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Scientific Computing
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Technical University of Munich

Multilevel Monte Carlo estimators for derivative-free optimization under uncertainty

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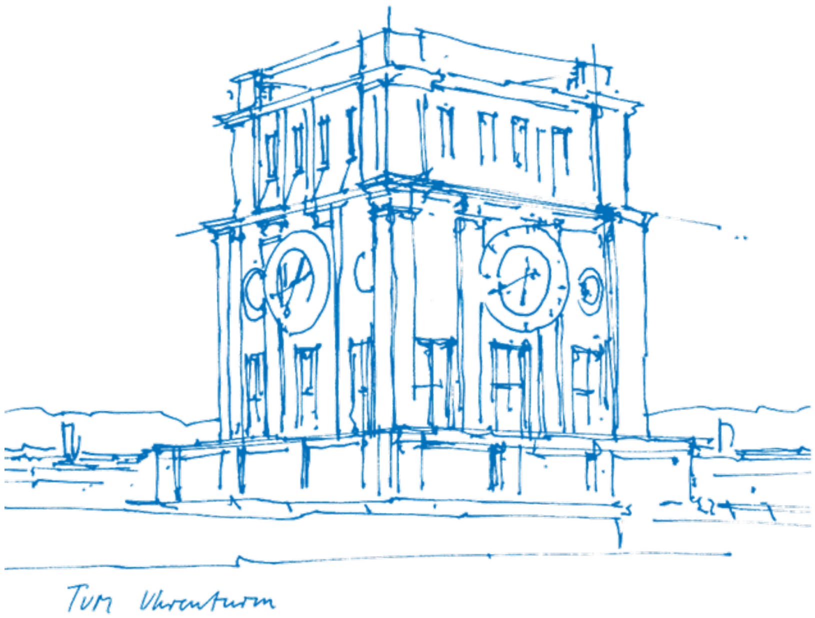
MS82

PDE-Constrained Optimization Under Uncertainty

April 13th, 2022



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Motivation

Robustness in OUU:

$$\min_x \mathscr{R}_{\text{Mean}} = \min_x \mathbb{E}[Q(x,\theta)]$$

Reliability in OUU:

$$\min_x \mathscr{R}_{\text{Scalar}} = \min_x \mathbb{E}[Q(x,\theta)] + \alpha\sigma[Q(x,\theta)]$$

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Solve using derivative-free optimization method SNOWPAC*

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BUT: Monte Carlo is very expensive ($\mathscr{O}(\frac{1}{\sqrt{N}})$)

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BUT: Original MLMC estimator not sufficient for $\mathscr{R}_{\text{Scalar}}$ formulation

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$\Rightarrow$ Need MLMC estimators for higher order moments

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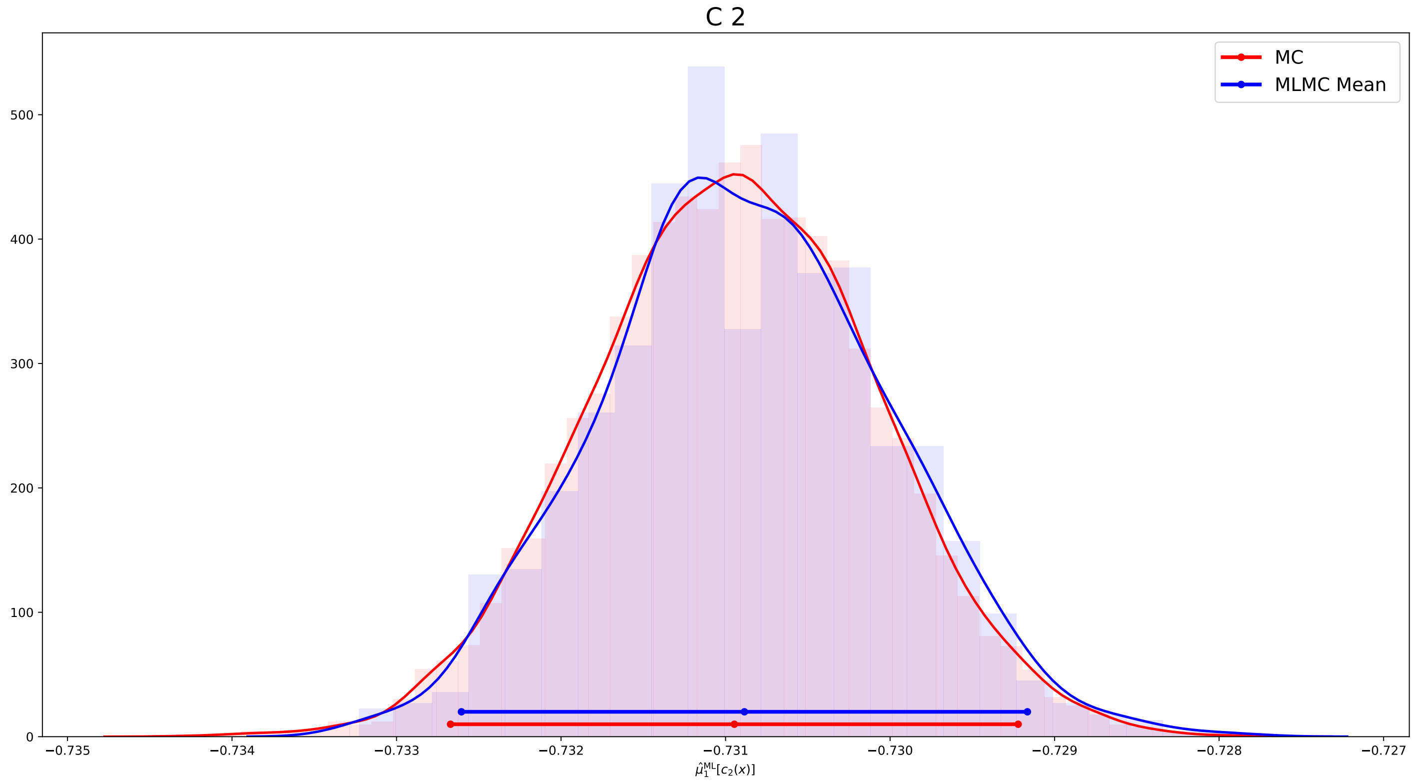
Motivation: Example

MLMC mean estimator for $\mathscr{R}_{\text{Mean}} \approx \widehat{\mu_1^{\text{ML}}}[Q(x,\theta)]$



- Good match between standard MC estimator and MLMC.

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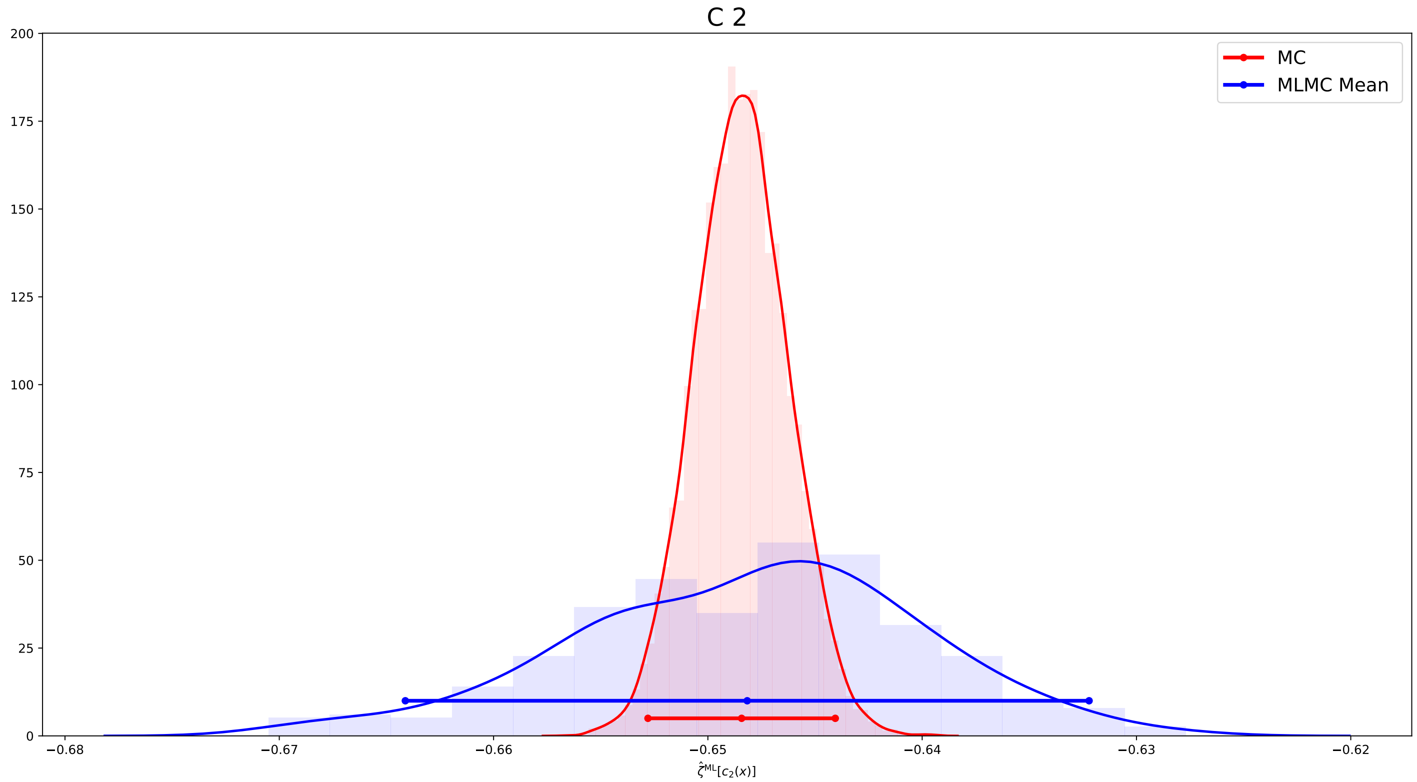
Motivation: Example

MLMC mean estimator for $\mathscr{R}_{\text{Scalar}} \approx \widehat{\mu_1^{\text{ML}}}[Q(x,\theta)] + \alpha\widehat{\sigma_{\text{biased}}^{\text{ML}}}[Q(x,\theta)]$



- MLMC estimator targeting the mean underestimates compared to MC.

