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

Peng Chen Omar Ghattas

Center for Computational Geosciences and Optimization The Institute for Computational Engineering and Sciences The University of Texas at Austin

QUIET 2017 - Quantification of Uncertainty: Improving Efficiency and Technology SISSA, International School for Advanced Studies, Trieste, 18-21 July 2017

P. Chen (ICES - UT Austin)

$$
\text { \# pixels } K=1^{2} \quad \text { \# modes } K=1
$$


\# pixels $K=2^{2}$

\# modes $K=2$

## Parametrization


\# pixels $K=4^{2}$

\# modes $K=4$

## Parametrization


\# pixels $K=8^{2}$

\# modes $K=8$

## Parametrization


\# pixels $K=16^{2}$

\# modes $K=16$

## Parametrization

Dimension
Information

\# pixels $K=32^{2}$

\# modes $K=32$

## Parametrization


\# pixels $K=64^{2}$

\# modes $K=64$

## Parametrization


\# pixels $K=128^{2}$

\# modes $K=128$

## Parametrization


\# pixels $K=256^{2}$

\# modes $K=256$

## Parametrization


\# pixels $K=512^{2}$

\# modes $K=512$

## Parametrization


\# pixels $K=1024^{2}$

\# modes $K=1024$

## Outline

(1) Model order reduction for parametric PDEs
(2) Hessian-based sampling
(3) Numerical experiments

## Parameters

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

$$
\boldsymbol{p}=\left(p_{1}, \ldots, p_{K}\right) \in P .
$$

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

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

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

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

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

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

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

which is self adjoint, positive, and of trace class.


## Parameters

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

$$
\boldsymbol{p}=\left(p_{1}, \ldots, p_{K}\right) \in P .
$$

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

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

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

- The parameter $p$ lives in the whole space, i.e., $P=\mathbb{R}^{K}$, with Gaussian distribution $\boldsymbol{p} \sim \mu=\mathcal{N}(\overline{\boldsymbol{p}}, \mathbb{C})$,
with mean $\overline{\boldsymbol{p}}$. and covariance $\mathbb{C}$. s.p.d.
- Eg., C is discretized from a covariance operator $\mathcal{C}$, given by

which is self adjoint, positive, and of trace class.


## Parameters

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

$$
\boldsymbol{p}=\left(p_{1}, \ldots, p_{K}\right) \in P .
$$

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

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

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

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

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

with mean $\overline{\boldsymbol{p}}$, and covariance $\mathbb{C}$, s.p.d.

- Eg., $\mathbb{C}$ is discretized from a covariance operator $\mathcal{C}$, given by
which is self adjoint, positive, and of trace class.


## Parameters

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

$$
\boldsymbol{p}=\left(p_{1}, \ldots, p_{K}\right) \in P .
$$

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

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

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

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

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

with mean $\overline{\boldsymbol{p}}$, and covariance $\mathbb{C}$, s.p.d.

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

$$
\mathcal{C}=(-\delta \triangle+\gamma I)^{-\alpha},
$$

which is self adjoint, positive, and of trace class.

## Parametric PDEs

- Let $V$ denote a Hilbert space with dual $V^{\prime}$. Given $\boldsymbol{p} \in P, \mu$-a.e., find $u \in V$ such that

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

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

$$
a(u, v ; \boldsymbol{p})=\int_{D} \kappa(\boldsymbol{p}) \nabla u \cdot \nabla v d x
$$



- $f(\cdot) \in V^{\prime}$ is a linear functional.
- $s(\boldsymbol{p})=s(u(\boldsymbol{p})) \in \mathbb{R}$ is a Qol.

Ex 1. heat conduction in thermal blocks

$$
\begin{gathered}
\kappa(p)=\sum_{k=1}^{K} k^{-\beta} \chi_{D_{k}}(x) p_{k} \\
p \sim \mathcal{U}\left([-\sqrt{3}, \sqrt{3}]^{K}\right)
\end{gathered}
$$



$$
K=16^{2}=256
$$

## Parametric PDEs

- Let $V$ denote a Hilbert space with dual $V^{\prime}$. Given $\boldsymbol{p} \in P, \mu$-a.e., find $u \in V$ such that

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

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

$$
a(u, v ; \boldsymbol{p})=\int_{D} \kappa(\boldsymbol{p}) \nabla u \cdot \nabla v d x
$$

- $f(\cdot) \in V^{\prime}$ is a linear functional.
- $s(\boldsymbol{p})=s(u(\boldsymbol{p})) \in \mathbb{R}$ is a Qol.

