UNIVERSITÉ DU LUXEMBOURG

European Research Council
Established by the European Commission

USING HIGHER-ORDER ADJOINTS TO ACCELERATE THE SOLUTION OF UQ PROBLEMS WITH RANDOM FIELDS

Jack S. Hale, Paul Hauseux, Stéphane P.A. Bordas.
Institute of Computational Engineering, University of Luxembourg.

AIMS

A powerful Monte Carlo variance reduction technique introduced in (Cao, M. Y. Hussaini, and Zhang, 2004) uses local derivatives to accelerate Monte Carlo estimation. This work aims to:

- develop a new derivative-driven estimator that works for SPDEs with uncertain data modelled as Gaussian random fields with Matérn covariance functions (infinite/high-dimensional problems) (Lindgren, Rue, and Lindström, 2011),
- use second-order derivative (Hessian) information for improved variance reduction over our approach in (Hauseux, Hale, and Bordas, 2017),
- demonstrate a software framework using FEniCS (Logg and Wells, 2010), dolfin-adjoint (Farrell et al., 2013) and PETSc (Balay et al., 2016) for automatic acceleration of MC estimation for a wide variety of PDEs on HPC architectures.

SETTING

A non-linear parametric (ω) PDE:

$$\text{Find } u \in U : F(u, \omega) = 0.$$

We solve using the finite element method and preconditioned Newton-Krylov methods. Uncertain parameter modelled by a Gaussian random field:

$$\omega \sim N(\bar{\omega}, C),$$

with mean $\bar{\omega}$ and covariance operator C.

A quantity of interest functional:

$$\psi : U \to \mathbb{R}.$$

MONTE CARLO

We want to find:

$$\mathbb{E}(\psi).$$

Classic approach:

$$\mathbb{E}^{\mathrm{MC}}(\psi) \approx \frac{1}{Z} \sum_{z=1}^{Z} \psi(\omega_z).$$

where ω_z are iid draws from ω.

VARIANCE REDUCTION

Standard error estimate for Monte Carlo:

$$||\mathbb{E}^{\mathrm{MC}}(\psi) - \mathbb{E}(\psi)|| \sim \nu \sqrt{\frac{V(\psi)}{Z}}, \qquad \nu \sim N(0,1).$$

Pros and cons:

- Non-intrusive $\Longrightarrow$ easy to implement.
- Independent of stochastic dimension $\Longrightarrow$ good for high-dimensional random field problems.
- Slow convergence $\Longrightarrow$ computational expense.

Options:

- More samples Z $\Longrightarrow$ more PDE solves.
- Reduce variance $V(\psi)$ $\Longrightarrow$ variance reduction techniques.

DERIVATIVES FOR VARIANCE REDUCTION

We take the N-th order Taylor expansion using the Fréchet derivatives D^N_ω of ψ with respect to ω about the mean parameter $\bar{\omega}$:

$$T_N(\omega) = \sum_{n=0}^{N} \frac{1}{n!} D^n_\omega \psi(\bar{\omega}) \left(\omega - \bar{\omega}\right)^n.$$

The N-th order sensitivity derivative Monte Carlo estimator can then be written:

$$\mathbb{E}^{\mathrm{SD-MC}}_N[\psi] := \mathbb{E}[T_N(\omega)] + \frac{1}{Z}\sum_{z=1}^{Z}[\psi(\omega_z) - T_N(\omega_z)].$$

This estimator can be shown to be unbiased, convergent, and have reduced variance under certain conditions (Jimenez, Liu, and M. Yousuff Hussaini, 2013).

SECOND ORDER VERSION

The second order sensitivity derivative Monte Carlo estimator can be written:

$$\mathbb{E}^{\mathrm{SD-MC}}_2[\psi] := \frac{1}{2}\mathbb{E}[D^2_\omega \psi(\bar{\omega})(\omega - \bar{\omega})(\omega - \bar{\omega})] + \frac{1}{Z}\sum_{z=1}^{Z}[\psi(\omega_z) - D^1_\omega \psi(\bar{\omega})(\omega_z - \bar{\omega}) - \frac{1}{2} D^2_\omega \psi(\bar{\omega})(\omega_z - \bar{\omega})(\omega_z - \bar{\omega})].$$

AUTOMATIC DIFFERENTIATION

We use dolfin-adjoint (Farrell et al., 2013) to automatically derive the adjoint and second-order adjoint equations and their finite element discretisation from their Unified Form Language description. This gives us access to routines for calculating the gradient and Hessian-vector action of ψ with respect to ω.

