



Multilevel Monte Carlo Methods for Parametric Expectations: Distribution and Robustness Measures

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Uncertainty Quantification



Mathematical models describing real-word phenomena are affected by uncertainties and incomplete knowledge.

Aerodynamic design





Rough contact mechanics (Lotus effect, rubber on concrete, ...)





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From models to data and back

Reliably using the models requires the study of the impact of all forms of error and uncertainty in models.



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Model-based (forward) Analysis

Today's focus: Forward Uncertainty Quantification — quantifying the effects of uncertainties on model predictions induced by model/input uncertainties

Forward Propagation of Uncertainties





Random input parameters $\boldsymbol{\xi}$, possibly infinite dimensional

• Model: for ξ given, find u s.t. $\mathcal{M}_{\xi}(u) = 0 \rightsquigarrow$ Quantity of interest: $Q(\xi) = Q(u(\xi))$



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- General purpose method to approximate moments of *Q_h* for *given discretization h*:
 - generate sample of *N* i.i.d. realizations $\boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(N)} \sim \mathbb{P}_{\boldsymbol{\xi}}$
 - compute corresponding model outputs $Q_h(\boldsymbol{\xi}^{(i)}), i = 1, ..., N$
 - approximate expectation of Q_h by sample average:

$$\mathbb{E}(Q) \approx \mathbb{E}(Q_h) \approx E_N(Q_h) := \frac{1}{N} \sum_{i=1}^N Q_h^{(i)}, \quad Q_h^{(i)} \equiv Q_h(\boldsymbol{\xi}^{(i)}) \text{ i.i.d. realizations}$$



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Question: How should we select *h* and *N* to ensure a certain *accuracy* at *minimal cost*?
 Mean squared error (MSE) accuracy of Monte Carlo method:

$$\mathsf{MSE} := \mathbb{E}\Big(\big|\mathbb{E}(Q) - E_N(Q_h)\big|^2\Big) = \underbrace{\big(\mathbb{E}(Q) - \mathbb{E}(Q_h)\big)^2}_{\text{squared bias}} + \underbrace{\frac{\mathsf{Var}(Q_h)}{N}_{\text{stat. error}}}_{\text{stat. error}}$$



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- That is, the parameters are implied by MSE tolerance with:
 - h dictated by the bias = discretization error of approximate model
 - sample size N given by the statistical error



Monte Carlo: cost vs. accuracy

Lemma: MSE complexity analysis MC (error vs. cost)

Suppose that:

•
$$|\mathbb{E}(Q - Q_h)| = \mathcal{O}(h^{\alpha}),$$

• $\operatorname{Var}(Q_h) = \mathcal{O}(1),$
• $\operatorname{cost}(Q_h^{(i)}) = \mathcal{O}(h^{-\gamma}).$

Achieving MSE $\leq \varepsilon^2$ requires $N = \mathcal{O}(\varepsilon^{-2})$ and $h = \mathcal{O}(\varepsilon^{1/\alpha})$, resulting in

comp. cost MC =
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Achieving MSE $< \varepsilon^2$ requires $N = \mathcal{O}(\varepsilon^{-2})$ and $h = \mathcal{O}(\varepsilon^{1/\alpha})$, resulting in

comp. cost MC = $N \operatorname{cost}(Q_h) = \mathcal{O}(\varepsilon^{-(2+\gamma/\alpha)})$.

• Another error criterion is the **probability of failure**: find (h, N) such that

$$\mathbb{P}ig(|\mathbb{E}(\mathcal{Q}) - \mathcal{E}_{\mathcal{N}}(\mathcal{Q}_{h})| \geq 2arepsilonig) \leq au \;, \quad ext{for } arepsilon > 0 ext{ and } au \in (0,1) \;.$$

• For $\varepsilon \ll 1$, the distribution of $E_N(Q_h)$ can be approximated in view of central limit theorem (CLT) as $Var(Q_h)$ is bounded.