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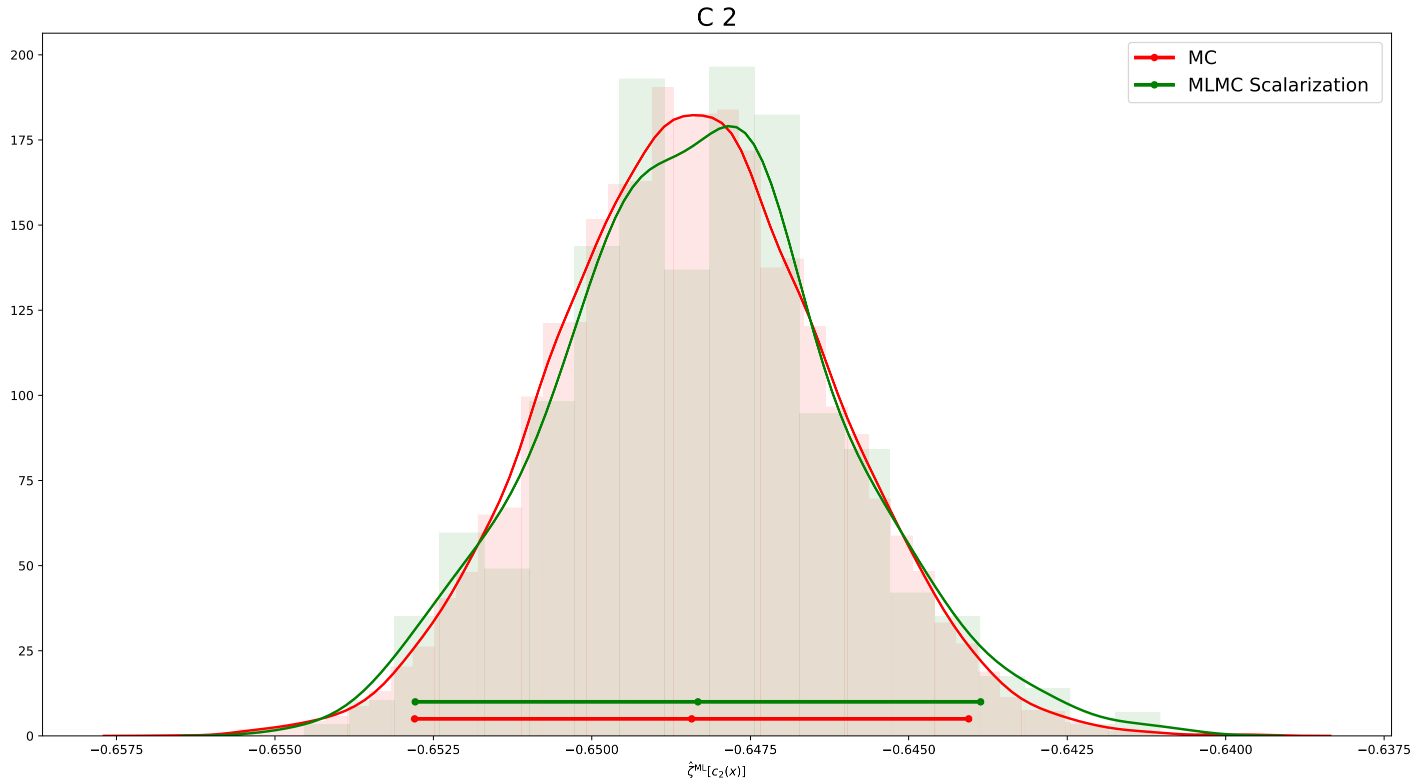
Motivation: Goal

MLMC scalarization estimator for $\mathscr{R}_{\text{Scalar}} \approx \widehat{\mu_1^{\text{ML}}}[Q(x,\theta)] + \alpha\widehat{\sigma_{\text{biased}}^{\text{ML}}}[Q(x,\theta)]$



- New MLMC estimator targeting the scalarization matches MC.

Up next:

Mean in OUU:

$$\min_x \mathscr{R}_{\text{Mean}} \approx \min_x \widehat{\mu_1^{\text{ML}}}[Q(x,\theta)]$$

Scalarization in OUU:

$$\min_x \mathscr{R}_{\text{Scalar}} \approx \min_x \widehat{\mu_1^{\text{ML}}}[Q(x,\theta)] + \alpha \widehat{\sigma_{\text{biased}}^{\text{ML}}}[Q(x,\theta)]$$

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Up next:

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Up next:

1. Recap (from literature): $\widehat{\mu_1^{\text{ML}}}[Q(x,\theta)]$

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1. Recap (from literature): $\widehat{\mu_1^{\text{ML}}}[Q(x,\theta)]$
2. (Our contribution) ML for Standard deviation: $\widehat{\sigma_{\text{biased}}^{\text{ML}}}[Q(x,\theta)]$

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2. (Our contribution) ML for Standard deviation: $\widehat{\sigma_{\text{biased}}^{\text{ML}}}[Q(x,\theta)]$
3. (Our contribution) ML for Scalarization: $\widehat{\mu_1^{\text{ML}}}[Q(x,\theta)] + \alpha \widehat{\sigma_{\text{biased}}^{\text{ML}}}[Q(x,\theta)]$

Multilevel Monte Carlo (MLMC) Estimator

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MLMC estimator: Mean

Mean in OUU:

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‡Giles, M.B., "Multilevel Monte Carlo methods," Acta Numerica, Vol.24, 2015, p.259–328

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MLMC estimator: Mean

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- Estimator[‡]:

$$\mathbb{E}[Q_L] = \mu_1^{\text{ML}}[Q_L] \approx \widehat{\mu_1^{\text{ML}}}[Q_L] = \sum_{\ell=0}^{L} \underbrace{\widehat{\mu_1}[Q^{(\ell)} - Q^{(\ell-1)}]}_{\text{telescopic sum}} = \sum_{\ell=0}^{L} \underbrace{\frac{1}{N_\ell} \sum_{i=1}^{N_\ell} (Q_i^{(\ell)} - Q_{i,\ell}^{(\ell-1)})}_{\text{estimator expansion}}, \quad Q_{i,0}^{(-1)} := 0$$

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- Sample allocation:

$$\min_{N_\ell^{\mathbb{E}}} \sum_{\ell=0}^{L} C_\ell N_\ell^{\mathbb{E}},$$

$$\text{s.t. } \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] = \varepsilon^2, \text{ where } \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] = \sum_{\ell=0}^{L} \mathbb{V}[\widehat{\mu_1^{(\ell)}} - \widehat{\mu_{1,\ell}^{(\ell-1)}}] = \sum_{\ell=0}^{L} \frac{\mathbb{V}[Q^{(\ell)} - Q^{(\ell-1)}]}{N_\ell}$$

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- Solution:

$$N_\ell^{\mathbb{E}} = \left\lceil \lambda \sqrt{\frac{\mathbb{V}[Q_\ell - Q_{\ell-1}]}{C_\ell}} \right\rceil, \text{ where } \lambda = \varepsilon^{-2} \sum_{\ell=0}^{L} \sqrt{\mathbb{V}[Q_\ell - Q_{\ell-1}] C_\ell}$$

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MLMC estimator: Standard deviation

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MLMC estimator: Standard deviation

- Estimator:

$$\sigma[Q_L] = \sqrt{\mathbb{V}[Q_L]} \approx \sqrt{\widehat{\mu_2^{\mathrm{ML}}}} := \widehat{\sigma^{\mathrm{ML}}_{\mathrm{biased}}}$$

where

$$\mathbb{V}[Q_L] \approx \widehat{\mu_2^{\mathrm{ML}}}[Q_L] = \sum_{\ell=0}^{L} \underbrace{\widehat{\mu_2}[Q^{(\ell)}] - \widehat{\mu_2}[Q^{(\ell-1)}]}_{\text{telescopic sum}}$$

$$= \sum_{\ell=0}^{L} \underbrace{\frac{1}{N_\ell - 1}\left(\sum_{i=1}^{N_\ell} (Q_i^{(\ell)} - \widehat{\mu_1^{(\ell)}})^2 - (Q_{i,\ell}^{(\ell-1)} - \widehat{\mu_{1,\ell}^{(\ell-1)}})^2\right)}_{\text{estimator expansion}}$$

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- Sample allocation:

$$\min_{N_\ell^\sigma} \sum_{\ell=0}^{L} C_\ell N_\ell^\sigma,$$

$$\text{s.t. } \mathbb{V}[\widehat{\sigma^{\text{ML}}_{\text{biased}}}] = \varepsilon^2, \text{ where } \mathbb{V}[\widehat{\sigma^{\text{ML}}_{\text{biased}}}] \approx \frac{1}{4}\frac{\mathbb{V}[\widehat{\mu_2^{\text{ML}}}]}{\widehat{\mu_2^{\text{ML}}}} \text{ (Delta Method)}$$

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- How to solve this?

MLMC sample allocation for higher order terms

1. Analytic approximation [§]
   - **Obs**: Decrease of variance of MLMC estimator $\mathcal{O}(\frac{1}{N})$ true also for higher order moments
   - **Idea**: Use similar analytic solution approach as for MLMC Mean:

$$\min_{N_\ell^{\mathbb{E}}} \sum_{\ell=0}^{L} C_\ell N_\ell^{\mathbb{E}},$$

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[§]Pisaroni, M., Krumscheid, S., and Nobile, F., "MATHICSE Technical Report : Quantifying uncertain system outputs via the multilevel Monte Carlo method - Part I: Central moment estimation," 2017, p. 29.

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$$\text{s.t. } \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] = \varepsilon^2, \text{ where } \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] = \sum_{\ell=0}^{L} \frac{\mathbb{V}[Q^{(\ell)} - Q^{(\ell-1)}]}{N_\ell}$$

$$N_\ell^{\mathbb{E}} = \left\lceil \lambda \sqrt{\frac{\mathbb{V}[Q_\ell - Q_{\ell-1}]}{C_\ell}} \right\rceil, \text{ where } \lambda = \varepsilon^{-2} \sum_{\ell=0}^{L} \sqrt{\mathbb{V}[Q_\ell - Q_{\ell-1}] C_\ell}$$

   - Introduce helper variance: $\mathbb{V}[\widehat{\mu_1^{(\ell)}}] = \frac{\mathscr{V}_\ell}{N_\ell} \Leftrightarrow \mathscr{V}_\ell = \mathbb{V}[\widehat{\mu_1^{(\ell)}}] N_\ell^{\mathbb{E}}$

[§] Pisaroni, M., Krumscheid, S., and Nobile, F., "MATHICSE Technical Report : Quantifying uncertain system outputs via the multilevel Monte Carlo method - Part I: Central moment estimation," 2017, p. 29.

