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Technical University of Munich

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Multifidelity Monte Carlo Estimators for Robust Formulations in Optimization under Uncertainty

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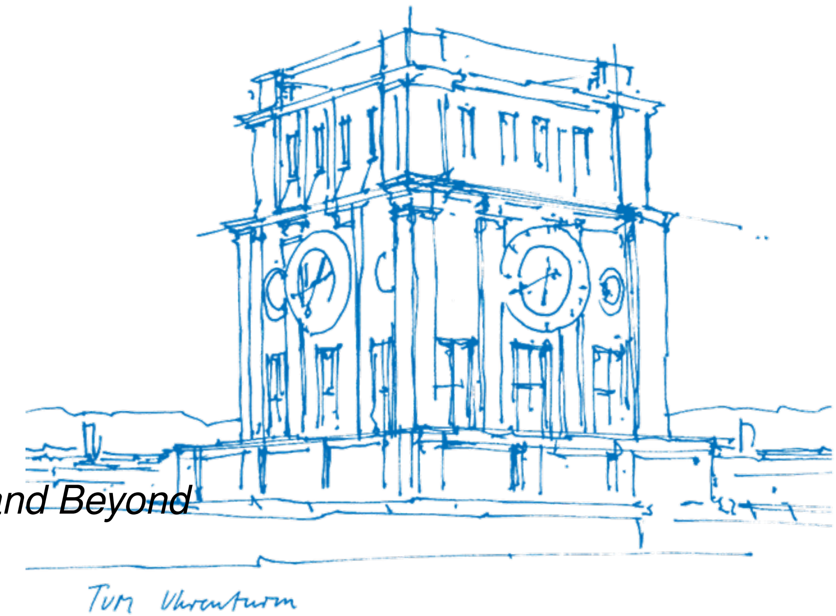

SIAM CSE 2021

MS18

Models, Layers, Levels, Fidelities: Hierarchies in UQ and Beyond

Virtual, Mar 1st, 2021

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Motivation: Design optimization of a wind power plant

Provided by NREL

Vattenfall's Horns Rev wind farm off Denmark*

Setup:

- Wakes of turbine upstream interfere with turbines downstream
- Task: Steer turbines to maximize total power production P_{total}

Challenges:

- Complex, computationally expensive CFD black box code
- Uncertain conditions
- No gradients available

*Figure from https://www.rechargenews.com/wind/will-wind-wake-slow-industrys-ambitions-offshore-/2-1-699430

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Mean in OUU:

$$\max_{\gamma} \mathscr{R}_{\text{Mean}} := \max_{\gamma} \mathbb{E}[P_{\text{total}}(\gamma, \theta)]$$

Scalarization in OUU:

$$\max_{\gamma} \mathscr{R}_{\text{Pback}} := \max_{\gamma} (\mathbb{E}[P_{\text{total}}(\gamma, \theta)] - 3\sigma[P_{\text{total}}(\gamma, \theta)])$$

- γ: yaw angles of turbines
- θ: uncertain/stochastic inputs (wind speed, sensor errors, etc.)
- $\mathscr{R}$: measure of robustness/reliability

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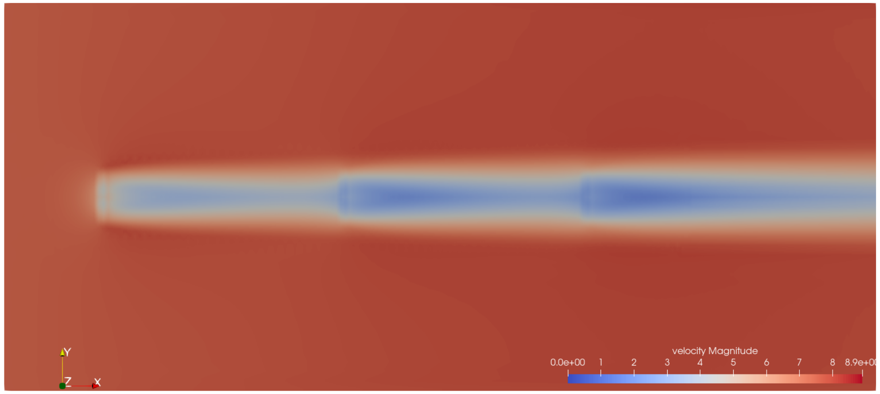

Mean in OUU:

$$\max_{\gamma} \mathbb{E}[P_{\text{total}}(\gamma, \theta)]$$
$$\approx \max_{\gamma} \frac{1}{N} \sum_{i=1}^{N} [P_{\text{total}}(\gamma, \theta_i)]$$

Scalarization in OUU:

$$\max_{\gamma} \mathbb{E}[P_{\text{total}}(\gamma, \theta)] - 3\sigma[P_{\text{total}}(\gamma, \theta)]$$
$$\approx \max_{\gamma} \frac{1}{N} \sum_{i=1}^{N} P_{\text{total}}(\gamma, \theta_i) - 3\sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (P_{\text{total}}(\gamma, \theta_i) - \hat{P})^2}$$

MC property: Error $\sim \mathcal{O}(\frac{1}{\sqrt{N}}) \Rightarrow N$ should be high but evaluations computationally expensive!

Motivation: Design optimization of a wind power plant

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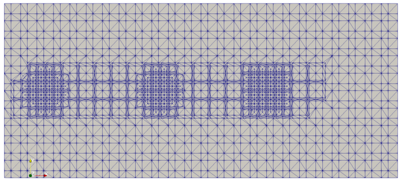
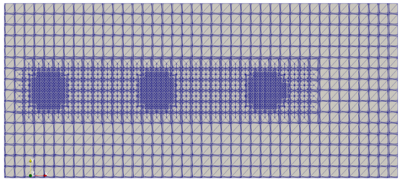
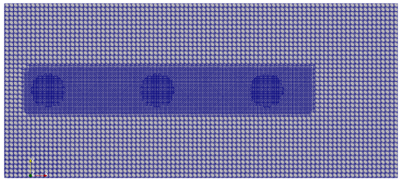
Hierarchies of levels and fidelities (future work) available:

- Discretization level:







- Model level:

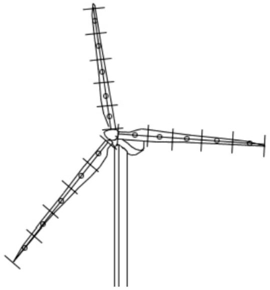


Image: Yu, Zheng, Ma, https://nwtc.nrel.gov/OpenFAST – Jason Jonkman, et al.

