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A fast Monte–Carlo method with a reduced basis of control variates applied to uncertainty propagation and Bayesian estimation

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A B S T R A C T

The reduced-basis control-variate Monte-Carlo method was introduced recently in [S. Boyaval, T. Lelièvre, A variance reduction method for parametrized stochastic differential equations using the reduced basis paradigm, Commun. Math. Sci. 8 (2010) 735–762 (Special issue "Mathematical Issues on Complex Fluids")] as an improved Monte-Carlo method, for the fast estimation of many parametrized expected values at many parameter values. We provide here a more complete analysis of the method including precise error estimates and convergence results. We also numerically demonstrate that it can be useful to some parametric frameworks in Uncertainty Quantification, in particular (i) the case where the parametrized expectation is a scalar output of the solution to a Partial Differential Equation (PDE) with stochastic coefficients (an Uncertainty Propagation problem), and (ii) the case where the parametrized expectation is the Bayesian estimator of a scalar output in a similar PDE context. Moreover, in each case, a PDE has to be solved many times for many values of its coefficients. This is costly and we also use a reduced basis of PDE solutions like in [S. Boyaval, C. Le Bris, Y. Maday, N. Nguyen, A. Patera, A reduced basis approach for variational problems with stochastic parameters: Application to heat conduction with variable robin coefficient, Comput. Methods Appl. Mech. Eng. 198 (2009) 3187–3206]. To our knowledge, this is the first combination of various reduced-basis ideas, with a view to reducing as much as possible the computational cost of a simple versatile Monte-Carlo approach to Uncertainty Quantification.

1. Introduction

The reduced-basis (RB) control-variate Monte-Carlo (MC) method was recently introduced in [1] to compute fast many expectations of scalar outputs of the solutions to parametrized ordinary Stochastic Differential Equations (SDEs) at many parameter values. But as a simple, generic MC method with reduced variance, the RB control-variate MC method can also be useful in other parametric contexts and the main goal of this article is to show that it can be useful to Uncertainty Quantification (UQ) too, possibly in combination with the standard RB method in a PDE context.

There is a huge literature on the UQ subject. Indeed, to be actually predictive in real-life situations [2], most numerical models require (i) to calibrate as much as possible the parameters and (ii) to quantify the remaining uncertainties propagated by the model. Besides, the latter two steps are complementary in an iterative procedure to improve numerical models using data from experiments: quantifying the variations of outputs generated by input parameters allows one to calibrate the input uncertainties with data and in turn reduces the epistemic uncertainty in outputs despite irreducible aleatoric uncertainty. Various numerical techniques have been developed to quantify uncertainties and have sometimes been used for years [3,4]. But there are still a number of challenges [5–7].

For PDEs in particular, the coefficients are typical sources of uncertainties. One common modelling of these uncertainties endows the coefficients with a probability distribution that presumably belongs to some parametric family and the PDEs solutions inherit the random nature of the uncertainty sources. A Bayesian approach is often favoured to calibrate the parameters in the probability law using observations of the reality [8,9]. But the accurate numerical simulation of the PDEs solutions as a function of parametrized uncertain coefficients is a computational challenge due to its complexity, and even more so is the numerical optimization of the parameters in uncertain models. That is why new/improved techniques are still being investigated [10,11]. Our goal in this work is to develop a practically useful numerical method that bases on the simple versatile MC approach to simulate the probability law of the uncertain coefficients. We suggest to use the RB control-variate MC method in some UQ frameworks to improve the computational cost of the naive MC method, in particular in

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contexts where some coefficients in a PDE are uncertain and others are controlled.

There exist various numerical approaches to UQ. The computational cost of MC methods is certainly not optimal when the random PDE solution is regular, see e.g. [12]. But we focus here on MC methods because they are (a) very robust, that is useful when the regularity of the solution with respect to the random variables degrades, and (b) very easy to implement (they are *non-intrusive* in the sense that they can use a PDE numerical solver as a black-box, with the values of the PDE coefficients as input and that of the discrete solution as output). Besides, note that even when the random PDE solution is very regular with respect to the random variables, it is not yet obvious how algorithms can take optimal profit of the regularity of random PDE solutions and remain practically efficient as the dimension of the (parametric) probability space increases, see e.g. [13]. So, focusing on a MC approach, our numerical challenge here is basically two-sided: (i) on the probabilistic side, one should sample fast the statistics of the random PDE solution (or of some random output that is the quantity of interest), and (ii) on the deterministic side, one has to compute fast the solution to a PDE for many realizations of the random coefficients. It was proposed in [14] to use the RB method in order to reduce the numerical complexity of (ii), but this does not fully answer the numerical challenge. In particular, although the RB method can improve naive MC approaches at no-cost (since the selection of the reduced basis for the PDE solutions at various coefficients values can be trained on the same large sample of coefficients values that is necessary to the MC sampling, see also [15]), the resulting MC approach might still be very costly, maybe prohibitively, due to the large number of realizations that is necessary to accurately sample the statistics of the PDE solution (side (i) of our challenge above). In this work, we thus tackle the question how to reduce the numerical complexity of (i). We have in mind the particular but useful case where one is interested in the expected value of a random scalar output of the random PDE solution as a function of a (deterministic) *control parameter*, typically another (deterministic) coefficient in the UQ problem which is "under control". (Think of the construction of response surfaces for a mean value as a function of control parameters.) A similar parametric context occurs in Bayesian estimation, sometimes by additionally varying the *hyper parameters* or the observations. In any case, our goal is to reduce the computational cost of a parametrized (scalar) MC estimation when the latter has to be done many times for many values of a parameter, and we illustrate it with examples meaningful in a UQ context.

