Sampling algorithms for generalized model ensembles in multifidelity uncertainty quantification

Workshop on Multilevel and multifidelity sampling methods in UQ for PDEs, Erwin Schrödinger Institute (Virtual)
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Alex Gorodetsky
joint work with Gianluca Geraci, Mike Eldred and John Jakeman (SNL)
Motivation

Observation: Many models and simulations are created over the course of analyzing a system.

Key idea: Usually, these models serve to develop the eventual high-fidelity model. How do we use them to also analyze the eventual high-fidelity model?

Information sources
- Hierarchy of fidelities
- Ensemble of peer models
- Discretization levels
- Experimental data
High-level modeling questions

1. How do we model the multi-fidelity uncertainty quantification problem?
   ▶ How is each simulation related? (Discretization hierarchies, physics
   hierarchies, “competing” peers (model selection), combination)
   ▶ How are relationships between models represented/exploited?
     (discrepancies, statistical correlations, probabilistic conditional
     dependencies, something else?)
High-level modeling questions

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2. What are the algorithmic objectives of multi-fidelity uncertainty quantification?
   - Variance/Bias reduction, MSE reduction (Frequentist)
   - Probabilistic predictions (Bayesian)
High-level modeling questions

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2. What are the algorithmic objectives of multi-fidelity uncertainty quantification?
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   - Probabilistic predictions (Bayesian)

3. Are there any general approaches for addressing these modeling questions, which can then be adapted to specific cases?
Algorithmic challenges

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   - Corrupted evaluations
   - Unconverged grids, because simulations tuned to fixed parameter settings
   - Problem geometry leads to meshing issues
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3. Nonlinearities in time-dependent problems (dynamical systems)
   - Correlations may not be the best “structure” to exploit here
   - How can chaotic systems be considered?
**Algorithmic challenges**

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4. Simulation models have different inputs
   - Extremely common in variety of physics domain where lower fidelities replace “physics” with “models”
   - Each low-fidelity may have its own set of uncertain model parameters, while all share uncertain environmental parameters (e.g., boundary conditions)
Dealing with general model ensembles

We present several **sampling** approaches that avoid explicit or implicit orderings based on model fidelity or correlations. We focus on **variance reduction**, with some broader ideas at the end.

1. Take an **optimality and convergence** viewpoint for variance reduction: What is the best possible performance when increasing the information from each low-fidelity information source?

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Gorodetsky, et. al. *A generalized approximate control variate framework for multifidelity uncertainty quantification*, JCP 2020

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1. Take an **optimality and convergence** viewpoint for variance reduction: What is the best possible performance when increasing the information from each low-fidelity information source?

2. Some commonly used existing approaches built on recursive-difference and recursive-nested estimators have limited variance reduction:
   - Low-fidelity sims can be infinitely evaluated with no further variance reduction
   - Arises because of orderings and recursive sampling strategies

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3. Convergent estimators can be derived

Outline

1. Notation: Monte Carlo and control variates
2. Recursive difference (MLMC) and nested difference estimators (MFMC)
3. Convergent approximate control variates
4. Probabilistic models
Monte Carlo

1. \( z \): input parameter uncertainties
2. \( Q \): quantity of interest evaluation

\[
\hat{Q}(z) = \frac{1}{N} \sum_{i=1}^{N} Q(z^{(i)})
\]

3. The estimator is unbiased

\[
\mathbb{E} \left[ \hat{Q}(z) \right] = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E} \left[ Q(z^{(i)}) \right] = \mathbb{E} [Q]
\]

4. The estimator variance decays like \( 1/N \):

\[
\text{Var}[\hat{Q}] = \frac{1}{N} \sum_{i=1}^{N} \text{Var} \left[ Q(z^{(i)}) \right] = \frac{\text{Var}[Q]}{N}
\]
Motivation
Control Variate Var. Reduction
Variance Reduction in UQ
Convergent estimators
Examples
Other models

