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Scientific Computing
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Technical University of Munich

Multilevel Estimators for Measures of Robustness in Optimization under Uncertainty

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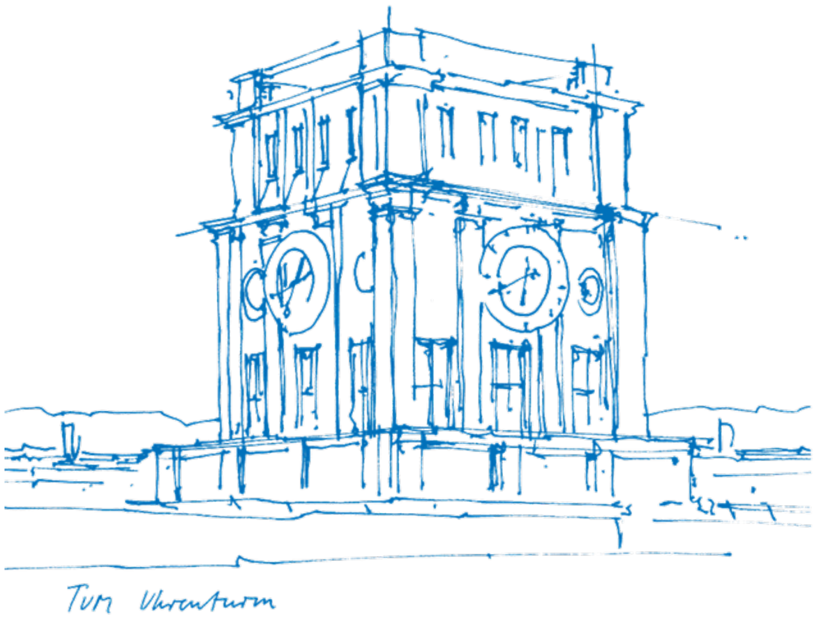
USNCCM 16, July 25-29, 2021

MS307

Data-Enhanced Modeling and Uncertainty Quantification of Systems with Multiple Fidelities

Virtual, Jul 26th, 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 upstream turbine 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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$\Rightarrow$ Results in **optimization under uncertainty (OUU)** problem

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Mean in OUU:

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

Scalarization (= Mean + α Sigma) in OUU:

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

- γ: yaw angles of turbines
- θ: uncertain/stochastic inputs (wind speed, sensor errors, etc.)
- P_{total}: Total (yearly) power production
- $\mathscr{R}_{\text{Mean}}$: measure to maximize mean

- $\mathscr{R}_{\text{Scalar}}$: measure to maximize mean while decreasing variance $\Rightarrow$ higher robustness/reliablity

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

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

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

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Leverage hierarchy using multilevel Monte Carlo estimators:

Mean in OUU:

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

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Up next:

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Up next:

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

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Up next:

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

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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

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

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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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Standard deviation in OUU:

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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

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

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

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

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

- Sample allocation:

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

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

MLMC estimator: Standard deviation

- Estimator:

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

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- Solution: Numerical Optimization (Different to the mean, no closed form available)

MLMC estimator: Standard deviation

- Estimator:

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

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- 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

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- Variance of scalarization:

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

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- Solution: Numerical Optimization

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MLMC estimator: Scalarization Covariance

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

Three (independent) solution strategies:

MLMC estimator: Scalarization Covariance

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Three (independent) solution strategies:

- Pearson correlation:

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

MLMC estimator: Scalarization Covariance

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- Jensen inequality:

$$\mathbb{C}\text{ov}[\widehat{\mu_1^{\text{ML}}}, \widehat{\sigma_{\text{biased}}^{\text{ML}}}] \leq \frac{1}{N_\ell}\Big((N_\ell - 6)(N_\ell - 2)\mathbb{E}[Q]^2\mathbb{E}[Q^2] + (N_\ell - 3)\mathbb{E}[Q^2]^2 + (2N_\ell - 4)\mathbb{E}[Q^3]\mathbb{E}[Q]$$
$$+ \mathbb{E}[Q^4] - (N_\ell - 2)(N_\ell - 3)\mathbb{E}[Q]^4\Big)^{\frac{1}{2}} - \widehat{\mu_1^{(\ell)}}\mathbb{E}[\widehat{\sigma_{\text{biased}}^{(\ell)}}]$$

$$\text{, since } \varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi[X]], X \text{ integrable}, \varphi \text{ convex.}$$

MLMC estimator: Scalarization Covariance

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

Three (independent) solution strategies:

- Pearson correlation: (easy to compute, **inequality**)
- Jensen inequality: (terms need numerical estimation, **inequality**)

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Three (independent) solution strategies:

- Pearson correlation: (easy to compute, **inequality**)
- Jensen inequality: (terms need numerical estimation, **inequality**)
- Bootstrapping (more expensive, **approximation**):

