Hessian-based sampling in high dimensions for goal-oriented model order reduction

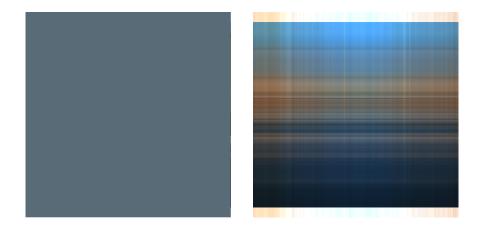
Peng Chen Omar Ghattas

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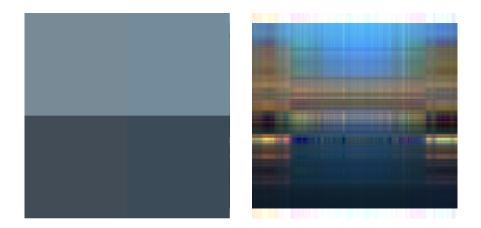
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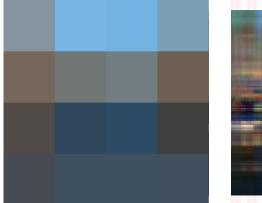


pixels
$$K = 1^2$$



pixels
$$K = 2^2$$

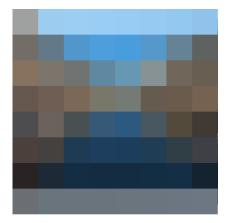
Information





pixels
$$K = 4^2$$

Information





pixels
$$K = 8^2$$

Information





pixels
$$K = 16^2$$

Parametrization

Dimension

Information





pixels
$$K = 32^2$$

Information





pixels
$$K = 64^2$$

Information





pixels
$$K = 128^2$$

Information





pixels
$$K = 256^2$$

Information





pixels
$$K = 512^2$$



pixels
$$K = 1024^2$$

Model order reduction for parametric PDEs

Hessian-based sampling

Numerical experiments

• Let $P \subset \mathbb{R}^{K}$ denote a *K*-dimensional parameter space, where $K \in \mathbb{N} \cup \infty$.

 $\boldsymbol{p}=(p_1,\ldots,p_K)\in P.$

• The parameter *p* lives in a box, w.l.o.g., $P = [-\sqrt{3}, \sqrt{3}]^K$, with uniform distribution

$$\boldsymbol{p} \sim \boldsymbol{\mu} = \mathcal{U}([-\sqrt{3},\sqrt{3}]^K),$$

with mean $\bar{p} = 0$, and covariance $\mathbb{C} = \mathbb{I}$.

• The parameter p lives in the whole space, i.e., $P = \mathbb{R}^{K}$, with Gaussian distribution

 $\boldsymbol{p} \sim \boldsymbol{\mu} = \mathcal{N}(\bar{\boldsymbol{p}}, \mathbb{C}),$

with mean \bar{p} , and covariance \mathbb{C} , s.p.d.

• Eg., \mathbb{C} is discretized from a covariance operator \mathcal{C} , given by

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Parametric PDEs

 Let V denote a Hilbert space with dual V'. Given p ∈ P, μ-a.e., find u ∈ V such that

$$a(u, v; \mathbf{p}) = f(v) \quad \forall v \in V.$$

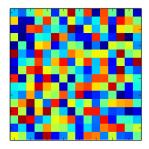
•
$$a(\cdot, \cdot; \mathbf{p}) : V \times V \to \mathbb{R}$$
 is a bilinear form, e.g.,

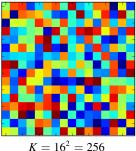
$$a(u,v;\boldsymbol{p}) = \int_D \kappa(\boldsymbol{p}) \nabla u \cdot \nabla v dx.$$

f(·) ∈ *V*′ is a linear functional.
 s(*p*) = *s*(*u*(*p*)) ∈ ℝ is a Qol.