CORRECTION TERM

The term:

$$\mathbb{E}[D^2_\omega \psi(\bar{\omega})(\omega - \bar{\omega})(\omega - \bar{\omega})],$$

can be written in a finite-dimensional Euclidean $\mathbb{R}^M$ setting as:

$$\mathbb{E}[(\omega - \bar{\omega})^T H \, (\omega - \bar{\omega})],$$

with $\omega, \bar{\omega} \in R^M$ and the Hessian $H \in \mathbb{R}^{M \times M}$ the usual matrix of second derivatives of the functional ψ with respect to the parameters ω. It can be shown that this term is equal to:

$$\mathrm{tr}(C^{1/2} H C^{1/2}).$$

Let (λ_i, v_i) be the $M - 1$ eigenvalue-eigenvector pairs of the operator $C^{1/2}HC^{1/2}$ with the ordering $|\lambda_i| > |\lambda_{i+1}|$. The operator $C^{1/2}HC^{1/2}$ has a compact spectrum, allowing us to take the leading $P \ll M - 1$ eigenvalues:

$$\mathbb{E}[(\omega - \bar{\omega})^T H \, (\omega - \bar{\omega})] = \mathrm{tr}(HC) \approx \sum_{i=1}^{P} \lambda_i.$$

In practice, we cannot explicitly form either $C^{1/2}$ or H as they are both very large and dense matrices. Therefore we choose to solve for (λ_i, v_i) in a completely matrix-free manner by wrapping multigrid preconditioned Krylov solvers $C^{1/2}$ and Hessian-vector actions H within a Krylov-Schur eigenvalue solver.

RESULTS

We solve a stochastic non-linear Burgers equation with uncertain viscosity coefficient ν modelled as a random field. *We can acheive variance reduction of three orders of magnitude over a standard MC method with only a few dozen extra PDE solves. We need far fewer realisations Z of the non-linear PDE to acheive convergence.*

Find $u \in H^1_D(\Omega_s)$ such that:

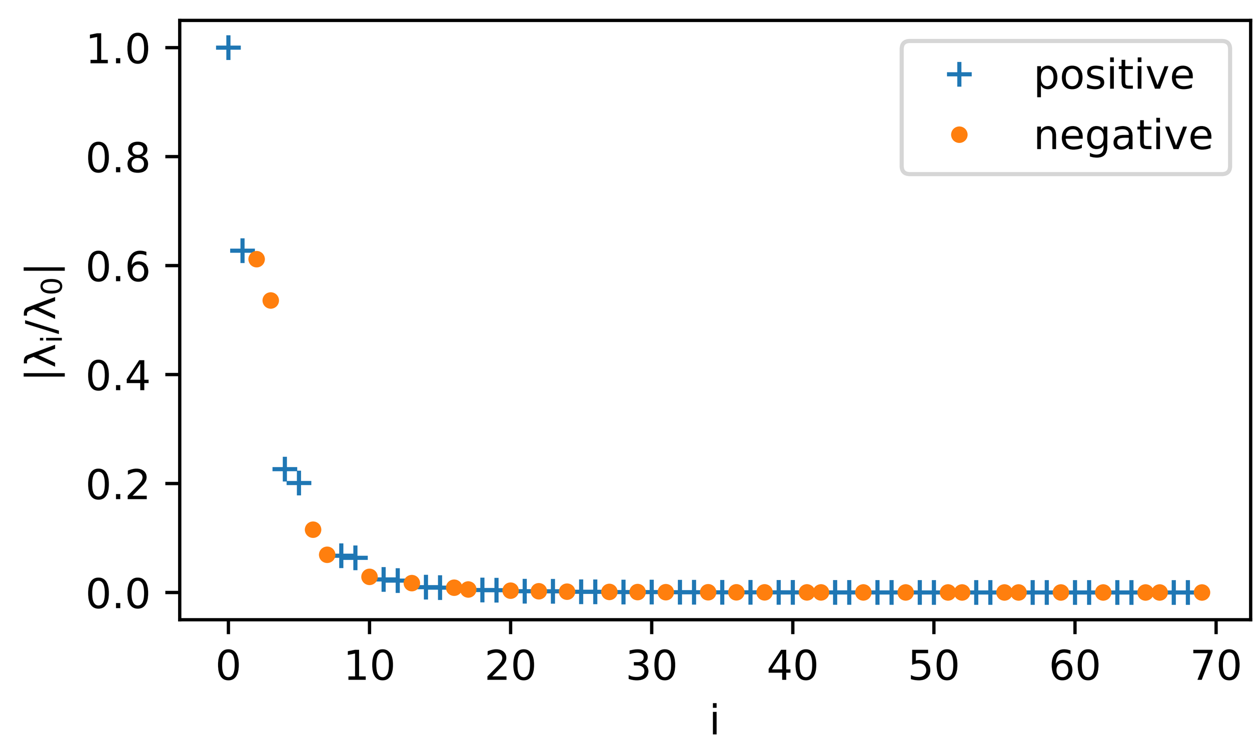
$$F(u, \nu; \tilde{u}) := \int_{\Omega_s} \nu \nabla u \cdot \nabla \tilde{u} - \frac{1}{2}\nabla(u^2 - u)\tilde{u} \; dx = 0 \quad \forall \tilde{u} \in H^1_0(\Omega_s), \tag{1}$$