To accelerate the convergence of MC methods as numerical quadratures for the expectation of a random variable, one idea is to tune the sampling for a given family of random variables like in the quasi-Monte-Carlo (qMC) methods [16–18]. Another common idea is to sample another random variable with same mean but with a smaller variance. Reducing the variance allows one to take smaller MC samples of realizations and yet get MC estimations with confidence intervals of similar (asymptotic) probability. Many techniques have been designed in order to reduce the variance in various contexts [19,20]. Our RB control-variate MC method bases on the so-called control-variate technique. It has a specific scope of application in parametric contexts. But it suits very well to some computational problems in mathematical finance and molecular dynamics as shown in [1], and can be useful in UQ as we are going to see.

The paper is organized as follows. In Section 2, we recall the RB control-variate technique as a general variance reduction tool for the MC approximation of a parametrized expected value at many values of the parameter. The presentation is a bit different to that in [1], which was more focused on SDEs. Moreover, we also give new error estimates and convergence results. In Section 3, the RB control-variate MC method is applied to compute the mean of a random scalar output in a model PDE with stochastic coefficients (the input uncertainty) at many values of a control parameter. In Section 4, it is applied to Bayes estimation, first for a toy model where various parametric contexts are easily discussed, then for the same random PDE as in Section 3.

We also note that this work does not only improve on the RB approach to UQ [14] but also on an RB approach to Bayesian estimation proposed in [21] with a deterministic quadrature formula to evaluate integrals. For both applications, to our knowledge, our work is the first attempt at optimally approximating the solution with a simple MC/FE method by combining RB ideas of two kinds, stochastic and deterministic ones [22]. Note that for convenience of the reader non-expert in RB methods, the standard RB method [23,24] is briefly recalled in Section 3.3.

2. The RB control-variate MC method

The RB control-variate technique is a generic variance reduction tool for the MC approximation of a parametrized expected value at many values of the parameter. In this section we recall the technique for the expectation $E(Z^\lambda)$ of a generic square-integrable random variable $Z^\lambda \in L^2_P$ parametrized by λ. The principle for the reduction of computations is based on the same paradigm as the standard RB method and allows one to accelerate the MC computations of many $E(Z^\lambda)$ at many values of λ. Our presentation is slightly different than the initial one in [1] and gives new elements of analysis (error estimates and convergence results).

2.1. Principles of RB control-variate MC method

Let P be a probability measure such that Z^λ is a random variable in L^2_P for all parameter values λ in a given fixed range Λ. Assume one has an algorithm to simulate the law of Z^λ whatever $\lambda \in \Lambda$. Then, at any $\lambda \in \Lambda$, one can define MC estimators $E_M(Z^\lambda)$ that provide useful approximations of $E(Z^\lambda) := \int Z^\lambda dP$, by virtue of the strong law of large numbers

$$E_M(Z^\lambda) := \frac{1}{M}\sum_{m=1}^{M} Z^\lambda_m \underset{M\to\infty}{\overset{P-a.s.}{\to}} E(Z^\lambda) \tag{2.1}$$

provided the number M of independent identically distributed (i.i.d.) random variables $Z^\lambda_m \sim Z^\lambda,\ m = 1\ldots M$, is sufficiently large. Here, the idea is: if $E(Z^{\lambda^I_i})$ is already known with a good precision for I parameter values $\lambda^I_i,\ i = 1\ldots I$, ($I \in \mathbb{N}_{>0}$) and if the law of Z^λ depends smoothly on λ then, given I well-chosen real values $\alpha^\lambda_i,\ i = 1\ldots I$, the standard MC estimator $E_M(Z^\lambda)$ could be efficiently replaced by a MC estimator for $E\left(Z^\lambda - \sum_{i=1}^I \alpha^\lambda_i Z^{\lambda^I_i}\right) + \sum_{i=1}^I \alpha^\lambda_i E\left(Z^{\lambda^I_i}\right)$ that is as accurate and uses much less than M copies of Z^λ.

In other words, if for some $\alpha^{\lambda^2}_i$ $(i = 1\ldots I)$ the random variable

$$\hat{Y}^\lambda = \sum_{i=1}^{I} \alpha^\lambda_i \left(Z^{\lambda^I_i} - E\left(Z^{\lambda^I_i}\right)\right) \tag{2.2}$$

is correlated with Z^λ (eq. $Z^\lambda - E(Z^\lambda)$) such that the control of Z^λ by $\hat{Y}^\lambda$ reduces the variance, that is if

$$V(Z^\lambda) := \int \left|Z^\lambda - E(Z^\lambda)\right|^2 dP \geqslant V\left(Z^\lambda - \hat{Y}^\lambda\right),$$

then the confidence intervals of MC estimations

$$E_M\left(Z^\lambda - \hat{Y}^\lambda\right) := \sum_{m=1}^{M} \frac{Z^\lambda_m - \hat{Y}^\lambda_m}{M} \underset{M\to\infty}{\overset{P-a.s.}{\to}} E\left(Z^\lambda\right) \tag{2.3}$$

with asymptotic probabilities erf a $(a > 0)$ converge faster with respect to the number M of realizations than the confidence intervals