

The application of Bayesian interpolation in Monte Carlo simulations

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ABSTRACT: To reduce the cost of Monte Carlo (MC) simulations for time-consuming processes (like Finite Elements), a Bayesian interpolation method is coupled with the Monte Carlo technique. It is, therefore, possible to reduce the number of realizations in MC by interpolation. Besides, there is a possibility of thought about priors. In other words, this study tries to speed up the Monte Carlo process by taking into the account the prior knowledge about the problem and reduce the number of simulations. Moreover, the information of previous simulations aids to judge accuracy of the prediction in every step. As a result, a narrower confidence interval comes with a higher number of simulations. This paper shows the general methodology, algorithm, and result of the suggested approach in the form of a numerical example.

1 INTRODUCTION

The so-called Monte Carlo (MC) technique helps engineers to model different phenomena by simulations. However, these simulations are sometimes expensive and time-consuming. This is because of the fact that the more accurate models, usually defined by finite elements (FE), are time-consuming process themselves. To overcome this problem the cheaper methods are generally used in the simulation of complicated problems and, consequently, less accurate results are obtained. In other words, implementing more accurate models in the Monte Carlo simulation technique provides more accurate and reliable results; by the reduction of calculation's cost to a reasonable norm, more accurate plans for risk management are possible.

To reduce the cost of Monte Carlo simulations for a time-consuming process (like FE), numerous research projects have been done, primarily in the structural reliability to get the benefits of not only a probabilistic approach but also to obtain accurate models. For instance, importance sampling and directional sampling are among those approaches implemented to reduce the cost of calculations. But still this coupling is a time-consuming process for practical purposes and it should be still modified. This research tries to speed up the Monte Carlo process by considering the assumption that the information of every point (pixel) can give an estimation of its neighboring pixels. Taking the advantage of this property, the Bayesian interpolation technique (Bretthorst 1992) is applied to our requirement of randomness of the generated data. In this study, we try to present a brief review of the method and important formulas. The application of the Bayesian interpolation into the MC for estimation

of randomly generated data in the unqualified area is presented by a numerical example.

2 GENERAL OUTLINES

In the interpolation problem, there is a signal U which is to be estimated at a number of discrete points. These discrete points will be called pixels, presented by u_i . These pixels are evenly spaced on a grid of pixels $\mathbf{u} \equiv (u_0, \dots, u_{v+1})$. Therefore, there are totally $v + 2$ pixels. The first and last pixels are called boundary pixels and are treated separately. These boundary pixels are presented by u_0 and u_{v+1} . As a result, v presents the number of interior pixels. The total number of observed data points is equal to n which are distributed in arbitrary (or random) locations among the pixels. Therefore, the maximum value of n is equal to $v + 2$ when there is an observed data point for each pixel ($n \leq v + 2$). The locations of the observed data points are collected in a vector \mathbf{c} , so this vector has n elements which are presented by c_i and $i = 1, 2, \dots, n$. The vector of observed data points is called $\mathbf{d} \equiv (d_1, \dots, d_n)$, and its elements are presented by d_i . Figure 1 presents an illustration of the internal and boundary pixels as well as data points. According to this figure $\mathbf{c} \equiv (1, v - 1, v + 2)$.

3 BAYESIAN INTERPOLATION

The univariate posterior probability density function (PDF) for an arbitrary pixel u_j , given the data \mathbf{d} and the prior information I , will be found by integrating out all pixels. In this case the sum rule is applied and the

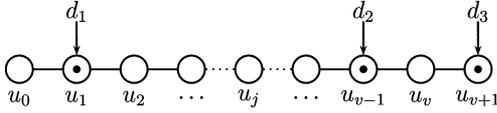


Figure 1. An illustration of the pixels which data points are assigned to.

product is integrated all over the multivariate posterior PDF of all pixels of \mathbf{u} except the required pixel u_j .

$$P(u_j|\mathbf{d}, I) = \int P(\mathbf{u}|\mathbf{d}, I) \underbrace{\dots du_i \dots}_{i \neq j} \quad (1)$$

Also, according to the Bayes' rule we have:

$$P(\mathbf{u}|\mathbf{d}, I) = \frac{P(\mathbf{d}|\mathbf{u}, I)P(\mathbf{u}|I)}{P(\mathbf{d}|I)} \quad (2)$$

