over the scenario index k. In Figure 12c, the variations of Z_1, Z_2, and a putative response $\hat{Y} = f\,(Z_1, Z_2)$ are displayed as a function of k. This figure shows that the oscillations of $\hat{Y}$ and those of the factor Z_2 are quite simultaneous. This result indicates that Z_2 has a strong influence on the response. With the FAST method, the sensitivity of the output to the factors is quantified by estimating a sensitivity index for a series of frequency (Figure 12d). If the factor Z_i has a strong influence on the model output, the index takes high values for $\omega = \omega_i$ and for its higher harmonics $(2\omega_i, 3\omega_i, \ldots)$. Figure 12d shows that the sensitivity index is higher for $\omega = \omega_2 = 5$ than for $\omega = \omega_1 = 2$. This result reveals that the model output is more sensitive to Z_2 than to Z_1.

4.2.5.3. Spectral decomposition of $f(z_{k,1}, z_{k,2})$ variability

The variability of $f(z_{k,1}, z_{k,2})$ is decomposed into components associated with each frequency ω from 1 to $N - 1$, defined by:

$$D_{[\omega]} = A_\omega^2 + B_\omega^2,$$

where

$$A_\omega = \frac{1}{2\pi}\sum_{k=1}^{N} f(z_{k,1}, z_{k,2})\cos(\omega u_k)$$

$$B_\omega = \frac{1}{2\pi}\sum_{k=1}^{N} f(z_{k,1}, z_{k,2})\sin(\omega u_k).$$

The scalar $D_{[\omega]}$ is called the spectral component of $\hat{Y}$ at frequency ω, while A_ω and B_ω are called the Fourier coefficients of $\hat{Y}$ at frequency ω. They are theoretically defined as integrals over $[-\pi, +\pi]$, but they are shown here in the discrete summation form imposed by the finite number of simulations. The scalar $S_{[\omega]} = D_{[\omega]}/(\sum D_{[\omega]})$ can then

be considered as the proportion of variability of $f(z_{k,1}, z_{k,2})$ associated with frequency ω. The values of $S_{[\omega]}$ are presented in Figure 12d.

4.2.5.4. The classical FAST method

The original FAST (Cukier et al., 1973, 1975; Schaibly and Shuler, 1978) is a method for estimating essentially the first-order sensitivity indices (or main effects) of the factors Z_i. The frequencies of the different factors are chosen so that the spectral components $D_{[\omega]}$ of $\hat{Y}$ at frequency ω_i and at its first higher harmonics depend on the effects of input factor Z_i only. It follows that the sensitivity index of Z_i can be estimated by

$$S_i = \sum_{p=1}^{M} S_{[p\omega_i]},$$

where M is the number of harmonics taken into account and is usually set to $M = 4$.

Adequate sets of frequencies have been proposed by Cukier et al. (1973) for up to 19 factors. In FAST, there is a minimum number of simulations which is equal to $2M\max(\omega_i) + 1$. For example, when there are $s = 8$ factors, the frequencies given by Cukier et al. (1973) are 23, 55, 77, 97, 107, 113, 121, 125, and so the minimum number of simulations is equal to $8 \times 125 + 1 = 1001$.

4.2.5.5. The extended FAST method

The extended FAST method (Saltelli et al., 1999) allows the estimation of the first-order *and* the total sensitivity indices. In a simulation study on a crop model, it appeared more efficient than the Monte Carlo approach to estimate first and total sensitivity indices (Makowski et al., 2004). As opposed to the classical FAST, it requires separate sets of simulations for each input factor Z_i of interest.

In the simulations dedicated to factor Z_i, the frequency ω_i must satisfy: $\omega_i \geq 2M\max(\omega_j)$ where $\max(\omega_j)$ denotes the largest frequency associated with a factor other than Z_i. As for classical FAST, there is a minimum number N_0 of simulations, equal to $2M\omega_i + 1$. In practice, N_0 is usually chosen first, ω_i is then chosen as the largest integer satisfying $2M\omega_i + 1 \leq N_0$ and the other frequencies ω_j are chosen to satisfy the constraint $\omega_i \geq 2M\max(\omega_j)$ as well as a few other favourable properties.