Courtesy of Barone and Maniaci, SNL

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Motivation: Design optimization of a wind power plant

Provided by NREL

Leverage hierarchy using multilevel Monte Carlo estimators:

Mean in OUU:

$$\min_x \mathscr{R}_{\text{Mean}} := \max_\gamma \mathbb{E}[P_{\text{total}}(\gamma,\theta)] \approx \widehat{\mu_1^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)]$$

Push back:

$$\min_x \mathscr{R}_{\text{Pback}} := \max_\gamma \mathbb{E}[P_{\text{total}}(\gamma,\theta)] - 3\sigma[P_{\text{total}}(\gamma,\theta)] \approx \max_\gamma \widehat{\mu_1^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)] - 3\widehat{\sigma^{\text{ML}}_{\text{biased}}}[P_{\text{total}}(\gamma,\theta)]$$

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Up next:

Motivation: Design optimization of a wind power plant

Provided by NREL

Leverage hierarchy using multilevel Monte Carlo estimators:

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Up next:

1. Recap: $\widehat{\mu_1^{\text{ML}}}[P_{\text{total}}(\gamma, \theta)]$

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$$\approx \max_\gamma \widehat{\mu_1^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)] - 3\widehat{\sigma_{\text{biased}}^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)]$$

Up next:

1. Recap: $\widehat{\mu_1^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)]$
2. (Our contribution) ML for Standard deviation: $\widehat{\sigma_{\text{biased}}^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)]$

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Up next:

1. Recap: $\widehat{\mu_1^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)]$
2. (Our contribution) ML for Standard deviation: $\widehat{\sigma_{\text{biased}}^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)]$
3. (Our contribution) ML for Scalarization: $\widehat{\mu_1^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)] - 3\widehat{\sigma_{\text{biased}}^{\text{ML}}}[P_{\text{total}}(\gamma,\theta)]$

Multilevel Monte Carlo (MLMC) Estimator

MLMC estimator: Mean

Mean in OUU:

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

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

MLMC estimator: Mean

Mean in OUU:

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

- Estimator[†]:

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

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

MLCC estimator: Mean

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

- Estimator[†]:

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

- Sample allocation:

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

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

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

MLMC estimator: Mean

Mean in OUU:

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

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

- Sample allocation:

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- Solution:

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

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

MLMC estimator: Standard deviation

Mean in OUU:

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

Standard deviation in OUU:

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

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MLMC estimator: Standard deviation

- Estimator:

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

where

$$\begin{aligned}
\mathbb{V}[Q_L] \approx \widehat{\mu_2^{\text{ML}}}[Q_L] &= \sum_{\ell=0}^{L} \widehat{\mu_2}[Q^{(\ell)}] - \widehat{\mu_2}[Q^{(\ell-1)}] \\
&= \sum_{\ell=0}^{L} \frac{1}{N_\ell - 1} \left(\sum_{i=1}^{N_\ell} (Q_i^{(\ell)} - \widehat{\mu_1^{(\ell)}})^2 - (Q_{i,\ell}^{(\ell-1)} - \widehat{\mu_{1,\ell}^{(\ell-1)}})^2 \right) \\
&= \sum_{\ell=0}^{L} (\widehat{\mu_2^{(\ell)}} - \widehat{\mu_{2,\ell}^{(\ell-1)}}), \quad Q_{i,0}^{(-1)} := 0
\end{aligned}$$

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MLMC estimator: Standard deviation

- Estimator:

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

where

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

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

$$= \sum_{\ell=0}^{L} (\widehat{\mu_2^{(\ell)}} - \widehat{\mu_{2,\ell}^{(\ell-1)}}), \quad Q_{i,0}^{(-1)} := 0$$

- Sample allocation:

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

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

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MLMC estimator: Standard deviation

- Estimator:

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

where

$$\begin{aligned}\mathbb{V}[Q_L] \approx \widehat{\mu_2^{\text{ML}}}[Q_L] &= \sum_{\ell=0}^{L} \widehat{\mu_2}[Q^{(\ell)}] - \widehat{\mu_2}[Q^{(\ell-1)}] \\ &= \sum_{\ell=0}^{L} \frac{1}{N_\ell - 1} \left(\sum_{i=1}^{N_\ell} (Q_i^{(\ell)} - \widehat{\mu_1^{(\ell)}})^2 - (Q_{i,\ell}^{(\ell-1)} - \widehat{\mu_{1,\ell}^{(\ell-1)}})^2 \right) \\ &= \sum_{\ell=0}^{L} (\widehat{\mu_2^{(\ell)}} - \widehat{\mu_{2,\ell}^{(\ell-1)}}), \quad Q_{i,0}^{(-1)} := 0\end{aligned}$$

- Sample allocation:

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

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

- Solution: Numerical Optimization

MLMC estimator: Standard deviation

- Estimator:

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

where

$$\begin{aligned}\mathbb{V}[Q_L] \approx \widehat{\mu_2^{\mathrm{ML}}}[Q_L] &= \sum_{\ell=0}^{L} \widehat{\mu_2}[Q^{(\ell)}] - \widehat{\mu_2}[Q^{(\ell-1)}] \\ &= \sum_{\ell=0}^{L} \frac{1}{N_\ell - 1}\left(\sum_{i=1}^{N_\ell} (Q_i^{(\ell)} - \widehat{\mu_1^{(\ell)}})^2 - (Q_{i,\ell}^{(\ell-1)} - \widehat{\mu_{1,\ell}^{(\ell-1)}})^2 \right) \\ &= \sum_{\ell=0}^{L} (\widehat{\mu_2^{(\ell)}} - \widehat{\mu_{2,\ell}^{(\ell-1)}}), \quad Q_{i,0}^{(-1)} := 0\end{aligned}$$

- Sample allocation:

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

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

- Solution: Numerical Optimization

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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:

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

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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- Estimator:

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- Sample allocation:

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

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- Variance of scalarization:

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

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

- Solution: Numerical Optimization

MLMC estimators: 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:

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

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

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

From work for higher order moments:

- 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.
- (Bierig, C., Chernov, A., “Estimation of arbitrary order central statistical moments by the multilevel Monte Carlo method,” Stochastics and Partial Differential Equations Analysis and Computations, Vol. 4, No. 1, 2016, pp. 3-40.)

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

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

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MLMC estimators: Analytic approximation

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- **Idea**: Use similar analytic solution approach as for MLMC Mean:

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

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

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

From work for higher order moments:

- 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.
- (Bierig, C., Chernov, A., “Estimation of arbitrary order central statistical moments by the multilevel Monte Carlo method,” Stochastics and Partial Differential Equations Analysis and Computations, Vol. 4, No. 1, 2016, pp. 3-40.)