Multilevel Monte Carlo for expected values



• Main idea: use a hierarchy of $L \in \mathbb{N}_0$ discretizations $h_0 > h_1 > \cdots > h_L$, instead of just one fine level:



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• The multilevel Monte Carlo (MLMC) estimator of $\mathbb{E}(Q)$ then is $(Q_{\ell} \equiv Q_{h_{\ell}})$:

$$\mathbb{E}(Q) \approx \mathbb{E}(Q_L) = \mathbb{E}(Q_0) + \sum_{\ell=1}^{L} \mathbb{E}(Q_\ell - Q_{\ell-1}) \approx E_{N_0}(Q_0) + \sum_{\ell=1}^{L} E_{N_\ell}(Q_\ell - Q_{\ell-1}) =: \hat{Q}_{N,L}$$

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MSE accuracy of multilevel Monte Carlo method is

$$\mathsf{MSE} \equiv \mathbb{E}\left(\left|\mathbb{E}(Q) - \hat{Q}_{\mathsf{N},L}\right|^{2}\right) = \underbrace{\left(\mathbb{E}(Q) - \mathbb{E}(Q_{L})\right)^{2}}_{\text{squared bias}} + \underbrace{\sum_{\ell=0}^{L} \frac{\mathsf{Var}(Q_{\ell} - Q_{\ell-1})}{N_{\ell}}}_{\text{statistical error}}, \quad Q_{-1} \equiv \mathbf{Q}_{\mathsf{N},L}$$

- Select parameters $L \in \mathbb{N}_0$ and $N \equiv (N_0, N_1, \dots, N_L)^T \in \mathbb{N}^{L+1}$ s.t. MSE criterion is met at minimal cost.
- Optimal parameters by balancing errors:
 - bias = discretization error $\rightsquigarrow L$,
 - determine N_{ℓ} by minimizing $\sum_{\ell=1}^{L} N_{\ell} C_{\ell}$ subject to MSE $\leq \varepsilon^2$,
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Theorem: Complexity analysis MLMC for $h_{\ell-1}/h_{\ell} = s > 1$

[Giles, 2008; Cliffe et al., 2011]

Suppose that: • $|\mathbb{E}(Q - Q_{\ell})| = \mathcal{O}(h_{\ell}^{\alpha}),$

•
$$\operatorname{Var}(Q_{\ell} - Q_{\ell-1}) = \mathcal{O}(h_{\ell}^{\beta}),$$

•
$$C_\ell = \mathcal{O}({h_\ell}^{-\gamma}).$$

If $2\alpha \geq \min\{\beta, \gamma\}$, then there exists an MLMC estimator $\hat{Q}_{N,L}$ that satisfies MSE $\leq \varepsilon^2$ with

$$\text{comp. cost MLMC} = \sum_{\ell=1}^{L} N_{\ell} C_{\ell} \lesssim \begin{cases} \varepsilon^{-2} , & \beta > \gamma ,\\ \varepsilon^{-2} \ln(\varepsilon)^{2} , & \beta = \gamma ,\\ \varepsilon^{-\left(2 + \frac{\gamma - \beta}{\alpha}\right)} , & \beta < \gamma . \end{cases}$$

Other error criteria are possible, e.g., tuning MLMC for probability of failure is possible thanks to CLT [Collier et al. 2015], [Hoel, K. 2019].



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One could estimate central moments of arbitrary order

$$\mu_{
ho}({\mathcal Q}) := \mathbb{E}ig[ig({\mathcal Q} - \mathbb{E}({\mathcal Q})ig)^{
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with MLMC [Bierig, Chernov. 2016], [K., Nobile, and Pisaroni. 2020]



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However, some applications require techniques that systematically go beyond using a few moments: characterization of entire distribution or applications in risk averse optimization, e.g., involving quantiles

$$rgmin_{z\in\mathbb{R}^d}\mathcal{R}(z)\ ,\quad \mathcal{R}(z)\equiv\mathcal{R}(z;\mathbb{P}_Q)\colon$$
 "risk" of design parameter z