Ex 2. subsurface flow in a porous medium

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

log-normal diffusion with

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



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

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

## Finite element approximation

Finite element space $V_{h}$,

$$
\operatorname{dim}\left(V_{h}\right)=N_{h}
$$

Given $\boldsymbol{p} \in P$, find $u_{h} \in V_{h}$ s.t.

$$
a\left(u_{h}, v_{h} ; \boldsymbol{p}\right)=f\left(v_{h}\right) \forall v_{h} \in V_{h}
$$

The algebraic system is

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

$$
\mathbb{V}^{T} \mathbb{A}_{h}(\boldsymbol{p}) \mathbb{V}=\mathbb{A}_{N}(\boldsymbol{p})
$$

$$
\begin{gathered}
\mathbb{V}=\left[\boldsymbol{\psi}_{1}, \ldots, \boldsymbol{\psi}_{N}\right] \\
\mathbb{V}^{T} \boldsymbol{u}_{h}=u_{N}
\end{gathered}
$$

Reduced basis approximation
Reduced basis space $V_{N} \subset V_{h}$,

$$
\operatorname{dim}\left(V_{N}\right)=N
$$

Given $\boldsymbol{p} \in P$, find $u_{N} \in V_{N}$ s.t.

$$
a\left(u_{N}, v_{N} ; \boldsymbol{p}\right)=f\left(v_{N}\right) \forall v_{N} \in V_{N}
$$

The algebraic system is

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

$$
\mathbb{V}^{T} \mathbf{f}_{h}=\mathbf{f}_{N}
$$



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

## POD/SVD

## Samples

$$
\Xi_{t}=\left\{\boldsymbol{p}^{n}, n=1, \ldots, N_{t}\right\}
$$

Compute snapshots

$$
\mathbb{U}=\left[\boldsymbol{u}_{h}\left(\boldsymbol{p}^{1}\right), \ldots, \boldsymbol{u}_{h}\left(\boldsymbol{p}^{N_{t}}\right)\right]
$$

Perform SVD

$$
\mathbb{U}=\mathbb{V} \Sigma \mathbb{W}^{T}
$$

Extract bases $\mathbb{V}[1: N,:]$
$N=\operatorname{argmin}_{n} \mathcal{E}_{n}(\Sigma) \geq 1-\varepsilon$

## Greedy algorithm

## Samples

$$
\Xi_{t}=\left\{\boldsymbol{p}^{n}, n=1, \ldots, N_{t}\right\}
$$

Initialize $V_{N}$ for $N=1$ as

$$
V_{N}=\operatorname{span}\left\{u_{h}\left(\boldsymbol{p}^{1}\right)\right\}
$$

Pick next sample such that

$$
\boldsymbol{p}^{N+1}=\operatorname{argmax}_{\boldsymbol{p} \in \Xi_{t}} \Delta_{N}(\boldsymbol{p})
$$

Update bases $V_{N+1}$ as

$$
V_{N} \oplus \operatorname{span}\left\{u_{h}\left(\boldsymbol{p}^{N+1}\right)\right\}
$$

## Offline-Online

Affine assumption/approx.

$$
a=\sum_{q=1}^{Q} \theta_{q}(\boldsymbol{p}) a_{q}
$$

Offline computation once

$$
\mathbb{A}_{N}^{q}=\mathbb{V}^{T} \mathbb{A}_{h}^{q} \mathbb{V}, \mathbf{f}_{N}=\mathbb{V}^{T} \mathbf{f}_{h}
$$

Online assemble

$$
\mathbb{A}_{N}(\boldsymbol{p})=\sum_{q=1}^{Q} \theta_{q}(\boldsymbol{p}) \mathbb{A}_{N}^{q}
$$

Online solve and evaluate
$\mathbb{A}_{N}(\boldsymbol{p}) \boldsymbol{u}_{N}=\mathbf{f}_{N}, s(\boldsymbol{p})=\mathbf{s}_{N}^{T} \boldsymbol{u}_{N}$