MLMC estimators: Analytic approximation

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

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

$$\text{s.t. } \mathbb{V}[\widehat{\mu_x^{\mathrm{ML}}}] = \varepsilon^2, \text{ where } \mathbb{V}[\widehat{\mu_x^{\mathrm{ML}}}] = \sum_{\ell=0}^{L} \frac{\mathscr{V}_\ell}{N_\ell}$$

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

- Introduce helper variance: $\mathscr{V}_\ell = \mathbb{V}[\widehat{\mu_x^{(\ell)}}] N_\ell^{\mathbb{X}} \Leftrightarrow \mathbb{V}[\widehat{\mu_x^{(\ell)}}] = \frac{\mathscr{V}_\ell}{N_\ell}$
- Disregard higher order terms in $\mathscr{V}_\ell \Rightarrow$ Analytic approximation

From work for higher order moments:

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Coupling ML with OUU

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SNOWPAC*

OUU problem statement

$$\mathcal{R}_\theta^* = \mathcal{R}^f(\mathbf{x}^*, \theta) = \min_{\mathcal{R}^c(\mathbf{x},\theta)\leq 0} \mathcal{R}^f(\mathbf{x}, \theta)$$

Features of SNOWPAC:

0. **Extension of NOWPAC**: Derivative-free nonlinear constraint optimization method using trust-regions (deterministic)
1. **Estimate robustness measures**: Use sampling, e.g.

$$\mathcal{R}_\theta^f = \mathbb{E}[f_\theta(\mathbf{x})] \approx R^f = \frac{1}{N}\sum_{i=1}^N f(\mathbf{x}, \theta_i) + \varepsilon_N$$

2. **Implement new trust region management**: Account for noise ε_N in objective/constraint evaluations
3. **Introduce Gaussian process surrogates**: Mitigate effect of noise ε_N
4. **Feasibility restoration mode**

*F. Augustin, Y. Marzouk, A trust-region method for derivative-free nonlinear constrained stochastic optimization. 2017

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SNOWPAC*

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$$\mathscr{R}^f_\theta = \mathbb{E}[f_\theta(\mathbf{x})] \approx R^f = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} (f^\ell(\mathbf{x}, \theta_i) - f^{\ell-1}(\mathbf{x}, \theta_i)) + \varepsilon_N$$

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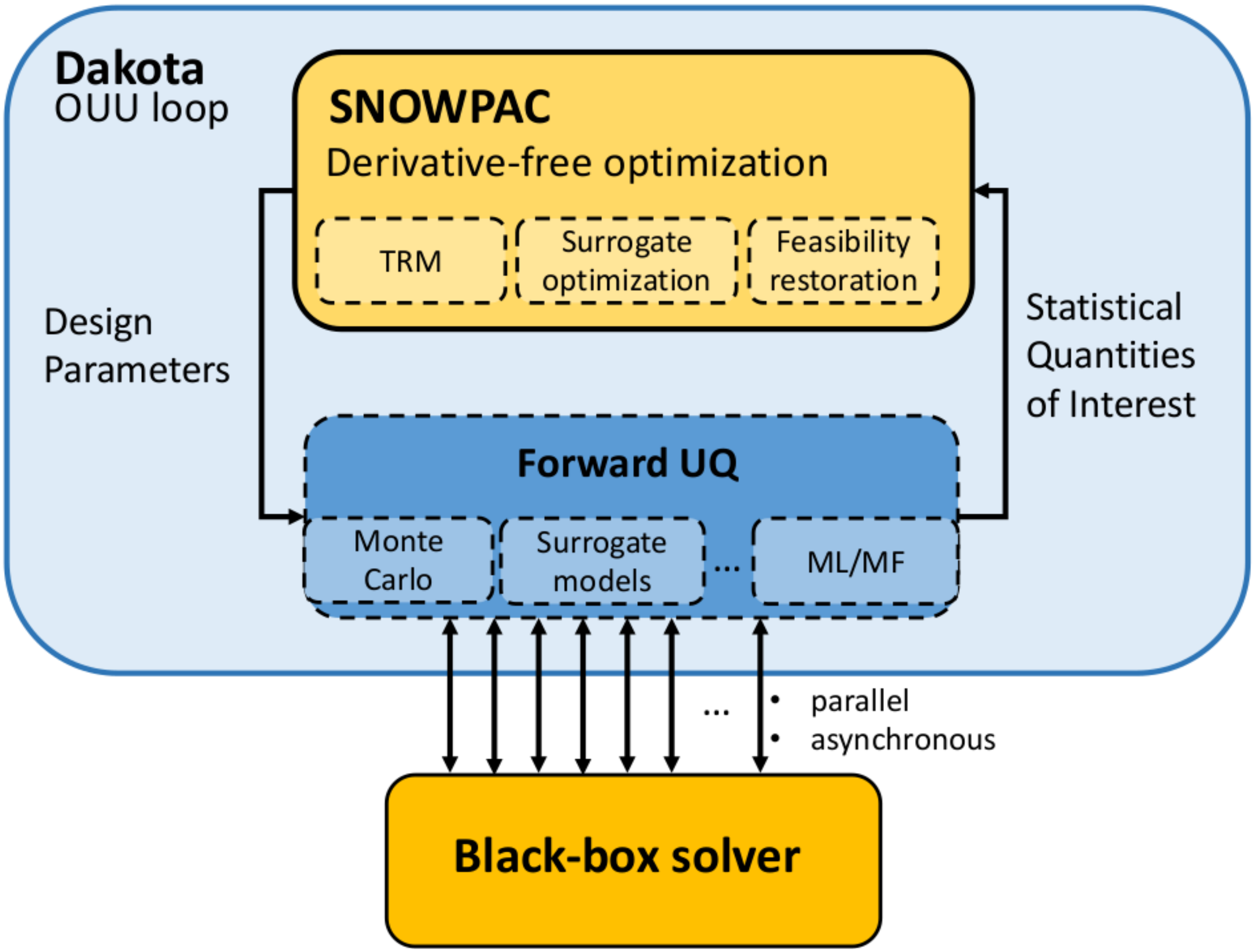
SNOWPAC in Dakota using MLMC



Benchmark Results

Problem statement

Objective:

$$f(x) = \begin{cases} (x-2)^2 & \text{if } x \leq 3 \\ 2\log(x-2)+1 & \text{if } x > 3 \\ x \in [0,6] \end{cases}$$

OUU:

$$\min_x f(x)$$

Mean:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)]$

Push back:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)] + 3\sigma[g_H(x,\xi)]$

