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MONTE CARLO ESTIMATION OF UNCERTAINTY CONTRIBUTIONS FROM SEVERAL INDEPENDENT MULTIVARIATE SOURCES

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Summary

An efficient random sampling method is introduced to estimate the contributions of several sources of uncertainty to prediction variance of (computer) models. Prediction uncertainty is caused by uncertainty about the initial state, parameters, unknown (e.g. future) exogenous variables, noises, etcetera. Such uncertainties are modelled here as random inputs into a deterministic model, which translates input uncertainty into output uncertainty. The goal is to pinpoint the major causes of output uncertainty. The method presented is particularly suitable for cases where uncertainty is present in a large number of inputs (such as future weather conditions). The expected reduction of output variance is estimated for the case that various (groups of) inputs should become fully determined. The method can be applied if the input sources fall into stochastically independent groups. The approach is more flexible than conventional methods based on approximations of the model. An agronomic example illustrates the method. A deterministic model is used to advise farmers on control of brown rust in wheat. Empirical data were used to estimate the distributions of uncertain inputs. Analysis shows that effective improvement of the precision of the model's prediction requires alternative submodels describing pest population dynamics, rather than better determination of initial conditions and parameters.

1. Introduction

After the structure of a deterministic model has been decided upon, much has to be done before the model can be used for prediction in a given situation. In this process random phenomena are encountered. Initial values are measured more or less accurately. Parameters have to be estimated, usually in a series of experiments on submodels. During the estimation of submodel parameters, for instance by regression, more random effects turn up. Often parameters will show 'natural' variation from case to case. The general setting of a parameter could be the population-parameter: the mean over a population of application-cases. The population-parameter is estimated with some error, and the parameters of particular cases will differ from the population-parameter. During submodel regression, lack of fit may become apparent, in the sense that differences between observations and fit are larger than can be ascribed to observation-error. If one does not succeed in modifying the regression equation so that the lack of fit disappears, and if the lack of fit is non-systematic, one might incorporate submodel-errors as random effects in an extended model (the case of systematic lack of fit will not be treated in this paper). One might, for instance, account for temporal

variability in subprocesses by white noise inputs. In addition, exogenous variables processed by the model may not be known when predictions are made. We will account for all such effects by assuming a deterministic model with random inputs. This enables an a priori investigation of prediction precision, based on the assumption that the structure of the model is correct.

Usually, the widely different nature of the inputs has implications for their mutual (in)dependency. The whole state of affairs will hinge on the model and its application, but we will try to give some examples. If various sets of parameters are estimated in different experiments, estimation errors of parameters from different sets are likely to be stochastically independent, whereas parameter estimation errors within a set will often be dependent. Natural variation of parameters has little to do with errors in estimating population means. Errors in the measurement of the initial state are independent of errors in parameter estimates. Random exogenous variables and noise inputs, in their turn, may often be assumed to be independent of errors in parameter estimation and in measurement of initial values.

The situation is formalized as follows. A scalar model output Y is assumed to depend on a number of stochastically independent random input vectors, say $X_1, X_2, \ldots X_n$:

$$Y = f(X_1, X_2, \ldots X_n).$$

The vectors X_i may have different lengths. The function f is deterministic, usually it is evaluated by simulation; f may represent a single output or a combination of outputs. Fixed inputs are not represented in the argument list, being of no interest in the present context.

In this paper, Y's variability will be characterized by its variance. It will be assumed that Y has finite mean and variance; this is guaranteed for instance when f is bounded. The use of the variance as measure of uncertainty has an economic rationale: if the loss caused by a prediction error is proportional to the square of that error, the expected loss is proportional to the variance.

Uncertainty analysis consists of the investigation of the output distribution, given the model and the distribution of the inputs. One may investigate the *full variance*, that is the variance of Y induced by all sources X_i collectively. Let U denote a group of one or more sources of uncertainty X_i; then, by assumption, U is independent of the complementary sources. With respect to U, two variance components are particularly interesting. Firstly, the *top marginal variance* from U, which is defined as the expected reduction of the variance of Y in case U should become fully known, whereas the other inputs remain as variable as before. Secondly, the *bottom marginal variance* from U, defined as the expected value of the variance of Y in case all inputs except U should become fully known, U remaining as variable as before. Since one does not know in advance at what value the sources will become fixed, one can only determine the distribution of the two variances mentioned; we will content ourselves with the mean of these distributions. Iman and Hora (1990) define uncertainty components in a similar way. A source will hardly ever become fully known, so the two variance components represent limits to what may be achieved: the top marginal variance is a maximal variance reduction, the bottom marginal variance is a minimal residual variance. It will appear that the top marginal variance from a source can never be greater than its bottom marginal variance.

