

Uncertainty propagation using the point estimate method

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Abstract The point estimate method is presented as an alternative to Monte Carlo simulation and the first-order second-moment method for propagating uncertainty with models containing a limited number of uncertain inputs. In this method, the model is evaluated at a discrete set of points in the uncertain parameter space, with the mean/variance of model predictions computed using a weighted average of these functional evaluations. The methodology is illustrated using an analytical model of health risk arising from water-borne radionuclide migration from a repository. Estimates of mean and variance for model-predicted risk, as obtained with the point estimate method, are found to compare well with those from a detailed Monte Carlo simulation study.

INTRODUCTION

In many engineering and scientific applications, Monte Carlo simulation (MCS) is typically the method chosen for evaluating the impacts of parameter uncertainty on model predictions (Morgan & Henrion, 1990). The MCS methodology allows a full mapping of the uncertainty in model inputs, expressed as probability distributions, into the corresponding uncertainty in model output which is also expressed in terms of a probability distribution. Often, however, it is sufficient to quantify the uncertainty in model predictions in terms of the mean and the variance rather than the full distribution. The first-order second-moment method (FOSM) is one such approach, entailing considerably less computational effort than MCS for problems with a small number of uncertain parameters (Benjamin & Cornell, 1970). Although this method is strictly applicable for linear problems, it has been shown to provide results of comparable accuracy for mildly nonlinear problems.

The point estimate method (PEM) was originally proposed by Rosenblueth (1975) to address the poor performance of FOSM for nonlinear models, as well as to avoid the computation of the gradients of model output with respect to the uncertain inputs required in the FOSM approach. Rosenblueth's method involved 2^n functional evaluations (n being the number of uncertain variables)—corresponding to the perturbation of each variable by ± 1 standard deviation from its mean value. Lind (1981) proposed an alternative requiring $2n$ estimates where the points are chosen near the centre of each face of the hypercube whose corners are the points of the Rosenblueth distribution. Harr (1989) presented a modified version of Lind's approach, also involving $2n$ functional evaluations but based on an eigen transformation of the correlation matrix, which is easier to implement.

The objective of this paper is to describe the theory behind Harr's PEM and associated implementation details. An example problem will be used to demonstrate the application of PEM and compare its performance with MCS and FOSM.

THEORETICAL DETAILS

The first step of Harr’s PEM algorithm requires an eigen transformation of the correlation matrix for the uncertain variables to estimate its eigenvalues (λ_i) and eigenvectors (e_{ij}). This information is utilized in the next step wherein each variable, x_j , is perturbed around its mean by a factor, Δx_j :

$$\Delta x_j = \pm e_{ij} \sqrt{n} \sigma [x_j] ; \quad j = 1, n \tag{1}$$

As depicted in Fig. 1, this amounts to locating the points for evaluating the function at the intersection of the eigenvectors of the correlation matrix and a hypersphere of radius $(n)^{1/2}$ centred at the origin of the standardized parameter space. Note that in the standardized space, the mean values of the parameters are located at the origin and distances are measured in standard deviation units.

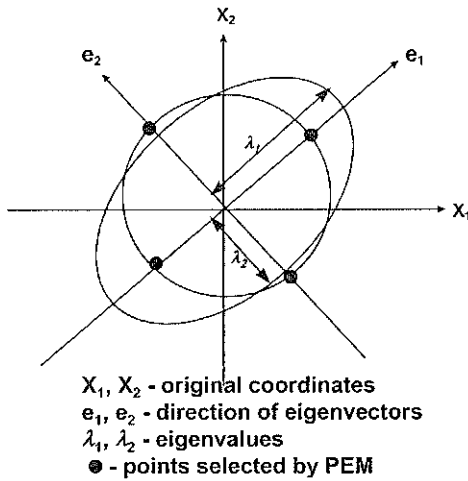


Fig. 1 Selection of points for functional evaluations in PEM.

The method thus results in $2n$ point estimates of the model, based on which the expected value (mean) of the output, $\mathbf{E}[F]$, is computed from:

$$\mathbf{E}[F] = \sum_i (F_i^+ + F_i^-) \frac{\lambda_i}{2n} ; \quad i = 1, n \tag{2}$$

The output variance, $V[F]$, is computed by first evaluating the second moment:

$$\mathbf{E}[F^2] = \sum_i [(F_i^+)^2 + (F_i^-)^2] \frac{\lambda_i}{2n} ; \quad i = 1, n \tag{3}$$

and using the relationship: $V[F] = \sigma^2[F] = \mathbf{E}[F^2] - (\mathbf{E}[F])^2$, where σ is the standard deviation. Here F_i^+ and F_i^- denote estimates of model output corresponding to the perturbation of each input parameter from its mean value by Δx_j in the positive and negative directions, and λ_i are the eigenvalues corresponding to each uncertain input.