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Examples:

- 1. Mean & variance: $\phi(\vartheta, Q) = (Q \vartheta)^2 \rightsquigarrow \text{Var}(Q) = \min_{\vartheta} \Phi(\vartheta), \mathbb{E}(Q) = \arg\min_{\vartheta} \Phi(\vartheta)$
- 1. Characteristic function of Q: $\phi(\vartheta, Q) = e^{i\vartheta Q} = \cos(\vartheta Q) + i\sin(\vartheta Q)$
- 2. Cumulative distribution function of *Q*: $\phi(\vartheta, Q) = I(Q \le \vartheta)$



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Difficulty for CDF: $\phi(\vartheta, \cdot)$ is **discontinuous**! Consequently, the variance Var $(\phi(\theta_j, Q_\ell) - \phi(\theta_j, Q_{\ell-1}))$ will decay slowly \rightsquigarrow Not much gain in MLMC.



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Remedies in the context of MLMC (cf. [Giles. 2023]):

- Regularizing ϕ to yield $\Phi(\vartheta) = \mathbb{E}(\phi(\vartheta, Q)) \approx \mathbb{E}(\phi_{\delta}(\vartheta, Q))$ [Giles, Nagapetyan, Ritter. 2015]
- Approximate CDF (PDF) based on MLMC estimates of moments [Bierig, Chernov. 2016]
- numerical smoothing via conditioning [Bayer, Ben Hammouda, Tempone. 2022]

Remedy for CDF: antiderivative/integration approach [K., Nobile. 2018] Katsuke of Technology

For any $au \in (0, 1)$ define

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Then

$$F(\vartheta) = (1 - \tau) \Phi'(\vartheta) + \tau \; ,$$

which is the starting point for the MLMC estimator:

 \rightsquigarrow requires effective estimator of Φ and its derivatives.

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This approach may also offer approximations for:

- PDF: $f(\vartheta) = F'(\vartheta) = (1 \tau)\Phi''(\vartheta)$
- τ -quantile: $q_{\tau} = \inf\{\vartheta \colon F(\vartheta) \ge \tau\} = \arg\min_{\vartheta \in \mathbb{R}} \Phi(\vartheta)$
- Conditional Value at Risk: $\text{CVaR}_{\tau} = \frac{1}{1-\tau} \int_{q_{\tau}}^{\infty} \vartheta \, dF(\vartheta) = \min_{\vartheta \in \mathbb{R}} \Phi(\vartheta)$



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Interpolation approach (e.g., splines or polynomials):

- introduce grid $\boldsymbol{\theta} = (\theta_1, \dots, \theta_n) \subset \Theta$
- compute MLMC estimate Φ^{MLMC}_L(θ_j) of Φ(θ_j), j = 1,..., n (same samples of Q_ℓ for every θ_j)
- interpolate values $\Phi_{L}^{\text{MLMC}}(\boldsymbol{\theta}) = (\Phi_{L}^{\text{MLMC}}(\theta_{j}))_{j=1}^{n}$: $\hat{\Phi}_{L} = \mathcal{I}_{n}(\Phi_{L}^{\text{MLMC}}(\boldsymbol{\theta}))$



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Exemplary **a-priori properties** for Spline interpolation \mathcal{I}_n :