Linear control variate
Single additional information source

Introduce a correlated information source $\hat{Q}_1(z)$

[Lavenberg and Welch 1981]
Motivation  Control Variate Var. Reduction  Variance Reduction in UQ  Convergent estimators  Examples  Other models

Linear control variate
Single additional information source

▶ Introduce a correlated information source $\hat{Q}_1(z)$
▶ Suppose we know the mean of $\mathbb{E} \left[ \hat{Q}_1(z) \right] = \mu_1$

\[
\hat{Q}^{CV} = \hat{Q}(z) + \alpha (\hat{Q}_1(z) - \mu_1)
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[Lavenberg and Welch 1981]
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Single additional information source

- Introduce a correlated information source $\hat{Q}_1(z)$
- Suppose we know the mean of $\mathbb{E} \left[ \hat{Q}_1(z) \right] = \mu_1$
  \[ \hat{Q}_{\text{CV}} = \hat{Q}(z) + \alpha (\hat{Q}_1(z) - \mu_1) \]
- Variance reduction effectiveness measured by correlation $\rho_1(\hat{Q}(z), \hat{Q}_1(z))$
  \[ \text{Var} [ \hat{Q}_{\text{CV}} ] = (1 - \rho_1^2) \text{Var} [ \hat{Q} ] \]

[Lavenberg and Welch 1981]
Several additional random variables $\hat{Q}_i(z)$ with known means $\mu_i$

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Optimal weights are

$$\alpha = -\text{Cov}[\hat{Q}, \hat{Q}]\text{Cov}[\hat{Q}, \hat{Q}]^{-1}$$

Optimal reduction is (note covariance amongst all low-fidelity sources)

$$R^2 = \frac{\text{Cov}[\hat{Q}, \hat{Q}]\text{Cov}[\hat{Q}, \hat{Q}]^{-1}\text{Cov}[\hat{Q}, \hat{Q}]}{\text{Var}[\hat{Q}]}$$

Adaptation to UQ

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- Approximate the control variate by generating estimators as (heuristic model of MFUQ)

\[ \tilde{Q}(z, z_1, \ldots, z_M) = \hat{Q}(z) + \sum_{i=1}^{M} \alpha_i (\hat{Q}_i(z_1^i) - \hat{\mu}_i(z_2^i)) \]
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▶ Single control variate case considered by [Pasupathy, Schmeiser, Taaffee, and Wang 2012] and [Ng and Willcox, 2014]
Multiple-model case

- Two families of recursive algorithms can be understood with this model
  - Recursive difference estimator (inner loop of MLMC and MIMC, [Giles, 2008], [Haji-Ali, Nobile, Tempone 2016])
  - Recursive nested estimator (Multifidelity Monte Carlo [Peherstorfer, Willcox, and Gunzberger 2016])

- Variance reduction of these recursive approaches do not converge to optimal control variate in the limit of infinite data

- Next: an interlude about robustness of some recursive approaches

- Eventual: Convergent and robust ACV estimators can be found
A limitation of some recursive schemes
Robustness to noise

- Stochastic ODE with payoff modeling European options (Giles 2008)
  \[ dS = rSdt + \sigma SdW \quad P = \exp(-r) \max(0, S(1) - 1) \]

- Euler-Maruyama for time integration at different resolutions

- Expectation is a telescopic sum —
  \[
  \mathbb{E}[P_L] = \mathbb{E}[P_1] + \sum_{\ell=2}^{L} \mathbb{E}[P_i - P_{i-1}] \quad \text{Var}[P_L] = \text{Var}[P_1] + \sum_{\ell=2}^{L} \text{Var}[P_i - P_{i-1}]
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Variance Decay → MLMC
A limitation of some recursive schemes

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Corrupt some level 3 evals.
Recursive differences *within* Multilevel Monte Carlo

1. Consider a sequence of LF sources

   \[ \{Q_1, \ldots, Q_M\} \]