Ex 1. heat conduction in thermal blocks

$$\kappa(\boldsymbol{p}) = \sum_{k=1}^{K} k^{-\beta} \chi_{D_k}(x) \boldsymbol{p}_k$$
$$\boldsymbol{p} \sim \mathcal{U}([-\sqrt{3}, \sqrt{3}]^K)$$





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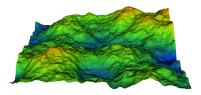
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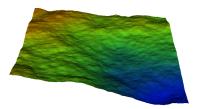
Ex 2. subsurface flow in a porous medium

$$\kappa(\mathbf{p}) = e^{\mathbf{k}}$$

log-normal diffusion with

$$\boldsymbol{p} \in \mathcal{N}(\bar{\boldsymbol{p}},\mathbb{C})$$







$$K = 129^2 = 16,641$$

Model order reduction - formulation (Maday, Patera, Rozza, et. al.)

Finite element approximation

Finite element space V_h ,

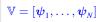
 $\dim(V_h) = N_h$

Given $p \in P$, find $u_h \in V_h$ s.t.

$$a(u_h, v_h; \boldsymbol{p}) = f(v_h) \ \forall v_h \in V_h$$

The algebraic system is

 $\mathbb{A}_h(\boldsymbol{p})\boldsymbol{u}_h = \mathbf{f}_h$



$$\mathbb{V}^T \boldsymbol{u}_h = \boldsymbol{u}_N$$

$$\mathbb{V}^T \mathbb{A}_h(\mathbf{p}) \mathbb{V} = \mathbb{A}_N(\mathbf{p})$$

 $\mathbb{V}^T \mathbf{f}_h = \mathbf{f}_N$

Reduced basis approximation

Reduced basis space $V_N \subset V_h$,

$$\dim(V_N) = N$$

Given $p \in P$, find $u_N \in V_N$ s.t.

$$a(u_N, v_N; \boldsymbol{p}) = f(v_N) \ \forall v_N \in V_N$$

The algebraic system is

 $\mathbb{A}_N(\boldsymbol{p})\boldsymbol{u}_N=\mathbf{f}_N$



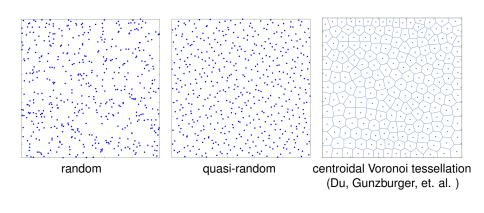
Model order reduction - algorithms (Maday, Patera, Rozza, et. al.)

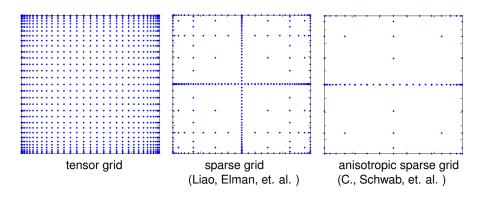
POD/SVD	Greedy algorithm	Offline-Online
Samples	Samples	Affine assumption/approx.
$\Xi_t = \{ \boldsymbol{p}^n, n = 1, \dots, N_t \}$	$\Xi_t = \{ \boldsymbol{p}^n, n = 1, \dots, N_t \}$	$a = \sum_{q=1}^{Q} heta_q({m p}) a_q$
Compute snapshots	Initialize V_N for $N = 1$ as	Offline computation once
$\mathbb{U} = [\boldsymbol{u}_h(\boldsymbol{p}^1), \dots, \boldsymbol{u}_h(\boldsymbol{p}^{N_t})]$	$V_N = \operatorname{span}\{u_h(p^1)\}$	$\mathbb{A}_N^q = \mathbb{V}^T \mathbb{A}_h^q \mathbb{V}, \mathbf{f}_N = \mathbb{V}^T \mathbf{f}_h$
Perform SVD	Pick next sample such that	Online assemble
$\mathbb{U} = \mathbb{V}\Sigma\mathbb{W}^T$	$p^{N+1} = \operatorname{argmax}_{p \in \Xi_t} \Delta_N(p)$	$\mathbb{A}_{\scriptscriptstyle N}({oldsymbol p}) = \sum_{q=1}^{\mathcal{Q}} heta_q({oldsymbol p}) \mathbb{A}_{\scriptscriptstyle N}^q$
Extract bases $\mathbb{V}[1:N,:]$	Update bases V_{N+1} as	Online solve and evaluate
$N = \operatorname{argmin}_n \mathcal{E}_n(\Sigma) \ge 1 - \varepsilon$	$V_N \oplus \operatorname{span}\{u_h(p^{N+1})\}$	$\mathbb{A}_N(\boldsymbol{p})\boldsymbol{u}_N = \mathbf{f}_N, s(\boldsymbol{p}) = \mathbf{s}_N^T \boldsymbol{u}_N$