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

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

similarly for $\widehat{\sigma_{\text{biased},b}^{(\ell)}}$ and $\overline{\widehat{\sigma_{\text{biased},b}^{(\ell)}}}$

Results

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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 and Analytic Approximation (AA)†

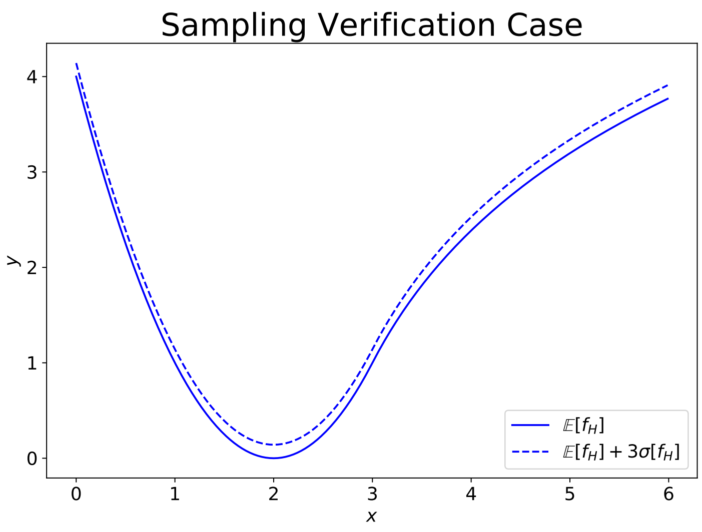
Test problem:

Deterministic:

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

Stochastic extension:

$$f_H(x,\xi) = f_{det}(x) + \xi^3$$
$$f_L(x,\xi) = f_{det}(x) + A(x)\xi^3, \xi \sim \mathscr{U}(-0.5, 0.5)$$
$$A(x) = \frac{1}{12}x + 0.4$$



†Pisaroni, M., Krumscheid, S., Nobile, Fabio. (2020). Quantifying uncertain system outputs via the multilevel Monte Carlo method — Part I: Central moment estimation. Journal of Computational Physics. 414.

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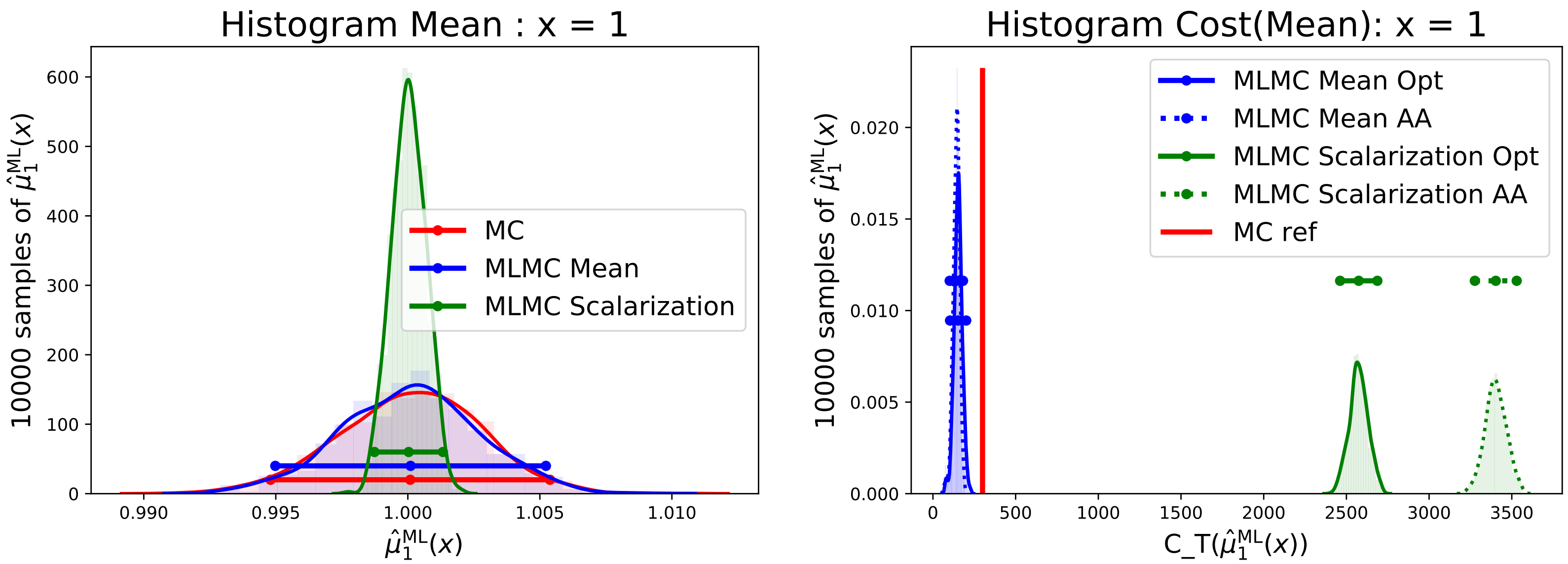
Sampling Results: Mean