Since the sources of uncertainty are closely related to the methods of data acquisition, knowledge of the variances mentioned can be used to assess the potential benefits of further research. One may pinpoint sources of uncertainty that are worthwhile to determine more

accurately, namely those sources that one *can* determine better, and that have a large top marginal variance. On the other hand, there may be sources which cannot become fixed; the bottom marginal variance from the collective of such sources is the best one could ever expect to reach.

In section 2 an overview is given of some current types of uncertainty analyses. The anatomy of uncertainty from two independent complementary sources is discussed in section 3. In section 4 we introduce a new sampling method for uncertainty analysis. The method is applied to an example from agronomy in section 5.

2. Taxonomy of uncertainty analyses

With respect to the *mathematical techniques* used, one may discern two major types of uncertainty analyses: analyses based on an approximation of the model (most often a low-order polynomial of the inputs, sometimes a nonparametric regression function), and analyses based directly on the model. Analyses based on an approximation may be attractive because of computational efficiency. Apart from that, an approximation may be interesting for its own sake. But an approximation-based analysis depends critically on the quality of the approximation. One has to check the approximation in each new case, and will not always be satisfied. A good linear approximation, for instance, may simply not exist over the entire range of the inputs. Moreover, if the model has high-dimensional inputs, such as exogenous variables or noises, an approximation is not readily available. (See also Iman & Helton, 1988, and Morris, 1991.) In contrast, methods based directly on the model are more easily applicable over a wide range of circumstances. They may require more computation, but in many cases this extra effort is far from unsurmountable.

With respect to the *questions* addressed, one may also distinguish two major types of uncertainty analyses: analyses in which only the full uncertainty is investigated, the uncertainty when all inputs are variable; and analyses in which one also investigates the decrease of uncertainty if one or more inputs were to become known more accurately. The latter subject is sometimes called the analysis of uncertainty contributions.

The *dependency* between the groups of inputs distinguished in the analysis of uncertainty contributions brings about another division in the realm of uncertainty analyses. Unfortunately, something simple like *the* uncertainty contribution of an input does not exist, except for rare occasions. Usually the variance reduction due to the fixing of an input depends on which inputs have already been fixed. The concept of uncertainty contribution of an input becomes extra complicated when the inputs distinguished are mutually dependent (Janssen, 1993). Latin hypercube samples, for instance, are often used as data for an uncertainty analysis (McKay & Beckman & Conover, 1979). This method was originally designed for independent scalar inputs: the samples being constructed by independent association of stratified samples of scalar inputs. Occasionally one may solve dependency problems by using a bit more technique or by giving up a bit of exactness (Iman & Conover, 1982; Stein, 1987). Technically and conceptually, uncertainty analysis becomes much simpler if one aggregates the inputs into independent groups, and restricts the analysis to those groups. By doing so one does not sacrifice relevance, since the dependencies are functionally linked with the current method of data acquisition.

The uncertainty analysis proposed will be restricted to independent groups of inputs: the smallest possible independent input sets are to the analysis like atoms to a chemist. This

restriction enables an analysis based directly on the model, in which one can estimate the top marginal variance and the bottom marginal variance from each source X_i and from some pooled sources. Thus, the analysis proposed calculates, without recourse to an approximation, the uncertainty contributions of stochastically independent groups of inputs while allowing for dependency within groups. As far as we know, such analyses do not yet exist.

3. Anatomy of uncertainty from independent sources

In this section we study the decomposition of the prediction variance caused by two stochastically independent vector inputs. Extension to a larger number of independent vector inputs is straightforward. Stochastic variables and vectors will be written in upper case letters, the values they assume in lower case. If an input vector, say U, becomes fully known at value u, whereas the other input vector, say V, independent of U, remains as uncertain as before, the best prediction of Y will be the mean of $f(u,V)$ (*best* in the least squares sense). The situation is illustrated in Table 1 for the case that U and V can assume a finite number of equiprobable values.