$$\begin{aligned} & \left\| f^{(m)} - \frac{d^m}{d\vartheta^m} \mathcal{I}_n(f(\theta)) \right\|_{L^{\infty}} \leq c_1 n^{m-(k+1)}, \text{ for any } f \in C^{k+1}(\bar{\Theta}), \, m \leq k \\ & \left\| \mathcal{I}_n(\mathbf{x}) \right\|_{L^{\infty}} \leq c_2 \|\mathbf{x}\|_{\ell^{\infty}}, \text{ for any } \mathbf{x} \in \mathbb{R}^n \\ & \quad \operatorname{cost}(\mathcal{I}_n(\mathbf{x})) \leq c_3 n, \, \mathbf{x} \in \mathbb{R}^n \\ & \quad \left\| \frac{d^m}{d\vartheta^m} \mathcal{I}_n(\mathbf{x}) \right\|_{L^{\infty}} \leq c_5 (n-1)^m \| \mathcal{I}_n(\mathbf{x}) \|_{L^{\infty}}, \, \mathbf{x} \in \mathbb{R}^n, \, m \geq 1 \text{ (inverse inequality)} \end{aligned}$$



Measure accuracy in terms of mean squared error:

$$\mathsf{MSE}(\hat{\Phi}_L^{(m)}) := \mathbb{E}\Big(\left\| \hat{\Phi}_L^{(m)} - \Phi^{(m)} \right\|_{L^\infty}^2 \Big) \;, \quad m \in \mathbb{N}_0 \;, \qquad L^\infty \equiv L^\infty(\Theta)$$



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$$\mathsf{MSE}(\hat{\Phi}_{L}^{(m)}) \leq 3 \underbrace{\left\| \Phi^{(m)} - \mathcal{I}_{n}^{(m)}(\Phi) \right\|_{L^{\infty}}^{2}}_{squared interpolation error} + 3 \underbrace{\left\| \mathcal{I}_{n}^{(m)}(\Phi - \Phi_{L}) \right\|_{L^{\infty}}^{2}}_{squared bias} + 3 \underbrace{\mathbb{E}\left(\left\| \mathcal{I}_{n}^{(m)}(\Phi_{L} - \Phi_{L}^{\mathsf{MLMC}}) \right\|_{L^{\infty}}^{2} \right)}_{stat. \ error}$$



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- Notation: $\operatorname{Var}(\boldsymbol{\xi}) = \mathbb{E}(\|\boldsymbol{\xi} \mathbb{E}(\boldsymbol{\xi})\|_{\ell^{\infty}}^2)$, for any r.v. $\boldsymbol{\xi}$ with values in \mathbb{R}^n
- Useful technical result: let $(\boldsymbol{\xi}^{(1)}, \dots, \boldsymbol{\xi}^{(N)}) \subset \mathbb{R}^n$ independent, then

$$\operatorname{Var}\left(\sum_{i=1}^{N} \boldsymbol{\xi}^{(i)}\right) \leq c \ln(n) \sum_{i=1}^{N} \operatorname{Var}\left(\boldsymbol{\xi}^{(i)}\right)$$

Theorem: A-priori MSE complexity ($h_{\ell-1}/h_{\ell} = s > 1$) for Spline interpolation [K., Nobile. 2018]

Suppose that: • $\sup_{\vartheta \in \Theta} |\Phi(\vartheta) - \mathbb{E}(\phi(\vartheta, Q_l))| = \mathcal{O}(h_l^{\alpha})$

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$$\mathbb{E}\left(\left\|\phi(\cdot, Q_l) - \phi(\cdot, Q_{l-1})\right\|_{L^{\infty}(\Theta)}^2\right) = \mathcal{O}(h_l^{\beta}),$$

• cost for each $(Q_{\ell}^{(i,\ell)}, Q_{\ell-1}^{(i,\ell)}) = \mathcal{O}(h_{\ell}^{-\gamma})$

Let m = 0. If $\Phi \in C^{k+1}(\Theta)$ and $2\alpha \ge \min\{\beta, \gamma\}$, then there exists an MLMC estimator $\hat{\Phi}_L$ of Φ such that $MSE(\hat{\Phi}_L) = \mathcal{O}(\varepsilon^2)$ with

$$\text{comp. cost} \lesssim \varepsilon^{-\left(2+\frac{1}{k+1}\right)} |\ln(\varepsilon)| + |\ln(\varepsilon)| \begin{cases} \varepsilon^{-2} , & \beta > \gamma , \\ \varepsilon^{-2} \ln(\varepsilon)^2 , & \beta = \gamma , \\ \varepsilon^{-\left(2+\frac{\gamma-\beta}{\alpha}\right)} , & \beta < \gamma . \end{cases}$$

■ NB: first term accounts for cost of computing interpolation: negligible for heavy computational models; systematically removable by n = n_ℓ (different interpolation grid on each level; Cor. 2.3 in [K., Nobile. 2018]).