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MLMC sample allocation for higher order terms

1. Analytic approximation [§]
   - **Obs**: Decrease of variance of MLMC estimator $\mathcal{O}(\frac{1}{N})$ true also for higher order moments
   - **Idea**: Use similar analytic solution approach as for MLMC Mean:

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$$N_\ell^{\mathbb{X}} = \left\lceil \lambda \sqrt{\frac{\mathscr{V}_\ell}{C_\ell}} \right\rceil, \text{ where } \lambda = \varepsilon^{-2} \sum_{\ell=0}^{L} \sqrt{\mathscr{V}_\ell C_\ell}$$

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   - Disregard higher order terms in $\mathscr{V}_\ell \Rightarrow$ Analytic approximation

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   - Disregard higher order terms in $\mathscr{V}_\ell \Rightarrow$ Analytic approximation
2. Numerical optimization
   - Solve $\min_{N_\ell^{\mathbb{X}}} \sum_{\ell=0}^{L} C_\ell N_\ell^{\mathbb{X}}$, s.t. $\mathbb{V}[\widehat{\mu_X^{\text{ML}}}] = \varepsilon^2$ numerically

[§] Pisaroni, M., Krumscheid, S., and Nobile, F., "MATHICSE Technical Report : Quantifying uncertain system outputs via the multilevel Monte Carlo method - Part I: Central moment estimation," 2017, p. 29.

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MLMC estimator: Scalarization

Mean in OUU:

$$\min_x \mathscr{R}_{\text{Mean}} \approx \min_x \widehat{\mu_1^{\text{ML}}}[Q(x,\theta)]$$

Scalarization in OUU:

$$\min_x \mathscr{R}_{\text{Scalar}} \approx \min_x \widehat{\mu_1^{\text{ML}}}[Q(x,\theta)] + \alpha \widehat{\sigma_{\text{biased}}^{\text{ML}}}[Q(x,\theta)]$$

MLMC estimator: Scalarization

- Estimator:

$$\mathbb{S}[Q_L] := \mathbb{E}[Q_L] + \alpha\sigma[Q_L] \approx \widehat{\mu_1^{\text{ML}}} + \alpha\widehat{\sigma_{\text{biased}}^{\text{ML}}} := \widehat{\zeta}^{\text{ML}}$$

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- Sample allocation:

$$\min_{N_\ell^{\mathbb{S}}} \sum_{\ell=0}^{L} C_\ell N_\ell^{\mathbb{S}},$$

$$\text{s.t. } \mathbb{V}[\widehat{\zeta^{\text{ML}}}] = \varepsilon^2, \text{ where } \mathbb{V}[\widehat{\zeta^{\text{ML}}}] \approx \mathbb{V}[\widehat{\mu_1^{\text{ML}}} + \alpha\widehat{\sigma_{\text{biased}}^{\text{ML}}}]$$

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$$\text{s.t. } \mathbb{V}[\widehat{\zeta^{\text{ML}}}] = \varepsilon^2, \text{ where } \mathbb{V}[\widehat{\zeta^{\text{ML}}}] \approx \mathbb{V}[\widehat{\mu_1^{\text{ML}}} + \alpha\widehat{\sigma_{\text{biased}}^{\text{ML}}}]$$

- Variance of scalarization:

$$\begin{aligned}\mathbb{V}[\widehat{\zeta^{\text{ML}}}] &= \mathbb{V}[\widehat{\mu_1^{\text{ML}}} + \alpha\widehat{\sigma_{\text{biased}}^{\text{ML}}}] \\ &= \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] + \alpha^2\mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}] + 2\alpha\mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}]\end{aligned}$$

- Solution: Numerical Optimization or analytic approximation

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MLMC estimator: Scalarization

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$$\min_{N_\ell^{\mathbb{S}}} \sum_{\ell=0}^{L} C_\ell N_\ell^{\mathbb{S}},$$
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- Variance of scalarization:

$$\begin{aligned}\mathbb{V}[\widehat{\zeta^{\text{ML}}}] &= \mathbb{V}[\widehat{\mu_1^{\text{ML}}} + \alpha\widehat{\sigma_{\text{biased}}^{\text{ML}}}] \\ &= \underbrace{\mathbb{V}[\widehat{\mu_1^{\text{ML}}}]}_{\text{known}} + \alpha^2\underbrace{\mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}]}_{\text{known}} + 2\alpha\underbrace{\mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}]}_{\text{up next}}\end{aligned}$$

- Solution: Numerical Optimization or analytic approximation

MLMC estimator: Scalarization Covariance

$$\mathbb{V}[\widehat{\zeta^{\text{ML}}}] = \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] + \alpha^2 \mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}] + 2\alpha \mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}]$$

$$= \sum_{\ell=0}^{L} \mathbb{V}\left[\widehat{\mu_1^{(\ell)}} - \widehat{\mu_{1,\ell}^{(\ell-1)}}\right] + \alpha^2 \mathbb{V}\left[\widehat{\sigma_{\text{biased}}^{(\ell)}} - \widehat{\sigma_{\text{biased},\ell}^{(\ell-1)}}\right] + 2\alpha \mathbb{C}\text{ov}\left[\widehat{\mu_1^{(\ell)}} - \widehat{\mu_{1,\ell}^{(\ell-1)}}, \widehat{\sigma_{\text{biased}}^{(\ell)}} - \widehat{\sigma_{\text{biased},\ell}^{(\ell-1)}}\right]$$

Three (independent) solution strategies:

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MLMC estimator: Scalarization Covariance

$$\mathbb{V}[\widehat{\zeta^{\text{ML}}}] = \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] + \alpha^2 \mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}] + 2\alpha \mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}]$$
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Three (independent) solution strategies:

1. Pearson correlation $\rho[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}]$:

$$\mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}] \leq \sqrt{\mathbb{V}[\widehat{\mu_1^{\text{ML}}}] \cdot \mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}]}, \text{ since} \qquad -1 \leq \frac{\mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}]}{\sqrt{\mathbb{V}[\widehat{\mu_1^{\text{ML}}}]\mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}]}} \leq 1$$

MLMC estimator: Scalarization Covariance

$$\mathbb{V}[\widehat{\zeta^{\text{ML}}}] = \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] + \alpha^2 \mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}] + 2\alpha \mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}]$$
$$= \sum_{\ell=0}^{L} \mathbb{V}\left[\widehat{\mu_1^{(\ell)}} - \widehat{\mu_{1,\ell}^{(\ell-1)}}\right] + \alpha^2 \mathbb{V}\left[\widehat{\sigma_{\text{biased}}^{(\ell)}} - \widehat{\sigma_{\text{biased},\ell}^{(\ell-1)}}\right] + 2\alpha \mathbb{C}\text{ov}\left[\widehat{\mu_1^{(\ell)}} - \widehat{\mu_{1,\ell}^{(\ell-1)}}, \widehat{\sigma_{\text{biased}}^{(\ell)}} - \widehat{\sigma_{\text{biased},\ell}^{(\ell-1)}}\right]$$

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2. Bootstrapping:

$$\mathbb{C}\text{ov}[\widehat{\mu_1^{(\ell)}}, \widehat{\sigma_{\text{biased}}^{(\ell)}}] \approx \frac{1}{B-1} \sum_{b=1}^{B} (\widehat{\mu_{1,b}^{(\ell)}} - \overline{\widehat{\mu_{1,b}^{(\ell)}}})(\widehat{\sigma_{\text{biased},b}^{(\ell)}} - \overline{\widehat{\sigma_{\text{biased},b}^{(\ell)}}})$$

$$\text{where e.g.} \widehat{\mu_{1,b}^{(\ell)}} = \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} Q_i^* \text{ and } \overline{\widehat{\mu_{1,b}^{(\ell)}}} = \frac{1}{B} \sum_{b=1}^{B} \widehat{\mu_{1,b}^{(\ell)}} \text{ and } Q_i^* \text{ iid from } \{Q_i\}_{i=1}^{N_\ell}$$

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MLMC estimator: Scalarization Covariance

$$\mathbb{V}[\widehat{\zeta^{\text{ML}}}] = \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] + \alpha^2 \mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}] + 2\alpha \mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}]$$
$$= \sum_{\ell=0}^{L} \mathbb{V}\left[\widehat{\mu_1^{(\ell)}} - \widehat{\mu_{1,\ell}^{(\ell-1)}}\right] + \alpha^2 \mathbb{V}\left[\widehat{\sigma_{\text{biased}}^{(\ell)}} - \widehat{\sigma_{\text{biased},\ell}^{(\ell-1)}}\right] + 2\alpha \mathbb{C}\text{ov}\left[\widehat{\mu_1^{(\ell)}} - \widehat{\mu_{1,\ell}^{(\ell-1)}}, \widehat{\sigma_{\text{biased}}^{(\ell)}} - \widehat{\sigma_{\text{biased},\ell}^{(\ell-1)}}\right]$$

Three (independent) solution strategies:

1. Pearson correlation: (easy to compute, **inequality**)
2. Bootstrapping (more expensive, **approximation**)

MLMC estimator: Scalarization Covariance

$$
\begin{aligned}
\mathbb{V}[\widehat{\zeta^{\text{ML}}}] &= \mathbb{V}[\widehat{\mu_1^{\text{ML}}}] + \alpha^2 \mathbb{V}[\widehat{\sigma_{\text{biased}}^{\text{ML}}}] + 2\alpha \mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}] \\
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\end{aligned}
$$

Three (independent) solution strategies:

1. Pearson correlation: (easy to compute, **inequality**)
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3. Correlation Lift:

$$
\text{Assume: } \rho[\widehat{\mu_1^{(\ell)}}, \widehat{\sigma_{\text{biased}}^{(k)}}] \approx \rho[\widehat{\mu_1^{(\ell)}}, \widehat{\mu_2^{(k)}}], (\ell - k) \in \{-1, 0, 1\}
$$

$$
\text{Then: } \mathbb{C}\text{ov}\left[\widehat{\mu_1^{(\ell)}}, \widehat{\sigma_{\text{biased}}^{(k)}}\right] \approx \mathbb{C}\text{ov}\left[\widehat{\mu_1^{(\ell)}}, \widehat{\mu_2^{(k)}}\right] \sqrt{\frac{\mathbb{V}[\widehat{\mu_2^{(k)}}]}{\mathbb{V}[\widehat{\sigma_{\text{biased}}^{(k)}}]}},
$$

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MLMC estimator: Scalarization Covariance

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MLMC estimator: Scalarization Covariance

- Same level[¶]:

$$\mathbb{C}\mathrm{ov}\left[\widehat{\mu_1^{(\ell)}}, \widehat{\mu_2^{(\ell)}}\right] = \frac{\mu_3^{(\ell)}}{N_\ell}$$