Where $P(\mathbf{d}|I)$ is a normalization constant called evidence. Therefore, combination of Equations 1 and 2 produces the following equation.

$$P(u_j|\mathbf{d}, I) \propto \int P(\mathbf{d}|\mathbf{u}, I)P(\mathbf{u}|I) \underbrace{\dots du_i \dots}_{i \neq j} \quad (3)$$

This equation presents that to obtain the posterior, we need to define our likelihood function and the prior. The likelihood, or in this case more appropriate the PDF of the data (\mathbf{d}) conditional on the pixels (\mathbf{u}), is constructed by making the standard assumptions of noise. Therefore, according to the Bayesian interpolation technique, there are three main steps should be taken into account:

1. All the pixels are connected to each other so each pixel is defined as a function of its neighboring pixels. This is the prior information which is formulated in Section 4.
2. For the pixels which take the corresponding data values, the data values are considered the best estimates. This is described in Section 5.
3. Then the outcome of the previous steps are combined so as to get an estimation of every pixel in grid, based on the data. In this case, Equation 3 is used and the result is presented in Section 6.

4 THE PRIOR

We expect some logical dependence between neighboring pixels and this expectation is translated in the

following model, f , for an arbitrary pixel u_i .

$$u_i = f(u_{i-1}, u_{i+1}) = \frac{u_{i-1} + u_{i+1}}{2} \quad (4)$$

Having the model defined, the error e_i also is implicitly defined by Equation 5.

$$e_i = u_i - f(u_{i-1}, u_{i+1}) = u_i - \frac{u_{i-1} + u_{i+1}}{2} \quad (5)$$

The only thing we know about this error is that the error has a mean of zero (the error is either positive or negative) with some unknown variance ϕ^2 . Using the principle of Maximum Entropy (Jaynes 2003), we find the well known Gaussian probability distribution function of e_i presented in Equation 6.

$$P(e_i|\phi) = \frac{1}{\sqrt{2\pi}\phi} \exp\left[-\frac{1}{2\phi^2}e_i^2\right] \quad (6)$$

Substituting Equation 5 into Equation 6 and making the appropriate change of variable from e_i to u_i , the PDF of the pixel u_i can be obtained by Equation 7.

$$\begin{aligned} P(u_i|u_{i-1}, u_{i+1}, \phi) \\ = \frac{1}{\sqrt{2\pi}\phi} \exp\left[-\frac{1}{2\phi^2}\left[u_i - \frac{u_{i-1} + u_{i+1}}{2}\right]^2\right] \end{aligned} \quad (7)$$

Assuming that there is no logical dependence between the errors e_1, \dots, e_v , the multivariate PDF of all the errors is a product of the univariate PDFs. Then, by making the change of variable from e_i to u_i we find the following multivariate PDF for the pixels u_1, \dots, u_v .

$$\begin{aligned} P(u_1, \dots, u_v|u_0, u_{v+1}, \phi) \\ = \frac{1}{(2\pi)^{v/2}\phi^v} \exp\left[-\frac{1}{2\phi^2}\sum_{i=1}^v\left[u_i - \frac{u_{i-1} + u_{i+1}}{2}\right]^2\right] \end{aligned} \quad (8)$$

The boundary pixels are treated separately. In fact, these two pixels are assigned to the first and last position and presented as $u_0 = v_1$ and $u_{v+1} = v_{v+2}$. As a result of using the principle of Maximum Entropy, the PDF of the boundary pixel u_0 is obtained in Equation 9. And a similar equation can be established for

the pixel u_{v+1} .

$$P(u_0|u_1, \phi) = \frac{1}{\sqrt{2\pi}\phi} \exp\left[-\frac{1}{2\phi^2} [u_0 - u_1]^2\right] \quad (9)$$