Table 1

	v_1	v_2	v_3	v_4	v_5	
u_1	y_{11}	y_{12}	y_{13}	y_{14}	y_{15}	$y_{1.}$
u_2	y_{21}	y_{22}	y_{23}	y_{24}	y_{25}	$y_{2.}$
u_3	y_{31}	y_{32}	y_{33}	y_{34}	y_{35}	$y_{3.}$
u_4	y_{41}	y_{42}	y_{43}	y_{44}	y_{45}	$y_{4.}$
	$y_{.1}$	$y_{.2}$	$y_{.3}$	$y_{.4}$	$y_{.5}$	$y_{..}$

A dot index indicates that the mean has been taken over the index; $f(u_i,v_j)$ is denoted by y_{ij}. The left column and the upper row contain the values assumed by U and V. The best predictions are conditional means of the model output Y. The bottom right element $y_{..}$ is the best prediction when neither U nor V are known. The right column and the bottom row contain the best predictions at the given value of U respectively V. The output y_{ij} can be decomposed into general mean, main effects and interactions, as usual in analysis of variance:

$$y_{ij} = y_{..} + (y_{i.}-y_{..}) + (y_{.j}-y_{..}) + [y_{ij}-y_{..}-(y_{i.}-y_{..})-(y_{.j}-y_{..})].$$

In the general case, the function $f(u,v)$ can be decomposed as follows. Let f_0 denote the best prediction when U and V are unknown:

$$f_0 = \mathrm{E}\, f(U,V).$$

The best predictions when U or V have become fixed at u or v respectively, are given by $\mathrm{E}\, f(u,V)$ and $\mathrm{E}\, f(U,v)$ respectively. Let $f_u(u)$ and $f_v(v)$ denote the corrections to f_0 when U respectively V get fixed:

$$f_u(u) = \mathrm{E}\, f(u,V) - f_0, \qquad f_v(v) = \mathrm{E}\, f(U,v) - f_0$$

and let $f_{uv}(u,v)$ denote what is left. Then $f(u,v)$ may be decomposed:

$$f(u,v) = f_0 + f_u(u) + f_v(v) + f_{uv}(u,v),$$

which is sometimes called the *analysis of variance decomposition* of f. Accordingly f_0 is called the general mean, $f_u(u)$ and $f_v(v)$ are called main effects of u and v, while $f_{uv}(u,v)$ is called the interaction of u and v. The *full variance* of f neatly falls apart:

$$\mathrm{Var}\, f(U,V) = \mathrm{Var}\, f_u(U) + \mathrm{Var}\, f_v(V) + \mathrm{Var}\, f_{uv}(U,V).$$

If U were to become fixed at u, the best prediction would be $f_0 + f_u(u)$, leaving $f_v(V) + f_{uv}(u,V)$ as prediction error, with reduced variance $\mathrm{Var}\, f_v(V) + \mathrm{Var}\, f_{uv}(u,V)$, which is a function of u. It is not known in advance at which value U should become fixed. One might wish to calculate the distribution of this reduced variance, but we will be content with the mean of the reduced variance over U, that is $\mathrm{Var}\, f_v(V) + \mathrm{Var}\, f_{uv}(U,V)$. Accordingly, the *top marginal variance* from U, the expected variance reduction due to the fixing of U while V remains as variable as before, is given by $\mathrm{Var}\, f_u(U)$. Similarly, the *bottom marginal variance* from V, the expected variance left over when only V remains uncertain, equals $\mathrm{Var}\, f_v(V) + \mathrm{Var}\, f_{uv}(U,V)$. The top marginal variance from U is seen to be the variance of the main effect of U, whereas the bottom marginal variance from V is equal to the sum of the variances of the main effect of V and the interaction between U and V.