2. Recursive difference est. [Owen 2013]

   \[ \tilde{Q} = (Q - Q_1) + \mu_1 \quad \text{so that} \quad \mathbb{E} \left[ \tilde{Q} \right] = \mathbb{E} [Q] \]
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3. Samples for each level partioned \( z_i = z_i^1 \cup z_i^2 \)

\[ \hat{Q}^{\text{MLMC}}(z) = \left( \hat{Q}(z) - \hat{Q}_1(z_1^1) \right) + \hat{\mu}_1(z_1^2) \]
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3. Samples for each level partitioned \( z_i = z_{i1} \cup z_{i2} \)

\[ \hat{Q}^{\text{MLMC}}(z) = \left( \hat{Q}(z) - \hat{Q}_1(z_{11}) \right) + \left( \hat{\mu}_1(z_{12}) - \hat{Q}_2(z_{12}) \right) + \hat{\mu}_2(z_{22}) + \ldots \]
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4. This is an ACV with \( \alpha = -1 \) and variance
   \[ \text{Var}[Q] = \text{Var}[Q_L] + \sum_{\ell=L-1}^{1} \text{Var}[Q_\ell - Q_{\ell+1}] + \text{Var}[Q - Q_1] \]
1. Consider a sequence of LF sources

\[ \{Q_1, \ldots, Q_M\} \]

2. Recursive nested estimator, base is the CV

\[ \tilde{Q} = \hat{Q} + \alpha (\hat{Q}_1 - \mu_1) \]

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Recursive-nested estimators within Multifidelity Monte Carlo

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3. ... however samples are nested
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**Potentially significant limitations to variance reduction**

- **Fix** number of HF evaluations
- Increase the number of LF evaluations
- \( Q = x^5, \ Q_1 = x^4, \ Q_2 = x^3, \ Q_3 = x^2, \ Q_4 = x \)
Sub-optimality of recursive estimators

**Theorem 2.4** (Maximum variance reduction of MLMC). The variance reduction of MLMC is bounded above by the optimal single CV i.e.,

\[ R_{\text{MLMC}}^2 < \rho_1^2. \]

(2.19)

**Theorem 2.7** (Maximum variance reduction of MFMC). The variance reduction of MFMC is bounded above by the optimal single CV, i.e.,

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**Why?** lack of consideration of all correlations

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R^2 = \frac{\text{Cov}[\hat{Q}, \hat{Q}] \text{Cov}[\hat{Q}, \hat{Q}]^{-1} \text{Cov}[\hat{Q}, \hat{Q}]}{\text{Var}[\hat{Q}]}
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\[ R^2 = \frac{\text{Cov}[\hat{\mathbb{Q}}, \mathbb{Q}]\text{Cov}[\hat{\mathbb{Q}}, \hat{\mathbb{Q}}]^{-1}\text{Cov}[\hat{\mathbb{Q}}, \hat{\mathbb{Q}}]}{\text{Var}[\mathbb{Q}]} \]
Approximate control variates

Estimator Ansatz

\[ \hat{Q}(z, z_1, \ldots, z_M) = \hat{Q}(z) + \sum_{i=1}^{M} \alpha_i (\hat{Q}_i(z) - \hat{\mu}_i(z_i^2)) \]

- Ests. distinguished by distribution of samples amongst \( \hat{Q}_i \) and \( \mu_i \)
- Includes previous recursive estimators as specific cases
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- We seek ACV estimators that converge to \( \gamma = 1 - R^2 \)
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- We seek ACV estimators that **converge** to \(\gamma = 1 - R^2\)
- The simplest such scheme is the following
  1. Use the same number of samples as the high fidelity model to compute \(\hat{Q}_i\)
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1. Use the same number of samples as the high fidelity model to compute \(\hat{Q}_i\)
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  1. Use the same number of samples as the high fidelity model to compute \( \hat{Q}_i \)
  2. Use the same and extra samples to compute \( \hat{\mu}_i \)
  3. Compute optimal weights (there is a formula)
- Converges because it maintains correlation amongst all \( \hat{Q}_i \)
Sample allocations for two (of many) variants