Combining Equations 8 and 7 using Bayes' Theorem, the next equation will be obtained. This equation is written in a matrix form where \mathbf{u} is vector of pixel positions,

$$P(u_0, u_1, \dots, u_{v+1}|\phi) = \frac{1}{(2\pi)^{(v+2)/2}\phi^{v+2}} \exp\left[-\frac{\mathbf{Q}}{2\phi^2}\right] \quad (10)$$

where

$$\mathbf{Q} = \mathbf{u}^T \mathbf{R} \mathbf{u}$$

and

$$\mathbf{R} \equiv \begin{pmatrix} 1 & -1.5 & 0.5 & 0 & \dots & \dots & 0 \\ -1.5 & 3 & -2 & 0.5 & 0 & \ddots & \vdots \\ 0.5 & -2 & 3 & -2 & 0.5 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0.5 & -2 & 3 & -2 & 0.5 \\ \vdots & \ddots & \ddots & 0.5 & -2 & 3 & -1.5 \\ 0 & \dots & \dots & 0 & 0.5 & -1.5 & 1 \end{pmatrix}$$

We have derived the above equation which provides the PDF for the pixels u_0, \dots, u_{v+1} using the assumed prior model presented in Equation 4.

If $\phi = 0$, we get to the conclusion that our model (Equation 4) holds exactly. So setting $\phi = 0$ produces an extremely informative prior which determines the values of the pixels. On the other hand, if $\phi \rightarrow \text{inf}$ then the prior relaxes to an extremely uninformative distribution which lets the values of the pixels totally free. So in a sense ϕ 'regulates' the freedom allowed to the pixels u_0, \dots, u_{v+1} .

5 THE LIKELIHOOD

Apart from our model and prior, we also have $n+2$ non-overlapping data points, $n \leq v$. These data points can be assigned arbitrarily to any pixel u_c where c is an element of the vector \mathbf{c} described in Section 2. The value of c corresponds with the location of the observed data regarding the pixel numbers (see Figure 2). The error of the model at the location of any observed data point is defined as:

$$e_c = u_c - d_c \quad (11)$$

Assuming that this error has a mean of zero (the error is either positive or negative) with some unknown variance σ^2 and using the principle of Maximum Entropy we find that this error has the following probability distribution function:

$$P(e_c|\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2\sigma^2} e_c^2\right] \quad (12)$$

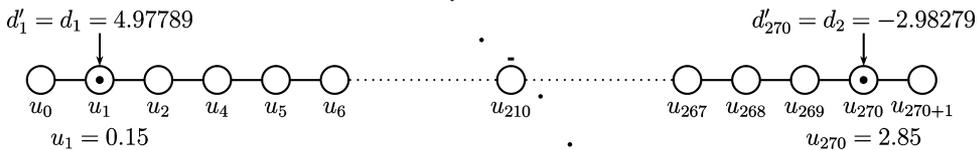


Figure 2. An illustration of the pixels which data points are assigned to. The '·' is a representation of the evaluated values in the pixels.

Substituting 11 into 12 and making a change of variable from the error e_c to the data d_c , the likelihood function can be obtained according to Equation 13.

$$P(d_c|u_c, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2\sigma^2}(d_c - u_c)^2\right] \quad (13)$$

Again by assuming logical independence between the errors and making the appropriate substitutions and changes of variables, the following likelihood function can be obtained.

$$P(d_1, \dots, d_n|u_0, u_1, \dots, u_{(v+1)}, \sigma) = \frac{1}{(2\pi)^{n/2}\sigma^n} \exp\left[-\frac{1}{2\sigma^2} \sum_{c \in \mathbf{c}} (d_c - u_c)^2\right] \quad (14)$$

Equation 14 can be rewritten in the matrix form as presented in Equation 15.

$$P(d_1, \dots, d_n|u_1, \dots, u_n, \sigma) = \frac{1}{(2\pi)^{n/2}\sigma^n} \exp\left[-\frac{1}{2\sigma^2} (\mathbf{d}' - \mathbf{S}\mathbf{u})^T (\mathbf{d}' - \mathbf{S}\mathbf{u})\right] \quad (15)$$

Where \mathbf{d}' is a padded vector of length $v + 2$ where the data points have been coupled with their corresponding pixels and \mathbf{S} is a diagonal matrix with entry 1 for pixels which data points are assigned to them and 0 everywhere else.