## Goal-oriented a-posteriori error estimate $\Delta_{N}(p)$ - dual weighted residual

$\Delta_{N}(\boldsymbol{p})=f\left(\varphi_{N}\right)-a\left(u_{N}, \varphi_{N} ; \boldsymbol{p}\right)$, where dual Prob.: $a\left(w_{N}, \varphi_{N} ; \boldsymbol{p}\right)=s\left(w_{N}\right) \forall w_{N} \in W_{N}$.

$$
\Delta_{N}(\boldsymbol{p})=\overline{\mathbf{f}}_{N}^{T} \boldsymbol{\varphi}_{N}-\sum_{q=1}^{Q} \theta_{q}(\boldsymbol{p}) \boldsymbol{\varphi}_{N}^{T} \overline{\mathbb{A}}_{N}^{q} \boldsymbol{u}_{N}, \text { where } \overline{\mathbf{f}}_{N}=\mathbb{W}^{T} \mathbf{f}_{h}, \text { and } \overline{\mathbb{A}}_{N}^{q}=\mathbb{W}^{T} \mathbb{A}_{h}^{q} \mathbb{V}
$$

## Model order reduction - samples


random

quasi-random

centroidal Voronoi tessellation (Du, Gunzburger, et. al. )

## Model order reduction - samples


tensor grid

sparse grid
(Liao, Elman, et. al. )

anisotropic sparse grid (C., Schwab, et. al. )

## Model order reduction - samples


hp-adaptive-rb
(Eftang, Patera, et. al. )

adaptive-add-remove (Hesthaven, Stamm, et. al.)

hybrid goal-oriented adaptive (C., Quarteroni, et. al. )

## Outline

## (1) Model order reduction for parametric PDEs

(2) Hessian-based sampling

## (3) Numerical experiments

## Hessian-based sampling - Hessian

- Hessian $\mathbb{H} \in \mathbb{R}^{K \times K}$, the second-order partial derivatives of $s$ with respect to $\boldsymbol{p}$, i.e.,

$$
\mathbb{H}_{k l}=\frac{\partial^{2} s}{\partial p_{k} \partial p_{l}}, \quad k, l \in 1, \ldots, K
$$

- The eigendirections corresponding to the leading eigenvalues of the Hessian are the directions along which the s changes the most

- Thus, sampling in the subspace of leading eigendirections presumably provide the most representative samples that capture the variation of the $s$, at least locally.
- It has been widely used in large-scale computation for


## Hessian-based sampling - Hessian

- Hessian $\mathbb{H} \in \mathbb{R}^{K \times K}$, the second-order partial derivatives of $s$ with respect to $\boldsymbol{p}$, i.e.,

$$
\mathbb{H}_{k l}=\frac{\partial^{2} s}{\partial p_{k} \partial p_{l}}, \quad k, l \in 1, \ldots, K
$$

- 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 provide the most representative samples that capture the variation of the $s$, at least locally.
- It has been widely used in large-scale computation for


## Hessian-based sampling - Hessian

- Hessian $\mathbb{H} \in \mathbb{R}^{K \times K}$, the second-order partial derivatives of $s$ with respect to $\boldsymbol{p}$, i.e.,

$$
\mathbb{H}_{k l}=\frac{\partial^{2} s}{\partial p_{k} \partial p_{l}}, \quad k, l \in 1, \ldots, K
$$

- 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 provide the most representative samples that capture the variation of the $s$, at least locally.
- It has been widely used in large-scale computation for


## Hessian-based sampling - Hessian

- Hessian $\mathbb{H} \in \mathbb{R}^{K \times K}$, the second-order partial derivatives of $s$ with respect to $\boldsymbol{p}$, i.e.,

$$
\mathbb{H}_{k l}=\frac{\partial^{2} s}{\partial p_{k} \partial p_{l}}, \quad k, l \in 1, \ldots, K
$$

- 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 provide the most representative samples that capture the variation of the $s$, at least locally.
- It has been widely used in large-scale computation for solving nonlinear problems, control/optimization, parameter estimation, data assimilation