$\mathbb{E}[f_H(x,\xi)] \approx \widehat{\mu_1^{\text{ML}}}[f_{H/L}(x,\xi)]$



- MLMC Mean distribution (blue) consistent with MC reference (red) (left) for lower cost (right)
- MLMC Scalarization (green) overresolves (left), results in higher computational cost (right)

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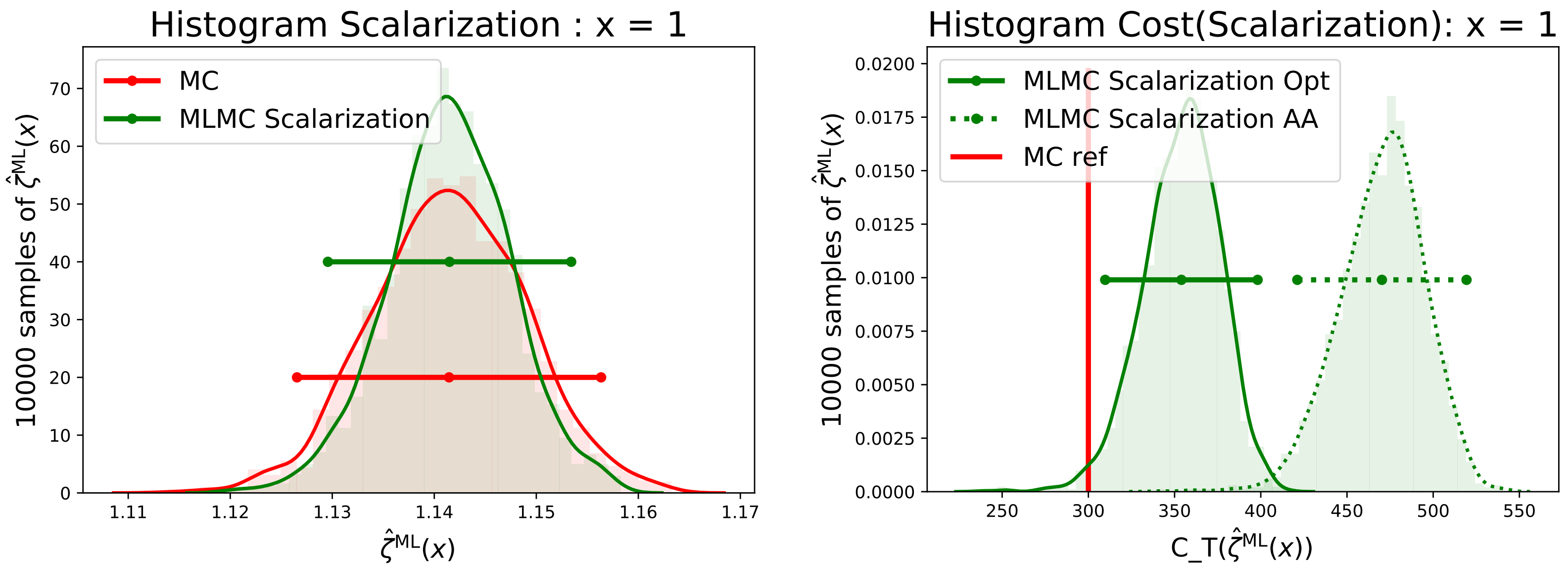
Sampling Results: Scalarization (Pearson)

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



- MLMC Scalarization (green) close to MC reference case (red)
- MLMC Scalarization overresolves due to upper bound in $\mathbb{C}$ov using Pearson property
- Results in higher computational cost than MC reference for $x = 1$