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- **NB:** first term accounts for cost of computing interpolation: negligible for heavy computational models; systematically removable by $n = n_{\ell}$ (different interpolation grid on each level; Cor. 2.3 in [K., Nobile. 2018]).
- Neglecting first term: complexity is the same as for expectations, up to extra log factor.

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$$\mathbb{E}\left(\left\|\phi(\cdot, Q_l) - \phi(\cdot, Q_{l-1})\right\|_{L^{\infty}(\Theta)}^2\right) = \mathcal{O}(h_l^{\beta}),$$

• cost for each $(Q_{\ell}^{(i,\ell)}, Q_{\ell-1}^{(i,\ell)}) = \mathcal{O}(h_{\ell}^{-\gamma})$

Let m = 0. If $\Phi \in C^{k+1}(\Theta)$ and $2\alpha \ge \min\{\beta, \gamma\}$, then there exists an MLMC estimator $\hat{\Phi}_L$ of Φ such that $MSE(\hat{\Phi}_L) = \mathcal{O}(\varepsilon^2)$ with

$$\text{comp. cost} \lesssim \varepsilon^{-\left(2+\frac{1}{k+1}\right)} |\ln(\varepsilon)| + |\ln(\varepsilon)| \begin{cases} \varepsilon^{-2} , & \beta > \gamma , \\ \varepsilon^{-2} \ln(\varepsilon)^2 , & \beta = \gamma , \\ \varepsilon^{-\left(2+\frac{\gamma-\beta}{\alpha}\right)} , & \beta < \gamma . \end{cases}$$

- **NB:** first term accounts for cost of computing interpolation: negligible for heavy computational models; systematically removable by $n = n_{\ell}$ (different interpolation grid on each level; Cor. 2.3 in [K., Nobile. 2018]).
- Neglecting first term: complexity is the same as for expectations, up to extra log factor.
- Similar complexity for Φ analytic and using an interpolation in global polynomials:

$$\begin{array}{ll} {\rm comp.\ cost} \lesssim \varepsilon^{-2} |\ln(\varepsilon)|^4 + |\ln(\varepsilon)|^3 \begin{cases} \varepsilon^{-2} \ , & \beta > \gamma \ , \\ \varepsilon^{-2} \ln(\varepsilon)^2 \ , & \beta = \gamma \ , \\ \varepsilon^{-(2+\frac{\gamma-\beta}{\alpha})} |\ln(\varepsilon)|^{\frac{\gamma-\beta}{\alpha}} \ , & \beta < \gamma \ . \end{cases}$$

Theorem (cont.)

If $\Phi \in C^{k+1}(\Theta)$ and $m \leq k$, then there exists $\hat{\Phi}_L$ such that $MSE(\hat{\Phi}_L^{(m)}) = \mathcal{O}(\varepsilon^2)$:

$$\begin{array}{ll} \text{comp. cost (no interp. cost)} \lesssim |\ln(\varepsilon)| \begin{cases} \varepsilon^{-2\frac{k+1}{k+1-m}}, & \beta > \gamma \ , \\ \varepsilon^{-2\frac{k+1}{k+1-m}} \ln(\varepsilon)^2 \ , & \beta = \gamma \ , \\ \varepsilon^{-\left(2+\frac{\gamma-\beta}{\alpha}\right)\frac{k+1}{k+1-m}}, & \beta < \gamma \ . \end{cases}$$

• Result applies to the approximation of CDF, quantiles and CVaR with m = 1, and with m = 2 for the PDF.