Independent Samples

\[ Q \]
\[ z \]
\[ z_1^1 \]
\[ z_2^1 \]
\[ z_1^2 \]
\[ z_2^2 \]
\[ \ldots \]
\[ Q_M \]
\[ z_1^M \]
\[ z_2^M \]

Shared Samples

\[ Q \]
\[ z \]
\[ z_1^1 \]
\[ z_2^1 \]
\[ z_1^2 \]
\[ z_2^2 \]
\[ \ldots \]
\[ Q_M \]
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\[ z_2^M \]
Sample allocations for two (of many) variants

**Independent Samples**

- $Q$
- $Q_1$
- $Q_2$
- ... $Q_M$

- $z^1$
- $z^2$
- $z^1$
- $z^2$
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V.S.

**Recursive Difference**

- $Q$
- $Q_1$
- $Q_2$
- ... $Q_M$

- $z^1$
- $z^2$
- $z^1$
- $z^2$
- $z^1$
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- $z^2$
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**MFMC**

- $Q$
- $Q_1$
- $Q_2$
- ... $Q_M$

- $z^1$
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- $z^2$
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- $z^2$
- $z^1$
- $z^2$
- $z^1$
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- $z^2$
We can prove convergence
Hybrid estimator to accelerate convergence

- Use the first $K$ control variates to accelerate the Qoi $Q$
- Use the last $M - K$ to accelerate the convergence of the $\mu_L$ for some $L$

$$\hat{Q}_{\text{ACV-KL}}(\alpha, z) = \hat{Q}(z) + \sum_{i=1}^{K} \alpha_i \left( \hat{Q}_i(z) - \hat{\mu}_i(z) \right) + \sum_{i=K+1}^{M} \alpha_i \left( \hat{Q}_i(z_L) - \hat{\mu}_i(z) \right)$$

$$\hat{Q}_{\text{ACV-KL}}(\alpha, z) = \hat{Q}_{K}^{\text{ACV-MF}}(\alpha_1, \ldots, \alpha_K, z, z_1, \ldots, z_k) + \sum_{i=K+1}^{M} \alpha_i \left( \hat{Q}_i(z_L) - \hat{\mu}_i(z) \right)$$
Accelerated convergence to target levels

\[ \log_2(r_i) - i \]

Variance reduction ratio \( \gamma \)

- MC
- OCV-1
- OCV-2
- OCV-3
- OCV
- W-RDiff
- MFMC
- ACV-MF

\((K, L) = (1, 1)\)
\((K, L) = (2, 1)\)
\((K, L) = (3, 1)\)
\((K, L) = (4, 1)\)
Sample Allocation

1. Optimize over distribution of samples to minimize variance for target cost

\[ J_{ACV}(N, r) = (1 - R^2_{ACV}) \frac{\text{Cov}[Q]}{N} \]

2. This is a mixed-integer nonlinear program (MINLP) where \( N \) is a non-categorical integer variable, \( r_iN \) are derived integer quantities, and, in the case of ACV-KL, \((K, L)\) are categorical integer variables.

\[
\min_{N, r, K, L} \log(J_{ACV}(N, r, K, L)) \quad \text{subject to}
\]

\[
N \left( w + \sum_{i=1}^{M} w_i r_i \right) \leq C, \quad N \geq 1, \quad r_1 \geq 1, \text{ and } r_i \geq r_{i-1}
\]

for \( i = 2, \ldots, M \)
**Viscous Burgers with uncertain boundaries**

- Compare recursive-difference, MFMC, and optimal ACV
- Viscous Burgers at 6 discretization levels
- Estimate mean of $u$ at a spatial location

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \kappa \frac{\partial^2 u}{\partial x^2} = 0
\]

(a) Number of high-fidelity is variable

(b) Number of high-fidelity is fixed
No Corruption
Back to the robustness issue
Considerable improvement by using full correlations

Corruption Rate: $10^{-5}$
Back to the robustness issue
Considerable improvement by using full correlations