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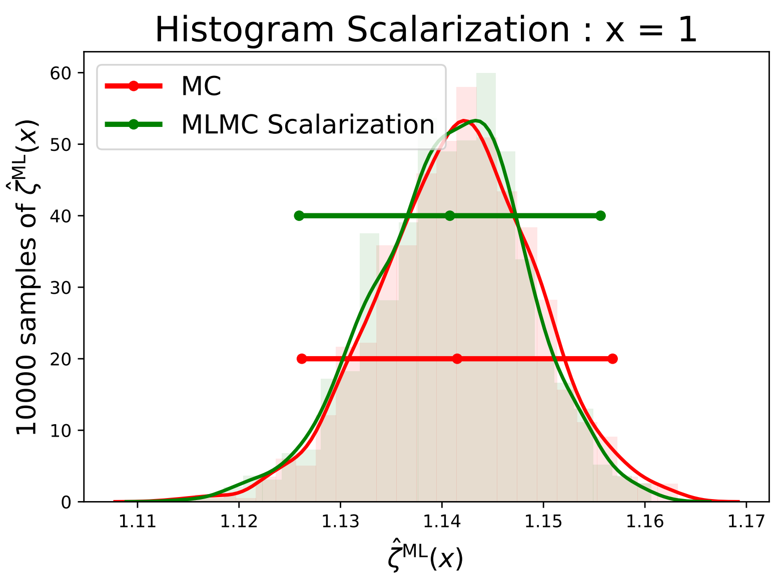
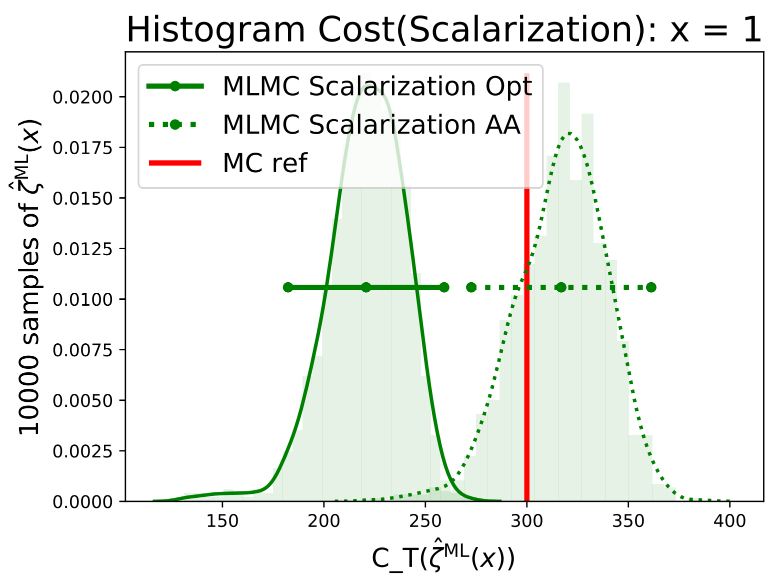
Sampling Results: Scalarization (Bootstrap)

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





- MLMC Scalarization (green) consistent with MC reference (red) (left) for lower cost (right) using Bootstrap.
- Numerical optimization (Opt) reduce cost compared to analytical approximation (AA)

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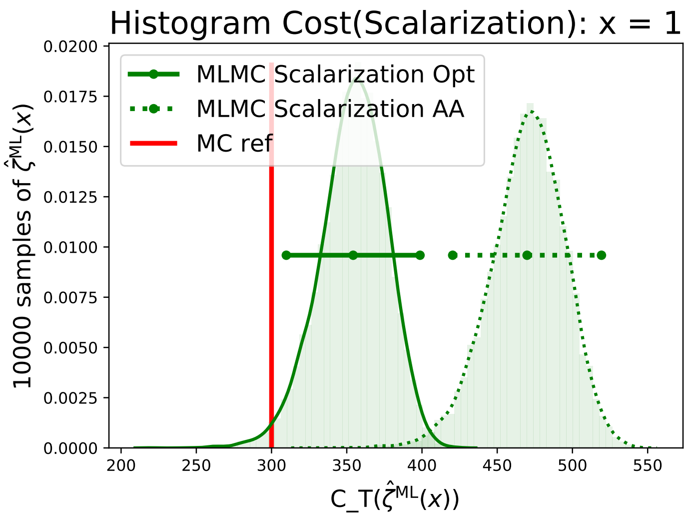
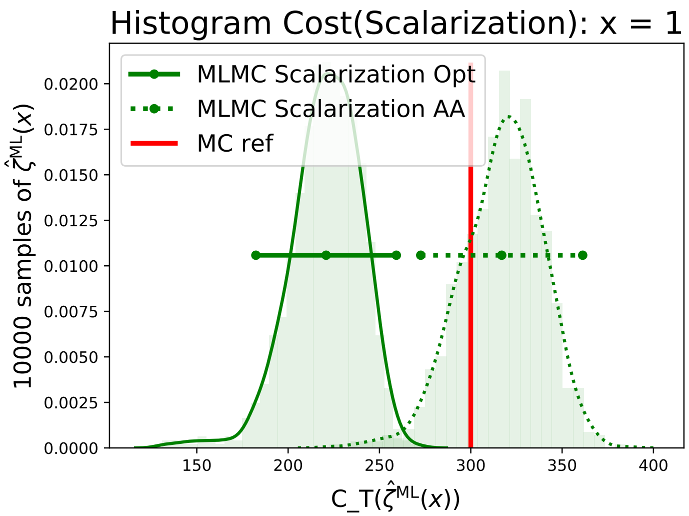
Sampling Summary

- MLMC targeting the respective formulation necessary for optimal result
- Covariance term approximation crucial in scalarization
- Bootstrap leads to consistently better results