- Lower level variance:

$$\mathbb{C}\mathrm{ov}\left[\widehat{\mu_1^{(\ell)}}, \widehat{\mu_{2,\ell}^{(\ell-1)}}\right] =$$

$$\frac{1}{N_\ell}\left[\mathbb{E}[Q^{(\ell)}(Q^{(\ell-1)})^2] - \mathbb{E}[Q^{(\ell)}]\mathbb{E}[(Q^{(\ell-1)})^2] - 2\mathbb{E}[Q^{(\ell-1)}]\mathbb{E}[Q^{(\ell)}Q^{(\ell-1)}] + 2\mathbb{E}[Q^{(\ell)}]\mathbb{E}[Q^{(\ell-1)}]^2\right]$$

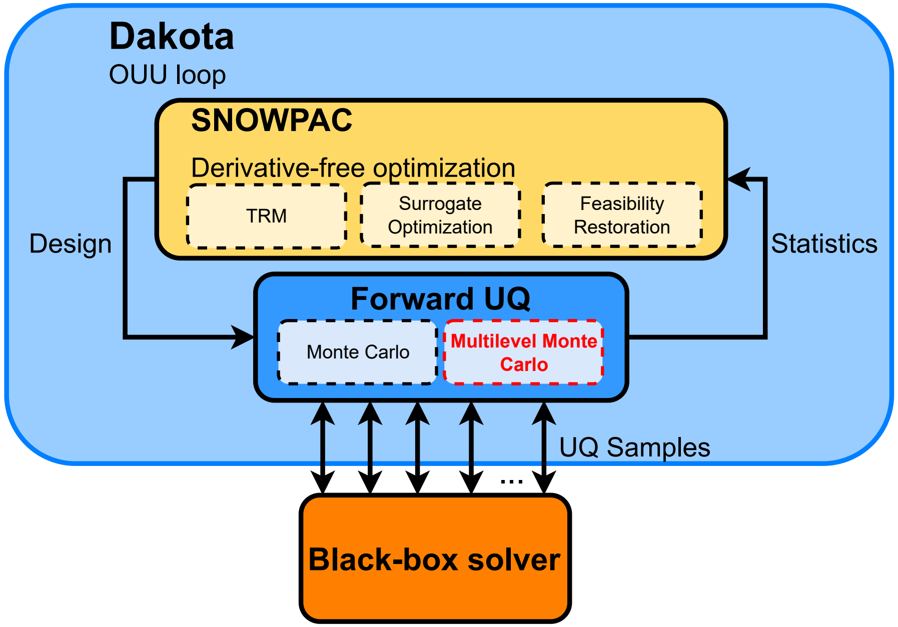
- Lower level mean:

$$\mathbb{C}\mathrm{ov}\left[\widehat{\mu_{1,\ell}^{(\ell-1)}}, \widehat{\mu_2^{(\ell)}}\right] =$$

$$\frac{1}{N_\ell}\left[\mathbb{E}[Q^{(\ell-1)}(Q^{(\ell)})^2] - \mathbb{E}[Q^{(\ell-1)}]\mathbb{E}[(Q^{(\ell)})^2] - 2\mathbb{E}[Q^{(\ell)}]\mathbb{E}[Q^{(\ell-1)}Q^{(\ell)}] + 2\mathbb{E}[Q^{(\ell-1)}]\mathbb{E}[Q^{(\ell)}]^2\right]$$

[¶]Dodge Y., Rousson V., The Complications of the Fourth Central Moment, The American Statistician, 1999

SNOWPAC in Dakota using MLMC



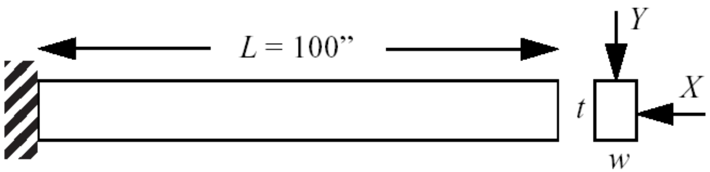
Algorithmic details:

- Iterative sample allocation
- Underrelaxation
- Choice of sample allocation strategy: Analytic approximation vs. numerical optimization
- Choice of covariance approximation: Pearson vs. Bootstrap vs. Correlation Lift

Results

Cantilever beam problem:

2 **design** parameters: w, t



Adams, B.M., et. al., Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.15 User's Manual

Objective: $\min_{w,t} wt$

4 **uncertain** parameters:

- Yield stress: $R \sim \mathcal{N}(40000, 200)$
- Young's modulus: $E \sim \mathcal{N}(2.9e7, 1.45e6)$
- Horizontal load: $X \sim \mathcal{N}(500, 100)$
- Vertical load: $Y \sim \mathcal{N}(1000, 100)$

- Level 3: Rectangle (Cost = 1)

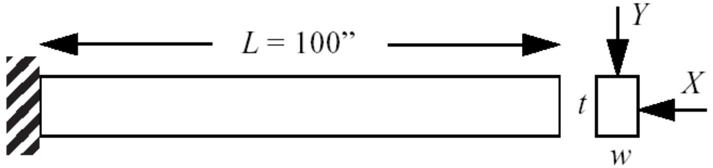
$$\text{stress} : (\frac{600}{wt^2}Y + \frac{600}{w^2 t}X)/R - 1 \leq 0$$

$$\text{displacement} : (\frac{4L^3}{Ewt}\sqrt{(\frac{Y}{t^2})^2 + (\frac{X}{w^2})^2})/D_0 - 1 \leq 0$$

- Level 2: Ellipse instead of rectangle (Cost = 1e-2)
- Level 1: Circle inscribed in rectangle instead of rectangle (Cost = 1e-4)
- Level 0: Circle with same area instead of rectangle (Cost = 1e-6)

Cantilever beam problem:

2 **design** parameters: w, t



Adams, B.M., et. al., Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.15 User's Manual

Objective: ~~$\min_{w,t}$~~ w t (Sampling only)

4 **uncertain** parameters:

- Yield stress: $R \sim \mathcal{N}(40000, 200)$
- Young's modulus: $E \sim \mathcal{N}(2.9e7, 1.45e6)$
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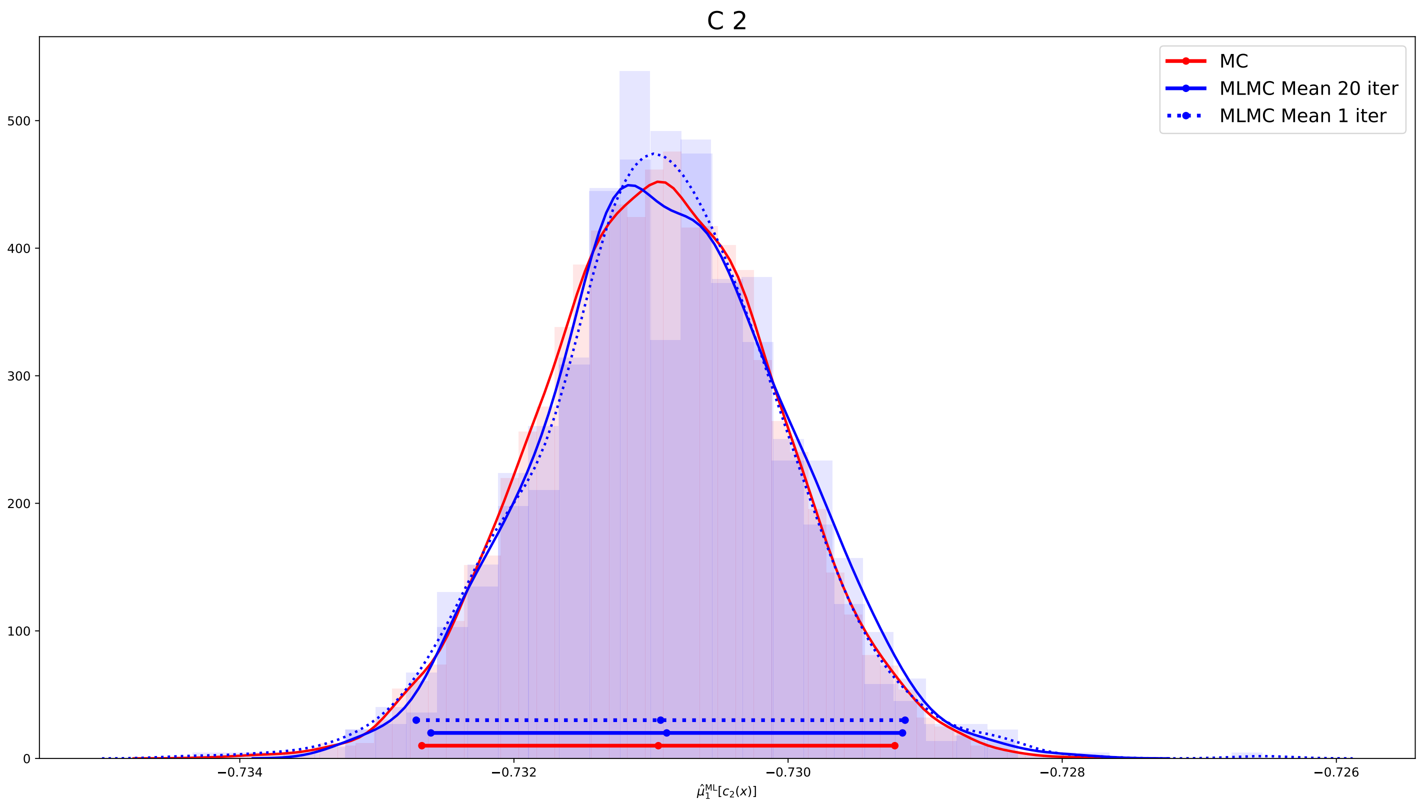
- Level 0: Circle with same area instead of rectangle (Cost = 1e-6)

Test results

1. Present sampling results by resampling estimators and plot histogram of **estimators**
2. Compare three strategies for estimating $\mathbb{C}$ov-term:
   - Pearson
   - Bootstrap
   - using $\rho[\widehat{\mu_1^{(\ell)}}, \widehat{\sigma_{\text{biased}}^{(k)}}] = \rho[\widehat{\mu_1^{(\ell)}}, \widehat{\mu_2^{(k)}}]$ (CorrLift)
3. Compare algorithmic strategies:
   - Iterations vs. no iterations
   - Analytics approximation (only) vs. numerical optimization

Sampling Results: Mean



- MLMC Mean distribution (blue) consistent with MC reference (red) for lower cost.

