Reactor Safety and Incomplete Information: Comparison of Extrapolation Methods for the Extension of Computational Codes

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Abstract – *The purpose of this paper is to present a comparative analysis of two extrapolation methods: Kriging (which is commonly used) and the EPH (a new method developed by SCM).*

I. INTRODUCTION

In order to investigate the safety properties of nuclear reactors, various software have been developed. One of the examples of such software is the computational code CATHARE (**C**ode for **A**nalysis of **TH**ermalhydraulics during an **A**ccident of **R**eactor and safety **E**valuation), which is the result of a joint effort of AREVA, CEA, EDF and IRSN. It represents a system code for PWR safety analysis, accident management, definition of plant operating procedures and for research and development. For instance, it calculates the temperature reached in a nuclear reactor in the case of an accident, taking into account a large number of parameters. Therefore, due to a large calculation time, the number of runs is limited: a few hundreds, sometimes a few thousands. From the precise values obtained by such simulations, there is a need to "propagate" the information to wider regions of the parameter space, which means, to obtain results where no computation has been made.

The classical way to proceed is by applying the Kriging methods. The aim of this paper is to compare these methods with a new one, called EPH (**E**xperimental **P**robabilistic **H**ypersurface) which was introduced by Societe de Calcul Mathematique, SA [PIT]. The comparison analysis we provide here is based on a series of tests, in which the response-surface is already given by a known function, so that the calculated values are compared directly to the true ones.

Both Kriging and EPH were also compared upon their abilities to investigate "unexplored" part of the configuration space, in order to optimise the choice of further measurements.

II. PROBLEM DESCRIPTION

The function Branin-Hoo is taken as a test-function defined in the two-dimensional space [0; 1]x[0; 1] as follows:

$$\begin{aligned} u_1 &= 15x_1 - 5 \\ u_2 &= 15x_2 \\ Branin(x) &= \left(u_2 - \tfrac{5}{4\pi^2}u_1 + \tfrac{5}{\pi}u_1 - 6\right)^2 + \\ &\quad +10\left(1 - \tfrac{1}{8\pi}\right)\cos(u_1) + 10 \end{aligned} \tag{1}$$

The comparison procedure will be carried out in 3 steps:

- Various quantities of the initial points will be generated using the Branin function: 3 points, then 9 points, and finally 16 points.

- Both methods will be applied in order to estimate 400 unknown configurations, chosen both regularly and randomly.

- The results of the estimates will be compared to the real values, taking into account the confidence intervals.

III. IMPLEMENTATION

III.A. Kriging method

Kriging (or Gaussian process regression) is a method of interpolation for which the interpolated values are modelled by a Gaussian process governed by prior covariance, that is a linear relationship between the variables. The outcome estimate always has a Gaussian form.

This procedure is frequently used in various situations, so that it was standardized and coded in R language. In the current situation, we used the DiceKriging package which is an open source code.

III.B. EPH method

As opposed to the Kriging method, the EPH relies only upon the data themselves: no artificial assumptions are made. The construction can be viewed in terms of propagation of information from available measurement points (given or calculated) to the unknown ones. This propagation is governed by a general principle of maximal entropy (or minimal information) which is itself an increasing function of the distance to the measurement points. A complete description of the construction is given in the book [PIT].

The EPH model requires to fix the input parameters such as the space boundaries:

- Boundary on each dimension;
- Boundary on the outcome range and discretisation path; it must be fixed because the resulting estimate has the form of a discrete probability law on the defined range;

The boundary values may come from expert knowledge, physical limits or be defined by a user.

The result is given under the form of a collection of discrete probability densities having a maximal variance for the fixed entropy. Such a density takes the form of a Dirac function at the measurement point location (the value is known precisely), and becomes less and less concentrated when moving further away from it.

Each of the measurement gives its own contribution to the final result, written under the following form:

$$p_{n,j}(X) = \frac{\tau}{\sigma\sqrt{2\pi}}\ exp\left\{-\frac{(j-C_n)^2}{2\sigma^2}\right\} \qquad (2)$$

$$\text{with } \sigma = \frac{\tau e^{\lambda d_n}}{\sqrt{2\pi e}} \qquad (3)$$

where X is point to be estimated; n is a measurement counter $n = 1, \dots, N$; C_n – the outcome value of the n-th configuration, j – discretisation of the result range with the step τ; d_n – distance between the unknown point and the n-th point; λ – parameter related to the entropy which is calculated so as to maintain the information minimal at every point [PIT].