Cost using Pearson:



Cost using Bootstrap:



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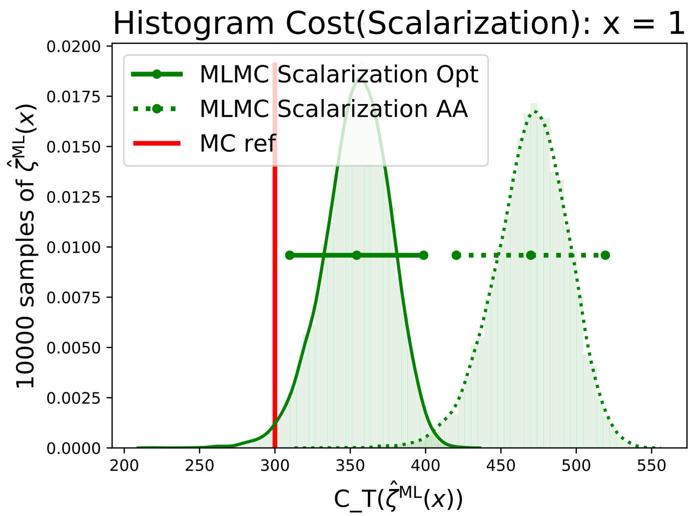
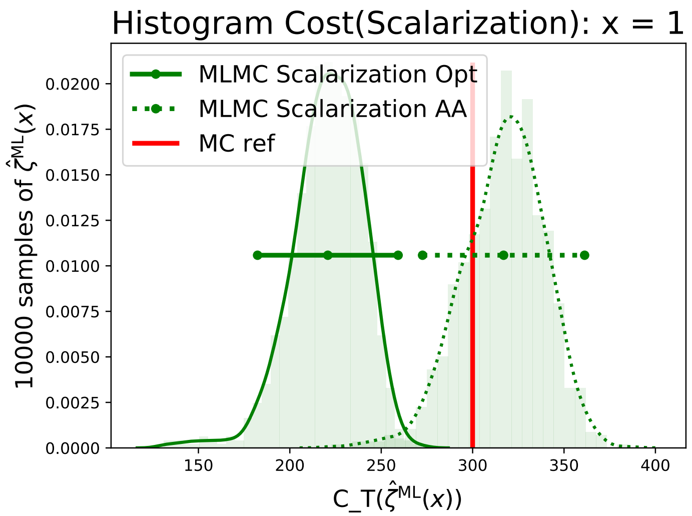


Cost using Bootstrap:



How does this translate to optimization?

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Extend problem statement for OUU

Objective:

$$f_H(x,\xi) = f_{det}(x) + \xi^3$$
$$f_L(x,\xi) = f_{det}(x) + A(x)\xi^3, \xi \sim \mathscr{U}(-0.5, 0.5)$$
$$A(x) = \frac{1}{12}x + 0.4$$

Constraint:

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

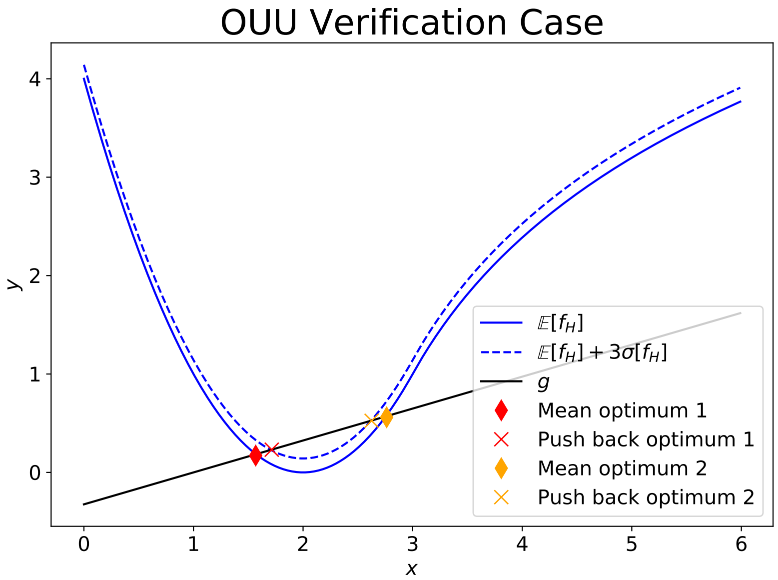
OUU:

1. Mean:

$$\min_x \mathbb{E}[f_H(x,\xi)]$$
$$\text{s.t. } f_{det}(x) \geq g(x)]$$

2. Scalarization:

$$\min_x \mathbb{E}[f_H(x,\xi)] + 3\sigma[f_H(x,\xi)]$$
$$\text{s.t. } f_{det}(x) \geq g(x)]$$