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Result applies to the approximation of CDF, quantiles and CVaR with *m* = 1, and with *m* = 2 for the PDF.
 Again, a similar complexity result is available for Φ analytic:

$$\begin{array}{l} \operatorname{comp. cost} \lesssim \varepsilon^{-2} |\ln(\varepsilon)|^{4(1+m)} + |\ln(\varepsilon)|^{3+4m} \begin{cases} \varepsilon^{-2} , & \beta > \gamma , \\ \varepsilon^{-2} \ln(\varepsilon)^2 , & \beta = \gamma , \\ \varepsilon^{-\left(2 + \frac{\gamma - \beta}{\alpha}\right)} |\ln(\varepsilon)|^{\frac{\gamma - \beta}{\alpha}} (1 + 2m) , & \beta < \gamma . \end{cases}$$

MLMC for CDF, quantile, and CVaR: error control



Recall that key quantities such as the CDF, quantile, and CVaR are all derived from the function

$$\Phi(\vartheta) = \mathbb{E}ig(\phi(artheta, oldsymbol{Q})ig) \quad ext{for} \quad \phi(artheta, oldsymbol{Q}) = artheta + rac{1}{1- au}(oldsymbol{Q} - artheta)^+.$$

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Corollary

For $\tau \in (0, 1)$, let $\hat{\Phi}$ be the MLMC estimator of $\Phi \in C^{k+1}(\Theta)$, $k \ge 1 = m$, so that $MSE(\hat{\Phi}') = \mathcal{O}(\varepsilon^2)$. If the true τ -quantile is an interior point of Θ , then

max{quantile MSE, CVaR MSE, unif. CDF MSE} = $\mathcal{O}(\varepsilon^2)$,

at a cost dominated by $cost(\hat{\Phi}') = cost(CDF \text{ est.}).$

Corollary provides an all-at-once approach for the simultaneous approximation of CDF, quantiles, and CVaR.

Toy example: the characteristic function



Let's consider the toy model to describe a European call option again, i.e., asset follows

$$dS = rS dt + \sigma S dW$$
, $S(0) = S_0$,

• Quantity of interest is the discounted "payoff": $Q := e^{-rT} \max(S(T) - K, 0)$

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- **But**: *Q* has a *mixed distribution*, in the sense that $\mathbb{P}(Q = 0) > 0$.
- Consequently, its CDF $F_Q := \mathbb{E}(I(Q \le \cdot))$ has a jump discontinuity at the origin:

 \rightsquigarrow we **cannot** guarantee a uniformly accurate MLMC CDF-approximation, if $0 \in \Theta$.

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But we can guarantee an accurate MLMC approximation of the characteristic function to characterize probability distribution of Q:

$$\varphi_{Q}(\vartheta) = \mathbb{E}(\underbrace{\cos(\vartheta Q)}_{=:\phi_{1}(\vartheta,Q)}) + i \mathbb{E}(\underbrace{\sin(\vartheta Q)}_{=:\phi_{2}(\vartheta,Q)}) \equiv \Phi_{1}(\vartheta) + i \Phi_{2}(\vartheta) ,$$

NB: functions φ_i are smooth, no derivatives required (i.e., m = 0), moment approximations via post-processing possible [K., Nobile. 2018].

• Milstein scheme with $h_{\ell} = 2^{-\ell}T$; $\Theta = [-1, 1]$, $r = \frac{1}{20}$, $\sigma = \frac{1}{5}$, T = 1, $K = 10 = S_0$.



Karlsruhe Institute of Technology

PDE toy example

Consider a simple Poisson equation

$$-\Delta u = f , \quad \text{in } D = (0,1)^2 ,$$

with homogeneous Dirichlet boundary conditions and random forcing term *f* given by $f(x) = -72\xi(x_1^2 + x_2^2 - x_1 - x_2), \xi \sim \chi_1^2$. Quantity of interest: $Q := \int_D u \, dx = \xi$.