Goal-oriented a-posteriori error estimate $\Delta_N(p)$ – dual weighted residual

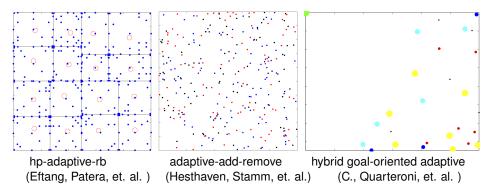
 $\Delta_N(\mathbf{p}) = f(\varphi_N) - a(u_N, \varphi_N; \mathbf{p}), \text{ where dual Prob.: } a(w_N, \varphi_N; \mathbf{p}) = s(w_N) \ \forall w_N \in W_N.$

$$\Delta_N(\boldsymbol{p}) = \overline{\mathbf{f}}_N^T \boldsymbol{\varphi}_N - \sum_{q=1}^Q heta_q(\boldsymbol{p}) \boldsymbol{\varphi}_N^T \overline{\mathbb{A}}_N^q \boldsymbol{u}_N, ext{ where } \overline{\mathbf{f}}_N = \mathbb{W}^T \mathbf{f}_h, ext{ and } \overline{\mathbb{A}}_N^q = \mathbb{W}^T \mathbb{A}_h^q \mathbb{V}$$





Model order reduction - samples



Model order reduction for parametric PDEs

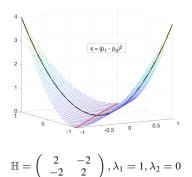
Hessian-based sampling

Numerical experiments

Hessian ℍ ∈ ℝ^{K×K}, the second-order partial derivatives of *s* with respect to *p*, i.e.,

$$\mathbb{H}_{kl} = \frac{\partial^2 s}{\partial p_k \partial p_l}, \quad k, l \in 1, \dots, K.$$

 The eigendirections corresponding to the leading eigenvalues of the Hessian are the directions along which the *s* changes the most in the parameter space.



Thus, sampling in the subspace of leading eigendirections presumably provid

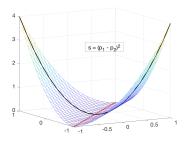
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$$\mathbb{H} = \begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix}, \lambda_1 = 1, \lambda_2 = 0$$

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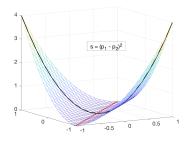
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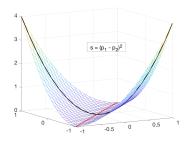
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$$s_{\text{quad}}(\boldsymbol{p}) = s(\bar{\boldsymbol{p}}) + \boldsymbol{g}_{\bar{\boldsymbol{p}}}^{T}(\boldsymbol{p} - \bar{\boldsymbol{p}}) + \frac{1}{2}(\boldsymbol{p} - \bar{\boldsymbol{p}})^{T} \mathbb{H}_{\bar{\boldsymbol{p}}}(\boldsymbol{p} - \bar{\boldsymbol{p}}),$$
(1)

where $g_{\bar{p}}$ and $\mathbb{H}_{\bar{p}}$ represent the **gradient** and the **Hessian** of *s* at \bar{p} .

The expectation of squad can be computed as

$$\mathbb{E}[s_{\text{quad}}] = s(\bar{p}) + \frac{1}{2} \text{tr}(\tilde{\mathbb{H}}_{\bar{p}}), \qquad (2$$

tr $(\hat{\mathbb{H}}_{\bar{p}})$: trace of the **covariance preconditioned Hessian** $\hat{\mathbb{H}}_{\bar{p}} = \mathbb{CH}_{\bar{p}}$ at the mean \bar{p} . • It is equivalent to the sum of all the eigenvalues, i.e.,

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Hessian-based sampling - from local to global Hessian