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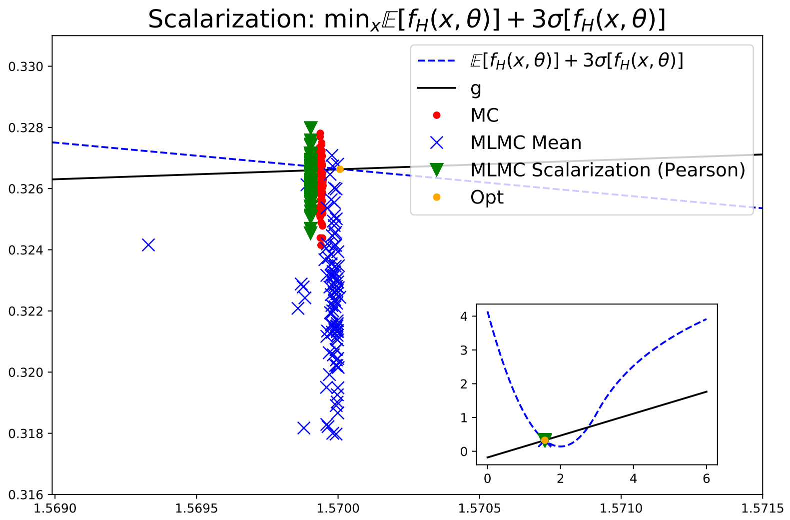
OUU Results

Scalarization: (Pearson)

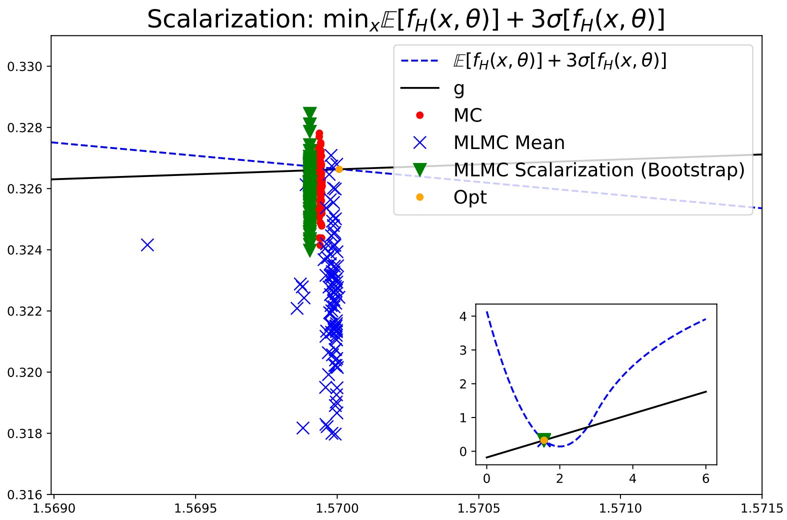
$$\min_x \mathbb{E}[f_H(x,\xi)] + 3\sigma[f_H(x,\xi)]$$



- More accurate result for MLMC Scalarization w.r.t. to MLMC Mean
- MLMC Mean underresolves

Scalarization: (Bootstrap)

$$\min_x \mathbb{E}[f_H(x,\xi)] + 3\sigma[f_H(x,\xi)]$$

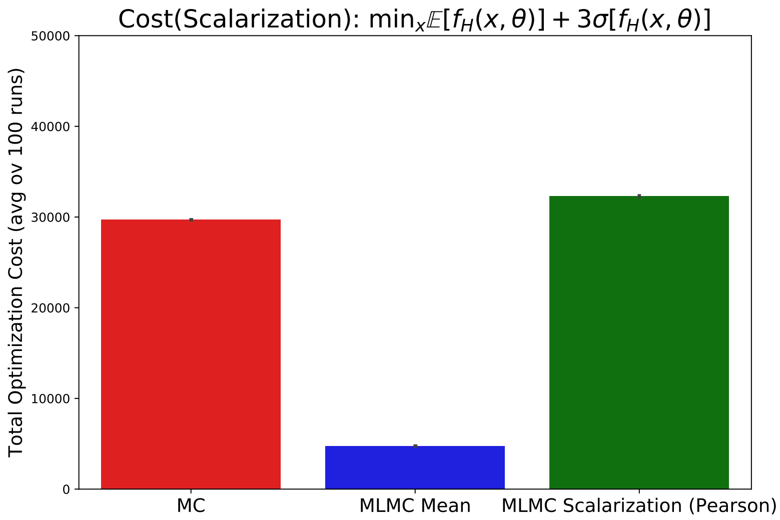


- Good match between MLMC Scalarization and MC

OUU Results

Scalarization: (Pearson)

