Data-Driven Multifidelity Methods for Monte Carlo Estimation

Benjamin Peherstorfer University of Wisconsin-Madison

Karen Willcox Massachusetts Institute of Technology

> Max Gunzburger Florida State University

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Outer loop applications



optimization



control



inference



visualization



model calibration



uncertainty quantification



Force/DLR

multi-discipline coupling

Surrogate models

Given is a high-fidelity model $f^{(1)}: \mathcal{D} \to \mathcal{Y}$

- Large-scale numerical simulation
- Achieves required accuracy
- Computationally expensive

Additionally, often have surrogate models

 $f^{(i)}: \mathcal{D} \to \mathcal{Y}, \qquad i=2,\ldots,k$

- Approximate high-fidelity $f^{(1)}$
- Often orders of magnitudes cheaper

Examples of surrogate models



data-fit models, response surfaces, machine learning



approximations



reduced basis, proper orthogonal decomposition



simplified models, linearized models



Replacing high-fidelity model with surrogate

Replace $f^{(1)}$ with a surrogate model

- Costs of outer loop reduced
- Often orders of magnitude speedups

Estimate depends on surrogate accuracy

- Control with error bounds/estimators
- Rebuild if accuracy too low
- No guarantees without bounds/estimators

Issues

- Propagation of surrogate error on estimate
- Surrogates without error control
- Costs of rebuilding a surrogate model



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Our approach: Multifidelity methods

Combine high-fidelity and surrogate models

- Leverage surrogate models for speedup
- Recourse to high-fidelity for accuracy

Multifidelity guarantees high-fidelity accuracy

- Occasional recourse to high-fidelity model
- High-fidelity model is kept in the loop
- Independent of error control for surrogates

Multifidelity speeds up computations

- Adapt, fuse, filter with surrogate models
- Balance #solves among models



[Brandt, 1977], [Hackbusch, 1985], [Bramble et al, 1990], [Booker et al, 1999], [Jones et al, 1998], [Alexandrov et al, 1998], [Christen et al, 2005], [Cui et al, 2014]

[P., Willcox, Gunzburger, Survey of multifidelity methods in uncertainty propagation, inference, and optimization; SIAM Review, 2018 (to appear)]

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[P., Willcox, Gunzburger, Survey of multifidelity methods in uncertainty propagation, inference, and optimization; SIAM Review, 2018 (to appear)]



- 1. Motivation for multifidelity methods
- 2. Multifidelity Monte Carlo estimation (MFMC)
- 3. Asymptotic analysis of MFMC
- 4. Adaptive surrogates and MFMC
- 5. Outlook and conclusions

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Uncertainty propagation as an outer loop application

High-fidelity ("truth") model with costs $w_1 > 0$

 $f^{(1)}:\mathcal{D}
ightarrow\mathcal{Y}$

Given random variable Z, estimate

$$s = \mathbb{E}[f^{(1)}(Z)]$$

Monte Carlo estimator with realizations z_1, \ldots, z_n of Z

$$\bar{y}_n^{(1)} = \frac{1}{n} \sum_{i=1}^n f^{(1)}(\boldsymbol{z}_i)$$

Uncertainty propagation with Monte Carlo is outer-loop application

- Each high-fidelity model solve is computationally expensive
- Repeated model solves become prohibitive

[Rozza, Carlberg, Manzoni, Ohlberger, Veroy-Grepl, Willcox, Kramer, Benner, Ullmann, Nouy, Zahm, etc]

MFMC: Control variates

Estimate $\mathbb{E}[A]$ of random variable A with Monte Carlo estimator

$$\bar{a}_n = \frac{1}{n} \sum_{i=1}^n a_i, \qquad a_1, \ldots, a_n \sim A$$

Unbiased estimator $\mathbb{E}[\bar{a}_n] = \mathbb{E}[A]$ with mean-squared error (MSE)

$$e(ar{a}_n) = rac{\mathsf{Var}[A]}{n}$$

Combine \bar{a}_n with Monte Carlo estimator \bar{b}_n of $\mathbb{E}[B]$ of random variable B

$$\hat{s}_{A} = \bar{a}_{n} + \gamma \left(\mathbb{E}[B] - \bar{b}_{n} \right) , \qquad \gamma \in \mathbb{R}$$

Control variate estimator \hat{s}_A is unbiased estimator $\mathbb{E}[\hat{s}_A] = \mathbb{E}[A]$ with MSE

$$e(\hat{s}_A) = (1 - \rho^2)e(\bar{a}_n)$$

- ▶ Correlation coefficient $-1 \le \rho \le 1$ of A and B
- If $\rho = 0$, same MSE as regular Monte Carlo
- If $|\rho| > 0$, lower MSE
- The higher correlated, the lower MSE of \hat{s}_A