• Hessian at the mean: let $(\lambda_k, \varphi_k)_{k=1}^K$ denote the eigenpairs of $\tilde{\mathbb{H}}_{\bar{p}} = \mathbb{CH}_{\bar{p}}$, or equivalently the generalized eigenpairs of $(\mathbb{H}_{\bar{p}}, \mathbb{C}^{-1})$ for computational efficiency

$$\mathbb{H}_{\bar{p}}\boldsymbol{\varphi}_{k} = \lambda_{k}\mathbb{C}^{-1}\boldsymbol{\varphi}_{k}.$$
(5)

Averaged Hessian: we can replace the Hessian at the mean by

$$\mathbb{H} = \int_{P} \mathbb{H}_{p} d\mu(p) \approx \frac{1}{M} \sum_{m=1}^{M} \mathbb{H}_{p^{m}}, \qquad (6)$$

with p^m sampled according to its probability distribution μ .

• Combined Hessian: we compute the eigenvectors of Hessian at different samples

$$\mathbb{H}_{p^m}\varphi_k^m = \lambda_k^m \mathbb{C}^{-1}\varphi_k^m, \quad m = 1, \dots, M.$$
(7)

Then we combine them with weights (e.g. $w_k^m = \sqrt{\lambda_k^m}$) and compress them by SVE

$$\Phi = (w_1^1 \varphi_1^1, \dots, w_{L_1}^1 \varphi_{L_1}^1, \dots, w_1^M \varphi_1^M, \dots, w_{L_M}^M \varphi_{L_M}^M).$$
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(8)

• We employ a Lagrange multiplier method to compute the action of Hessian:

$$\mathcal{L}(u, v, \boldsymbol{p}) = s(u) + f(v) - a(u, v; \boldsymbol{p}), \tag{9}$$

where v is the adjoint variable or the Lagrange multiplier.

• With first order variation, we obtain the adjoint problem: find $v \in V$ such that

$$a(w, v; \boldsymbol{p}) = s(w) \quad \forall w \in V.$$
(10)

• Given (u, v, p), we compute the Hessian action in \hat{p} by the second order variation

$$\begin{pmatrix} \partial_{uu}\mathcal{L} & \partial_{uv}\mathcal{L} & \partial_{up}\mathcal{L} \\ \partial_{vu}\mathcal{L} & \partial_{vv}\mathcal{L} & \partial_{vp}\mathcal{L} \\ \partial_{pu}\mathcal{L} & \partial_{pv}\mathcal{L} & \partial_{pp}\mathcal{L} \end{pmatrix} \begin{pmatrix} \hat{u} \\ \hat{v} \\ \hat{p} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \mathbb{H}_p \hat{p} \end{pmatrix},$$
(11)

the **incremental adjoint problem**: find $\hat{v} \in V$ such that

$$a(\tilde{u}, \hat{v}; \boldsymbol{p}) = -\partial_{\boldsymbol{p}} a(\tilde{u}, v; \boldsymbol{p}) \hat{\boldsymbol{p}} \quad \forall \tilde{u} \in V,$$
(12)

the **incremental state problem**: find $\hat{u} \in V$ such that

$$a(\hat{u},\tilde{v};\boldsymbol{p}) = -\partial_{\boldsymbol{p}}a(\boldsymbol{u},\tilde{v};\boldsymbol{p})\hat{\boldsymbol{p}} \quad \forall \tilde{v} \in V,$$
(13)

and the **Hessian action** in direction \hat{p} as

$$\mathbb{H}_{p}\hat{p} = -\partial_{p}a(\hat{u}, v; p) - \partial_{p}a(u, \hat{v}; p) - \partial_{pp}a(u, v; p)\hat{p}.$$
(14)

Hessian-based sampling – Hessian action

• We employ a Lagrange multiplier method to compute the action of Hessian:

$$\mathcal{L}(u, v, \boldsymbol{p}) = s(u) + f(v) - a(u, v; \boldsymbol{p}),$$
(9)

where v is the adjoint variable or the Lagrange multiplier.