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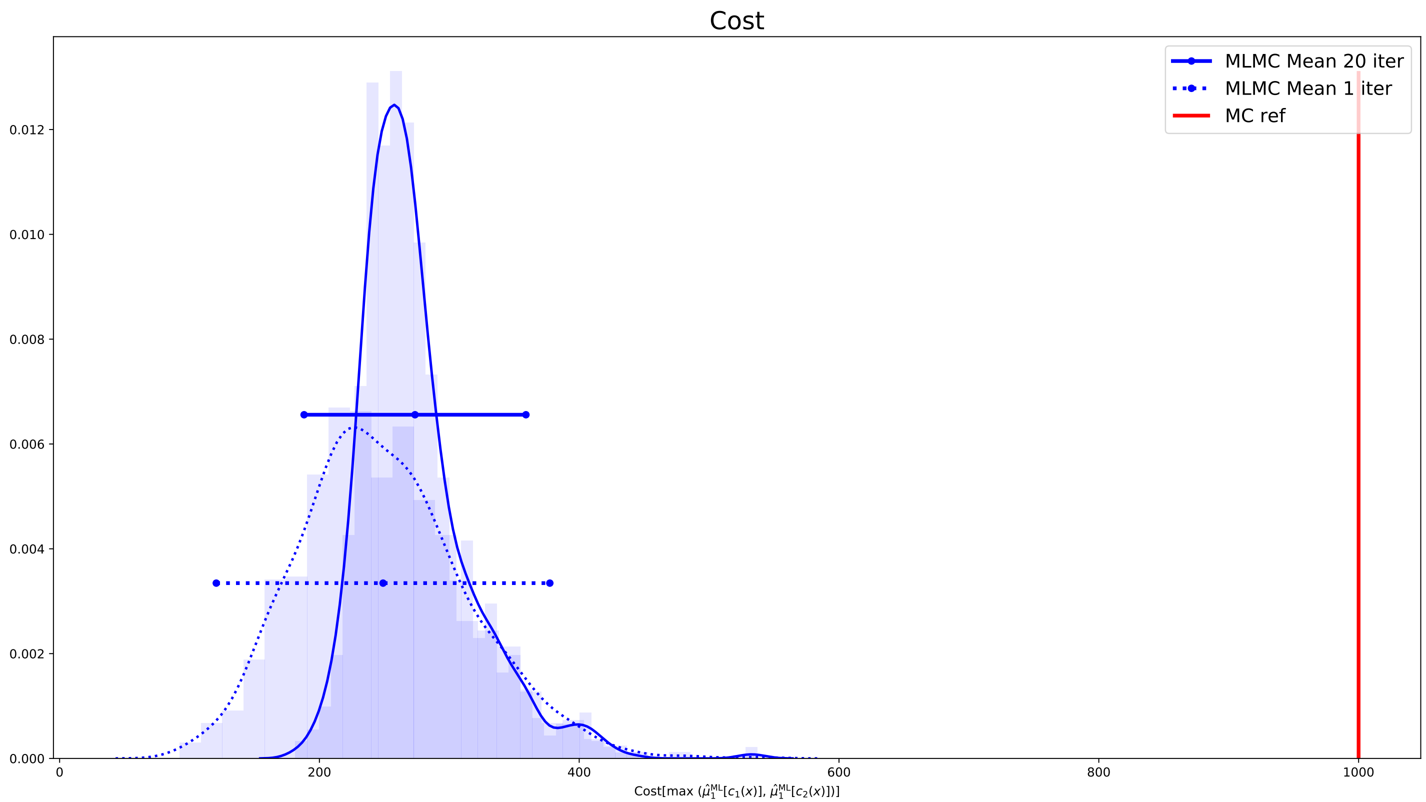
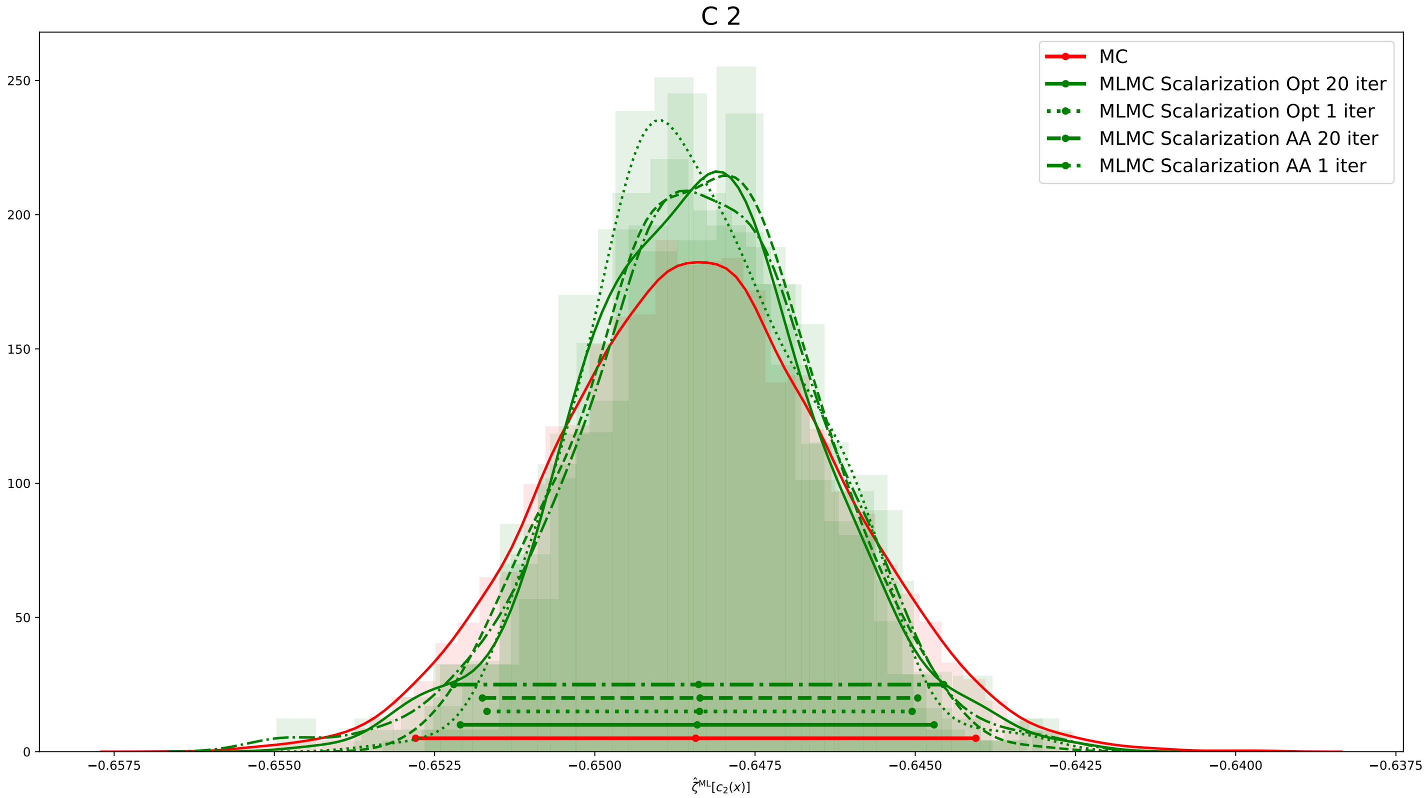
Sampling Results: Mean



- MLMC Mean distribution (blue) consistent with MC reference (red) for lower cost.

Sampling Results: Scalarization (Pearson)



- MLMC Scalarization (green) close but overresolves to MC reference case (red).