Recall that $2n$ model evaluations are required to compute the mean and variance via PEM using equations (2)–(3). However, it has been pointed out that in many cases

the eigen transformation of the correlation matrix results in only a few dominant eigenvalues (Harr, 1989). Thus, it is possible to use this subset of eigenvalues for uncertainty propagation without any significant loss of accuracy. Note also that when the uncertain variables are uncorrelated, the correlation matrix reduces to the identity matrix with unit eigenvalues/vectors, which simplifies the evaluation of equation (1), and hence, of the mean and variance of model output.

EXAMPLE PROBLEM

The methodology is illustrated using an analytical "screening" model of health risk arising from water-borne radionuclide migration (Robinson & Hodgkinson, 1986). This simple model contains components representing source release, geosphere transport and biosphere transport for a single member radionuclide chain. The source term is described by an initial containment time followed by radionuclide release at a rate specified as a fraction of the current nuclide inventory, with radioactive decay occurring all along. The geosphere term includes one-dimensional transport with advection, dispersion, equilibrium sorption and decay. The biosphere term is based on a stream being the principal groundwater pathway, and includes the rate of drinking water intake by an individual, the stream flow rate, the activity-to-dose factor, and the risk factor for radiation induced cancer fatality. As described in the original reference, intermediate expressions for the source term, the geosphere term and the biosphere term can be combined using the Laplace transformation technique to yield a time-dependent consequence, $C(t)$, given by:

$$C(t) = \frac{1}{2} B k M_0 e^{-\lambda(T_0+t)} e^{L/2d} e^{-RL^2/4dvt} e^{-vt/4dR} \left[\phi \left\{ \left(\frac{RL^2}{4dvt} \right)^{1/2} + \left(\frac{vt}{4dR} - kt \right)^{1/2} \right\} + \phi \left\{ \left(\frac{RL^2}{4dvt} \right)^{1/2} - \left(\frac{vt}{4dR} - kt \right)^{1/2} \right\} \right] \quad (4)$$

where $\phi(z) = \exp(z^2)\text{erfc}(z)$, and the other symbols are as defined in Table 1. Note also that the consequence, $C(t)$, is a risk term which expresses the probability of deaths per year beyond the initial containment period (i.e. for $t > T_0$).

Table 1 Parameter distributions used in the example problem.

Parameter	Symbol	Distribution	Median value	Standard dev.
Initial inventory	M_0 (Bq)	Fixed	1.0×10^{16}	—
Release rate	k (year ⁻¹)	Lognormal	3.16×10^{-5}	0.333
Containment time	T_0 (year)	Fixed	316	—
Decay constant	λ (year ⁻¹)	Fixed	3.25×10^{-6}	—
Retardation factor	R (—)	Fixed	10.0	—
Groundwater velocity	v (m year ⁻¹)	Lognormal	0.1	0.167
Dispersivity	d (m)	Fixed	20.0	—
Geosphere path length	L (m)	Fixed	316	—
Biosphere conv. term	B (deaths Bq ⁻¹)	Lognormal	1.0×10^{-18}	0.083

Note: Standard deviation is calculated for the log₁₀-transformed parameters.

This simple model is used to compute human health risk (and its associated uncertainty) after 20 000 years of waste emplacement due to the migration of a single radionuclide from a hypothetical repository. The uncertain parameters in the model are taken to be: (a) fractional release rate, k , (b) groundwater velocity, v , and (c) biosphere conversion term, B . Each of these parameters is assigned a lognormal distribution with prescribed first and second moments, as given in Table 1. Also tabulated therein are the fixed values assigned to all other parameters. Note that the correlation coefficient between $\log(k)$ and $\log(v)$ is specified as 0.80, and that between $\log(v)$ and $\log(B)$ is given as 0.30.

RESULTS AND DISCUSSION

For calculation purposes, a logarithmic transformation of the risk model given in equation (4) was used. As the first step of the PEM technique, an eigen transformation of the correlation matrix was carried out to yield the following eigenvalues, $\lambda_1 = 1.8544$, $\lambda_2 = 0.1456$ and $\lambda_3 = 1$. The eigen vectors corresponding to these eigenvalues were: $(0.6621, 0.7071, 0.2483)^T$, $(0.6621, -0.7071, 0.2483)^T$ and $(0.3511, 0, -0.9363)^T$. Application of equation (1) then yielded the magnitude of the perturbation around the mean value for each of three uncertain parameters in log-space, e.g. $\Delta\log(k) = 0.3819$, $\Delta\log(v) = 0.2045$, and $\Delta\log(B) = 0.0357$ for the first eigenvalue, $\lambda_1 = 1.8544$. With these "points", a total of six ($2n = 2 \times 3 = 6$) functional evaluations were carried out in order to estimate the mean and variance of $\log C$, with the risk term as given by equation (4) normalized to a nominal value of 10^{-6} deaths year⁻¹. Using equations (2)–(3), the mean and standard deviation of $\log C$ were then computed as: $E[\log C] = -1.04$, and $\sigma[\log C] = 1.11$.