• With first order variation, we obtain the adjoint problem: find $v \in V$ such that

$$a(w, v; \boldsymbol{p}) = s(w) \quad \forall w \in V.$$
(10)

• Given (u, v, p), we compute the Hessian action in \hat{p} by the second order variation

$$\begin{pmatrix} \partial_{uu}\mathcal{L} & \partial_{uv}\mathcal{L} & \partial_{up}\mathcal{L} \\ \partial_{vu}\mathcal{L} & \partial_{vv}\mathcal{L} & \partial_{vp}\mathcal{L} \\ \partial_{pu}\mathcal{L} & \partial_{pv}\mathcal{L} & \partial_{pp}\mathcal{L} \end{pmatrix} \begin{pmatrix} \hat{u} \\ \hat{v} \\ \hat{p} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \mathbb{H}_p \hat{p} \end{pmatrix},$$
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(14)

Algorithm 1 Randomized SVD for generalized eigenvalue problem $(\mathbb{H}_p, \mathbb{C}^{-1})$

Input: \mathbb{H}_{p} , \mathbb{C}^{-1} , the number of eigenpairs *L*, an oversampling factor $l = 5 \sim 10$. **Output:** eigenpairs (Λ_{L}, Ψ_{L}) with $\Lambda_{L} = \text{diag}(\lambda_{1}, \ldots, \lambda_{L})$ and $\Psi_{L} = (\psi_{1}, \ldots, \psi_{L})$. 1. Draw a Gaussian random matrix $\Omega \in \mathbb{R}^{K \times (L+l)}$.

- 2. Compute $Y = \mathbb{C}(\mathbb{H}_p\Omega)$.
- 3. Compute *QR*-factorization Y = QR such that $Q^{\top} \mathbb{C}^{-1} Q = I_{L+l}$.
- 4. Form $T = Q^{\top} \mathbb{H}_p Q$ and compute eigendecomposition $T = S \Lambda S^{\top}$.
- 5. Extract $\Lambda_L = \Lambda(1:L, 1:L)$ and $\Psi_L = QS_L$ with $S_L = S(:, 1:L)$.

Computational cost is dominated by two (so-called double pass algorithm)

 $\mathbb{H}_p\Omega, \quad \mathbb{H}_pQ$

which needs 4(L+l) linearized PDE solves, i.e., incremental problems.

• Approximation error is bounded by remaining eigenvalues $\leq C(L, l) (\sum_{l>L} \lambda_l^2)^{1/2}$.

Nathan Halko, Per-Gunnar Martinsson, and Joel A. Tropp. "Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions." SIAM review 53.2 (2011): 217-288.

Algorithm 2 Randomized SVD for generalized eigenvalue problem $(\mathbb{H}_p, \mathbb{C}^{-1})$

Input: \mathbb{H}_{p} , \mathbb{C}^{-1} , the number of eigenpairs *L*, an oversampling factor $l = 5 \sim 10$. **Output:** eigenpairs (Λ_{L}, Ψ_{L}) with $\Lambda_{L} = \text{diag}(\lambda_{1}, \ldots, \lambda_{L})$ and $\Psi_{L} = (\psi_{1}, \ldots, \psi_{L})$. 1. Draw a Gaussian random matrix $\Omega \in \mathbb{R}^{K \times (L+l)}$.

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Input: \mathbb{H}_{p} , \mathbb{C}^{-1} , the number of eigenpairs *L*, an oversampling factor $l = 5 \sim 10$. **Output:** eigenpairs (Λ_{L}, Ψ_{L}) with $\Lambda_{L} = \text{diag}(\lambda_{1}, \ldots, \lambda_{L})$ and $\Psi_{L} = (\psi_{1}, \ldots, \psi_{L})$. 1. Draw a Gaussian random matrix $\Omega \in \mathbb{R}^{K \times (L+l)}$.

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Model order reduction for parametric PDEs

Hessian-based sampling

3 Numerical experiments

Heat conduction in thermal blocks

 Let V denote a Hilbert space with dual V'. Given p ∈ P, μ-a.e., find u ∈ V such that

$$a(u,v;\mathbf{p}) = f(v) \quad \forall v \in V.$$

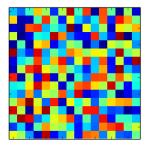
• $a(\cdot, \cdot; \mathbf{p}) : V \times V \to \mathbb{R}$ is a bilinear form, e.g.,