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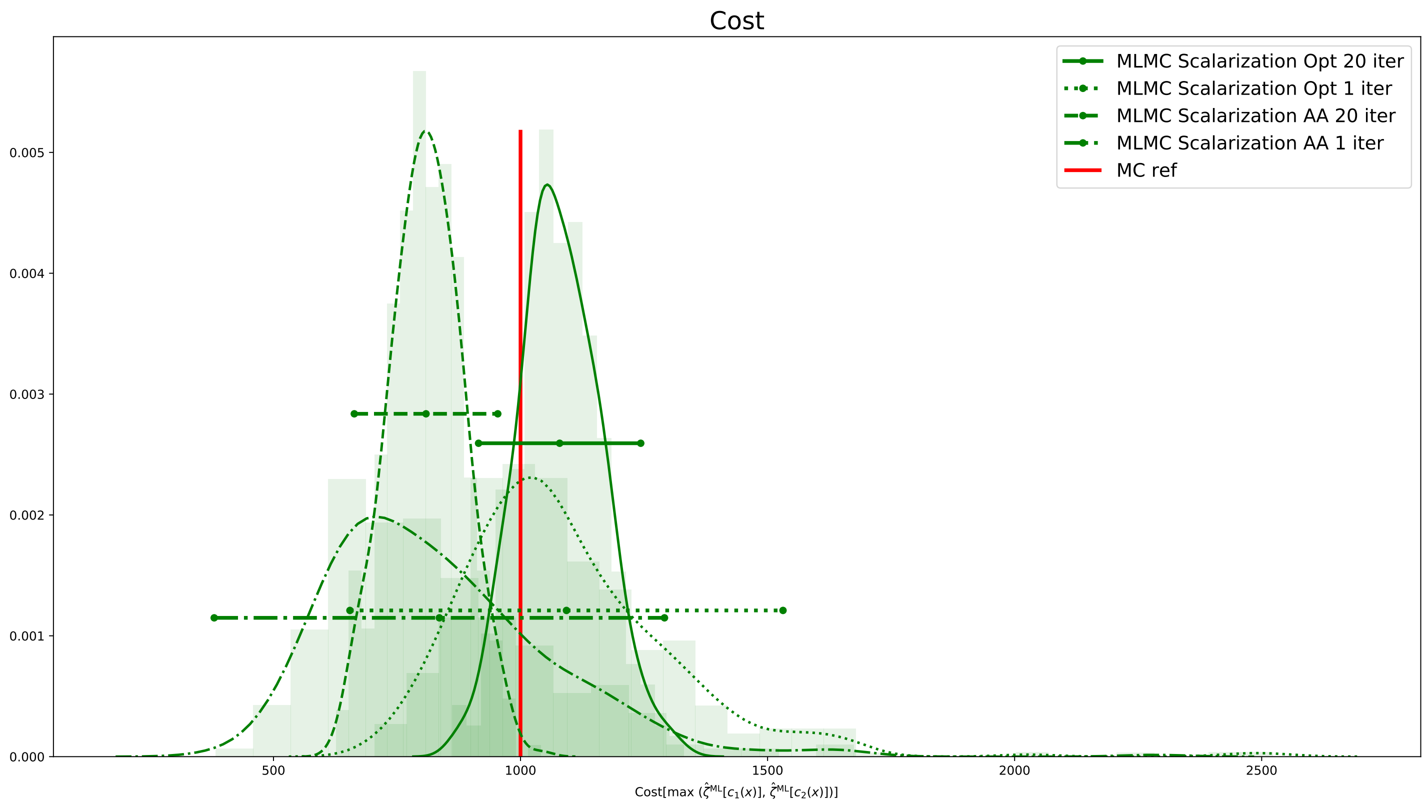
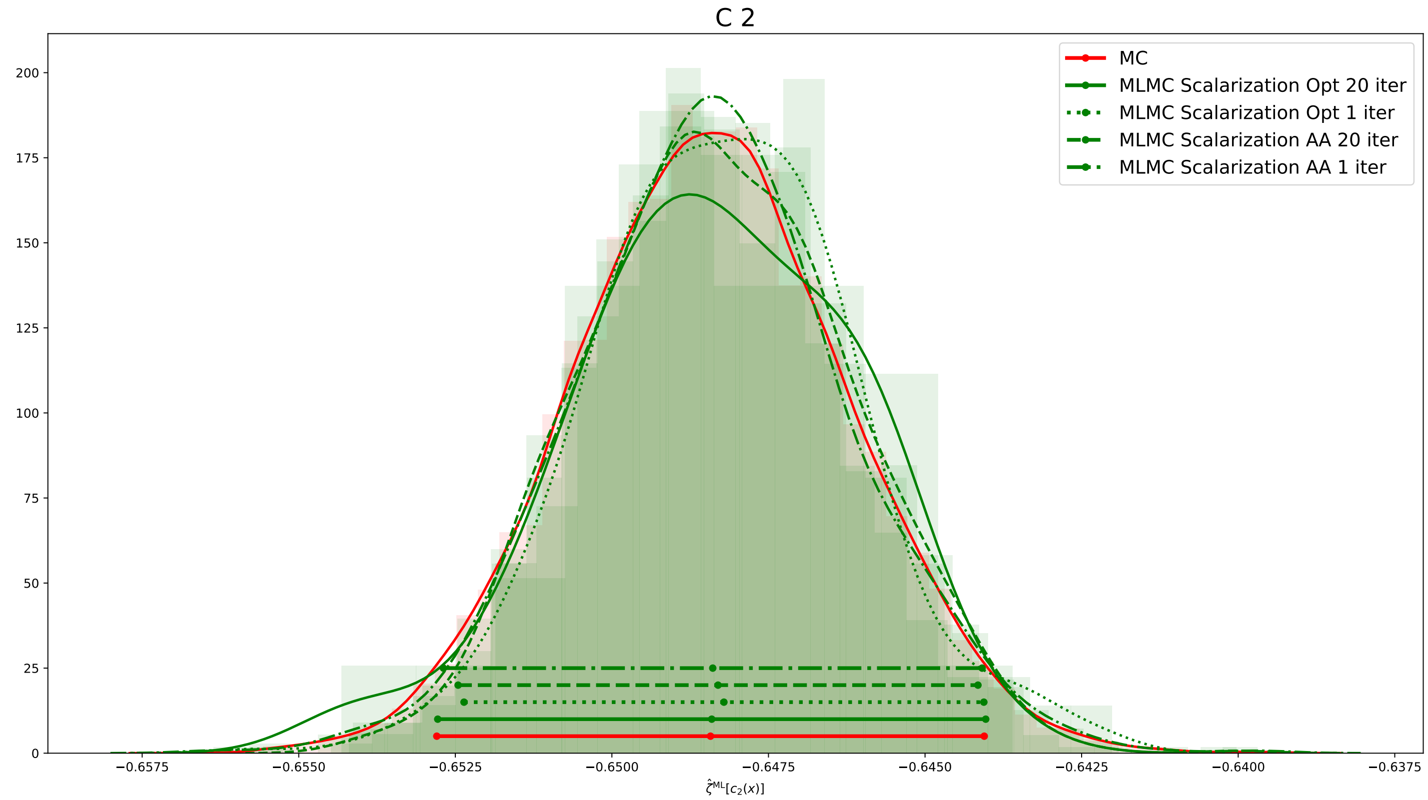
Sampling Results: Scalarization (Pearson)



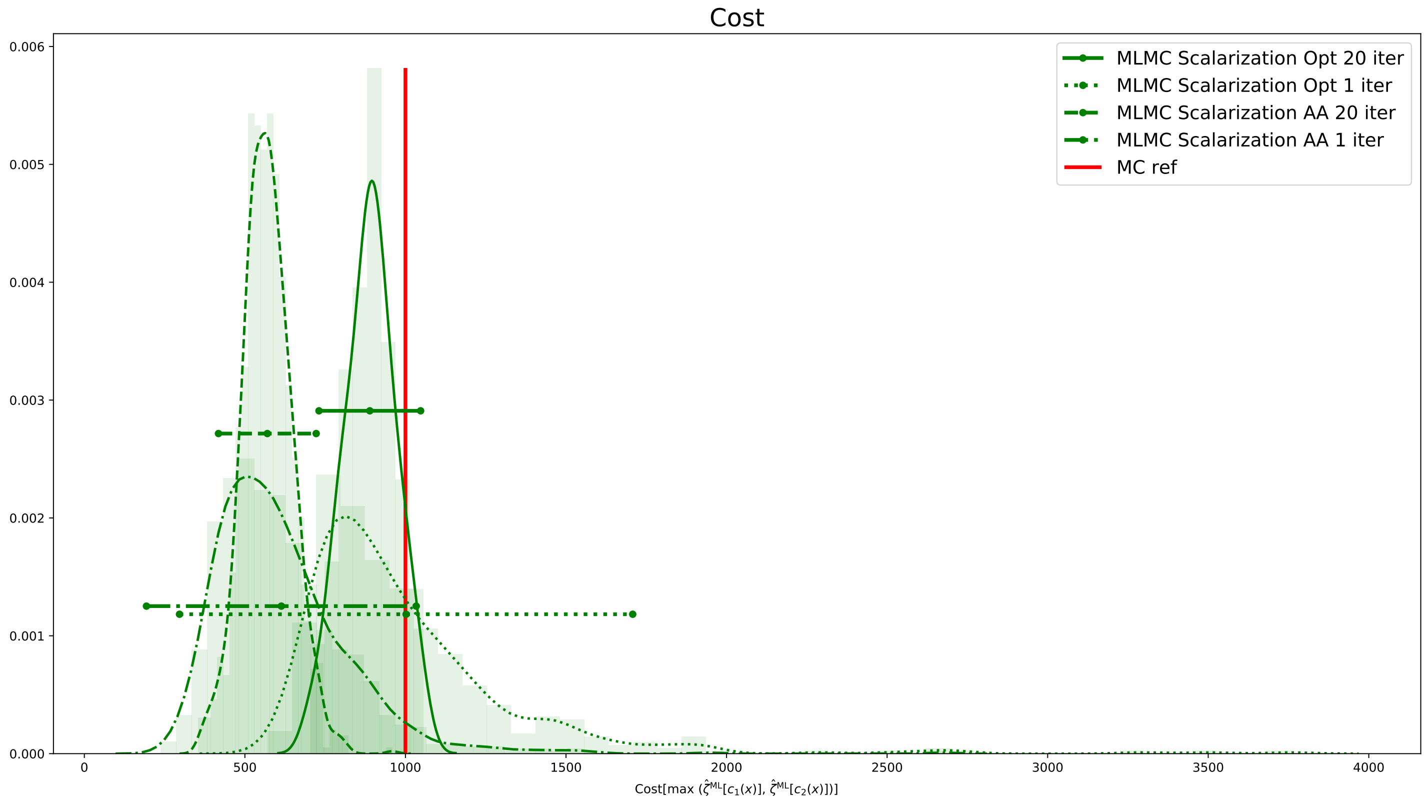
- MLMC Scalarization (green) close but overresolves to MC reference case (red).
- Results in higher computational cost than MC reference.

Sampling Results: Scalarization (Bootstrap)



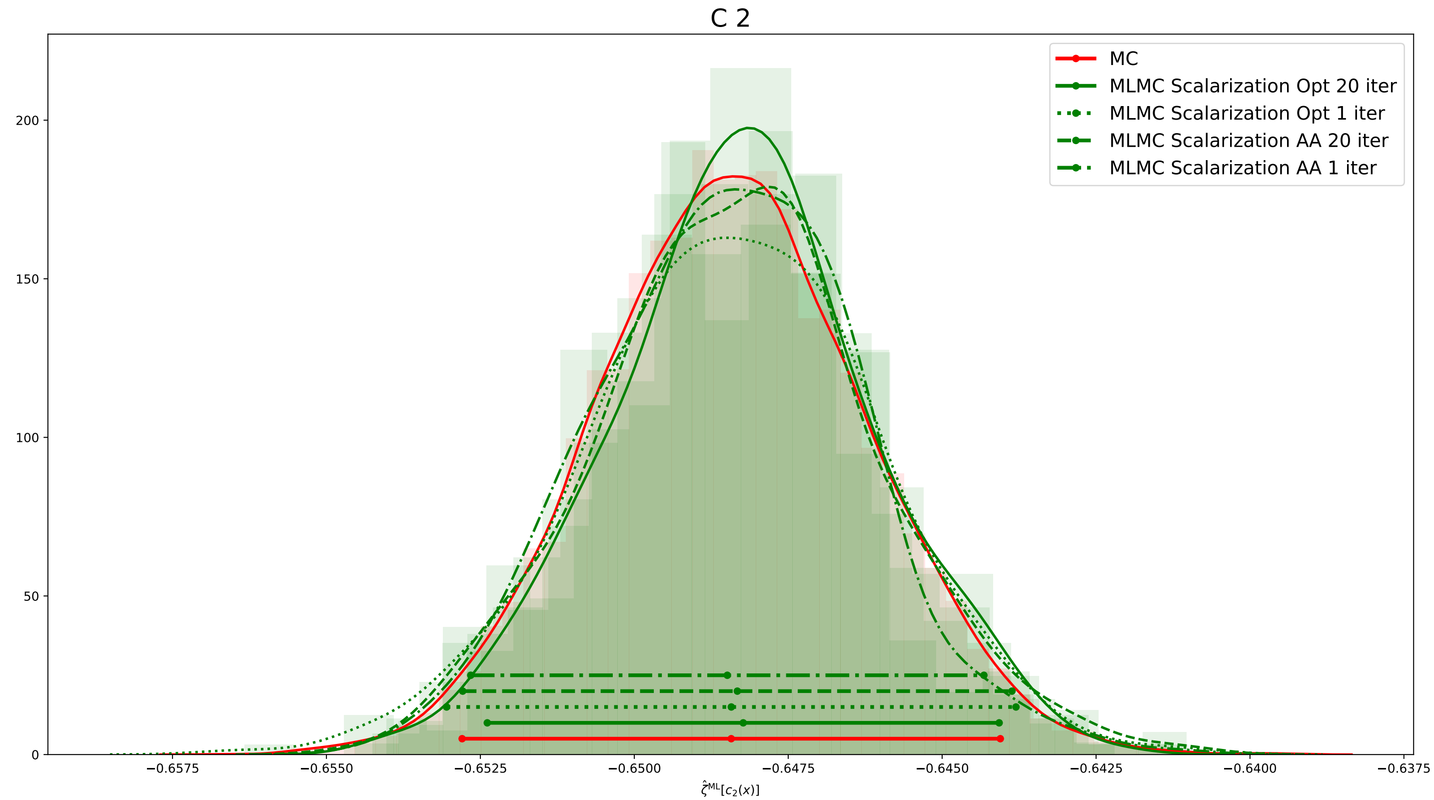
- MLMC Scalarization (green) consistent with MC reference (red) using Bootstrap.
- Cost reduced compared to Pearson
- BUT bootstrapping itself becomes computational bottleneck