The first-order sensitivity index of Z_i is estimated by

$$S_i = \sum_{p=1}^{M} S_{[p\omega_i]},$$

as in classical FAST. The total sensitivity index of Z_i is estimated by

$$TS_i = 1 - \sum_{\omega=1}^{M\max(\omega_j)} S_{[\omega]},$$

since all frequencies lower than $M\omega_{\max(j)}$ correspond to the factorial terms not involving Z_i.

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Example on the winter wheat dry matter (continued):

Figure 13 displays results of an extended FAST sensitivity analysis for the model, repeated twenty times. For each replication and each input factor, a FAST sample of size 1000 was generated. Thus, the number of model simulations needed to estimate first-order and total indices was equal to 8×1000 per replication. For each replication, the phase-shift parameters ϕ were drawn at random, and the frequencies were randomly allocated to all factors except the one under study. The ranges of the estimates over the 20 series of simulations are displayed in Figure 13.

The results are very coherent with the Sobol estimates (Fig. 11). However they show much less variability between replications and a practical advantage is that the sensitivity indices are always positive, as expected.

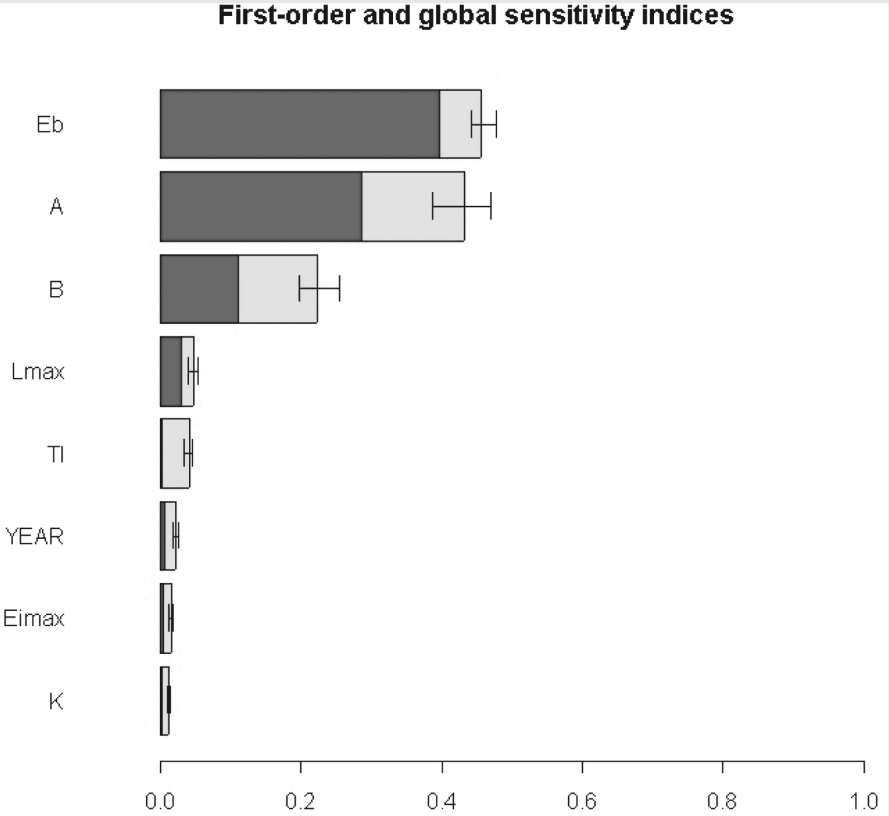

Figure 13. First-order and total sensitivity indices estimated by the extended FAST; there were 20 runs with 8×1000 model simulations for each run; the first part of the bars corresponds to the average (over the 20 runs) estimate of the first-order index, the full bars indicate average estimates of total indices, while the lines indicate extreme estimates of total indices.

5. Discussion

Which method to choose?