Constraint:

$$g_{det}(x) = \frac{2.log(1.5)}{2.5}x - \frac{2.log(1.5)}{2.5}$$

$$g_H(x,\xi) = g_{det}(x) + \xi^3$$

$$g_L(x,\xi) = g_{det}(x) + A(x)\xi^3, \xi \sim \mathscr{U}(-0.5, 0.5)$$

$$A(x) = \frac{1}{12}x + 0.4$$

Algorithmic comparison:

- AA: Analytic Approximation
- Opt: Numerical Optimization

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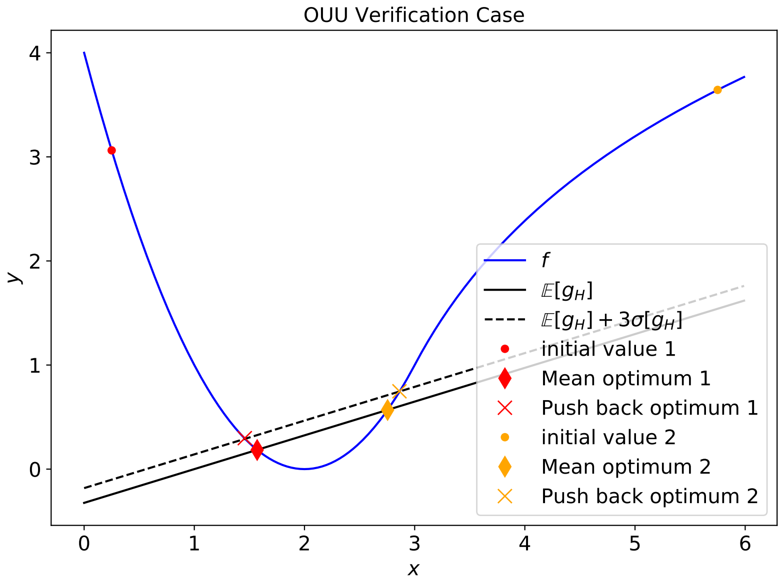

Sampling Results: Sample allocation

- Mean

$$\mathbb{E}[g_H(x,\xi)] \approx \widehat{\mu_1^{\mathrm{ML}}}[g_{H/L}(x,\xi)]$$

N_{MC}		$x=1$	3	5
200	N_L	213	236	233
	N_H	69	39	16
300	N_L	309	354	350
	N_H	103	58	24

- Scalarization

$$\mathbb{E}[g_H(x,\xi)] + 3\sigma[g_H(x,\xi)] \approx \widehat{\zeta^{\mathrm{ML}}}[g_{H/L}(x,\xi)]$$

N_{MC}		$x=1$	3	5
200	N_L	303	384	419
	N_H	190	121	63
300	N_L	456	579	626
	N_H	285	180	90

- Total computational cost: $C_T = 1.0 N_L + 1.1 N_H$
- Computational cost decrease for increasing x $\Leftrightarrow$ Higher correlation due to $A(x)$
- Overall higher computational cost for scalarization $\Leftrightarrow$ Need for higher resolution
- Cost for scalarization for $x = 1$ even higher than for standard MC $\Leftrightarrow$ Upper bound on $\mathbb{C}$ov

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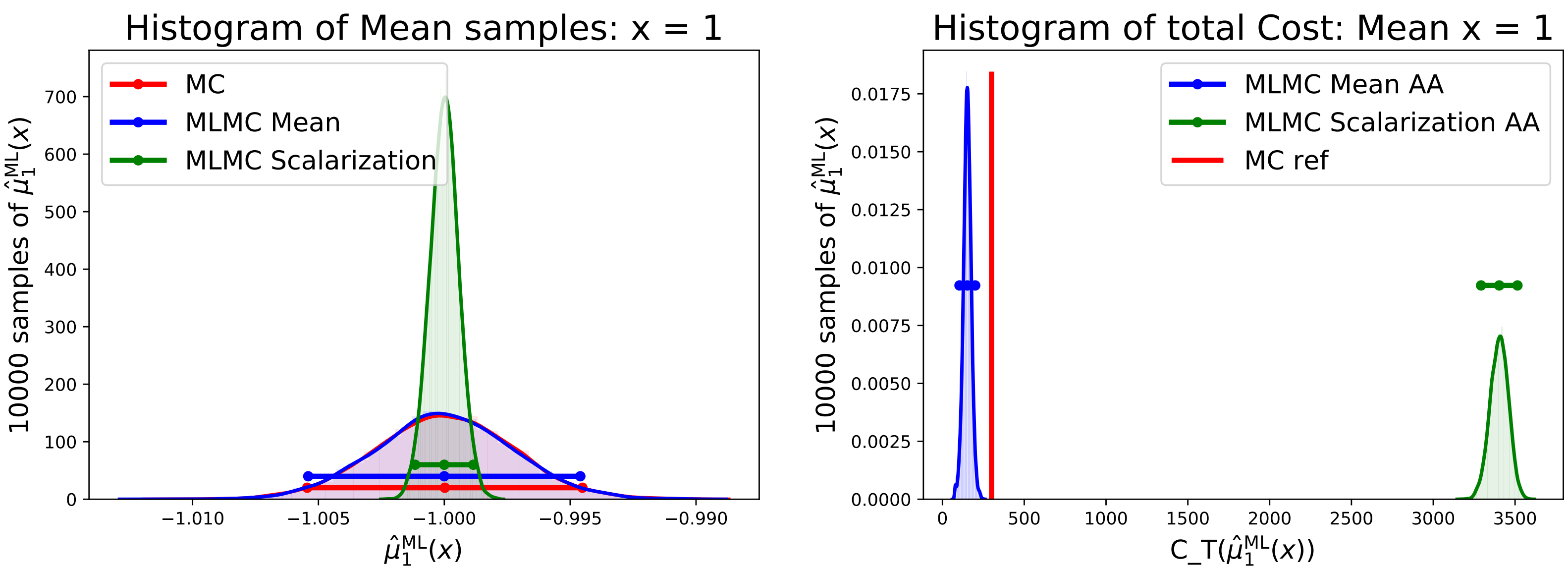
Sampling Results



Mean: $\widehat{\mu_1^{ML}}[g_{H/L}(x,\xi)]$

- MLMC Mean distribution consistent with MC reference
- MLMC Scalarization overresolves, results in higher computational cost

