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Uncertainty Quantification

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

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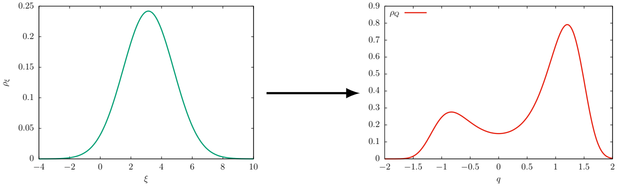
joint work with: Q. Ayoul-Guilmard, S. Ganesh, and F. Nobile

Forward propagation of Uncertainties

random input: ξ $\longrightarrow$ Model $\longrightarrow$ quantity of interest: $Q \equiv Q(\xi)$

- Random input parameters ξ, possibly infinite dimensional
- **Model**: for ξ given, find u s.t. $\mathcal{M}_{\xi}(u) = 0 \rightsquigarrow$ **Quantity of interest:** $Q(\xi) = Q\big(u(\xi)\big)$



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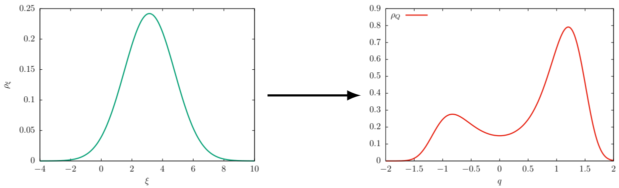

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Model ↓ approximations

computational Model → $Q_h \equiv Q_h(\boldsymbol{\xi})$

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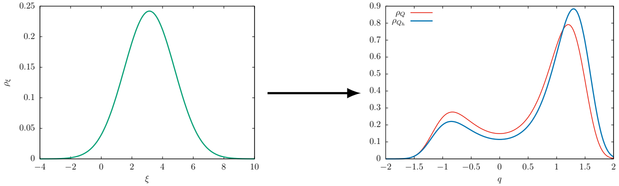

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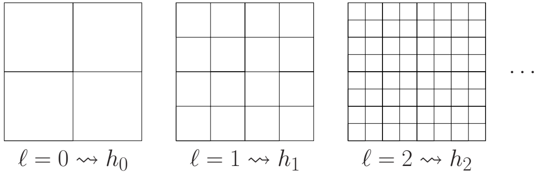
Multilevel Monte Carlo for expected values

- **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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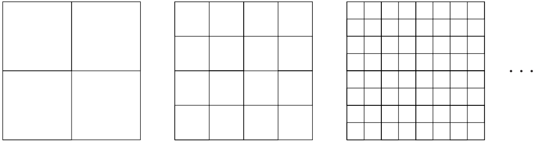

$\ell = 0 \rightsquigarrow h_0$ $\quad$ $\ell = 1 \rightsquigarrow h_1$ $\quad$ $\ell = 2 \rightsquigarrow h_2$

- 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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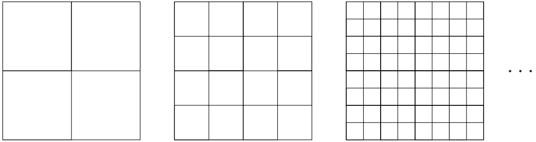

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- MSE accuracy of multilevel Monte Carlo method is

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

- 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:
- $\left|\mathbb{E}(Q - Q_\ell)\right| = \mathcal{O}(h_\ell{}^\alpha)$,
- $\mathrm{Var}(Q_\ell - Q_{\ell-1}) = \mathcal{O}(h_\ell{}^\beta)$,
- $C_\ell = \mathcal{O}(h_\ell{}^{-\gamma})$.