At the end of the process, the individual discrete laws we have been obtained are recombined in order to get a single one depending on the distance of the target-point from each measurement.

The resulting probability is given by the formula:

$$p_j(x) = \frac{1}{\sum_{i=1}^{N} 1/d_i}\left(\frac{1}{d_1}p_{1,j} + \cdots + \frac{1}{d_N}p_{N,j}\right) \qquad (4)$$

This formula is adjusted when dealing in a high-dimensional space [PIT].

The EPH method was coded in R language, in order to get a package similar with the Kriging package.

III.C. Major advantages of the EPH

The main advantages of EPH model compared to Kriging are the following:

- The outcome estimate does not have a Gaussian form (see fig.1. below), which enables to calculate not only the expectation but the median, the most probable value and so on (for Gaussian, they have the same value);

- The construction does not rely on a linear dependence of variables or on any other type of artificial assumptions;

- Being of probabilistic type, the EPH is very robust in terms of uncertainties: upon the value of a measurement, upon the points' disposition and so on;

- The method can be applied to a space of any dimension considering any number of measurement points without affecting significantly the calculation time;

- Propagation of information using the EPH can be extended to a non-homogeneous or/and isotropic space.

III.D. Comparison tools

In order to compare the results, in terms of precision, the absolute and squared differences are considered with the following notations:

- N number of test points to be reconstructed;
- X_n value estimated by the EPH model;
- Y_n value estimated by the Kriging model;
- R_n value of the Branin-Hoo function;

The distance *Dist_1* represents the mean difference between the expectation value calculated by each of the methods and the true value:

$$Dist_1 = \frac{1}{N}\sum_{n=1}^{N}|X_n - R_n| \quad \text{for the EPH} \quad (4)$$

$$Dist_1 = \frac{1}{N}\sum_{n=1}^{N}|Y_n - R_n| \quad \text{for the Kriging} \quad (5)$$

The distance *MSE_2* represents the mean squared error:

$$MSE_2 = \frac{1}{N}\sum_{n=1}^{N}(X_n - R_n)^2 \quad \text{for the EPH} \quad (6)$$

$$MSE_2 = \frac{1}{N}\sum_{n=1}^{N}(Y_n - R_n)^2 \quad \text{for the Kriging} \quad (7)$$

III.E. Extrapolation based on 16 measurement points

We have 16 regularly positioned measurement points and their $Branin(x)$ values were calculated. This case may be considered as "sufficiently explored" because the number of initial points is relatively high.

Then, the 400 unknown regular configurations were generated; the value for each will be estimated by both methods relying on 16 given values.

Fig.1 presents the example of the reconstruction of an unexplored configuration (0.8; 0.6) by means of the EPH method:

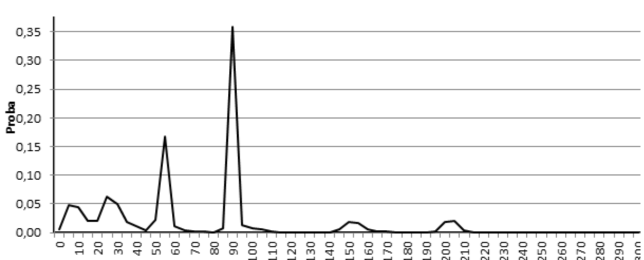

Fig.1. Discrete probability law estimated at the point (0.8; 0.6) by means of the EPH method relying on 16 given ones

The mathematical expectation is taken as the estimated value, which is equal to 73.12 in our case. The same procedure is applied to the next 399 points.

The same 400 configurations were estimated by means of Kriging method and the Table I provides the result of comparison of the two methods:

TABLE I

Kriging and EPH comparison based on 400 reconstructed values relying on 16 ones

	Dist_1	MES_2
Kriging	11	605
EPH	24	4 779

Conclusion: Kriging gives more precise estimates than EPH in this case.

III.F. Extrapolation based on 9 and 3 measurement points

Now, we have 9 and then 3 measurement points. This case may be considered as "poorly explored" because the number of initial points is relatively low.

Tables II and III show the result of comparison:

TABLE II

Kriging and EPH comparison based on 400 reconstructed values and relying on 9 ones

	Dist_1	MES_2
Kriging	45	36 254
EPH	32	4 880

TABLE III

Kriging and EPH comparison based on 400 reconstructed values and relying on 3 ones

	Dist_1	MES_2
Kriging	119	32 296
EPH	100	3 998

Conclusion: EPH gives more precise estimates than Kriging in these 2 cases.