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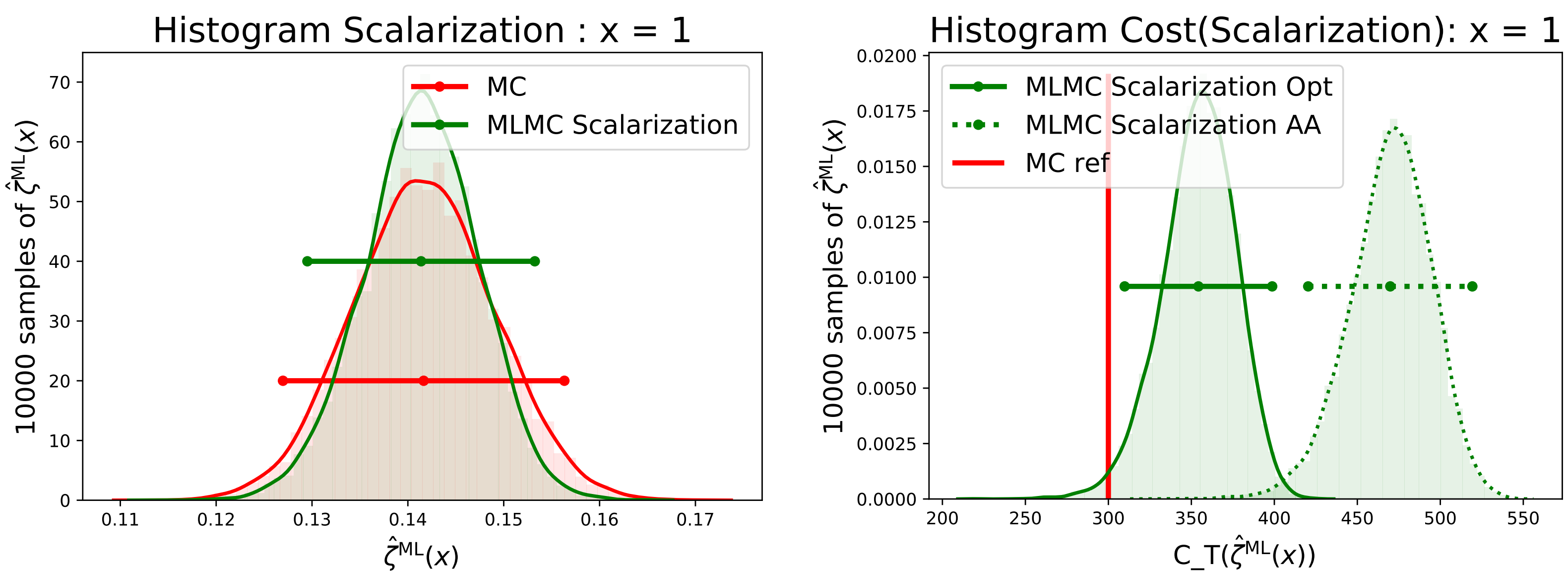
Sampling Results



Scalarization: $\widehat{\zeta^{\mathrm{ML}}}[g_{H/L}(x,\xi)]$

- MLMC Scalarization close to MC reference case
- MLMC Scalarization overresolves due to upper bound in $\mathbb{C}$ov
- Numerical optimization reduce cost compared to analytical approximation
- Results in higher computational cost than MC reference for $x = 1$

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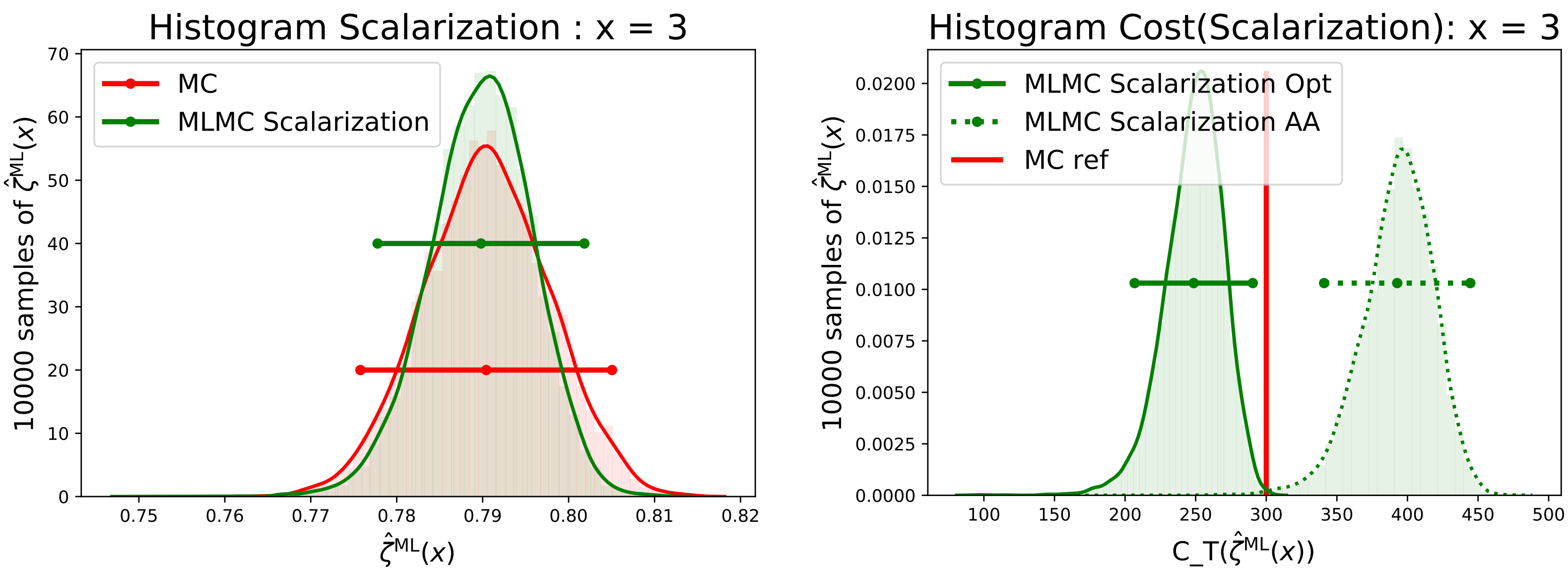
Sampling Results



Scalarization: $\widehat{\zeta^{\mathrm{ML}}}[g_{H/L}(x,\xi)]$

- MLMC Scalarization close to MC reference case
- MLMC Scalarization overresolves due to upper bound in $\mathbb{C}$ov
- Numerical optimization reduce cost compared to analytical approximation
- Decrease in cost and lower than MC reference for increase in x