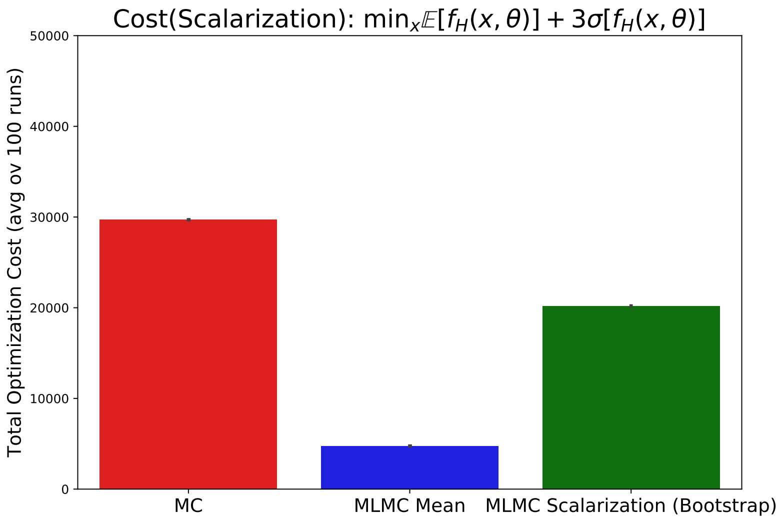
$$\min_x \mathbb{E}[f_H(x,\xi)] + 3\sigma[f_H(x,\xi)]$$



- Similar cost between Scalarization and MC (due to numerical opt)
- MLMC targeting mean uses too few runs

Scalarization: (Bootstrap)

$$\min_x \mathbb{E}[f_H(x,\xi)] + 3\sigma[f_H(x,\xi)]$$



- Use of bootstrap prevents us from over-resolving the statistics
- $\Rightarrow$ overall smaller computational burden

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Conclusion

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

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

Future work and open questions:

- Near future: More levels and wind application
- Outlook: From multilevel to multifidelity

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

Appendix

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

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

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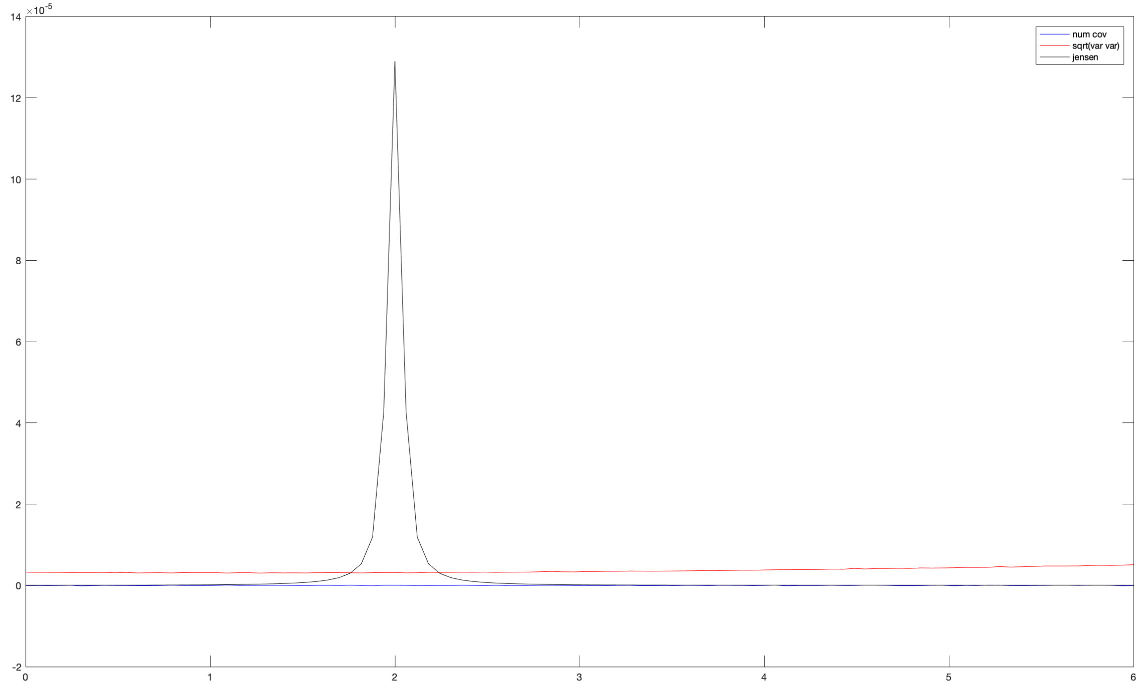
Sampling Results: Scalarization (Jensen)

To be explored. Does it even make sense?