Corruption Rate: $10^{-4}$
Elastic wave equation

Hypercubic equations

- Elastic wave propagation in two dims. with two materials
- Two numerical schemes, each scheme has different discretizations (10 total simulations)
  - Schemes: High-res second-order scheme, and first-order Godunov scheme
  - Discretizations: $200 \times 200, 100 \times 100, 50 \times 50, 25 \times 25, 10 \times 10$

$$q_t + A(q)q_x + B(q)q_y = 0,$$
Robust to aggressive coarsening

1. Left: single-fidelity with discretization hierarchy
2. Right: multi-fidelity with discretization hierarchies
3. Bottom: multi-fidelity with aggressive coarsening
Observations:

1. The ACV is a heuristic ansatz, but a useful one as it captures many existing methods.
2. Recursive approaches often work really well, general case not always needed.
3. Computational gains can be gained by imposing additional structure *when it is there*.
4. Pilot sample are needed for many algorithms, their effect is poorly studied.
Type of question we want to answer

- Can the ACV ansatz be *derived* from first principles rather than obtained from intuition? (yes)

Alternatives

Type of question we want to answer

▶ Can the ACV ansatz be *derived* from first principles rather than obtained from intuition? (yes)

▶ Can better, problem-dependent, estimator ansatz be obtained? (probably, ongoing)

Type of question we want to answer

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**Modeling idea**

1. Parameterize a set of model relationships, then use first principle inference instead of heuristic approach
2. Will present this from a Bayesian perspective, as it provides a way to incorporate prior knowledge

Network models

- Model multi-fidelity relationships through conditional independence relations of latent variables
- Fuse multiple models by learning their statistical relationships via network inference

Hierarchy

Low-fidelity peers
Graphs encode structure, enable scaling to many LV

Peer low-fidelity models
Example: M1 uses a composite turbulence model, M2 and 3 use components

\[ p(\theta_1, \theta_2, \theta_3) = p(\theta_3)p(\theta_2)p(\theta_1|\theta_2, \theta_3) \]
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Distinct model hierarchies
Example: refined discretization as in a multilevel scheme

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Peer high fidelity models
Example: independent high-fidelity models with an overlapping prediction

\[ p(\theta_1, \theta_2, \theta_3) = p(\theta_3)p(\theta_1 | \theta_3)p(\theta_2 | \theta_3) \]
Bayesian updating and recovering control variates

▶ Single fidelity:

\[ y = \theta + \xi \]
Bayesian updating and recovering control variates

- Single fidelity:

\[ y = \theta + \xi \]

- Prior is \( \mathcal{N}(\mu_{\text{prior}}, \sigma_{\text{prior}}^2) \) and likelihood is \( \mathcal{N}(\theta, \sigma_1^2) \)

- Posterior mean:

\[ \mu_{\text{post}} = (1 - \nu)\mu_{\text{prior}} + \nu\hat{\theta}^{\text{MC}} \]
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- **Bi-fidelity:**
  \[ y_1 = \theta_1 + \xi, \quad y_2 = \theta_2 + \xi, \text{ and } \theta_1 = a\theta_2 + b + \xi \]
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  - Compare with CV: recover the CV formula with weight \( B \) defined by first principles
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▶ Compare with CV: recover the CV formula with weight \( B \) defined by first principles

▶ See paper for theory where we recover CV for the general case
Back to noise robustness example

- Bayesian inference with model selection
- Common marginal priors on all models

No perturbation
Back to noise robustness example

- Bayesian inference with model selection
- Common marginal priors on all models

1/100 perturbation
Back to noise robustness example

- Bayesian inference with model selection
- Common marginal priors on all models

1/10 perturbation

Quantiles of MSE

Number of lowest fidelity samples

10^{-4}  10^{-3}  10^{-2}  10^{-1}
We have developed an approximate control variate framework for multifidelity UQ

- Works with generic model “fidelities”, without ordering based on discretization or correlation
- Includes recursive difference estimator and MFMC as subsets
- Enables the development of convergent schemes
Summary

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  - Adaptation to discretization-based schemes for “bias” reduction (like MLMC, MIMC, and related)
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- Papers links: see my website
  https://www.alexgorodetsky.com/publications
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