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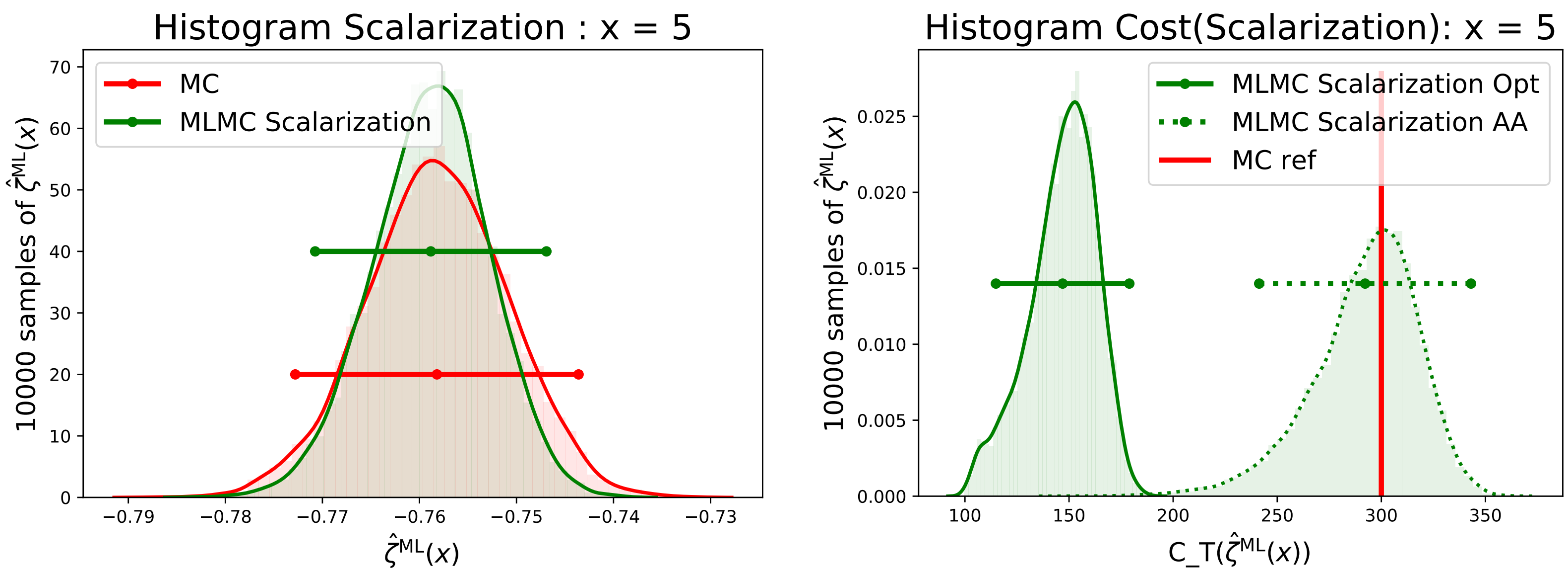
Sampling Results



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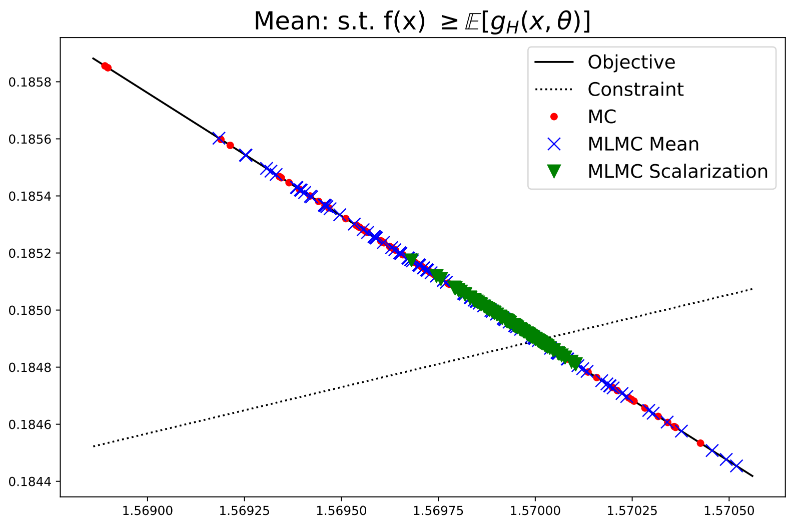
- MLMC Scalarization close to MC reference case
- MLMC Scalarization overresolves due to upper bound in $\mathbb{C}$ov
- Numerical optimization reduce cost compared to analytical approximation
- Decrease in cost and lower than MC reference for increase in x

OUU Results

Mean:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)]$



- Consistent match between MLMC Mean and MC
- Scalarization overresolves

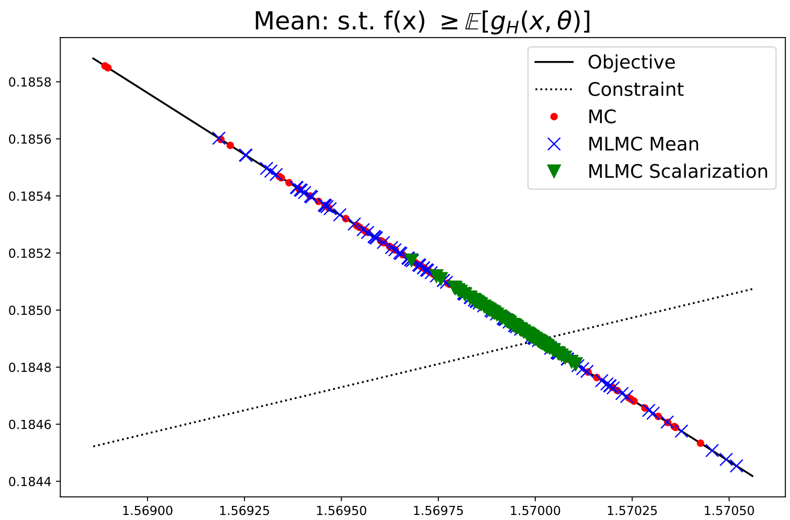
OUU Results

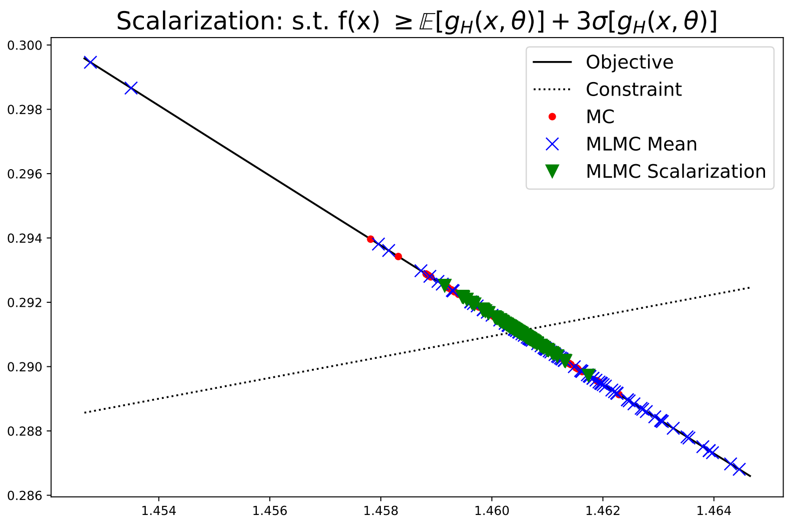
Mean:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)]$