## Hessian-based sampling - $\mathbb{C}$-preconditioned Hessian

- Let $s_{q u a d}$ denote the quadratic/Taylor approximation of $s$ given by

$$
\begin{equation*}
s_{\mathrm{quad}}(\boldsymbol{p})=s(\overline{\boldsymbol{p}})+\boldsymbol{g}_{\overline{\boldsymbol{p}}}^{T}(\boldsymbol{p}-\overline{\boldsymbol{p}})+\frac{1}{2}(\boldsymbol{p}-\overline{\boldsymbol{p}})^{T} \mathbb{H}_{\overline{\boldsymbol{p}}}(\boldsymbol{p}-\overline{\boldsymbol{p}}), \tag{1}
\end{equation*}
$$

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

- The expectation of $s_{\text {quad }}$ can be computed as

$\operatorname{tr}\left(\tilde{\mathbb{H}}_{\bar{p}}\right)$ : trace of the covariance preconditioned Hessian $\tilde{\mathbb{H}}_{\bar{p}}=\mathbb{C} \mathbb{H}_{\bar{p}}$ at the mean $\bar{p}$.
- It is equivalent to the sum of all the eigenvalues, i.e.,

- If $\lambda_{k}$ decay fast, sampling in a low-dimensional subspace of eigenvectors:



## Hessian-based sampling - $\mathbb{C}$-preconditioned Hessian

- Let $s_{\text {quad }}$ denote the quadratic/Taylor approximation of $s$ given by

$$
\begin{equation*}
s_{\text {quad }}(\boldsymbol{p})=s(\overline{\boldsymbol{p}})+\boldsymbol{g}_{\overline{\boldsymbol{p}}}^{T}(\boldsymbol{p}-\overline{\boldsymbol{p}})+\frac{1}{2}(\boldsymbol{p}-\overline{\boldsymbol{p}})^{T} \mathbb{H}_{\overline{\boldsymbol{p}}}(\boldsymbol{p}-\overline{\boldsymbol{p}}), \tag{1}
\end{equation*}
$$

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

- The expectation of $s_{\text {quad }}$ can be computed as

$$
\begin{equation*}
\mathbb{E}\left[s_{\text {quad }}\right]=s(\overline{\boldsymbol{p}})+\frac{1}{2} \operatorname{tr}\left(\tilde{\mathbb{H}}_{\overline{\boldsymbol{p}}}\right), \tag{2}
\end{equation*}
$$

$\operatorname{tr}\left(\tilde{H}_{\bar{p}}\right)$ : trace of the covariance preconditioned Hessian $\tilde{\mathbb{H}}_{\bar{p}}=\mathbb{C} \mathbb{H}_{\bar{p}}$ at the mean $\overline{\boldsymbol{p}}$.

- It is equivalent to the sum of all the eigenvalues, i.e.,

- If $\lambda_{k}$ decay fast, sampling in a low-dimensional subspace of eigenvectors:



## Hessian-based sampling - $\mathbb{C}$-preconditioned Hessian

- Let $s_{\text {quad }}$ denote the quadratic/Taylor approximation of $s$ given by

$$
\begin{equation*}
s_{\text {quad }}(\boldsymbol{p})=s(\overline{\boldsymbol{p}})+\boldsymbol{g}_{\overline{\boldsymbol{p}}}^{T}(\boldsymbol{p}-\overline{\boldsymbol{p}})+\frac{1}{2}(\boldsymbol{p}-\overline{\boldsymbol{p}})^{T} \mathbb{H}_{\overline{\boldsymbol{p}}}(\boldsymbol{p}-\overline{\boldsymbol{p}}), \tag{1}
\end{equation*}
$$

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

- The expectation of $s_{\text {quad }}$ can be computed as

$$
\begin{equation*}
\mathbb{E}\left[s_{\text {quad }}\right]=s(\overline{\boldsymbol{p}})+\frac{1}{2} \operatorname{tr}\left(\tilde{\mathbb{H}}_{\overline{\boldsymbol{p}}}\right) \tag{2}
\end{equation*}
$$

$\operatorname{tr}\left(\tilde{H}_{\bar{p}}\right)$ : trace of the covariance preconditioned Hessian $\tilde{\mathbb{H}}_{\bar{p}}=\mathbb{C} \mathbb{H}_{\bar{p}}$ at the mean $\overline{\boldsymbol{p}}$.