For example, the \mathbf{S} matrix for the grid in Figure 1, $\mathbf{d}' = (0, d_1, 0, \dots, 0, d_2, 0, d_3)$ becomes:

$$\mathbf{S} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & \dots & 0 \\ 0 & 1 & 0 & 0 & 0 & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & 0 & 1 & 0 & 0 \\ \vdots & \dots & \ddots & 0 & 0 & 0 & 0 \\ 0 & \dots & \dots & 0 & 0 & 0 & 1 \end{pmatrix} \quad (16)$$

6 THE POSTERIOR

Combining the prior in Equation 10 and with the likelihood presented in Equation 15 we get a function which is proportional to the posterior PDF of all the pixels

(Sivia 1996). Equation 19 presents the matrix form of this function.

$$P(\mathbf{u}|\mathbf{d}, \sigma, \phi) \propto P(\mathbf{u}|\phi)P(\mathbf{d}|\mathbf{u}, \sigma) = \frac{1}{\phi^{v+2}\sigma^n} \exp\left[-\frac{(\mathbf{d}' - \mathbf{S}\mathbf{u})^T (\mathbf{d}' - \mathbf{S}\mathbf{u})}{2\sigma^2} - \frac{\mathbf{u}^T \mathbf{R}\mathbf{u}}{2\phi^2}\right] \quad (17)$$

Equation 19 is conditional on unknown parameters ϕ and σ , but since we don't know these parameters we will want to integrate them eventually out as 'nuisance' parameters. We first assign Jeffery's prior to these unknown parameters:

$$P(\phi) = \frac{1}{\phi} \quad P(\sigma) = \frac{1}{\sigma} \quad (18)$$

Using Bayes' theorem we can combine the priors in Equation 18 with Equation 19 to get the following equation.

$$P(\mathbf{u}, \sigma, \phi|\mathbf{d}) = P(\sigma)P(\phi)P(\mathbf{u}|\mathbf{d}, \sigma, \phi) \propto \frac{1}{\phi^{v+3}\sigma^n} \exp\left[-\frac{(\mathbf{d}' - \mathbf{S}\mathbf{u})^T (\mathbf{d}' - \mathbf{S}\mathbf{u})}{2\sigma^2} - \frac{\mathbf{u}^T \mathbf{R}\mathbf{u}}{2\phi^2}\right] \quad (19)$$

By integrating over all pixel except the target pixel, u_j , the probability distribution function of just one pixel (u_j) is given as

$$P(u_j|\mathbf{d}, \sigma, \phi) = \int P(u_0, \dots, u_{v+1}|\mathbf{d}, \sigma, \phi) \underbrace{du_0 \dots du_{v+1}}_{\text{except } du_j} = \int \exp\left[-\frac{(\mathbf{d}' - \mathbf{S}\mathbf{u})^T (\mathbf{d}' - \mathbf{S}\mathbf{u})}{2\sigma^2} - \frac{\mathbf{u}^T \mathbf{R}\mathbf{u}}{2\phi^2}\right] \times \frac{1}{(\phi)^{v+3}\sigma^n} \underbrace{du_0 \dots du_{v+1}}_{\text{except } du_j} \quad (20)$$

For actual evaluation of Equation 20, we refer the interested reader to (Bretthorst 1992).

7 ALGORITHM

To couple the Bayesian interpolation approach with Monte Carlo techniques the following algorithm is suggested:

1. Define the interval of variation and the length of pixels for the variable X . Totally, $v + 2$ pixels are to be defined in this interval.

2. A random number is generated according to the PDF of the variable X , and according to its value, its assigned to a certain location. This location which is the j th pixel (as presented in Figure 1) is called u_j .
3. According to the information of the other pixels and our assumed model, the PDF of the u_j is calculated by Equation 20.
4. According to the accepted tolerance criteria, it is decided whether there is a need to calculate the limit state equation for the j th point or the accuracy is enough.
5. The calculations are iterated from step 3 and continues to meet the simulation criteria.

8 NUMERICAL EXAMPLE

One of the important research topics in hydraulic engineering focuses on the impact of water waves on walls and other coastal structures, which create velocities and pressure with magnitudes much larger than those associated with the propagation of ordinary waves under gravity. The impact of a breaking wave can generate pressures of up to 1000 kN/m^2 which is equal to 100 meters of water head. Although many coastal structures are damaged by breaking waves, very little is known about the mechanism of impacts. Insight into the wave impacts has been gained by investigating the role of entrained and trapped air in wave impacts. In this case, a simplified model of maximum pressure of ocean waves on the coastal structures is presented by Equation 21.