Push back:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)] + 3\sigma[g_H(x,\xi)]$





- Consistent match between MLMC Mean and MC
- Scalarization overresolves

- More accurate result for MLMC Scalarization cmp to MC
- MLMC Mean underresolves

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Mean:

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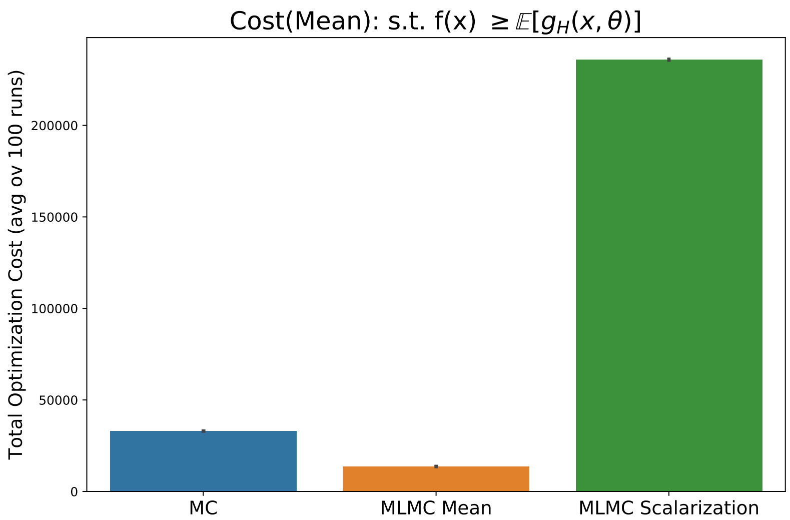
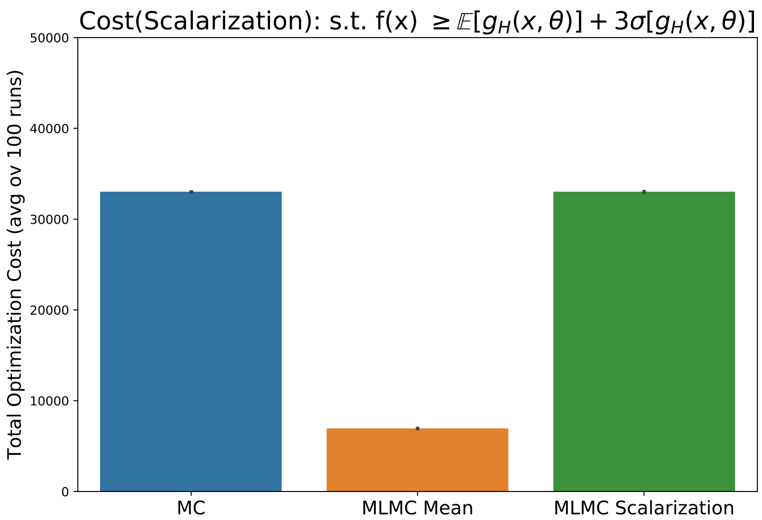




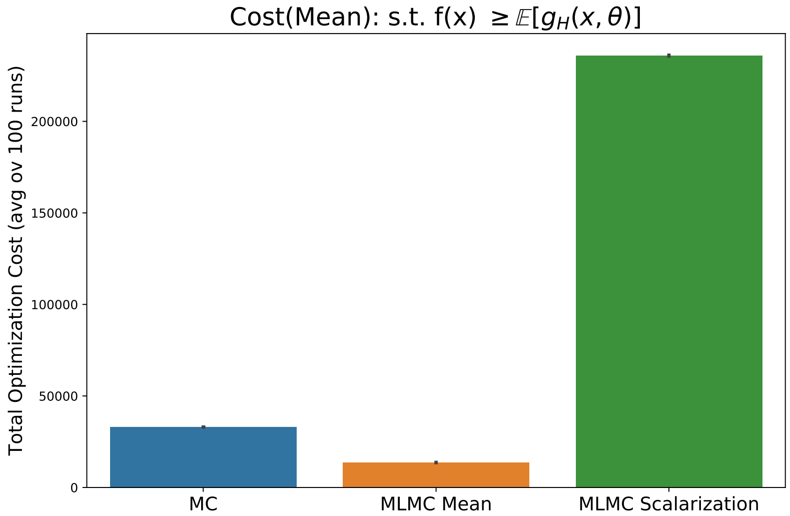
- Lower cost for MLMC Mean
- High cost for MLMC Scalarization

- Similar cost between Scalarization and MC (due to numerical opt)
- Too low cost for MLMC Mean

OUU Results

Mean:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)]$



- Lower cost for MLMC Mean
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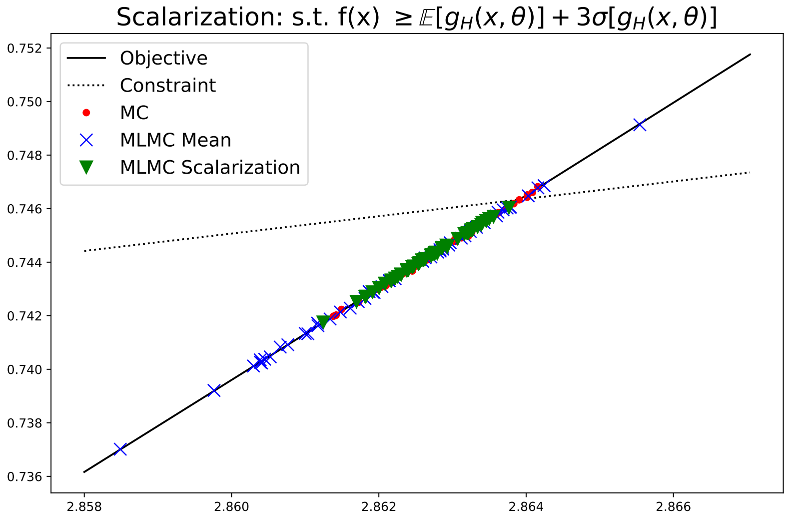
Push back:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)] + 3\sigma[g_H(x,\xi)]$