[Nelson, 87]

MFMC: Control variates and surrogate models

Models

- High-fidelity model $f^{(1)}: \mathcal{D} \to \mathcal{Y}$
- Surrogates $f^{(2)}, \ldots, f^{(k)} : \mathcal{D} \to \mathcal{Y}$

P., Willcox, Gunzburger, Optimal model management for multifidelity Monte Carlo estimation. SISC, 2016

Exploit correlation of $f^{(1)}(Z)$ and $f^{(i)}(Z)$ for reducing MSE

$$\rho_i = \frac{\text{Cov}[f^{(1)}(Z), f^{(i)}(Z)]}{\sqrt{\text{Var}[f^{(1)}(Z)]} \text{Var}[f^{(i)}(Z)]}, \qquad i = 2, \dots, k$$

Related work: Combine multiple models for Monte Carlo estimation

- Multilevel Monte Carlo [Giles 2008], [Heinrich 2001], [Speight, 2009]
- ▶ RBM and control variates [Boyaval et al, 2010, 2012], [Vidal et al 2015]
- Data-fit models and control variates [Tracey et al 2013]
- Monte Carlo with low-/high-fidelity model [Ng & Eldred 2012]
- Two models and control variates [Ng & Willcox 2012, 2014]

\Rightarrow Need for arbitrary number of surrogates, any type of surrogates

MFMC: Multifidelity Monte Carlo estimator

Take realizations of input random variable Z

 $\textbf{z}_1, \textbf{z}_2, \textbf{z}_3, \dots$

Evaluate model $f^{(i)}$ at first m_i realizations z_1, \ldots, z_{m_i} of Z

$$f^{(i)}(z_1),\ldots,f^{(i)}(z_{m_i}), \qquad i=1,\ldots,k$$

Multifidelity Monte Carlo (MFMC) estimator

$$\hat{s} = \underbrace{\bar{y}_{m_{1}}^{(1)}}_{\text{from HFM}} + \sum_{i=2}^{k} \gamma_{i} \underbrace{\left(\bar{y}_{m_{i}}^{(i)} - \bar{y}_{m_{i-1}}^{(i)}\right)}_{\text{from surrogates}}$$

- MFMC estimator \hat{s} is unbiased estimator of $s = \mathbb{E}[f^{(1)}(Z)]$
- ▶ Costs of each model evaluation $0 < w_1, \ldots, w_k \in \mathbb{R}$ give costs of MFMC

$$c(\hat{s}) = \sum_{i=1}^{k} m_i w_i$$

Selection of coefficients $\gamma_2, \ldots, \gamma_k$ and model evaluations m_1, \ldots, m_k ?

Comparison in terms of costs/MSE to regular Monte Carlo estimation?

P., Willcox, Gunzburger, Optimal model management for multifidelity Monte Carlo estimation. SISC, 2016

MFMC: Balancing work among models

Variance of MFMC estimator \hat{s} is

$$e(\hat{s}) = \operatorname{Var}[\hat{s}] = \frac{\sigma_1^2}{m_1} + \sum_{i=2}^k \left(\frac{1}{m_{i-1}} - \frac{1}{m_i}\right) \left(\gamma_i^2 \sigma_i^2 - 2\gamma_i \rho_i \sigma_1 \sigma_i\right)$$

- Variance σ_i^2 of $f^{(i)}(Z)$
- Correlation coefficient ρ_i between $f^{(1)}(Z)$ and $f^{(i)}(Z)$

Find m and γ that minimize MSE for given computational budget q

arg min

$$m \in \mathbb{R}^{k}, \gamma_{2}, ..., \gamma_{k} \in \mathbb{R}$$

subject to
 $m_{i-1} - m_{i} \leq 0, \quad i = 2, ..., k,$
 $-m_{1} \leq 0,$
 $\boldsymbol{w}^{T} \boldsymbol{m} = q.$

Theorem 1 (P., Willcox, Gunzburger, 2016).