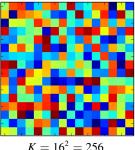
$$a(u,v;\boldsymbol{p}) = \int_D \kappa(\boldsymbol{p}) \nabla u \cdot \nabla v dx.$$

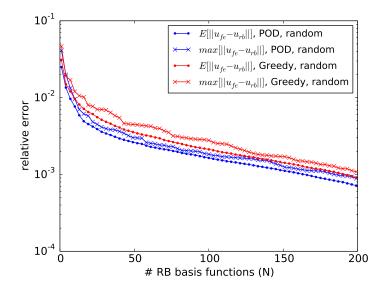
- f = 0, u = 1 on top, u = 0 on bottom.
- The Qol $s(u(\mathbf{p})) = 100 \int_{[0,0.1]^2} u(\mathbf{p}) dx.$
- $N_t = 1000$, uniform mesh of 65×65 .

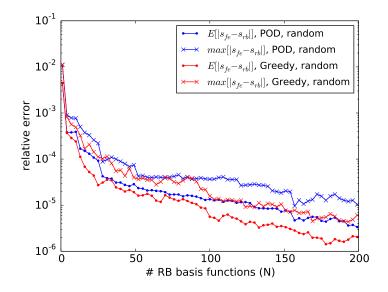
Ex 1. heat conduction in thermal blocks

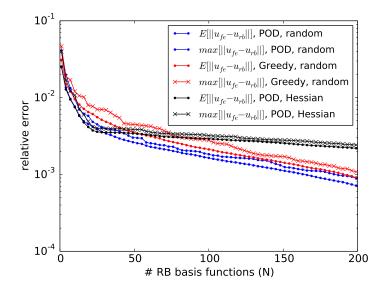
$$\kappa(\mathbf{p}) = \sum_{k=1}^{K} k^{-\beta} \chi_{D_k}(x) \mathbf{p}_k, \quad \beta = 1$$
$$\mathbf{p} \sim \mathcal{U}([-\sqrt{3}, \sqrt{3}]^K)$$

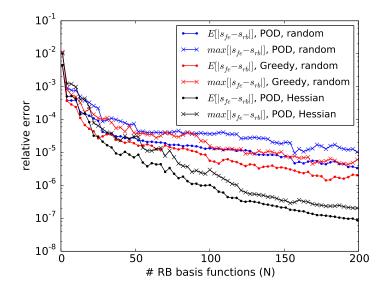


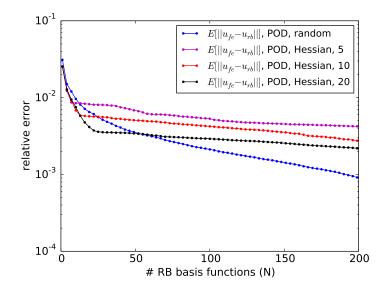


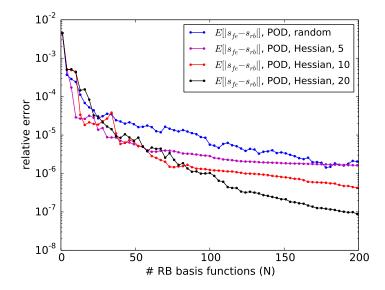


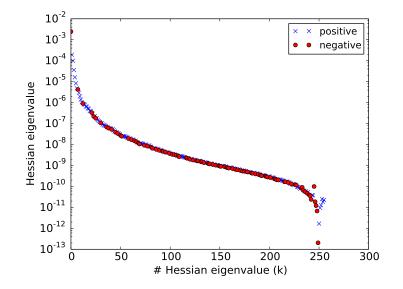


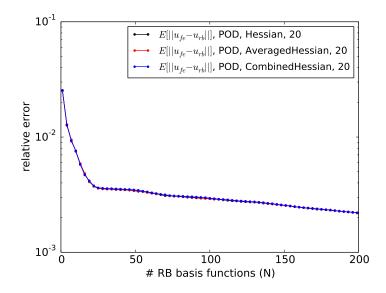


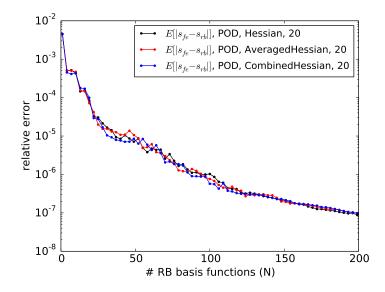












Subsurface flow in porous medium

 Let V denote a Hilbert space with dual V'. Given p ∈ P, μ-a.e., find u ∈ V such that