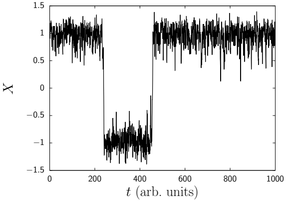
If $2\alpha \geq \min\{\beta, \gamma\}$, then there exists an MLMC estimator $\hat{Q}_{N,L}$ that satisfies MSE $\leq \varepsilon^2$ with

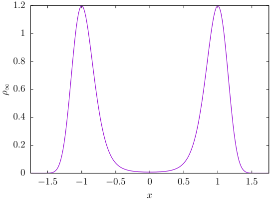
$$\text{comp. cost MLMC} = \sum_{\ell=1}^{L} N_\ell C_\ell \lesssim \begin{cases} \varepsilon^{-2}\,, & \beta > \gamma\,, \\ \varepsilon^{-2} \ln(\varepsilon)^2\,, & \beta = \gamma\,, \\ \varepsilon^{-\left(2+\frac{\gamma-\beta}{\alpha}\right)}\,, & \beta < \gamma\,. \end{cases}$$

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

Assessing the distribution beyond moments

- Expectation is a **good starting point**, but we would like more: **assessing the distribution**





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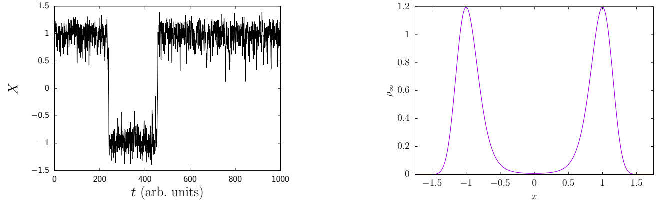

- One could estimate central moments of arbitrary order

$$\mu_p(Q) := \mathbb{E}\left[\left(Q - \mathbb{E}(Q)\right)^p\right], \quad p \in \mathbb{N}$$

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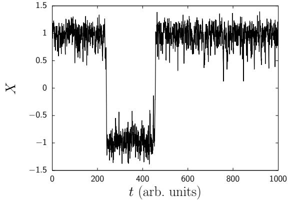

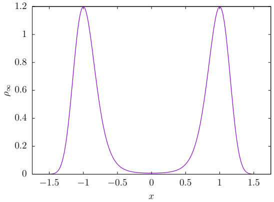

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- However, some applications require techniques that systematically go **beyond using a few moments**: characterization of entire distribution or applications in risk averse optimization, e.g., involving quantiles.

Parametric Expectations

- Many such distributional assessments are related to **parametric expectations** of the form

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Examples:

1. **Mean & variance**: $\phi(\vartheta, Q) = (Q - \vartheta)^2 \rightsquigarrow \mathrm{Var}\,(Q) = \min_\vartheta \Phi(\vartheta), \mathbb{E}(Q) = \arg\min_\vartheta \Phi(\vartheta)$
1. **Characteristic function** of Q: $\phi(\vartheta, Q) = e^{i\vartheta Q} = \cos(\vartheta Q) + i\sin(\vartheta Q)$
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Difficulty for CDF: $\phi(\vartheta, \cdot)$ is **discontinuous**! Consequently, the variance $\mathrm{Var}\,\big(\phi(\theta_j, Q_\ell) - \phi(\theta_j, Q_{\ell-1})\big)$ 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 $\Phi(\vartheta) = \mathbb{E}\big(\phi(\vartheta, Q)\big) \approx \mathbb{E}\big(\phi_\delta(\vartheta, Q)\big)$ [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]

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

$$\Phi(\vartheta) = \mathbb{E}\big(\phi(\vartheta, Q)\big) \ , \quad \phi(\vartheta, Q) = \vartheta + \frac{1}{1-\tau}(Q - \vartheta)^{+} \ .$$

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:

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- τ-quantile: $q_\tau = \inf\{\vartheta \colon F(\vartheta) \geq \tau\} = \arg\min_{\vartheta \in \mathbb{R}} \Phi(\vartheta)$
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MLMC method for parametric expectations

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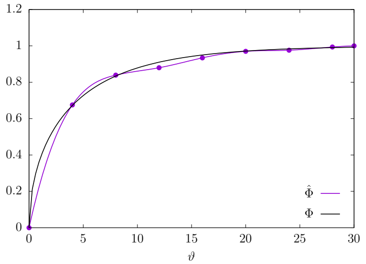

Interpolation approach (e.g., splines or polynomials):