$$P_{max} = C \times \frac{\rho \times k \times u^2}{d} \quad (21)$$

Where the ρ is density of water, k is the length of hypothetical piston, d is the thickness of air cushion, u is the horizontal velocity of the advancing wave, and C is a constant parameter and equal to $2.7 \text{ s}^2/\text{m}$. Having this knowledge, we are willing to find the probability of the event, when the maximum impact pressure exceeds $5 \times 10^5 \text{ N/m}^2$ for a specific case. The one dimensional limit state function (LSF) can be defined by Equation 22, where the velocity parameter is assumed to be normally distributed as $N(1.5, 0.45)$.

$$G(u) = 5 - 0.98280 \times u^2 \quad (22)$$

We consider the variation of the variable u in the interval of $[\mu - 3\sigma, \mu + 3\sigma]$ where μ is the mean value and σ is the standard deviation of variable u . This interval is divided to the finite pixels with an equal distance of 0.01. As a result, there are totally 270 internal pixels defined in this interval. A schematic view of the all pixels is presented in Figure 2. Pixel 210 is considered as a sample pixel in which we are going

to monitor the change of its PDF during Monte Carlo process. In this figure, the measured (or observed) data point is assigned to the first and last internal pixels.

Before we proceed to the simulation process, we would like to present the probable values of pixel 210 or u_{210} with the suggested model. Therefore, we need to use Equation 20 in order to get the required PDF. Nevertheless, this equation contains σ and ϕ . As a matter of fact, σ can be integrated out of the equation, but we need to estimate a value for the ϕ . In this case, we define $\epsilon = \frac{1}{\phi}$ which is called regularizer. Then we can get the PDF of our regularizer to find its optimal value which leads to the most narrow PDF. The reader who is interested in this process is referred to (Bretthorst 1992). The most probable value of ϵ is estimated to be 2.6 and we use this value during the rest of this work. As a result, Equation 20 will lead to Equation 23 for pixel number 210 given two data points: d_1 and d_2 .

$$P(u_{j=210}|d_1, d_2) = \frac{0.3126 \cdot 10^9}{0.5897 \cdot 10^{10} + 0.5265 \cdot 10^{10} u_j + 0.1339 \cdot 10^{10} u_j^2} \quad (23)$$

The PDF of u_{210} given d_1 and d_2 is depicted in Figure 3. This figure is a plot of Equation 23. The mean value of this PDF is -1.97 by assuming a symmetrical PDF. Besides, the 95% accuracy by assuming a symmetrical distribution leads to the values in the interval of $[-11.28, 7.35]$. This interval was obtained by solving the equation which defines the integration of a symmetrical area around mean value should be equal to 0.95. It is a wide PDF and its tails are much more informative than the Gaussian. In other words, we expect value of this pixel vary within the interval having the prior information about the model and just 2 data points.

It is useful to compare this result with the traditional interpolation problem. In fact, by considering two data points, there is no other way than we assume a linear relationship which leads to the value of -1.21 for this pixel while we do not have any estimation about the uncertainty. Now, the distinction between two methods is obvious; the applied method enables us to get a criterion for the uncertainty of the estimated value of each pixel. This is an huge advantage in the simulation process. This comparison is depicted in Figure 4. In this figure there are two data points called **A** and **B**. These two points are the only information which provide point **e** using a linear interpolation for the pixel 210, where $\mathbf{e} = -1.21$. This is not close to real value of the limit state function $\mathbf{g} = 0.0246$. Nevertheless, there is no information over the certainty of the estimated point **e** from the interpolation. In the other hand, point **f** is the mean value of the PDF calculated by the

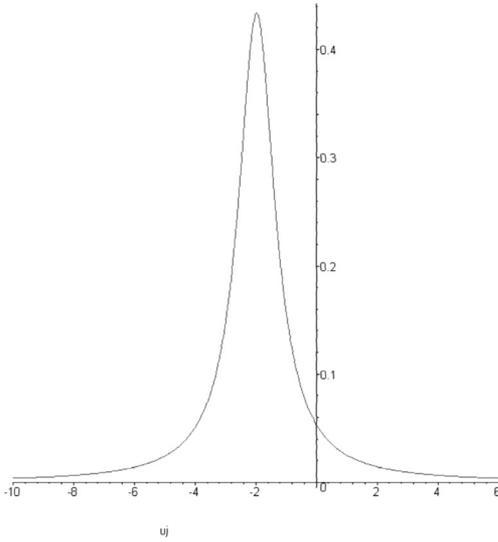


Figure 3. This figure presents the probability distribution function (PDF) of the u_{210} given 2 measured data points: d_1 and d_{270} .