III.G. Taking the uncertainties into account

A 95% confidence interval was fixed in order to check if the value of the Branin function falls into it. Both methods pass the test: in all cases the true value belongs to this interval.

Comparing the uncertainty amplitude, it should be mentioned that in most cases, the EPH gives a wider uncertainty range.

III.H. General comparison

Numerous tests were performed in order to check these conclusions. These tests were based on:

- using a various number of points, both initial and target ones;

- different choices of point disposition in the space: regular and random one;

- employing another function that is:

$$f(x_1, x_2) = \sin(5.5x_1)\cos(5x_2) + x_1^2 + 1$$

All results are similar to those presented above.

IV. OPTIMISATION ALGORITHMS

Both methods use algorithms designed in order to optimise the choice of the next measurement.

Kriging uses the Efficient Global Optimization (EGO) which is an optimisation algorithm based on the points aggregation which maximises the Expected Improvement at each iteration. This algorithm is designed to find local maxima and minima of the given function. It must be repeated a number of times, until the function increment reaches an epsilon value (sufficiently small value chosen by a user).

The EPH uses a different principle in order to localise the next investigation point.

In the case of the computational code which calculates the temperature in a nuclear reactor, we introduced a concept of search of a “dangerous zone”. They are the zones, in the configuration space, where the temperature may be high (that is, above a certain threshold).

The main feature of our search algorithm is that, from a small number of runs, the EPH allows us to find these dangerous zones. Once these zones are characterized, one may concentrate further runs of the code inside them. In other terms, the EPH allows a preliminary characterization, which will save time and efforts, in terms of number of runs: they will be concentrated where the true need is.

An essential point is as follows: the dangerous zones are first characterized by a mathematical property (greater proximity to points having high temperature than to points having low one), which is quite analogous to Voronoï diagrams ([BKOS]). But these diagrams cannot be explicitly constructed if the dimension d is high and the number of points n is large, since the complexity of the construction is in $n^{d/2}$.

In order to find the points situated at maximal distance to a given “hot” point, inside a diagram, we have to use a construction of probabilistic nature: we choose a random direction and we measure the distance attained, still remaining inside the hypercube.

The search algorithm may be iterated; the second step occurs inside an hyperplane, the third inside a space of co-dimension 2, and so on. Modifications must be brought to the algorithms in order to execute further steps.

Such an algorithm also helps to identify the zones with “poor” information. It helps not only to assess the local maxima and minima but also to insure that all parts of the space have the same quantity of information.

V. CONCLUSIONS

The usual Kriging method is more efficient when dealing with phenomena or functions where the variables dependence is more or less simple, the amount of observations is rather high, the number of parameters is small. In such cases, the estimates given by Kriging will be more precise than those coming from the EPH.

The explanation to this fact is quite simple: the EPH provides a "minimal information" model which uses nothing else but the existing data. If a lot of information is available, EPH is not the best model in order to handle it.

Conversely, the EPH method is advantageous in the case when a phenomenon (or a process) is very poorly studied, so that the result is a priori unexpected.
A parallel can be drawn with a blackbox: we know nothing about what is inside. So, applying the EPH propagation, we are sure that we are considering only genuine information, so that the result of estimate is not distorted by any external a priori assumptions. Still, if some of rules are imposed (for example, physical laws) they are easily incorporable into general construction; see [PIT].

Another technical remark is as follows: when dealing with just a few measurements, the Kriging method experiences problems in inversing matrixes when the covariance is calculated. The response-surface has a very irregular form. It is easy detectable in two or three dimensional space, but not in high dimensions.

This kind of failure is absolutely excluded in EPH model, because the principle of extrapolation is fundamentally different.

REFERENCES

[BBZB] Bernard Beauzamy, Hélène Bickert, Olga Zeydina (SCM), Giovanni Bruna (IRSN) : Probabilistic Safety Assessment and Reliability Engineering: Reactor Safety and Incomplete Information; Proceedings of ICAPP 2011 Nice, France, May 2-5, 2011 Paper 11399.

[BKOS] Mark de Berg, Marc van Kreveld, Mark Overmars and Otfried Schwarzkopf: Computational Geometry, 2nd revised edition, Springer-Verlag, 2000.

[PIT] Olga Zeydina and Bernard Beauzamy: Probabilistic Information Transfer SCM SA. ISBN: 978-2-9521458-6-2, ISSN : 1767-1175. May 2013.