- introduce grid $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_n) \subset \Theta$
- compute MLMC estimate $\Phi_L^{\mathrm{MLMC}}(\theta_j)$ of $\Phi(\theta_j)$, $j = 1, \ldots, n$ (same samples of Q_ℓ for every θ_j)
- interpolate values $\Phi_L^{\mathrm{MLMC}}(\boldsymbol{\theta}) = \big(\Phi_L^{\mathrm{MLMC}}(\theta_j)\big)_{j=1}^n$:
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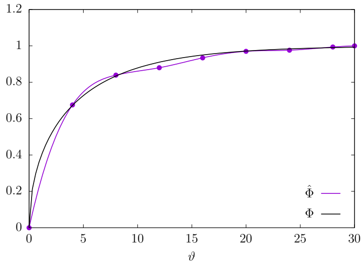

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Exemplary **a-priori properties** for Spline interpolation $\mathcal{I}_n$:

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

Complexity Analysis

- Measure accuracy in terms of mean squared error:

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

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- Using the notation $\Phi_L = \mathbb{E}\big(\phi(\cdot, Q_L)\big)$, the MSE can be decomposed as:

$$\mathrm{MSE}\big(\hat{\Phi}_L^{(m)}\big) \leq 3 \underbrace{\big\|\Phi^{(m)} - \mathcal{I}_n^{(m)}(\Phi)\big\|_{L^\infty}^2}_{\text{squared interpolation error}} + 3 \underbrace{\big\|\mathcal{I}_n^{(m)}(\Phi - \Phi_L)\big\|_{L^\infty}^2}_{\text{squared bias}} + 3 \underbrace{\mathbb{E}\big(\big\|\mathcal{I}_n^{(m)}(\Phi_L - \Phi_L^{\mathtt{MLMC}})\big\|_{L^\infty}^2\big)}_{\text{stat. error}}$$

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

$$\mathrm{Var}\Big(\sum_{i=1}^N \xi^{(i)}\Big) \leq c\ln(n) \sum_{i=1}^N \mathrm{Var}\big(\xi^{(i)}\big)$$

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

Suppose that:

- $\sup_{\vartheta\in\Theta}\left|\Phi(\vartheta) - \mathbb{E}\big(\phi(\vartheta, Q_l)\big)\right| = \mathcal{O}({h_l}^{\alpha})$
- $\mathbb{E}\Big(\big\|\phi(\cdot, Q_l) - \phi(\cdot, Q_{l-1})\big\|^2_{L^\infty(\Theta)}\Big) = \mathcal{O}({h_l}^{\beta})$,
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Let $m = 0$. If $\Phi \in C^{k+1}(\Theta)$ and $2\alpha \geq \min\{\beta, \gamma\}$, then there exists an MLMC estimator $\hat{\Phi}_L$ of Φ such that $\mathrm{MSE}\big(\hat{\Phi}_L\big) = \mathcal{O}(\varepsilon^2)$ with

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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]).

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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.

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

Suppose that:

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

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

Theorem (cont.)

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

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

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

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- Again, a similar complexity result is available for Φ analytic:

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

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

$$\Phi(\vartheta) = \mathbb{E}\big(\phi(\vartheta, Q)\big) \quad \text{for} \quad \phi(\vartheta, Q) = \vartheta + \frac{1}{1-\tau}(Q - \vartheta)^+ .$$

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Corollary

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

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

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

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

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

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

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Karlsruhe Institute of Technology