As the previous sections have shown, there is a large diversity of methods to perform sensitivity analyses. When choosing which one to use for a specific problem, important points to consider are the objectives of the study, the number of input factors to vary, the degree of regularity of the model and the computing time for individual model simulations.

If the objective is to screen for the most influential ones among a large number of input factors, the method of Morris or factorial designs are well adapted. Factorial designs with two-level factors are very efficient, but they give information only on the linear trends associated with each input factor. The method of Morris, by contrast, allows the investigation on the whole uncertainty ranges of the input factors.

When the objective is to quantify the influence of several input factors, experimental designs are very flexible, but once again, they give information on the model behaviour only for specific values of the input factors. Thus, it is necessary to assume, often implicitly, that the model is well-behaved and quite regular (for example, linear or near-linear if factors take two levels; near-quadratic if the factors take three levels, etc.). Methods based on intensive sampling, such as those described in the section on variance-based methods, have the advantage of being "model-free", that is, they do not rely on model approximations and they explore the full uncertainty ranges of the input factors. However, they require a large number of simulations.

In fact, there is no best method for all situations, and the differences between methods are less crucial than the accurate description of the uncertainty sources. A good understanding of the techniques and the ability to adapt them to one's situations is another key element.

Additional aspects of sensitivity analysis

Some key aspects of sensitivity analysis have been mentioned only briefly above but can be of great importance for a crop model.

The ability to take correlations into account between input factors, when generating scenarios, can make simulations much more representative of the phenomena under study. It was shown that such correlations can be taken into account in an uncertainty analysis. This is much more difficult for sensitivity analysis. There is a need to develop methods of sensitivity analysis that would take such correlations into account when interpreting simulation results.

It is often of great interest to consider the sensitivity of a response to a whole group of input factors (climatic/soil variables, or parameters associated with a specific growth stage). For most methods presented above, this can be done by summing the factorial indices associated with all factors within the group under consideration. The analogue of a first-order index is then the sum of all factorial indices involving only factors within the group. The analogue of a total index is the sum of all factorial indices involving at least one factor within the group. Note that this is not equal to the sum of the total indices of

the factors within the group, because interactions are counted several times within a sum of total indices.

The sensitivity analysis of dynamic responses $\hat{Y}(t)$ has not been considered explicitly in this chapter. The methods described above can be applied to time t separately, and it may then be interesting to follow how sensitivity indices change with time. However, it is often more useful to perform sensitivity analyses on meaningful characteristics of the response time series. These characteristics can be either chosen by the modeller or determined by applying multivariate techniques such as the Principal Components Analysis or the Partial Least Squares to the simulated response time series (Campbell et al., 2004).

For all the methods considered until now, only one level of uncertainty was considered for each factor. However, it happens quite frequently that distinct levels of uncertainty need to be considered: for example, climate uncertainty at a local scale *versus* a regional scale; or uncertainty in parameters at present and after further experiments; or simply uncertainties in the true levels of uncertainty on some parameters. An application in forestry is presented by Gertner et al. (1996).

Software

General statistical packages make it possible to implement the methods of analysis based on experimental design, analysis of variance and regression. But it is necessary to be aware of some interpretations: the meaning of a significance test is dubious when the responses come from a perfectly deterministic model. The SAS QC (SAS/QC User's guide, 1999) module includes procedures to construct factorial and optimal designs (proc factex, proc optex).

Some software packages for general modeling or for risk analysis include methods for sensitivity or uncertainty analysis (Crystall Ball, Risk). There is also softwares dedicated to sensitivity analysis. These software packages are restricted to the calculation of local sensitivity, but one exception is Simlab, which includes the main methods of global sensitivity analysis (see Saltelli et al., 2004).