- Start at $x = 5.75$
- Consistent match between MLMC Scalarization and MC

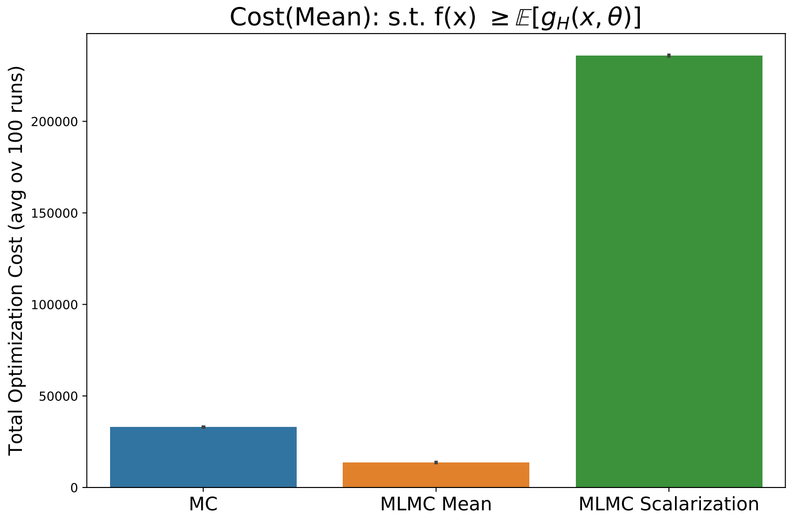
OUU Results

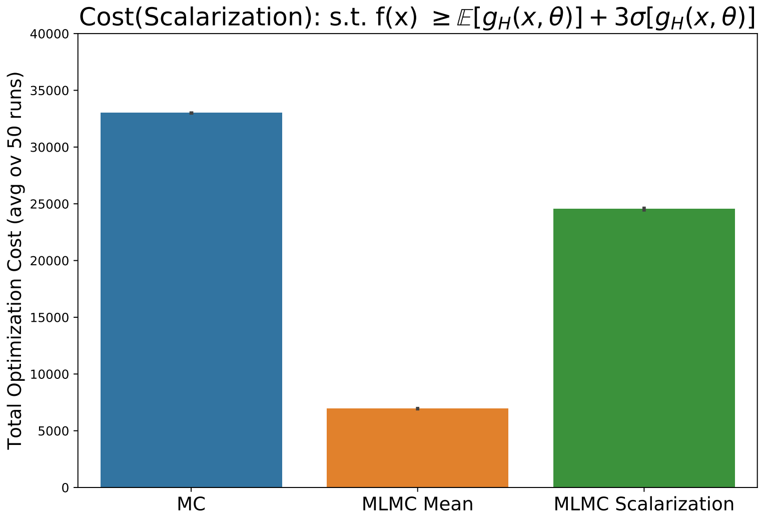
Mean:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)]$

Push back:

s.t. $f(x) \geq \mathbb{E}[g_H(x,\xi)] + 3\sigma[g_H(x,\xi)]$





- Lower cost for MLMC Mean
- High cost for MLMC Scalarization

- Start at $x = 5.75$
- Computational cost now lower than MC reference

Conclusion

- **NOWPAC** – Derivative-free trust region methods for constrained nonlinear optimization
- **SNOWPAC** – Stochastic derivative-free optimization using Gaussian process surrogates
- **DAKOTA** – Design Analysis Kit for Optimization and Terascale Applications

$\Rightarrow$ New MLMC estimators for Standard Deviation and Scalarization coupled with **SNOWPAC**.

Future work and open questions:

- Investigate bound for scalarization
- From MLMC to ACV

Links:

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

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References:

- FM, GG, DTS, MSE, RNK, HJB, YMM, Higher moment multilevel estimators for optimization under uncertainty applied to wind plant design. AIAA 2020
- F. Menhorn, F. Augustin, HJB, YMM, A trust-region method for derivative-free nonlinear constrained stochastic optimization. to be submitted

Multilevel Monte Carlo estimator: Standard deviation

Variance of variance:

$$\mathbb{V}[\widehat{\mu_2^{\text{ML}}}] = \sum_{\ell=0}^{L} \mathbb{V}[\widehat{\mu_2^{(\ell)}}] + \mathbb{V}[\widehat{\mu_{2,\ell}^{(\ell-1)}}] - 2\mathbb{C}\text{ov}[\widehat{\mu_2^{(\ell)}}, \widehat{\mu_{2,\ell}^{(\ell-1)}}]$$

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- $\mathbb{V}[\widehat{\mu_2}] = \frac{(N-1)}{N^2-2N+3}\left(\widehat{\mu_4} - \frac{N-3}{N-1}\widehat{\mu_2}^2\right)$

$$\text{where } \widehat{\mu_4} = \frac{1}{(N^2-3N+3) - \frac{(6N-9)(N^2-N)}{N(N^2-2N+3)}}\left(\frac{N^3}{N-1}\widehat{\mu_{4,\text{biased}}} - \frac{(6N-9)(N^2-N)}{N^2-2N+3}\widehat{\mu_2}^2\right)$$

- $\mathbb{C}\text{ov}[\widehat{\mu_2^{(\ell)}}, \widehat{\mu_{2,\ell}^{(\ell-1)}}] = \frac{1}{N_\ell}\mathbb{E}[\widehat{\mu_2^{(\ell)}}\widehat{\mu_{2,\ell}^{(\ell-1)}}] + \frac{1}{N_\ell(N_\ell-1)}(\widehat{\mu_1^{(\ell)}}[Q^{(\ell)}Q^{(\ell-1)}] - \widehat{\mu_1^{(\ell)}}\widehat{\mu_{1,\ell}^{(\ell-1)}})^2$

$$\begin{aligned}\text{where } \mathbb{E}[\widehat{\mu_2^{(\ell)}}\widehat{\mu_{2,\ell}^{(\ell-1)}}] = {} & \widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)2}Q^{(\ell-1)2}\right] - 2\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)2}Q^{(\ell-1)}\right]\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell-1)}\right] \\ & + 2\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell-1)}\right]^2\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)2}\right] - 2\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)}\right]\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)}Q^{(\ell-1)2}\right] \\ & + 4\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell-1)}\right]\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)}\right]\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)}Q^{(\ell-1)}\right] + 2\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)}\right]^2\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell-1)2}\right] \\ & - 4\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)}\right]^2\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell-1)}\right]^2 - \widehat{\mu_1^{(\ell)}}\left[Q^{(\ell)2}\right]\widehat{\mu_1^{(\ell)}}\left[Q^{(\ell-1)2}\right].\end{aligned}$$