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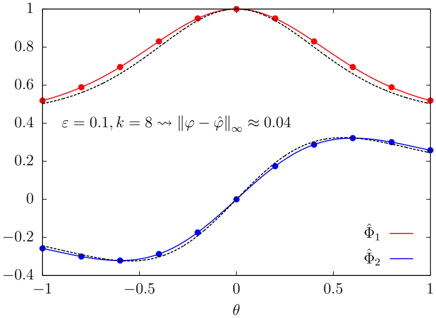
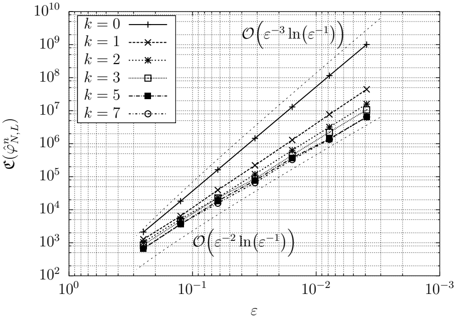
  $\rightsquigarrow$ we **cannot** guarantee a uniformly accurate MLMC CDF-approximation, if $0 \in \Theta$.
- But we **can** guarantee an accurate MLMC approximation of the **characteristic function** to characterize probability distribution of Q:

$$\varphi_Q(\vartheta) = \mathbb{E}\big(\underbrace{\cos(\vartheta Q)}_{=:\phi_1(\vartheta,Q)}\big) + \mathrm{i}\,\mathbb{E}\big(\underbrace{\sin(\vartheta Q)}_{=:\phi_2(\vartheta,Q)}\big) \equiv \Phi_1(\vartheta) + \mathrm{i}\,\Phi_2(\vartheta)\ ,$$

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





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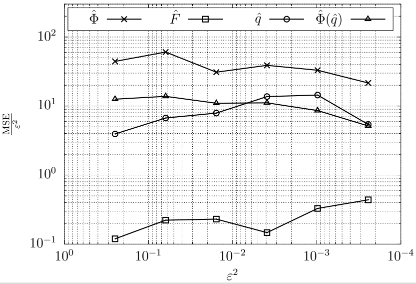
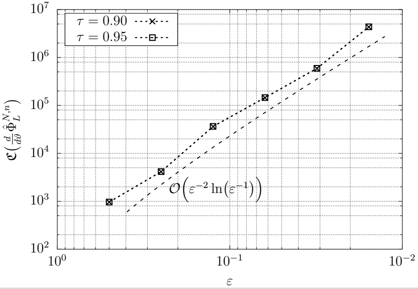
We approximate $\Phi(\vartheta) = \vartheta + \frac{1}{1-\tau}\mathbb{E}\left[(Q-\vartheta)^+\right]$ with $\tau = 0.95$ on $\vartheta \in \Theta = [0,10]$ for $k = 3 \rightsquigarrow$ theory predicts cost $= \mathcal{O}\left(\varepsilon^{-2.3}\ln(\varepsilon^{-1})\right)$, appears to be conservative.





Practical bottleneck: a-priori bounds

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

$$\frac{\mathrm{MSE}\big(\hat{\Phi}_L^{(m)}\big)}{3} \leq \big\|\Phi^{(m)} - \mathcal{I}_n^{(m)}(\Phi)\big\|_{L^\infty}^2 + \big\|\mathcal{I}_n^{(m)}(\Phi - \Phi_L)\big\|_{L^\infty}^2 + \mathbb{E}\Big(\big\|\mathcal{I}_n^{(m)}(\Phi_L - \Phi_L^{\mathtt{MLMC}})\big\|_{L^\infty}^2\Big)$$

$$\lesssim C_1(m)^2 n^{-2(k+1-m)} + C_2(m)^2 (n-1)^{2m} b_L{}^2 + C_2(m)^2 (n-1)^{2m} \log(n) \sum_{\ell=0}^{L} \frac{V_\ell}{N_\ell}$$

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

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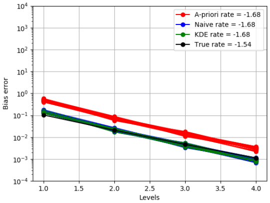
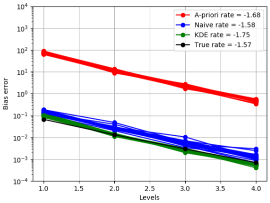
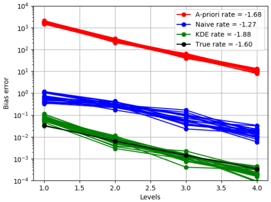
In particular, the *inverse inequality* makes error bound **severely conservative**. For example, the bias decay:



$m = 0$



$m = 1$



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Refined a-posterior error estimators

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}):

$$\left\|\mathcal{I}_n^{(m)}(\Phi - \Phi_L)\right\|_{L^\infty}^2 \approx \frac{1}{s^\alpha - 1}\left\|\mathcal{I}_n^{(m)}(\mathbb{E}(\phi_L - \phi_{L-1}))\right\|_{L^\infty}$$

$$\left\|\mathcal{I}_n^{(m)}(\mathbb{E}(\phi_L - \phi_{L-1}))\right\|_{L^\infty} \approx \left\|\mathcal{I}_n^{(m)}\left(\mathbb{E}^{\text{kde}}\left(\phi_L - \phi_{L-1}\right)\right)\right\|_{L^\infty}$$

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

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  where the *bivariate KDE approximates* the joint PDF of $(Q_\ell, Q_{\ell-1})$ using the N_ℓ correlated samples.
- **Error estimator for statistical error via bootstrapping MLMC estimators**:
  - "Observation": an MLMC estimator is defined through the hierarchy of samples

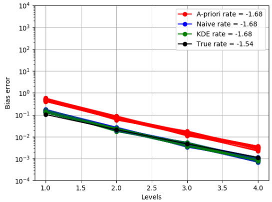
$$\left\{\left\{Q_\ell^{(i,\ell)}, Q_{\ell-1}^{(i,\ell)}\right\}_{i=1}^{N_\ell}\right\}_{\ell=0}^{L}$$

  - Idea: resample $N_{\text{bs}} \gg 1$ "new" MLMC estimators Ψ_j

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

Effects of refined a-posterior error estimators

Bias estimation:



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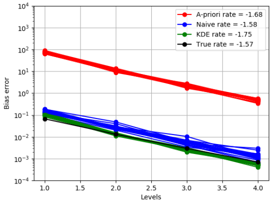

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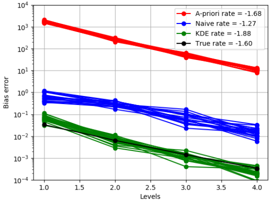

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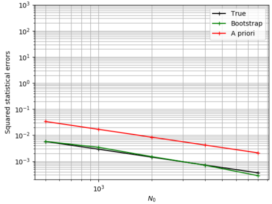
Estimation of statistical error:



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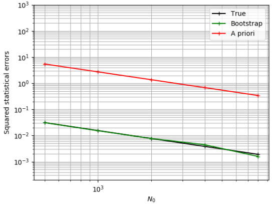

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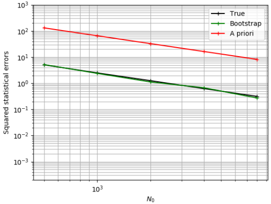

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Computational Example

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.

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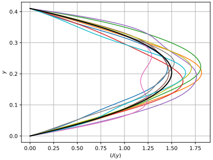
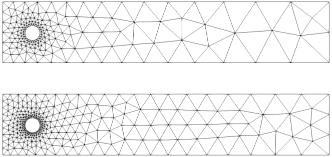
Example: (steady incompressible) Navier-Stokes Flow over a Cylinder in a Channel





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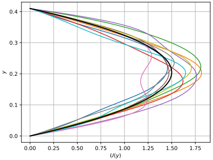

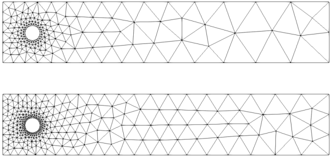

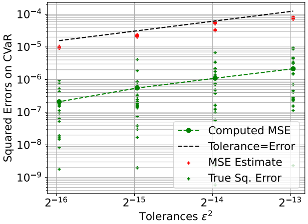

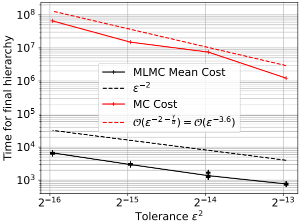

Take home message:

- 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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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.

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