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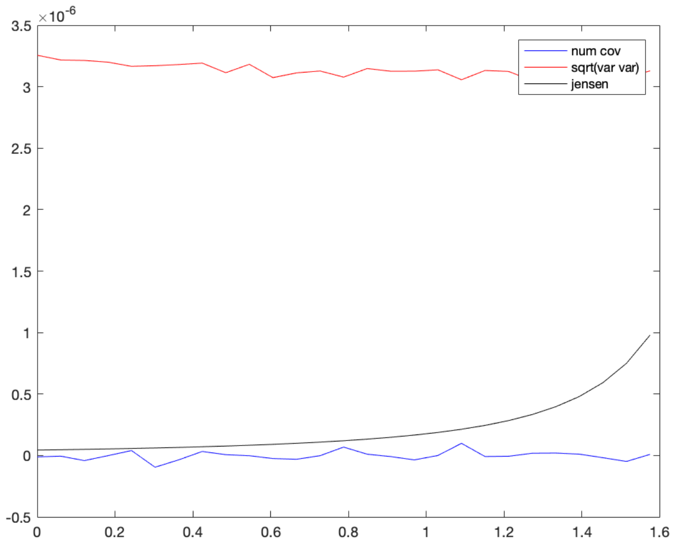

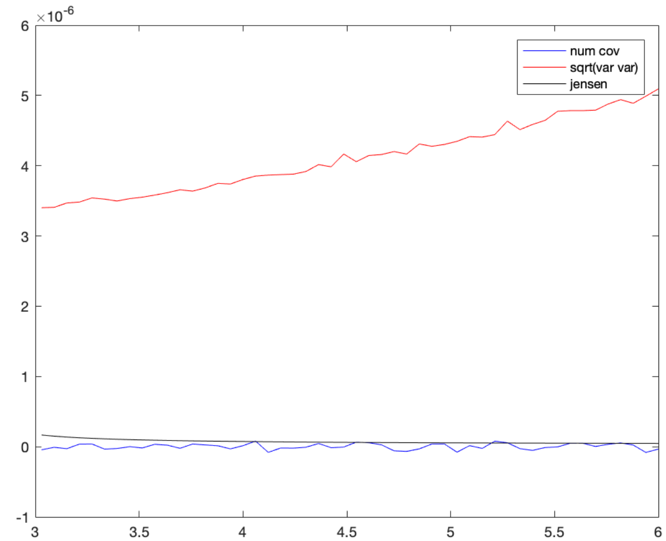

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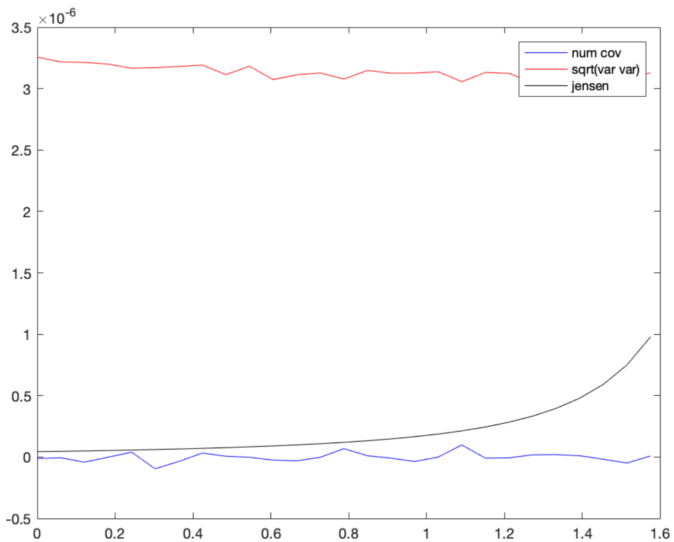

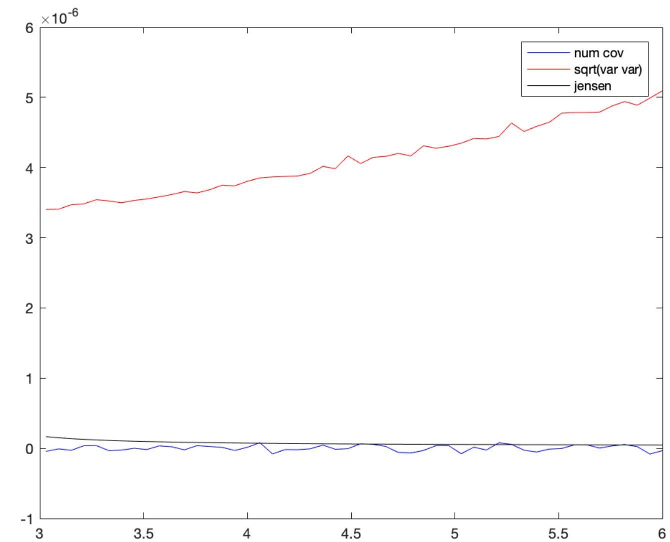

But:

- Problem18 is a very simple problem
- Bound needs to be numerically estimated