Optimization problem has unique (analytic) solution if $ho_1^2 > \dots >
ho_k^2 > 0$ and

$$\frac{w_{i-1}}{w_i} > \frac{\rho_{i-1}^2 - \rho_i^2}{\rho_i^2 - \rho_{i+1}^2}, \qquad i = 2, \dots, k$$
(1)

Sketch of proof

- Establish necessary condition for local optima with Karush-Kuhn-Tucker
- Only one local optima with $m_1 < m_2 < \cdots < m_k$
- ▶ This local optima has smaller objective value than any with "≤"

Variance reduction of MFMC \hat{s} w.r.t. benchmark Monte Carlo $\bar{y}_q^{(1)}$

$$e(\hat{s}) = \left(\sum_{i=1}^{k} \sqrt{\frac{w_i}{w_1} \left(\rho_i^2 - \rho_{i+1}^2\right)}\right)^2 e(\bar{y}_q^{(1)})$$

[P., Willcox & Gunzburger Optimal model management for multifidelity Monte Carlo estimation. SISC, 2016.]

MFMC: Numerical example

Locally damaged plate in bending

- Inputs: nominal thickness, load, damage
- Output: maximum deflection of plate
- Only distribution of inputs known
- Estimate expected deflection

Six models

- High-fidelity model: FEM, 300 DoFs
- Reduced model: POD, 10 DoFs
- Reduced model: POD, 5 DoFs
- Reduced model: POD, 2 DoFs
- Data-fit model: linear interp., 256 pts
- Support vector machine: 256 pts

Var, corr, and costs est. from 100 samples





MFMC: Speedups in uncertainty propagation



► Monte Carlo needs 12h runtime for estimate with error below 10⁻⁷

• Multifidelity provides estimator with error below 10^{-7} after 9 seconds

MFMC: Combining many models



 \blacktriangleright Largest improvement from "single \rightarrow two" and "two \rightarrow three"

Adding yet another reduced/SVM model reduces variance only slightly

MFMC: Distribution of #evals among models



- MFMC distributes #evals among models depending on corr/costs
- Number of evaluation changes exponentially between models
- Highest #evals in data-fit models (cost ratio $w_1/w_6 \approx 10^6$)

MFMC: Who else is using MFMC?

Multifidelity sensitivity analysis

- Identify the parameters of model with largest influence on quantity of interest
- Large-scale variance estimation problem
- Multifidelity makes tractable global sensitivity analysis with expensive models
- \rightarrow Qian (MIT) with Earth Science at LANL

Uncertainty quantification in flutter problem

- Highly flexible, high-aspect-ratio wing
- Air density and root angle of attack uncertain
- Estimate expected flutter speed
- MFMC reduced runtime by more than 3 orders of magnitude
- \rightarrow with Air Force Research Laboratory



Figure: Philip S. Beran

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MFMC: Asymptotic analysis

Properties of MFMC in setting with $f^{(1)}, f^{(2)}, \ldots, f^{(k)}$

- Existence and uniqueness
- Unbiased estimator of statistics of high-fidelity model f⁽¹⁾
- MSE in terms of costs and correlation coefficients

Now ("exact") f and sequence $f^{(1)}, f^{(2)}, \ldots$

Estimate

 $\mathbb{E}[f(Z)]$

• MSE of MFMC estimator \hat{s} that uses $f^{(1)}, \ldots, f^{(L)}$ is

$$e(\hat{s}) = \underbrace{\operatorname{Var}[\hat{s}]}_{\text{variance}} + \underbrace{\mathbb{E}[f(Z) - f^{(L)}(Z)]^2}_{\text{bias w.r.t. } f}$$

Example: $f^{(1)}, f^{(2)}, \ldots$ correspond to multilevel discretization of f

Goal: Given tolerance $\epsilon > 0$

- ▶ Find $L \in \mathbb{N}$, #model evaluations **m**, coefficients γ such that $e(\hat{s}) \lesssim \epsilon$
- ▶ Bound costs c(ŝ)

[Brandt, 1977], [Goodman et al, 1989], [Heinrich, 2001], [Giles, 2008], [Cliffe, 2011]

MFMC: Asymptotic results

Assumption: There exists $1 < h \in \mathbb{R}$ and rates $0 < \alpha, \beta, \tau \in \mathbb{R}$ such that

$$\blacktriangleright |\mathbb{E}[f - f^{(\ell)}]| \lesssim h^{-\alpha \ell}, \quad \ell \in \mathbb{N}$$

$$\blacktriangleright \ w_{\ell} \lesssim h^{\beta \ell} \,, \quad \ell \in \mathbb{N}$$

► Var
$$\left[f^{(\ell)} - f^{(\ell-1)}\right] \lesssim h^{-\tau \ell}, \quad \ell \in \mathbb{N}$$

(Regular) Monte Carlo estimator $\bar{y}_q^{(L)}$ achieves $e(\bar{y}_q^{(L)}) \lesssim \epsilon$ with

 $c(ar{y}_q^{(L)}) \lesssim \epsilon^{-1} \epsilon^{-eta/(2lpha)}$

Theorem 2 (P., Gunzburger, Willcox, 2018).