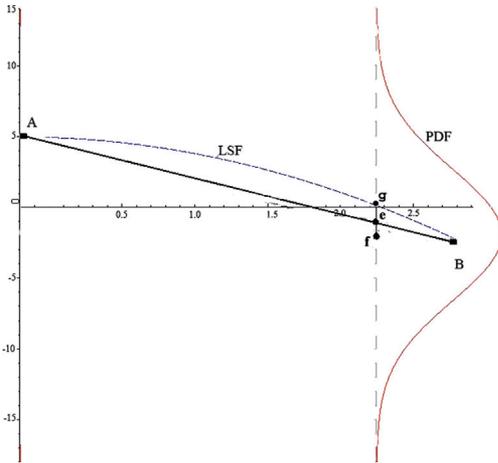


Figure 4. A comparison between linear interpolation and the Bayesian technique for the pixel u_{210} , given 2 measured data points: d_1 and d_{270} . The exact value of the function (Equation 22) is depicted by dashed line.

Bayesian technique ($\mathbf{f} = -1.97$). The uncertainty is shown by its PDF. Having a look at the presented PDF, a rather wide PDF can be seen; and both of positive and negative values are expected for this pixel.

From now on we start the Monte Carlo simulation by generating random numbers. However, before we run the limit state equation for each random number which

is assigned to a pixel u_j , we check if it is necessary to run the limit state equation, or we can assign its value regarding our tolerance. To investigate the changes, we monitor the u_{210} after 20 realizations of the LSE (or 20 data points) which are assigned to their location. As a result, the calculated PDF of u_{210} given 20 data points is obtained and depicted in Figure 5. The mean value of this PDF is 0.013, and the 95% accuracy by assuming a symmetrical distribution leads to the values in the interval of $[-0.16, 0.19]$. This shows that by implementing more data points, we get a more precise PDF.

The difference of the results of linear and Bayesian interpolation at this case is because of the value of the regularizer (ϵ). In this case study its value is set to be $\epsilon = 2.60$. The effect of epsilon (or ϕ which is inversely related to it) was previously described. In fact, we can have two extreme situations when we consider two extreme values for Φ . These extreme values are 0 and infinity. In the first case we just stick to our data values and in the second case we just consider our model assumption and leave the other information. Therefore, the difference between \mathbf{e} and \mathbf{f} should be related to the value of regularizer.

Since we are not satisfied with the accuracy we continue to generate more data points. Figure 6 presents the PDF of u_{210} having 90 data points measured or calculated. The mean value of this PDF is 0.025, and the 95% accuracy by assuming a symmetrical distribution leads to the values in the interval of $[0.014, 0.035]$. This shows that by implementing more data

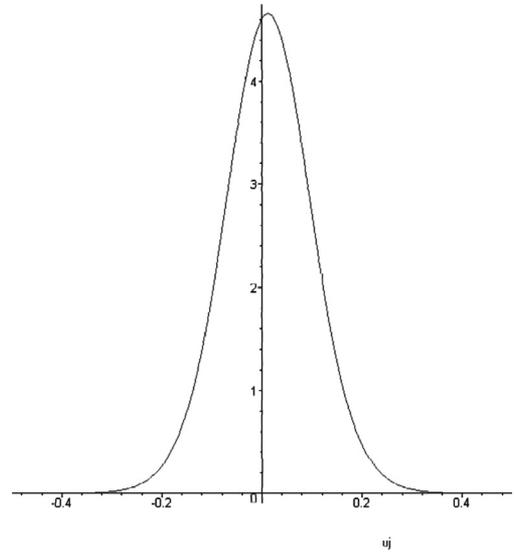


Figure 5. This figure presents the probability distribution function (PDF) of the u_{210} given 20 measured data points given in random locations.

points, we get a more precise PDF. Since this interval is small enough, we can assume that we have got the enough accuracy. Therefore, the simulation effort has been reduced by 67% for the presented numerical example.

In fact, the number of simulations in the Monte Carlo technique depends on several factors. The most important ones are the tolerance and the distance between pixels defined for the analysis. In other words, to get a more precise result we need to implement more data points. Meanwhile, a higher number of pixels lead to a higher accuracy.