- It is equivalent to the sum of all the eigenvalues, i.e.,

$$
\begin{equation*}
\operatorname{tr}\left(\tilde{\mathbb{H}}_{\bar{p}}\right)=\sum_{k=1}^{K} \lambda_{k}\left(\tilde{\mathbb{H}}_{\bar{p}}\right) \tag{3}
\end{equation*}
$$

- If $\lambda_{k}$ decay fast, sampling in a low-dimensional subspace of eigenvectors:


## Hessian-based sampling - $\mathbb{C}$-preconditioned Hessian

- Let $s_{\text {quad }}$ denote the quadratic/Taylor approximation of $s$ given by

$$
\begin{equation*}
s_{\text {quad }}(\boldsymbol{p})=s(\overline{\boldsymbol{p}})+\boldsymbol{g}_{\overline{\boldsymbol{p}}}^{T}(\boldsymbol{p}-\overline{\boldsymbol{p}})+\frac{1}{2}(\boldsymbol{p}-\overline{\boldsymbol{p}})^{T} \mathbb{H}_{\overline{\boldsymbol{p}}}(\boldsymbol{p}-\overline{\boldsymbol{p}}), \tag{1}
\end{equation*}
$$

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

- The expectation of $s_{\text {quad }}$ can be computed as

$$
\begin{equation*}
\mathbb{E}\left[s_{\text {quad }}\right]=s(\overline{\boldsymbol{p}})+\frac{1}{2} \operatorname{tr}\left(\tilde{\mathbb{H}}_{\overline{\boldsymbol{p}}}\right) \tag{2}
\end{equation*}
$$

$\operatorname{tr}\left(\tilde{H}_{\bar{p}}\right)$ : trace of the covariance preconditioned Hessian $\tilde{\mathbb{H}}_{\bar{p}}=\mathbb{C} \mathbb{H}_{\bar{p}}$ at the mean $\overline{\boldsymbol{p}}$.

- It is equivalent to the sum of all the eigenvalues, i.e.,

$$
\begin{equation*}
\operatorname{tr}\left(\tilde{\mathbb{H}}_{\bar{p}}\right)=\sum_{k=1}^{K} \lambda_{k}\left(\tilde{\mathbb{H}}_{\bar{p}}\right) \tag{3}
\end{equation*}
$$

- If $\lambda_{k}$ decay fast, sampling in a low-dimensional subspace of eigenvectors:

$$
\begin{equation*}
\boldsymbol{p}_{L}=\sum_{l=1}^{L}\left(\boldsymbol{p}, \boldsymbol{\varphi}_{l}\right)_{2} \boldsymbol{\varphi}_{l} \tag{4}
\end{equation*}
$$

## Hessian-based sampling - from local to global Hessian

- Hessian at the mean: let $\left(\lambda_{k}, \boldsymbol{\varphi}_{k}\right)_{k=1}^{K}$ denote the eigenpairs of $\tilde{\mathbb{H}}_{\bar{p}}=\mathbb{C} \mathbb{H}_{\bar{p}}$, or equivalently the generalized eigenpairs of $\left(\mathbb{H}_{\bar{p}}, \mathbb{C}^{-1}\right)$ for computational efficiency

$$
\begin{equation*}
\mathbb{H}_{\bar{p}} \boldsymbol{\varphi}_{k}=\lambda_{k} \mathbb{C}^{-1} \boldsymbol{\varphi}_{k} . \tag{5}
\end{equation*}
$$

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

with $p^{m}$ sampled according to its probability distribution $\mu$.
- Combined Hessian: we compute the eigenvectors of Hessian at different samples


Then we combine them with weights (e.g. $w_{k}^{m}=\sqrt{\lambda_{k}^{m}}$ ) and compress them by SVD


## Hessian-based sampling - from local to global Hessian

- Hessian at the mean: let $\left(\lambda_{k}, \boldsymbol{\varphi}_{k}\right)_{k=1}^{K}$ denote the eigenpairs of $\tilde{\mathbb{H}}_{\bar{p}}=\mathbb{C} \mathbb{H}_{\bar{p}}$, or equivalently the generalized eigenpairs of $\left(\mathbb{H}_{\bar{p}}, \mathbb{C}^{-1}\right)$ for computational efficiency

$$
\begin{equation*}
\mathbb{H}_{\overline{\boldsymbol{\rho}}} \boldsymbol{\varphi}_{k}=\lambda_{k} \mathbb{C}^{-1} \boldsymbol{\varphi}_{k} . \tag{5}
\end{equation*}
$$