If MFMC estimator exists and $\tau > \beta$, then MFMC achieves $e(\hat{s}) \lesssim \epsilon$ with

$$c(\hat{s}) \lesssim \epsilon^{-1}$$

- \blacktriangleright Costs bound independent of rates α and β
- Agrees with results in multilevel Monte Carlo estimation [Giles, 2008]

[P., Gunzburger & Willcox: Convergence analysis of multifidelity Monte Carlo estimation. Numerische Mathematik, 2018]

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online budget



- ► Trade off adaptation ("deterministic approximation") and sampling
- Surrogate model is constructed with outer-loop result in mind
- ▶ Related to "exploration vs. exploitation" in Bayesian optimization
- Constructing goal-oriented surrogates [Oden et al, 2000], [Bui-Thanh et al, 2007], [Lieberman and Willcox, 2013], [Spantini et al, 2017], [Li et al, 2018]

high-fidelity model surrogate model

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Construct goal-oriented and context-aware surrogate for outer-loop application at hand

- Goal is outer-loop result
- Other models set the context in which surrogate model will be used

Cheap surrogate with poor approximation quality might be more useful than an expensive one that is more accurate

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AMFMC: Problem setup

High-fidelity model with normalized evaluation costs $w_0 = 1$

 $f: \mathcal{D} \to \mathcal{Y}$

Surrogate model with $n \in \mathbb{N}$

$$f^{(n)}:\mathcal{D}
ightarrow\mathcal{Y}$$

Surrogate model approximates high-fidelity model in the sense

$$1 - \rho_n^2 \le c_1 n^{-\alpha} \,, \qquad 0 < c_1, \alpha$$

Evaluation costs of surrogate model may grow with n as

$$w_n \leq c_2 n^\beta \,, \qquad 0 < c_2, \beta$$

Costs of constructing surrogate $f^{(n)}$ are $w_0 n = n$

- Constructing $f^{(n)}$ requires *n* evaluations of *f*
- Evaluations of f dominate construction costs
- Construct costs are significant (e.g., model reduction)

AMFMC: Trading off construction costs and sampling costs

MFMC estimator \hat{s} with f and $f^{(n)}$ and ("online") budget q has MSE

$$e(\hat{s}) = rac{\sigma^2}{q} \left(\sqrt{1-
ho_n^2} + \sqrt{w_n
ho_n^2}
ight)^2$$

AMFMC splits total budget p between construction and sampling

• If spend *n* for constructing $f^{(n)}$, budget q = p - n remains for sampling

$$e(\hat{s}_n) = \frac{\sigma^2}{\rho - n} \left(\sqrt{1 - \rho_n^2} + \sqrt{w_n \rho_n^2}\right)^2$$

- Measures error with respect to goal of estimating $\mathbb{E}[f(Z)]$
- Takes construction costs n into account

1

Measures efficacy of surrogate model for variance reduction (context)

Upper bound on $e(\hat{s}_n)$

$$e(\hat{s}_n) \lesssim \frac{1}{p-n} \left(c_1 n^{-\alpha} + c_2 n^{\beta} \right)$$

AMFMC: Existence, uniqueness, and convexity

Consider the objective function

$$g(n) = \frac{1}{p-n} \left(c_1 n^{-\alpha} + c_2 n^{\beta} \right)$$

Find *n* such that g(n) is minimized

$$\min_{n\in(0,p)} g(n)$$

Theorem 3 (P., 2017).

The objective g is convex in (0, p) and therefore there exists a unique $\hat{n}^* \in (0, p)$ that minimizes $g(n) \Rightarrow$ there is an optimal trade-off

Define the AMFMC estimator \hat{s}_n^*

- Computes \hat{n}^* evaluations of f to construct surrogate $f^{(\hat{n}^*)}$
- Use MFMC to combine f and surrogate $f^{(\hat{n}^*)}$ with budget $p \hat{n}^*$

[[]P., Multifidelity Monte Carlo estimation with adaptive low-fidelity models, 2017 (submitted)]

AMFMC: Adaptive multifidelity Monte Carlo estimator

Upper bound for \hat{n}^* that is useful for "small" budgets p

$$\hat{n}^* \leq \frac{\alpha}{\alpha+1}p$$

There exists $\bar{n}^* \in \mathbb{N}$ independent of p such that $\hat{n}^* \leq \bar{n}^*$ for p > 0

- Number of adaptations \hat{n}^* is bounded with respect to p
- \blacktriangleright Stop adapting surrogate model even with unlimited budget $p
 ightarrow \infty$
- Surrogate models can be "too accurate" for multifidelity methods

Corollary 4 (P., 2017).