$$\nu \sim N(1, C), \qquad C := A^{-\alpha}, \quad A := \kappa - \nabla^2. \tag{2}$$

TABLE 1

Method	Normalised Variance of Estimator
Standard Monte Carlo	1.0
Sensitivity derivative Monte Carlo $N = 1$	1.80×10^{-2}
Sensitivity derivative Monte Carlo $N = 2$	1.13×10^{-3}

FIGURE 1



Normalised spectrum of operator $C^{1/2}HC^{1/2}$ for non-linear Burgers problem with stochastic viscosity.

REFERENCES

Balay, Satish et al. (2016). *PETSc Users Manual*. Tech. rep. ANL-95/11 - Revision 3.7. Argonne National Laboratory. URL: http://www.mcs.anl.gov/petsc.

Cao, Y., M. Y. Hussaini, and T. A. Zhang (2004). "Exploitation of sensitivity Derivates for Improving Sampling Methods". In: *AIAA Journal* 42.2, pp. 815–822. DOI: 10.2514/1.2820.

Farrell, P. et al. (2013). "Automated Derivation of the Adjoint of High-Level Transient Finite Element Programs". In: *SIAM Journal on Scientific Computing* 35.4, pp. C369–C393. ISSN: 1064-8275. DOI: 10.1137/120873558.

Hauseux, Paul, Jack S. Hale, and Stéphane P. A. Bordas (2017). "Accelerating Monte Carlo estimation with derivatives of high-level finite element models". In: *Computer Methods in Applied Mechanics and Engineering* 318.Supplement C, pp. 917–936. ISSN: 0045-7825. DOI: 10.1016/j.cma.2017.01.041.

Jimenez, Edwin, Yaning Liu, and M. Yousuff Hussaini (2013). "Variance Reduction Method Based on Sensitivity Derivatives, Part 2". In: *Appl. Numer. Math.* 74, pp. 151–159. ISSN: 0168-9274. DOI: 10.1016/j.apnum.2012.07.010.

Lindgren, Finn, Håvard Rue, and Johan Lindström (2011). "An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach". en. In: *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 73.4, pp. 423–498. ISSN: 1467-9868. DOI: 10.1111/j.1467-9868.2011.00777.x.

Logg, Anders and Garth N. Wells (2010). "DOLFIN: Automated Finite Element Computing". In: *ACM Trans. Math. Softw.* 37.2, 20:1–20:28. ISSN: 0098-3500. DOI: 10.1145/1731022.1731030.