UQOP 2019
Uncertainty Quantification & Optimization Conference
18-20 March, Paris, France

Multilevel Monte Carlo estimation of Sobol' indices for sensitivity analysis

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Keywords: Monte Carlo, Multilevel Monte Carlo, Covariance estimation, Sensitivity analysis, Sobol' indices.

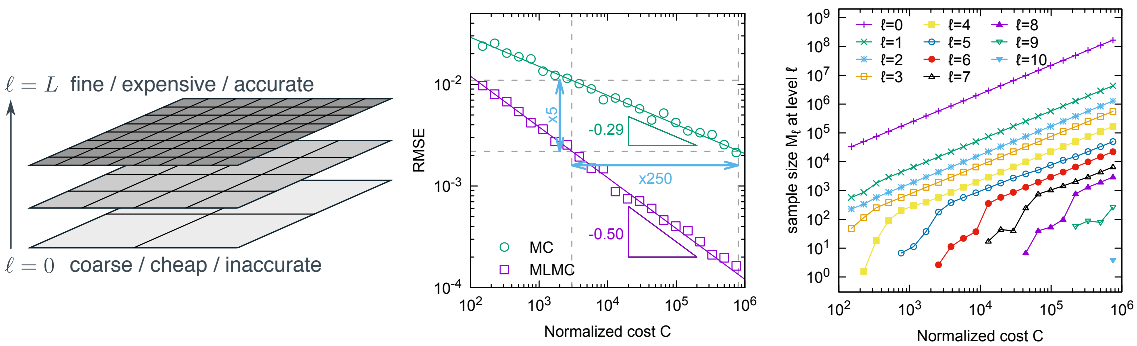
ABSTRACT

We consider an abstract numerical simulator described by the function:

$$\begin{aligned} f\colon \mathcal{X} &\to \mathbb{R} \\ \mathbf{x} &\mapsto f(\mathbf{x}) \equiv y, \end{aligned} \tag{1}$$

whose scalar input parameters $(x_1, \dots, x_d) = \mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d$ are uncertain, leading to an uncertainty in the output value y. In a probabilistic uncertainty quantification (UQ) framework, these uncertain input parameters are commonly described by random variables defined on a probability space $(\Omega, \mathcal{A}, \mathbb{P})$. The input vector $\mathbf{x}$ is then replaced by a $\mathcal{X}$-valued random vector $\mathbf{X}\colon \Omega \to \mathcal{X}$ whose components X_i are independent random variables with probability distributions given by expert knowledge; as a consequence, $Y \equiv f(\mathbf{X})$ is a random variable whose distribution is unknown. In UQ studies, we are often interested in the first central moments of Y. Moreover, sensitivity measures such as Sobol' indices are commonly computed to quantify the shares of output variability attributable to the different input parameters.

Monte Carlo (MC) methods are popular and powerful approaches for the estimation of statistical parameters (expectations, variances, covariances). However, it is well-known that the root mean square error ε of the MC estimator of the expectation converges slowly as a function of the sample size M, specifically $\varepsilon = \mathcal{O}(1/\sqrt{M})$ for the sample mean estimator of the expectation. Reducing this error by a factor of r thus implies increasing the sample size by a factor of r^2. In practice, for the quantity of interest $Y = f(\mathbf{X})$, obtaining a realization of the expectation estimator $E_M[Y]$ requires M calls to the numerical simulator f. This slow convergence may thus become a critical issue, especially if sampling involves computationally expensive operations, such as solving a (discretized) partial differential equation.



(a) *Illustrative MLMC mesh hierarchy* **(b)** *MLMC vs MC convergence* **(c)** *Sample size per level*

Figure 1

Multilevel Monte Carlo (MLMC) methods [1] were developed to improve the overall computational cost of MC sampling by introducing a sequence of so-called levels ℓ, usually corresponding to a hierarchy of numerical simulators $\{f_\ell\}_{\ell\geq 0}$ with increasing accuracy and corresponding cost of individual simulations (see Fig. 1(a)). Typically, an efficient MLMC estimation will require a large number of samples on the coarsest (cheapest) levels and fewer samples on finer (more expensive) levels. Originally designed for the estimation of expectations, MLMC was recently extended to the estimation of higher-order statistical moments such as variances [2]. We focus here on the MLMC estimation of covariances, which are particularly interesting for the computation of Sobol' indices in the context of sensitivity analysis [3]. Indeed, the first-order Sobol' index S_i associated to the i-th random input X_i can be written in "pick-and-freeze" formulation as

$$S_i \equiv \frac{\mathbb{V}[\mathbb{E}[f(\mathbf{X})|X_i]]}{\mathbb{V}[f(\mathbf{X})]} = \frac{\mathbb{C}[f(\mathbf{X}), f(\mathbf{X}^{[i]})]}{\mathbb{V}[f(\mathbf{X})]}, \quad \mathbf{X}^{[i]} \equiv (X'_1, \dots, X'_{i-1}, X_i, X'_{i+1}, \dots, X'_d), \tag{2}$$

where $\mathbf{X}^{[i]}$ denotes the random vector whose i-th component is X_i ("frozen"), while its j-th component ($j \neq i$) is X'_j, where X'_j is an i.i.d. copy of X_j.

We applied the MLMC methodology to the estimation of the covariance term in the numerator of S_i, for the output of a discretized ordinary differential equation with random parameters. Fig. 1(b) shows that MLMC has a better convergence rate compared to standard MC, specifically $\varepsilon_{\mathrm{ML}} = \mathcal{O}(C^{-1/2})$ and $\varepsilon_{\mathrm{MC}} = \mathcal{O}(C^{-1/3})$, leading to a significant reduction of the overall estimation cost. Indeed, using standard MC sampling to obtain an RMSE of 2×10^{-3} is about 250 times more expensive than using MLMC. Fig. 1(c) confirms that more samples are required on cheaper levels. Moreover, as we increase the computational budget, finer (more expensive) levels are considered.

References

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