Cost complexity of AMFMC with $w_n = 0$ is

$$e(\hat{s}_n^*) \in \mathcal{O}(p^{-1-lpha})$$

• Can interpret $w_n = 0$ as $\mathbb{E}[f^{(\hat{n}^*)}(Z)]$ is known

 \Rightarrow control functionals [Oates, Girolami, Chopin, 2016]

• Helps to understand case $w_n \ll 1$ ($f^{(\hat{n}^*)}$ much cheaper than f)

AMFMC: Anemometer

Anemometer problem

- Measure velocity of fluid
- Three inputs uniformly distributed in

 $[0,10]\times[0.1,10]\times[1,10]$

- Output is velocity
- Estimate expected velocity

High-fidelity model

- Based on convection-diffusion equation
- Discretized with finite elements
- High-fidelity model has 29008 DoFs







AMFMC: Surrogate model for anemometer problem

Surrogate model

- Gaussian process regression
- Take n realizations of Z
- Train on corresponding n outputs of f

Optimizing for \hat{n}^*

- One dimensional convex problem
- Numerically solve for \hat{n}^*

Adaptation of surrogate in AMFMC

- Numerically estimate rates from pilot runs
- Optimize for \hat{n}^* with Matlab's fmincon





AMFMC: Anemometer results



Speedups of up to 3 orders of magnitude compared crude Monte Carlo
 MSE of AMFMC decays with p^{-1-α} in pre-asymptotic regime

AMFMC: Anemometer optimal trade-off



- Approximation of n^{*} is bounded
- Lower and upper bounds seem tight in pre-asymptotic regime

AMFMC: Comparison to static models



AMFMC optimally trades off adaptation and sampling costs

Up to two orders of magnitude speedups compared to static models

AMFMC: Beam example

Beam problem

Length and height uniformly distributed

 $[0.8, 1.2] \times [5 \times 10^{-4}, 5 \times 10^{-3}]$

- Output is displacement of beam
- Estimate expected displacement

Models

- High-fidelity finite element model
- Surrogate is Gaussian process model
- Measure rates numerically





AMFMC: Beam results



AMFMC achieves about an order of magnitude speedup

• Decay of MSE slows down from $p^{-1-\alpha}$ to p^{-1}

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Outlook

Optimization under uncertainty

- Estimate statistics in optimization iteration
- Robust optimization

Rare event simulation

- Estimate probability of rare event
- Crucial for risk-averse optimization

Sensitivity analysis

- Identify parameters of model that lead to largest variance in quantity of interest
- Large-scale variance estimation problem

Bayesian inverse problems

- Markov chain Monte Carlo sampling
- Increase acceptance probability of moves

[P., Willcox, Gunzburger, Survey of multifidelity methods in uncertainty propagation, inference, and optimization; SIAM Review, 2018 (to appear)]





Figure: Elizabeth Qian

Conclusions



Multifidelity methods

- Leverage surrogate models for runtime speedup
- Recourse to high-fidelity model for accuracy guarantees
- Optimally trade off approximation, sampling, and construction
- Context aware construction of surrogate models

Our references

- 1 P., Willcox & Gunzburger Optimal model management for multifidelity Monte Carlo estimation. SISC, 2016.
- 2 P., Gunzburger & Willcox: Convergence analysis of multifidelity Monte Carlo estimation. Numerische Mathematik, 2018
- 3 P. Multifidelity Monte Carlo estimation with adaptive low-fidelity models. submitted, 2017.

MFMC: Wing flutter problem setup

Flutter problem

- Uncertain inputs
 - Angle of attack from 0.5° to 2.5°
 - Air density, mass of tip vary by 5%
- Estimate expected flutter speed

High-fidelity model

- Based on Hodges-Dowell equations
- ► Nonlinear terms of ≥3rd order ignored
- FEM discretization with 10 elements

Low-fidelity models

- Spline interpolants on equidistant grid
- Low-fidelity model f⁽²⁾ from 343 points
- Low-fidelity model $f^{(3)}$ from 125 points





collaboration with Philip Beran (Air Force Research Laboratory)

[Stanford and Beran, 2013], [Beran, Stanford, and Wang, 2017]

[P., Beran, Willcox, 2018]

MFMC: Wing flutter speedup results



MFMC achieves significant speedup

- Low-fidelity models are 8 orders of magnitude cheaper than $f^{(1)}$
- MFMC achieves about 7 orders of magnitude speedup



- With $f^{(2)}$, model $f^{(3)}$ is evaluated more often
- Demonstrates that interactions between models drives efficiency of MFMC



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