Let u_1 and u_2 denote two independent realizations of U, and let v denote some fixed value that can be assumed by V. Then $f(u_1,v)$ and $f(u_2,v)$ are independent realizations of $f(U,V)$ given $V=v$. Thus $d \equiv f(u_1,v) - f(u_2,v)$ has expectation 0, while its variance, i.e. its expected square, is twice the variance of $f(U,V)$ given $V=v$. So $\frac{1}{2}d^2$ is an unbiased estimate of this latter variance. It follows that if v is a random realization of V, $\frac{1}{2}d^2$ is an unbiased estimate of what we defined as the bottom marginal variance from source U. The top marginal variance from U is obtained by subtracting the bottom marginal variance from V from the full variance of Y.

4. A new sampling method

In order to estimate top marginal variances and bottom marginal variances, we need a sample with frequent occurrences of blocks with values of $f(X_1, X_2, \ldots X_n)$ within which one argument is constant while all other arguments vary randomly; and of blocks within which one argument varies randomly while all other arguments are constant. The arguments that are constant within blocks should vary randomly between blocks.

In an ordinary Monte Carlo sample a new realization of the model output f is obtained by drawing new values for the inputs $X_1 \ldots X_n$, and calculating the output f after *all* new drawings. Such a sample contains no information about the role of the individual inputs. In the method introduced here, f is calculated after *each* drawing of a new value of an individual source. New input values are sampled in some fixed *cyclic* order. In this way, one obtains a stationary sequence y_i (i=1,2...) of realizations of Y. After each cycle, n steps, an independent

realization is obtained. Differences between realizations within a cycle hold information about the contributions of the various inputs to the full variance. Such a sample will be called a *winding stairs* sample. Although the sample is best represented on a cylinder (the 'wall of the staircase') it may well be represented in rows and columns, as illustrated in Table 2. A row consists of the steps required to make a full turn, so that a column consists of steps connected by a vertical line on the wall of the staircase.

Table 2. A winding stairs sample for a model with three random inputs X_1, X_2 and X_3. Independent realizations of X_i are denoted by $x_{i,1}$, $x_{i,2}$, etcetera. The sample consists of eight cycles.

$f(x_{1,1}, x_{2,1}, x_{3,1})$	$f(x_{1,1}, x_{2,2}, x_{3,1})$	$f(x_{1,1}, x_{2,2}, x_{3,2})$
$f(x_{1,2}, x_{2,2}, x_{3,2})$	$f(x_{1,2}, x_{2,3}, x_{3,2})$	$f(x_{1,2}, x_{2,3}, x_{3,3})$
$f(x_{1,3}, x_{2,3}, x_{3,3})$	$f(x_{1,3}, x_{2,4}, x_{3,3})$	$f(x_{1,3}, x_{2,4}, x_{3,4})$
$f(x_{1,4}, x_{2,4}, x_{3,4})$	$f(x_{1,4}, x_{2,5}, x_{3,4})$	$f(x_{1,4}, x_{2,5}, x_{3,5})$
$f(x_{1,5}, x_{2,5}, x_{3,5})$	$f(x_{1,5}, x_{2,6}, x_{3,5})$	$f(x_{1,5}, x_{2,6}, x_{3,6})$
$f(x_{1,6}, x_{2,6}, x_{3,6})$	$f(x_{1,6}, x_{2,7}, x_{3,6})$	$f(x_{1,6}, x_{2,7}, x_{3,7})$
$f(x_{1,7}, x_{2,7}, x_{3,7})$	$f(x_{1,7}, x_{2,8}, x_{3,7})$	$f(x_{1,7}, x_{2,8}, x_{3,8})$
$f(x_{1,8}, x_{2,8}, x_{3,8})$	$f(x_{1,8}, x_{2,9}, x_{3,8})$	$f(x_{1,8}, x_{2,9}, x_{3,9})$

4.1. Variance estimation

We will show that a winding stairs sample enables unbiased estimation of the full variance, of the top marginal variance and of the bottom marginal variance, for single inputs as well as for groups of adjacent inputs. A more detailed discussion, including consideration of sample size requirements, will be given elsewhere.

The first column, the sequence y_{kn+1} (k=0,1,2...), consist of mutually independent realizations of Y. So the variance of this sequence estimates the *full variance*. The same applies to the other columns, leading to n (dependent) estimates which can be pooled.