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We approximate $\Phi(\vartheta) = \vartheta + \frac{1}{1-\tau}\mathbb{E}[(Q-\vartheta)^+]$ with $\tau = 0.95$ on $\vartheta \in \Theta = [0, 10]$ for $k = 3 \rightsquigarrow$ theory predicts $\cot \theta = \mathcal{O}(\varepsilon^{-2.3} \ln(\varepsilon^{-1}))$, appears to be conservative.



Practical bottleneck: a-priori bounds



Asymptotic complexity analysis is based on a-priori upper bounds for error estimates:

$$\frac{\mathsf{MSE}(\hat{\Phi}_{L}^{(m)})}{3} \leq \left\|\Phi^{(m)} - \mathcal{I}_{n}^{(m)}(\Phi)\right\|_{L^{\infty}}^{2} + \left\|\mathcal{I}_{n}^{(m)}(\Phi - \Phi_{L})\right\|_{L^{\infty}}^{2} + \mathbb{E}\left(\left\|\mathcal{I}_{n}^{(m)}(\Phi_{L} - \Phi_{L}^{\mathsf{MLMC}})\right\|_{L^{\infty}}^{2}\right)$$
$$\leq C_{1}(m)^{2}n^{-2(k+1-m)} + C_{2}(m)^{2}(n-1)^{2m}b_{L}^{2} + C_{2}(m)^{2}(n-1)^{2m}\log(n)\sum_{\ell=0}^{L}\frac{V_{\ell}}{N_{\ell}}$$

where $b_L = \|\Phi(\theta) - \Phi_L(\theta)\|_{\ell^{\infty}}$ and $V_\ell = \operatorname{Var}(\phi(\theta, Q_\ell) - \phi(\theta, Q_{\ell-1}))$.

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In particular, the *inverse inequality* makes error bound severely conservative. For example, the bias decay:





Refined a-posterior error estimators I: bias



- Starting point: derive error estimators based on *first error splitting* directly:
- Simplifications: interpolation in cubic Splines

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- Error estimator for bias via bivariate kernel smoothing of empirical measure of (Q_L, Q_{L-1}):

$$\begin{aligned} \left\|\mathcal{I}_{n}^{(m)}(\Phi-\Phi_{L})\right\|_{L^{\infty}}^{2} &\approx \frac{1}{s^{\alpha}-1} \left\|\mathcal{I}_{n}^{(m)}(\mathbb{E}(\phi_{L}-\phi_{L-1}))\right\|_{L^{\infty}} \\ \mathcal{I}_{n}^{(m)}(\mathbb{E}(\phi_{L}-\phi_{L-1}))\right\|_{L^{\infty}} &\approx \left\|\mathcal{I}_{n}^{(m)}(\mathbb{E}^{\mathsf{kde}}(\phi_{L}-\phi_{L-1})))\right\|_{L^{\infty}} \end{aligned}$$

where the *bivariate KDE approximates* the joint PDF of $(Q_{\ell}, Q_{\ell-1})$ using the N_{ℓ} correlated samples.

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A-posteriori bias error estimation:



Refined a-posterior error estimators II: statistical error

Idea: Statistical error estimator via bootstrapping MLMC estimators:

• "Observation": an MLMC estimator is defined through the hierarchy of samples

$$\left\{\{Q_{\ell}^{(i,\ell)}, Q_{\ell-1}^{(i,\ell)}\}_{i=1}^{N_{\ell}}\right\}_{\ell=0}^{L}$$

• Bootstrap principle: resample $N_{bs} \gg 1$ "new" MLMC estimators Ψ_j

$$\mathbb{E}\big(\big\|\mathcal{I}_n^{(m)}(\Phi_L - \Phi_L^{\texttt{MLMC}})\big\|_{L^\infty}^2\big) \approx \frac{1}{N_{\texttt{bs}}} \sum_{j=1}^{N_{\texttt{bs}}} \big\|\mathcal{I}_n^{(m)}(\Psi_j(\theta) - \bar{\Psi}(\theta)\big\|_{L^\infty}^2$$