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

$$
\begin{equation*}
\mathbb{H}=\int_{P} \mathbb{H}_{p} d \mu(\boldsymbol{p}) \approx \frac{1}{M} \sum_{m=1}^{M} \mathbb{H}_{p^{m}}, \tag{6}
\end{equation*}
$$

with $\boldsymbol{p}^{m}$ sampled according to its probability distribution $\mu$.

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

Then we combine them with weights (e.g. $w_{k}^{m}=\sqrt{\lambda_{k}^{m}}$ ) and compress them by SVD

## Hessian-based sampling - from local to global Hessian

- Hessian at the mean: let $\left(\lambda_{k}, \boldsymbol{\varphi}_{k}\right)_{k=1}^{K}$ denote the eigenpairs of $\tilde{\mathbb{H}}_{\bar{p}}=\mathbb{C} \mathbb{H}_{\bar{p}}$, or equivalently the generalized eigenpairs of $\left(\mathbb{H}_{\bar{p}}, \mathbb{C}^{-1}\right)$ for computational efficiency

$$
\begin{equation*}
\mathbb{H}_{\bar{p}} \boldsymbol{\varphi}_{k}=\lambda_{k} \mathbb{C}^{-1} \boldsymbol{\varphi}_{k} . \tag{5}
\end{equation*}
$$

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

$$
\begin{equation*}
\mathbb{H}=\int_{P} \mathbb{H}_{p} d \mu(\boldsymbol{p}) \approx \frac{1}{M} \sum_{m=1}^{M} \mathbb{H}_{p^{m}}, \tag{6}
\end{equation*}
$$

with $\boldsymbol{p}^{m}$ sampled according to its probability distribution $\mu$.

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

$$
\begin{equation*}
\mathbb{H}_{p^{m}} \boldsymbol{\varphi}_{k}^{m}=\lambda_{k}^{m} \mathbb{C}^{-1} \boldsymbol{\varphi}_{k}^{m}, \quad m=1, \ldots, M . \tag{7}
\end{equation*}
$$

Then we combine them with weights (e.g. $w_{k}^{m}=\sqrt{\lambda_{k}^{m}}$ ) and compress them by SVD

$$
\begin{equation*}
\Phi=\left(w_{1}^{1} \boldsymbol{\varphi}_{1}^{1}, \ldots, w_{L_{1}}^{1} \boldsymbol{\varphi}_{L_{1}}^{1}, \ldots, w_{1}^{M} \boldsymbol{\varphi}_{1}^{M}, \ldots, w_{L_{M}}^{M} \boldsymbol{\varphi}_{L_{M}}^{M}\right) \tag{8}
\end{equation*}
$$

## Hessian-based sampling - Hessian action

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

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

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

the incremental adjoint problem: find $\hat{v} \in V$ such that
$a(\tilde{u}, \hat{v} ; \boldsymbol{p})=-\partial_{p} a(\tilde{u}, v ; \boldsymbol{p}) \hat{\boldsymbol{p}}$
the incremental state problem: find $\hat{u} \in V$ such that
$a(\hat{u}, \tilde{v} ; \boldsymbol{p})=-\partial_{p} a(u, \tilde{v} ; \boldsymbol{p}) \hat{\boldsymbol{p}}$
and the Hessian action in direction $\hat{p}$ as



## Hessian-based sampling - Hessian action

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

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

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

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

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

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

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

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

## Hessian-based sampling - Hessian action

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

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

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

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

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

$$
\left(\begin{array}{ccc}
\partial_{u u} \mathcal{L} & \partial_{u v} \mathcal{L} & \partial_{u p} \mathcal{L}  \tag{11}\\
\partial_{v u} \mathcal{L} & \partial_{v v} \mathcal{L} & \partial_{v p} \mathcal{L} \\
\partial_{p u} \mathcal{L} & \partial_{p v} \mathcal{L} & \partial_{p p} \mathcal{L}
\end{array}\right)\left(\begin{array}{c}
\hat{u} \\
\hat{v} \\
\hat{\boldsymbol{p}}
\end{array}\right)=\left(\begin{array}{c}
0 \\
0 \\
\mathbb{H}_{p} \hat{\boldsymbol{p}}
\end{array}\right),
$$