The sequence $d_k \equiv y_{kn} - y_{kn+1}$ (k=1,2,3...) consists of differences between two values of the output with independent realizations of X_1, the other inputs having the same random value. The expectation of d_k equals 0. The expectation of $\frac{1}{2}d_k^2$ is equal to the *bottom marginal variance* from X_1; so the latter is estimated without bias by the mean of the sequence $\frac{1}{2}d_k^2$. Successive values of $\frac{1}{2}d_k^2$ are dependent. However, d_k and d_{k+m} are independent if $|m| > 1$; the dependence has a short range, from which it follows that the variance estimator is asymptotically normal. The accuracy of the variance estimator can also be estimated from the sequence $\frac{1}{2}d_k^2$. The range-1 dependence has to be taken into account in the calculations, which can be done with techniques similar to those used with first order moving-average time-series: the correlation matrix has the same form as in such series.

The *top marginal variance* from X_1 can be estimated similarly from the differences $\delta_k \equiv y_{kn+1} - y_{(k+1)n}$ (k=0,1,2...). Subtracting the mean of $\frac{1}{2}\delta_k^2$ from the full variance estimate produces an estimate of the top marginal variance from X_1. The same procedure can be applied to the other inputs, and to groups of adjacent inputs.

A significance test on the difference of two variance estimates is possible, since the estimates are asymptotically normally distributed, and since the accuracy of a sample difference can be estimated just as before, with the only modification that the dependence in the sequence used may now have range 2.

4.2. Efficiency

The efficiency of our sampling method is of a different type than the efficiency of, say, block designs or the latin hypercube method, where adverse effects on the accuracy are suppressed. The efficiency of our method lies mainly in the multiple use of model evaluations: one evaluation is used six times if all kinds of uncertainty contributions are estimated. The price paid is a dependency between estimates and within the sequences that provide the estimates. But these dependencies pose no serious problems. The extensibility of the sample also contributes to the efficient use of the method. One may start with a moderately small sample and append more cycles only if necessary in view of the accuracy of the results. Moreover, one may start with a small number of steps in a cycle, inserting new steps only at places where the effect of current steps is found to be large.

4.3. Related approaches

Owen (1992) shows how to estimate variances of latin hypercube sample means. A remarkable spin-off of Owen's exercise is a method to estimate top marginal variances of independent one-dimensional inputs.

Morris (1991) introduces random sampling plans for sensitivity analysis. The plans are made for independent one-dimensional inputs. Apart from these differences in application, the plans show a great similarity with our winding stairs samples: both consist of one-factor-at-a-time designs, and the efficiency of both methods lies in the multiple use of function evaluations.

5. Example

The winding stairs method is applied to a model used to advise farmers on control of brown rust in winter wheat. The model calculates the loss due to brown rust in Dutch guilders per hectare. We will very briefly sketch the model; a detailed description is given in Rossing *et al.* 1993a, 1993b and 1993c. The *incidence* of brown rust is observed as the number of leaves with rust spots in a sample of 160 leaves. By an empirical relation, the incidence is translated into a *density* (mean number of spots per leaf); a random effect is added to account for lack of fit in the density function. The density grows exponentially, the relative growth rate varying in time as a constant plus a white noise. The growth stops when the crop is harvested, that is when the crop reaches the mature stage of development. The stage of development is a function of the cumulative temperature, with a random effect to account for lack of fit. Finally, the loss is calculated as a bounded function of the integral over time of the number of brown rust spots.

The relations used in the model have been investigated experimentally. The parameters were estimated by regression: the resulting parameter error distributions are used in the uncertainty

analysis. In some submodels, undeniable lack of fit showed up, which appeared to be non-systematic and could not be ascribed, for instance, to natural parameter variation (which we did not observe). The variances were estimated, and the effects were incorporated as random inputs. The temperature uncertainty is represented by 36 years of historical temperature data.

The construction of an approximation of the model was hampered by the numerous temperature data and even more by the noise inputs. These problems were aggravated by the fact that the analyses had to be performed under a broad range of circumstances, each of which required construction and quality inspection of an approximation. For these reasons, an analysis without an approximation was attractive.