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AQ: pl. check the year (1978 in the text)

Exercises

Uncertainty and sensitivity analysis with a model predicting the percentage of diseased plants

We consider a model simulating the percentage of plants with eyespot pathogen (*Pseudocercosporella hypotrichosises*) in a field in function of cumulative degrees–days since sowing. The model is defined by

$$\hat{Y}(t) = 100 \times \frac{1 - \exp\left[-(c_1 + c_2)\, t\right]}{1 + \frac{c_2}{c_1} \exp\left[-(c_1 + c_2)\, t\right]}$$

where $\hat{Y}(t)$ is the predicted percentage of diseased plants when the cumulative degrees–days is equal to t, and $\theta = (c_1, c_2)$ are the model parameters.

AQ: pl. clarify whether the insertion of symbol is Ok here

Here, the objective is to predict the percentage for a field located in the Paris Basin at $t = 2300$C°day. The values of the two model parameters were studied previously (Colbach and Meynard, 1995) but accurate results are not known. In this study, we consider that the uncertainty ranges of c_1 and c_2 are $[4.5 \times 10^{-8} - 3.5 \times 10^{-4}]$ and $[4 \times 10^{-4} - 6.5 \times 10^{-3}]$ respectively. The nominal values of c_1 and c_2 are equal to 1.75×10^{-4} and 3.5×10^{-3} respectively.

1. We assume that the uncertainty in c_1 and c_2 is modelled by uniform distributions over the parameter uncertainty ranges. A sample of ten values of $\theta = (c_1, c_2)$ is generated by Monte Carlo sampling and is reported in Table 8. Each value of θ defines an input scenario.
   (a) Calculate $\hat{Y}(2300)$ for each one of the ten scenarios presented Table 8.
   (b) Estimate the expected value and standard deviation of $\hat{Y}(2300)$ from the ten computed values of $\hat{Y}(2300)$.

Table 8. Ten values of c_1 and c_2 generated by Monte Carlo sampling.

c_1	c_2
1.71×10^{-4}	6.42×10^{-3}
1.25×10^{-4}	2.52×10^{-3}
9.65×10^{-5}	1.67×10^{-3}
3.38×10^{-4}	4.79×10^{-3}
2.97×10^{-4}	4.39×10^{-3}
4.88×10^{-5}	5.51×10^{-3}
1.36×10^{-4}	5.94×10^{-4}
2.99×10^{-5}	1.11×10^{-3}
1.97×10^{-4}	3.36×10^{-3}
3.17×10^{-4}	5.93×10^{-4}

(c) Estimate the probability $P[\hat{Y}(2300) \geq 80\%]$ from the ten computed values of $\hat{Y}(2300)$.
(d) The procedure described above is repeated 5 times leading to a 5 samples of 10 values of $\theta = (c_1, c_2)$. Each sample is used to estimate the expected value of $\hat{Y}(2300)$. The 5 estimated values of $E[\hat{Y}(2300)]$ are 93.59, 88.47, 95.28, 92.02, 96.48, 79.03. How do you explain this large variability?
(e) Define a procedure to choose the size of the sample of values of θ in order to estimate accurately $E[\hat{Y}(2300)]$ and $P[\hat{Y}(2300) \geq 80\%]$?

2. (a) Perform a local sensitivity analysis of $\hat{Y}(2300)$ with respect to c_1 and c_2 at the nominal parameter values. Which parameter has the highest relative sensitivity?
(b) Calculate five equispaced values of c_1 and c_2 from the minimal to the maximal parameter values.
(c) Set c_2 equal to its nominal value and calculate $\hat{Y}(2300)$ for the five values of c_1 defined above. Then, set c_1 equal to its nominal value and calculate $\hat{Y}$ (2300) for the five values of c_2.
(d) Calculate the sensitivity index of Bauer and Hamby (1991) (see textbook) for each parameter from the computed values obtained in 2.(c). Which parameter has the highest index?
(e) Calculate the sensitivity index of Bauer and Hamby (1991) for c_2 when c_1 is set equal to its minimal value. Compare this index value with the value obtained in 2.(d).