In order to verify these results, a Monte Carlo analysis was carried out with Crystal Ball, a commercial spreadsheet add-in to MS-EXCEL for performing probabilistic risk assessment calculations. On the basis of 5000 Latin Hypercube samples, we obtained $E[\log C] = -1.05$, and $\sigma[\log C] = 1.20$, both values being in excellent agreement with the PEM results. Figure 2 shows a graphical comparison between the PEM and MCS results for the moments of $\log C$.

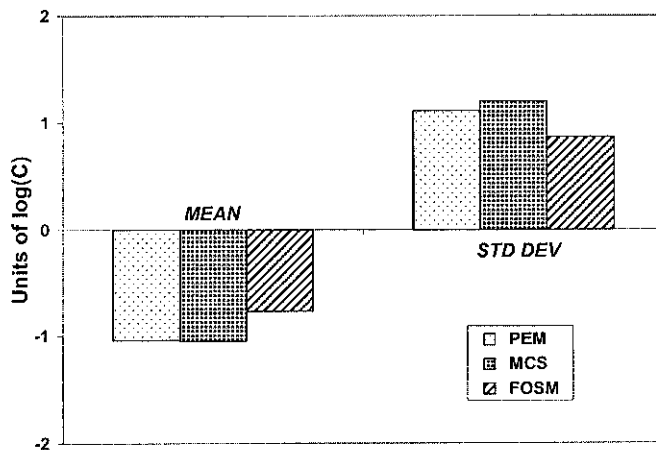


Fig. 2 Comparison of mean and std dev of $\log C$ from PEM, MCS and FOSM.

Also shown in Fig. 2 for comparative purposes are the FOSM estimates of $\mathbf{E}[\log C] = -0.77$, and $\sigma[\log C] = 0.86$, which are clearly inferior to those obtained with the PEM and MCS techniques. Note that $\mathbf{E}[\log C]$ is obtained by evaluating the model with all parameters held at their median values. The evaluation of $\sigma[\log C]$ requires a knowledge of the variance of the uncertain parameters, as well as the sensitivity of the model output with respect to these parameters (which were obtained using a forward finite difference approximation). A total of four ($n + 1 = 3 + 1 = 4$) functional evaluations was thus required for the FOSM approach.

CONCLUDING REMARKS

Although the example problem is characterized by a high degree of nonlinearity, as well as large variability in the output (i.e. $CV[\log C] \sim 1$), it is encouraging to note the robust performance of PEM upon quasi-linearization of the inputs and the output using a simple logarithmic transformation. It may also be pointed out that the same transformations failed to produce satisfactory results with the FOSM approach. In general, it is often helpful to transform the input distributions into symmetric distributions so that the original PEM methodology can be directly applied.

Typical MCS applications require ~ 100 to 1000 model runs to obtain stable estimates of the mean and variance. In this regard, the computational burden of $2n$ functional evaluations with PEM makes it particularly attractive, and competitive with MCS, for computationally intensive models with a small number of uncertain parameters (~ 10 to 20). The computational advantage of $(n + 1)$ functional evaluations offered by FOSM is offset by its poor performance for nonlinear models.

REFERENCES

- Benjamin, J. R. & Cornell, C. A. (1970) *Probability, Statistics and Decisions for Civil Engineers*. McGraw-Hill, New York.
- Harr, M. E. (1989) Probabilistic estimates for multivariate analysis. *Appl. Math. Modelling* 13(5), 313–318.
- Lind, N. C. (1981) Modeling of uncertainty in discrete dynamical systems. *Appl. Math. Modelling* 7(6), 146–152.
- Morgan, M. G. & Henrion, M. (1990) *Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk Assessment and Policy Analysis*. Cambridge University Press, New York.
- Robinson, P. C. & Hodgkinson, D. P. (1986) Exact solutions for radionuclide transport in the presence of uncertainty. *UK Atomic Energy Agency Report No. AERE R 12125*.
- Rosenblueth, E. (1975) Point estimates for probability moments. *Proc. US National Academy of Sciences* 72, 3812–3814.