Sampling Results: Scalarization (Bootstrap)



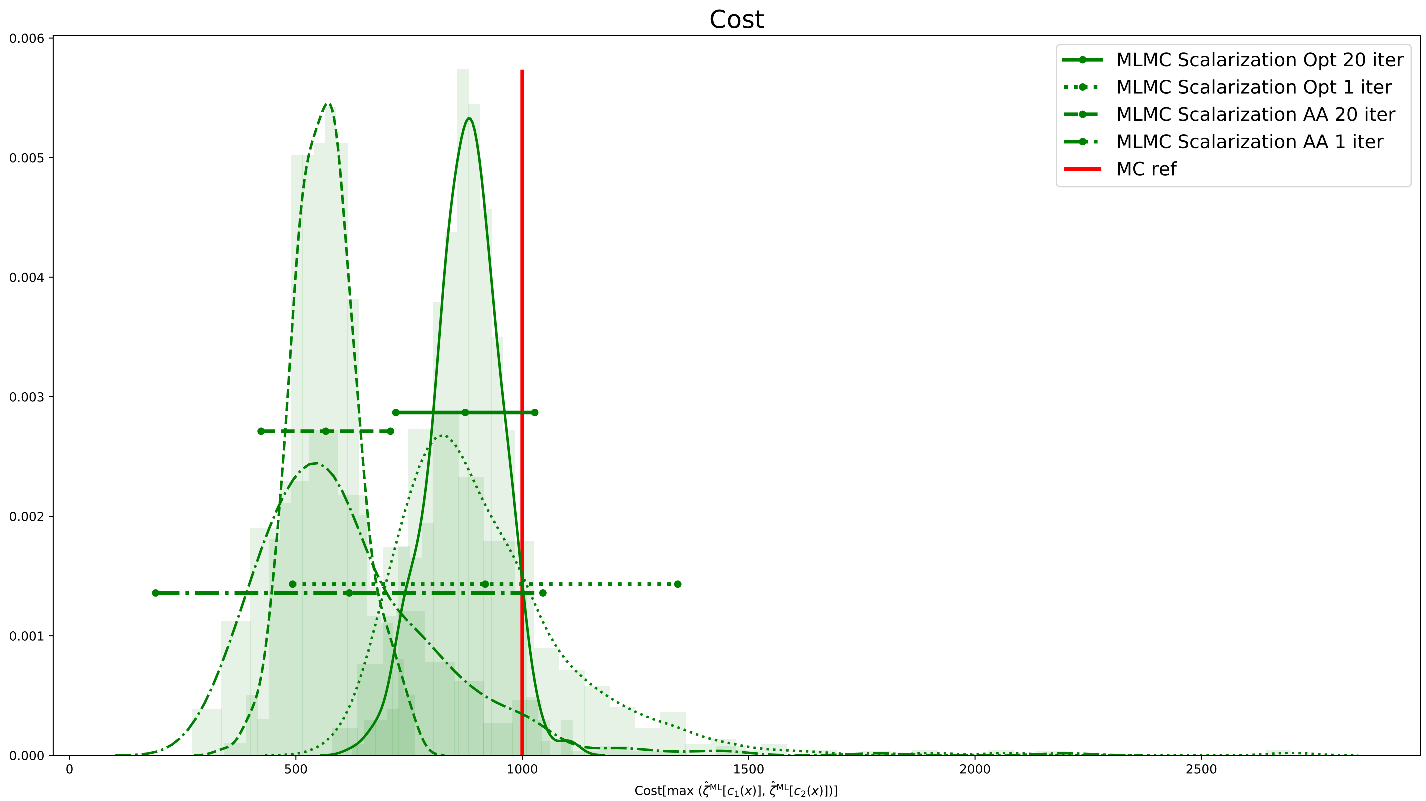
- MLMC Scalarization (green) consistent with MC reference (red) using Bootstrap.
- Cost reduced compared to Pearson
- BUT bootstrapping itself becomes computational bottleneck

Sampling Results: Scalarization (CorrLift)



- MLMC Scalarization (green) consistent with MC reference (red) (left) for lower cost (right) using CorrLift.
- Computational effort similar to Pearson and $<<$ Bootstrap

Sampling Results: Scalarization (CorrLift)



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Sampling Summary

- MLMC targeting the respective formulation necessary for optimal result
- Covariance term approximation crucial in scalarization
- Bootstrap leads to consistently better results but non-negligible computational cost
- ”Best of both worlds” achieved using CorrLift approach

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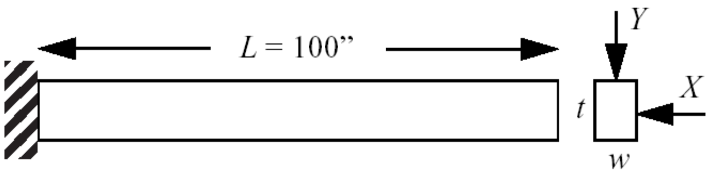
How does this translate to optimization?

Cantilever beam problem:

2 **design** parameters: w, t



Adams, B.M., et. al., Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.15 User's Manual

Objective: $\min_{\mathbf{w},\mathbf{t}} wt$

4 **uncertain** parameters:

- Yield stress: $R \sim \mathcal{N}(40000, 200)$
- Young's modulus: $E \sim \mathcal{N}(2.9e7, 1.45e6)$
- Horizontal load: $X \sim \mathcal{N}(500, 100)$
- Vertical load: $Y \sim \mathcal{N}(1000, 100)$

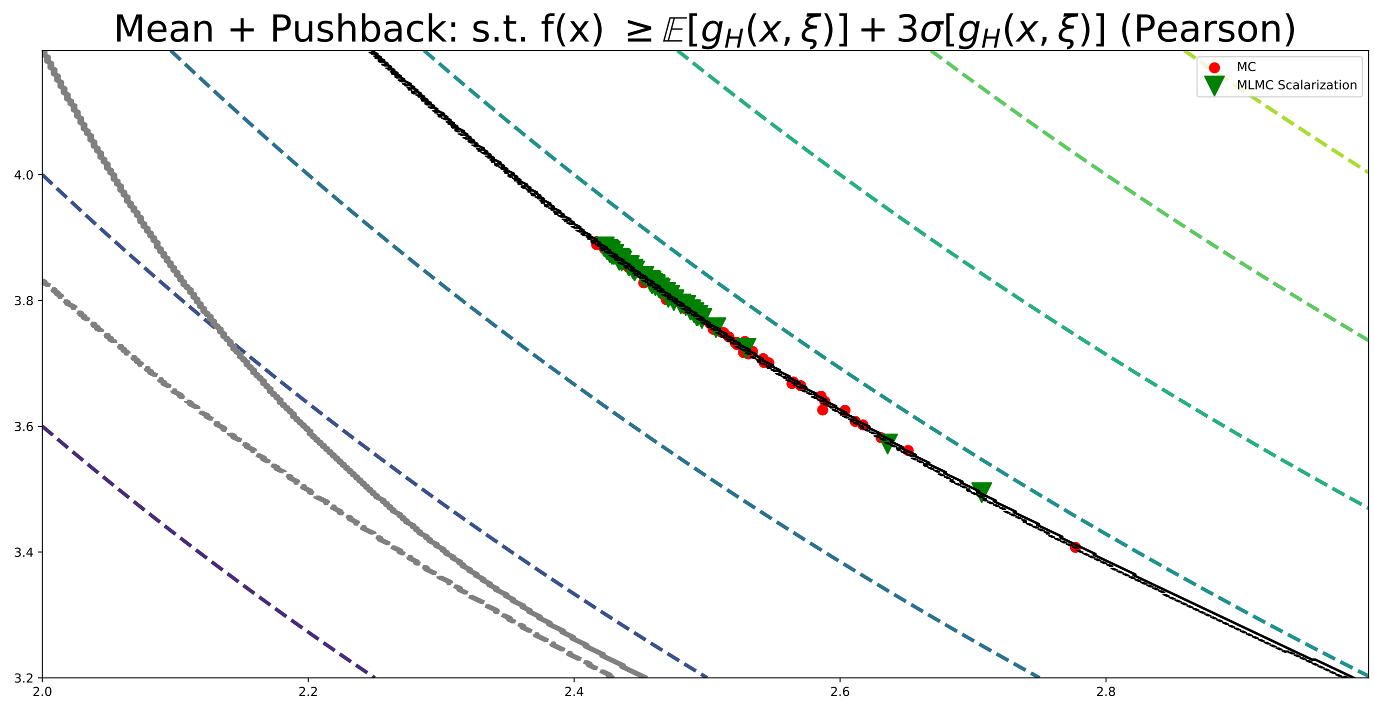
- Level 3: Rectangle (Cost = 1)

$$\text{stress}: \left(\frac{600}{wt^2}Y + \frac{600}{w^2t}X\right)/R - 1 \leq 0$$

$$\text{displacement}: \left(\frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2}\right)/D_0 - 1 \leq 0$$