A-posteriori statistical error estimation:





Implication for an (adaptive) MLMC implementation



• A-priori bounds yield error estimator that is convenient for an (adaptive) implementation:

$$\mathbb{E}\big(\left\|\mathcal{I}_{n}^{(m)}(\Phi_{L}-\Phi_{L}^{\mathsf{MLMC}})\right\|_{L^{\infty}}^{2}\big) \leq K(n,m)\sum_{\ell=0}^{L}\frac{V_{\ell}}{N_{\ell}} \approx K(n,m)\sum_{\ell=0}^{L}\frac{\hat{V}_{\ell}}{N_{\ell}}$$

The a-posterior error bound does not provide level-wise errors

$$\mathbb{E}\big(\left\|\mathcal{I}_{n}^{(m)}(\Phi_{L}-\Phi_{L}^{\text{MLMC}})\right\|_{L^{\infty}}^{2}\big)\approx\frac{1}{N_{\text{bs}}}\sum_{j=1}^{N_{\text{bs}}}\left\|\mathcal{I}_{n}^{(m)}(\Psi_{j}(\theta)-\bar{\Psi}(\theta)\right\|_{L^{\infty}}^{2}=:\left(\hat{\boldsymbol{e}}_{a-\text{post}}^{(m)}\right)^{2}$$

• Rescaling idea: we aim for redefined levelwise variances \tilde{V}_{ℓ} such that $\left(\hat{e}_{a-post}^{(m)}\right)^2 = \sum_{\ell=0}^{L} \frac{\tilde{V}_{\ell}}{N_{\ell}}$

Lemma

There exist positive constants $\mathfrak{K}_1(n)$ and $\mathfrak{K}_2(n)$: $\mathfrak{K}_1(n) \sum_{\ell=0}^{L} \frac{V_\ell}{N_\ell} \leq \sum_{m=0}^{2} k_m \left(\hat{e}_{exact}^{(m)}\right)^2 \leq \mathfrak{K}_2(n) \sum_{\ell=0}^{L} \frac{V_\ell}{N_\ell}$

1

Rescaling heuristic:
$$\tilde{V}_{\ell} = r_e \hat{V}_{\ell}$$
, $r_e = rac{\sum_{k=0}^{2} k_m \left(\hat{e}_{k\text{-post}}^{(m)} \right)}{\sum_{k=0}^{L} \hat{V}_k / N_k}$

Computational Example



In [Ayoul-Guilmarda, Ganesh, K., Nobile. 2023] we combine these with an adaptive, *continuation MLMC framework* for an efficient implementation (Python library XMC) that can be tuned to target CDF, VaR, or CVaR.

Computational Example



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Example: (steady incompressible) Navier-Stokes Flow over a Cylinder in a Channel



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24/25 DA Days 2023 Sebastian Krumscheid: MLMC for Parametric Expectations

Take home message:

- we introduced a uniformly accurate MLMC estimator for a parametric expectation and its derivatives
- the approach enables approximating the characteristic function as well as CDF, PDF, VaR, and CVaR
- refined, a-posterior error estimates are required for computationally "heavy" problems when derivatives are required.

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- the approach enables approximating the characteristic function as well as CDF, PDF, VaR, and CVaR
- refined, a-posterior error estimates are required for computationally "heavy" problems when derivatives are required.

Thank you for your attention.

Further details:

SK and F. Nobile. Multilevel Monte Carlo Approximation of Functions. *SIAM/ASA J. Uncertain. Quantif.*, **3**(6):1256–1293, 2018.

Q. Ayoul-Guilmard, S. Ganesh, SK, and F. Nobile. Quantifying uncertain system outputs via the multi-level Monte Carlo method – distribution and robustness measures. *Int. J. Uncertain. Quantif.*, **13**(5):61–98, 2023.