$$a(u,v;\mathbf{p}) = f(v) \quad \forall v \in V.$$

• $a(\cdot, \cdot; \boldsymbol{p}) : V \times V \to \mathbb{R}$ is a bilinear form, e.g.,

$$a(u,v;\boldsymbol{p}) = \int_D \kappa(\boldsymbol{p}) \nabla u \cdot \nabla v dx.$$

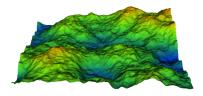
- f = 0, u = 1 on top, u = 0 on bottom.
- The Qol $s(u(\mathbf{p})) = 100 \int_{[0,0.1]^2} u(\mathbf{p}) dx.$
- $N_t = 1000$, uniform mesh of 129×129 .

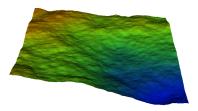
Ex 2. subsurface flow in a porous medium

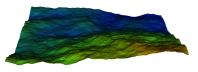
$$\kappa(\mathbf{p}) = e$$

log-normal diffusion with

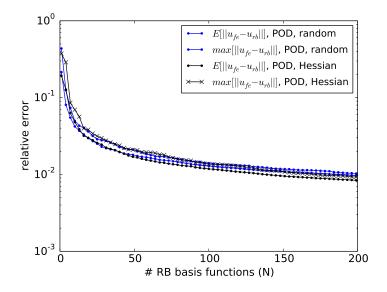
$$\boldsymbol{p} \in \mathcal{N}(\bar{\boldsymbol{p}},\mathbb{C}), \quad \mathcal{C} = (-\Delta + 0.5I)^{-2}$$

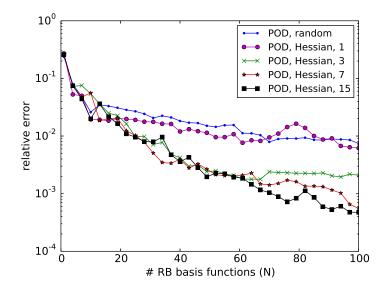


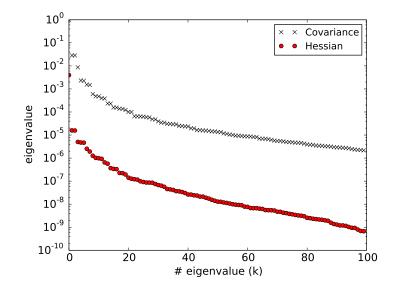


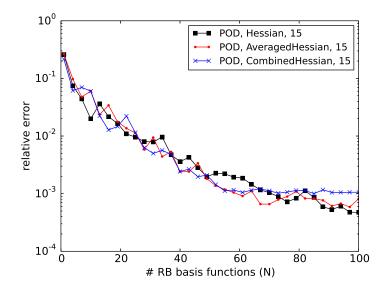


$$K = 129^2 = 16,641$$









- Even the solution manifold is high-dimensional, the manifold of the QoI may be **low-dimensional**, which can be detected by the **eigenvalues of the Hessian**.
- A scalable Hessian-based sampling algorithm is developed, whose cost is independent of the nominal dimensions but only intrinsic dimensions for Qol.
- Further investigation on adaptive Hessian sampling, local–global sampling, empirical interpolation, nonlinear problems, properties of different Qol.
- **Rigorous analysis** of goal-oriented error estimate for Hessian-based sampling.

P. Chen, and O. Ghattas. Hessian-based sampling in high-dimensional parameter space for goal-oriented model order reduction, preprint, 2017.

P. Chen, U. Villa, and O. Ghattas. Hessian-based adaptive sparse quadrature for infinite-dimensional Bayesian inverse problems, preprint, 2017.

P. Chen, U. Villa, and O. Ghattas. Taylor approximation and variance reduction for PDE-constrained optimal control problems under uncertainty, preprint, 2017.

Dimension

Information





pixels
$$K = 64^2$$

modes K = 64