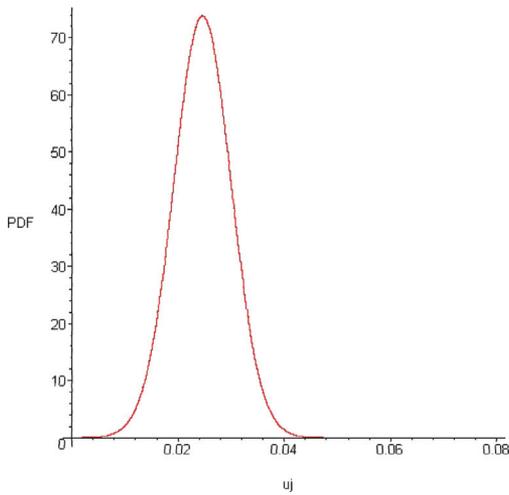


Figure 6. This figure presents the probability distribution function (PDF) of the u_{210} given 90 measured data points given in random locations.

It is useful to compare the calculated PDFs in another figure with the same scale. Figure 7 provides this comparison in which figure (a) presents the PDF of the pixel at the beginning of simulation where there are just two data points. Figure 7 (b) presents the PDF of the same pixel, u_{210} , when there are 20 data points randomly generated and assigned to the related pixels. Figure 7(c) again presents the PDF of the same pixel where the information of ninety pixels are implemented. In this figure, the same scale of axis is selected to clarify the change of the PDF during the simulation process.

9 DISCUSSION

The Bayesian interpolation is a technique which can be nicely coupled with Monte Carlo simulation. In this study, an attempt is made to have the prior information of the model incorporated to the current level of the analysis. This is a step forward in Monte Carlo simulations. In fact, the \mathbf{R} in Equation 10 provides a link between the information of each pixel with its neighborhood. In other words, information of each point passes through this link and effect the others. Besides, this approach provides a nice tool to get the other priors incorporated to the Monte Carlo simulations. For instance, the limit bounds method (Rajabalinejad et al.2007 assumes some other prior information which can be implemented in this approach.

Nevertheless, the approach presented in this paper has got two main limitations. The first one is that we need to use a grid and divide the interval of variation of the variable to finite number of pixels. The second limitation is that the pixel are evenly spaced. These conditions impose large matrices for a large interval, a small step size, or higher dimensions.

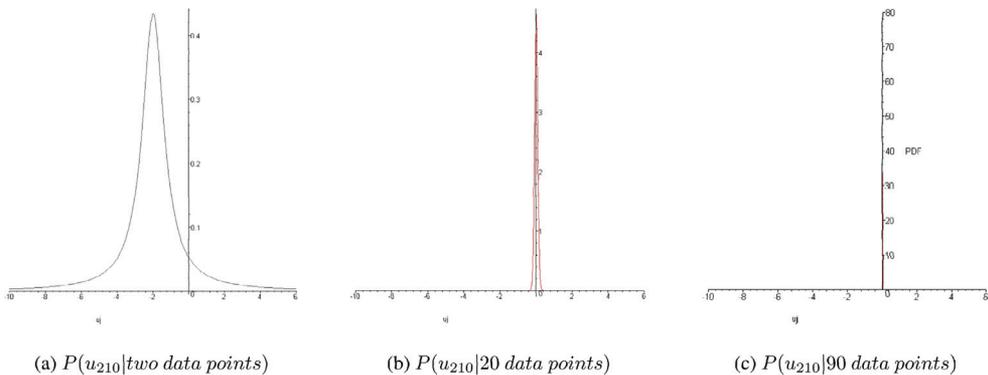


Figure 7. This figure shows the probability distribution function of variable which is assigned to the pixel $j = 210$. In Figure (a) Just the information of 2 data points are considered while in Figure (b) and (c), the information of 20 and 90 pixels are considered, respectively.

10 CONCLUSION

The suggested procedure can speed up the Monte Carlo simulations integrated with finite elements or the other highly complicated and time consuming processes. However, in this paper we have limited ourselves into the finite number of pixels. The proposed method also provides a tool for implementing informative priors regarding the considered model. The extension of this work with an arbitrary length and location of pixels can provide a more powerful tool and is recommended for future research projects.

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