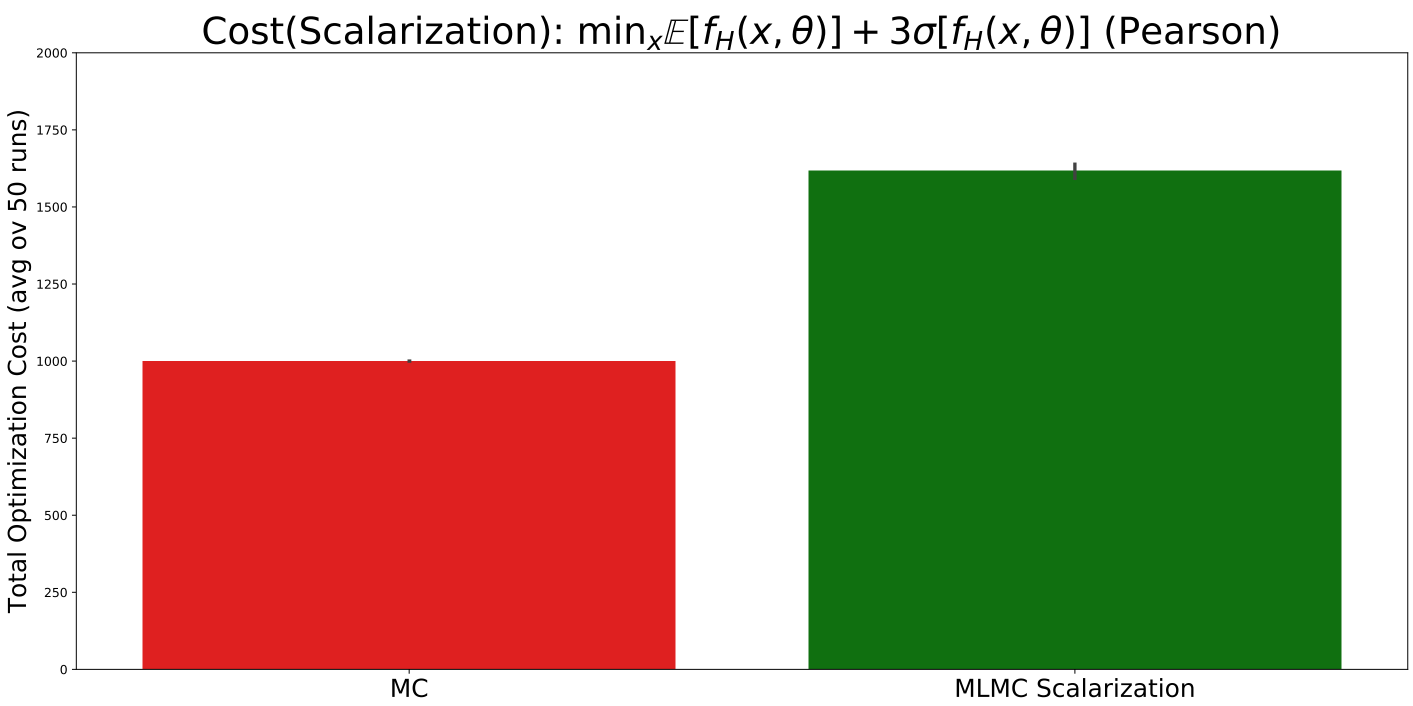
- Level 2: Ellipse instead of rectangle (Cost = 1e-2)
- ~~Level 1: Circle inscribed in rectangle instead of rectangle (Cost = 1e-4)~~
- ~~Level 0: Circle with same area instead of rectangle (Cost = 1e-6)~~

OUU Results (Pearson)



- Pearson approximation results in overestimation
- At the price of higher computational cost

OUU Results (Pearson)



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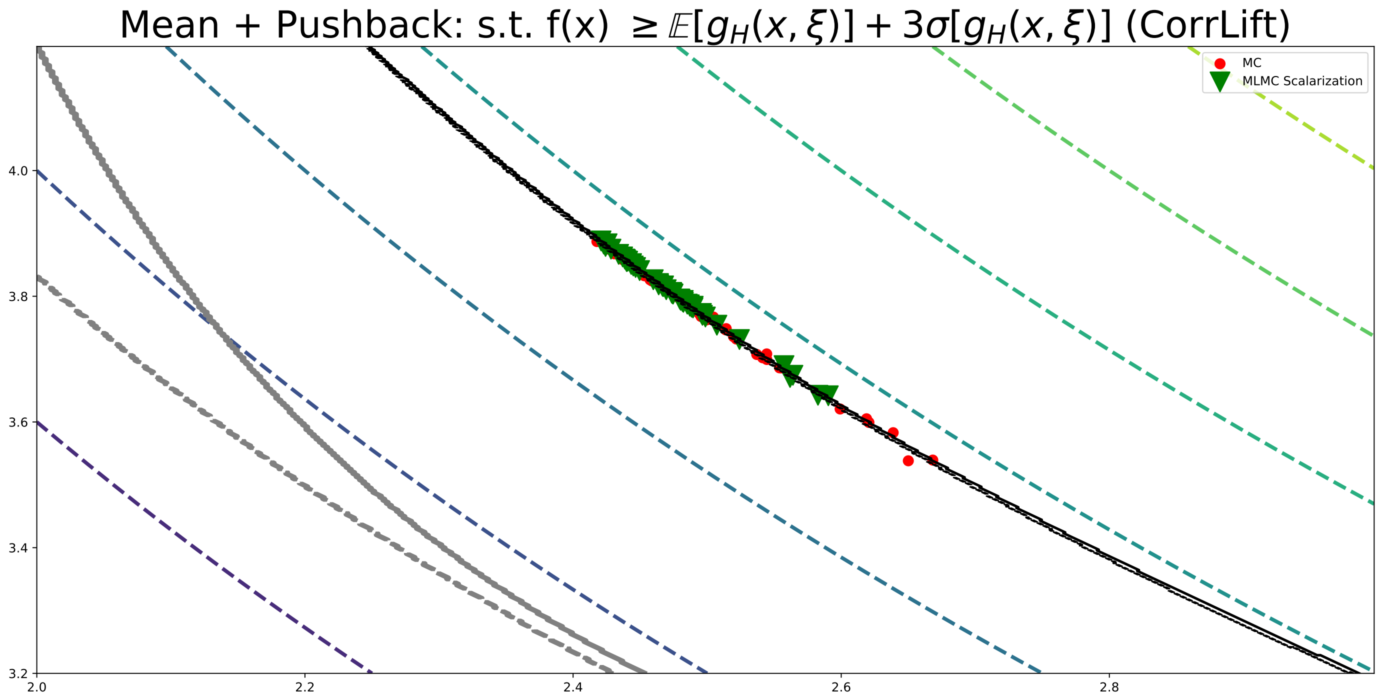
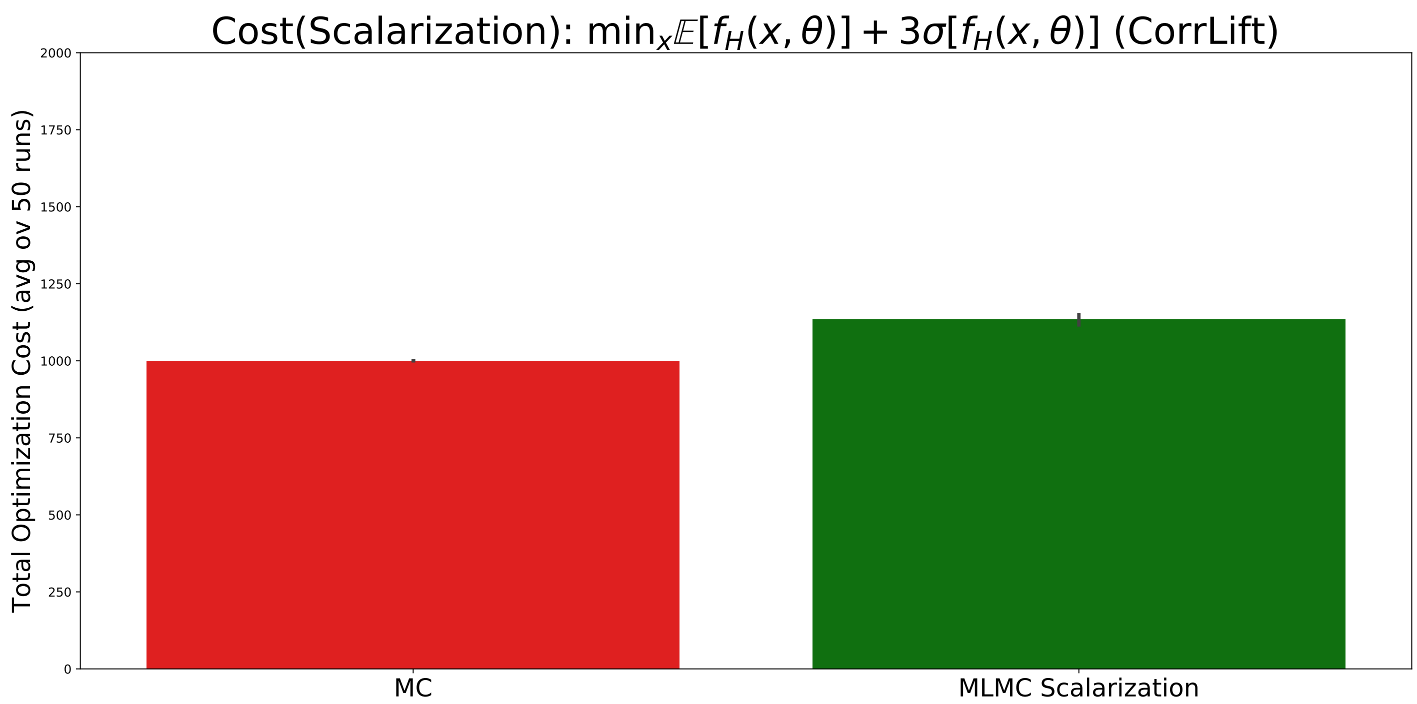
OUU Results (CorrLift)



- CorrLift can reduce costs and improve the results
- Still higher computational cost compared to MC

OUU Results (CorrLift)



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Conclusion

⇒ New MLMC estimators for Standard Deviation and Scalarization coupled with **SNOWPAC**.

⇒ New approximations for $\mathbb{C}$ov-Term in Scalarization.

Future work and open questions:

- Investigate cost increase in Cantilever case
- Near future: Wind application

Links:

- SNOWPAC: github.com/snowpac/snowpac
- Dakota: dakota.sandia.gov

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References:

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