In the uncertainty analysis the following six inputs were assumed independent, and were randomly sampled in the following cyclic order: (1) errors in estimating parameters; (2) error in estimation of initial state; (3) noise on relative growth rate; (4) non-systematic error in crop development function; (5) non-systematic error in the incidence-density relation; (6) a season of daily temperatures. The sampling order was chosen to enable the grouping of inputs into methodologically interesting classes. With some effort, the first two inputs might well become known more accurately. The subprocess errors and noises, however, will remain in force as long the model's structure is not modified; and the temperature is notoriously unpredictable.

The logarithm of the loss due to brown rust appears to be approximately normally distributed, although the right tail is somewhat shortened. In Table 3 we give the results of the analysis of a 250-cycle winding stairs sample of the (base 10) logarithm of the loss for one specific situation. The results of the analysis are formulated in terms of top marginal variances. This is always possible, since the top marginal variance of a source is complementary to the bottom marginal variance of the complementary sources.

Table 3. Estimated top marginal variances of various groups of uncertainty sources. The top marginal variances are expressed in percents of the estimated full variance (.544 with a relative standard error of 8%). The greatest variance in a column is marked with an asterisk if it is significantly greater than the other variances (separate tests, 5%-two-sided).

1. estimation error in parameters	80*	11	11
2. measurement error in initial value			
3. noise on relative growth rate		63*	45*
4. error on crop development function			7
5. error on density function			22
6. temperature	20	20	20

From the first column in Table 3 it may be seen that the full variance might be reduced up to some 80% in the imaginary case that all inputs could be fixed except the totally unpredictable temperature. Thus a worthwhile variance reduction is not a priori impossible. Subsequently the non-temperature sources are inspected more closely: a split is made between parameters and initial values on the one hand and subprocess errors and noise on the other

hand. From the second column it is seen that one will reach a reduction of some 11% at most by very accurate experiments to determine parameters and very accurate measurement of the initial conditions. For that reason these two sources were not considered separately. A reduction of the submodel errors and noise, representing imperfections in the current model structure, is much more promising. These three sources are separated in the third column. The non-systematic error on the incidence-density relation appears to be of some importance. But the noise on the relative growth rate is seen to be the main offender: up to 45% reduction of prediction variance might possibly be obtained if this 'noise' could be deterministically accounted for. That can only be imagined, however, with a more comprehensive model.

The sum of the true relative top marginal variances in a column is at most 100%, the deficit being caused by interactions, but due to sampling error the sum of the estimates of the relative top marginal variances may be greater than 100%. In Table 3 the column sums are close to 100%: the interaction between the sources is small. This implies that the logarithm of the loss can be well approximated by a sum of the form $\Sigma\, g_i(X_i)$, in which X_i denote the sources of variation distinguished, while the functions $g_i()$ denote arbitrary, presumably non-linear, functions.

Better prediction precision leads to more adequate control of brown rust, which implies less spraying. Rossing *et al.* (1993a) contains an investigation of some economic consequences of the current uncertainty. It remains an open question, however, whether a more comprehensive model can be constructed which would realize the maximal uncertainty reductions calculated above.

6. Discussion

The winding stairs uncertainty analysis proposed in this paper enables assessment of uncertainty contributions from stochastically independent sources while allowing for dependency within sources. The restriction to independent sources is no sacrifice of practical relevance since the dependencies are functionally linked with the method of data acquisition. The analysis is not based on an approximation of the model. A good approximation enables a very efficient uncertainty analysis. Occasionally, however, one will not succeed in obtaining an adequate approximation. Large input variation and model non-linearities may frustrate the construction of approximations. The presence of uncertainty in a large number of inputs, such as noise signals, may pose additional problems. Except for the case when the approximation is overwhelmingly good, one will always have to deal with the question wether the approximation is adequate for the analysis. All such problems can be circumvented with Monte Carlo techniques, at the price of a larger computational effort. The winding stairs strategy is a Monte Carlo sampling technique designed to capitalize on the computations. This is achieved by multiple use of model evaluations and by the extensibility of the sample. One may start with a moderately small sample and append new cycles if required in view of the precision of the uncertainty estimates. Moreover, one may start with a small number of steps in a cycle, inserting new steps only at places where the effect of current steps is found to be large.

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