3. Consider a complete factorial design with three modalities per factor.

(a) How many distinct scenarios (i.e. values of $\theta = (c_1, c_2)$) are included in this design?
(b) Define a complete factorial design with three modalities per factor using only the minimal, nominal and maximal parameter values.
(c) Calculate the general mean of $\hat{Y}_i(2300)$ where $\hat{Y}_i(2300)$ is the value of $\hat{Y}(2300)$ obtained with the ith scenario.
(d) The total variability of $\hat{Y}(2300)$ can be measured by $\text{var}[\hat{Y}(2300)] = \frac{1}{N}\sum_{i=1}^{N}[\hat{Y}_i(2300) - \bar{Y}]^2$ where $\bar{Y}$ is the mean of $\hat{Y}_i(2300)$ and N the number of scenarios in the factorial design. Calculate $\text{var}[\hat{Y}(2300)]$.
(e) Estimate $E[\hat{Y}(2300)|c_1]$ for each value of c_1 considered in the factorial design.
(f) Estimate $E[\hat{Y}(2300)|c_2]$ for each value of c_2 considered in the factorial design.
(g) Estimate $\text{var}\{E[\hat{Y}(2300)|c_1]\}$ and then $\frac{\text{var}\{E[\hat{Y}(2300)|c_1]\}}{\text{var}[\hat{Y}(2300)]}$.
(h) Estimate $\text{var}\{E[\hat{Y}(2300)|c_2]\}$ and then $\frac{\text{var}\{E[\hat{Y}(2300)|c_2]\}}{\text{var}[\hat{Y}(2300)]}$.
(i) To which sensitivity indices do $\frac{\text{var}\{E[\hat{Y}(2300)|c_1]\}}{\text{var}[\hat{Y}(2300)]}$ and $\frac{\text{var}\{E[\hat{Y}(2300)|c_2]\}}{\text{var}[\hat{Y}(2300)]}$ correspond?
(j) Estimate $\text{var}[\hat{Y}(2300)|c_1]$ for each value of c_1 considered in the factorial design.
(k) Estimate $\text{var}[\hat{Y}(2300)|c_2]$ for each value of c_2 considered in the factorial design.
(l) Estimate $E\{\text{var}[\hat{Y}(2300)|c_1]\}$ and then $\frac{E\{\text{var}[\hat{Y}(2300)|c_1]\}}{\text{var}}[\hat{Y}(2300)]$.

(m) Estimate $E\{\text{var}[\hat{Y}(2300)|c_2]\}$ and then $\frac{E\{\text{var}[\hat{Y}(2300)|c_2]\}}{\text{var}[\hat{Y}(2300)]}$.

(n) To which sensitivity indices do $\frac{E\{\text{var}[\hat{Y}(2300)|c_1]\}}{\text{var}[\hat{Y}(2300)]}$ and $\frac{E\{\text{var}[\hat{Y}(2300)|c_2]\}}{\text{var}[\hat{Y}(2300)]}$ correspond?

(o) Compare the indices calculated in 3.(n) and those calculated in 3.(i). Are they different? Why?

Answers

Only the numerical results are supplied.

1.(b) The expected value and standard deviation are equal to 81.15 and 27, respectively.

1.(c) About 0.6.

2.(d) 0.96 for c_1 and 0.51 for c_2.

3.(a) 9.

3.(c) 68.82.

3.(d) 1545.9.

3.(e) 33.15, 82.89 and 90.42.

3.(f) 40.18, 67.76 and 98.52.

3.(g) $\frac{\text{var}\left\{E[\hat{Y}(2300)|c_1]\right\}}{\text{var}[\hat{Y}(2300)]} = 0.42.$

3.(h) $\frac{\text{var}\left\{E[\hat{Y}(2300)|c_2]\right\}}{\text{var}[\hat{Y}(2300)]} = 0.37.$

3.(j) 2925.01, 855.51 and 271.1.

3.(k) 1333.82, 3060.91 and 6.57.

3.(l) $\frac{E\left\{\text{var}[\hat{Y}(2300)|c_1]\right\}}{\text{var}[\hat{Y}(2300)]} = 0.88.$

3.(m) $\frac{E\left\{\text{var}[\hat{Y}(2300)|c_2]\right\}}{\text{var}[\hat{Y}(2300)]} = 0.48.$