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

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

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

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

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

$$
\begin{equation*}
\mathbb{H}_{p} \hat{\boldsymbol{p}}=-\partial_{p} a(\hat{u}, v ; \boldsymbol{p})-\partial_{p} a(u, \hat{v} ; \boldsymbol{p})-\partial_{p p} a(u, v ; \boldsymbol{p}) \hat{\boldsymbol{p}} \tag{14}
\end{equation*}
$$

## Hessian-based sampling - Randomized SVD

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 $\left(\Lambda_{L}, \Psi_{L}\right)$ with $\Lambda_{L}=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{L}\right)$ and $\Psi_{L}=\left(\psi_{1}, \ldots, \psi_{L}\right)$. 1. Draw a Gaussian random matrix $\Omega \in \mathbb{R}^{K \times(L+l)}$.
2. Compute $Y=\mathbb{C}\left(\mathbb{H}_{p} \Omega\right)$.
3. Compute $Q R$-factorization $Y=Q R$ 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 $\Psi_{L}=Q S_{L}$ with $S_{L}=S(:, 1: L)$.

- Computational cost is dominated by two (so-called double pass algorithm)
which needs $4(L+l)$ linearized PDE solves, i.e., incremental problems.
- Approvimation error is bounded by remaining eigenvalues $\leq C(I, I) / \sum$

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.

## Hessian-based sampling - Randomized SVD

Algorithm 2 Randomized SVD for generalized eigenvalue problem $\left(\mathbb{H}_{p}, \mathbb{C}^{-1}\right)$
Input: $\mathbb{H}_{p}, \mathbb{C}^{-1}$, the number of eigenpairs $L$, an oversampling factor $l=5 \sim 10$. Output: eigenpairs $\left(\Lambda_{L}, \Psi_{L}\right)$ with $\Lambda_{L}=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{L}\right)$ and $\Psi_{L}=\left(\psi_{1}, \ldots, \psi_{L}\right)$. 1. Draw a Gaussian random matrix $\Omega \in \mathbb{R}^{K \times(L+l)}$.
2. Compute $Y=\mathbb{C}\left(\mathbb{H}_{p} \Omega\right)$.
3. Compute $Q R$-factorization $Y=Q R$ 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 $\Psi_{L}=Q S_{L}$ with $S_{L}=S(:, 1: L)$.

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

$$
\mathbb{H}_{p} \Omega, \quad \mathbb{H}_{p} Q
$$

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

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.

## Hessian-based sampling - Randomized SVD

Algorithm 3 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 $\left(\Lambda_{L}, \Psi_{L}\right)$ with $\Lambda_{L}=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{L}\right)$ and $\Psi_{L}=\left(\psi_{1}, \ldots, \psi_{L}\right)$. 1. Draw a Gaussian random matrix $\Omega \in \mathbb{R}^{K \times(L+l)}$.
2. Compute $Y=\mathbb{C}\left(\mathbb{H}_{p} \Omega\right)$.
3. Compute $Q R$-factorization $Y=Q R$ 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 $\Psi_{L}=Q S_{L}$ with $S_{L}=S(:, 1: L)$.

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

$$
\mathbb{H}_{p} \Omega, \quad \mathbb{H}_{p} Q
$$

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

- Approximation error is bounded by remaining eigenvalues $\leq C(L, l)\left(\sum_{l \geq L} \lambda_{l}^{2}\right)^{1 / 2}$.

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.

## Outline

## (1) Model order reduction for parametric PDEs

(2) Hessian-based sampling
(3) Numerical experiments

## Heat conduction in thermal blocks

- Let $V$ denote a Hilbert space with dual $V^{\prime}$. Given $\boldsymbol{p} \in P, \mu$-a.e., find $u \in V$ such that

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

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

$$
a(u, v ; \boldsymbol{p})=\int_{D} \kappa(\boldsymbol{p}) \nabla u \cdot \nabla v d x
$$

- $f=0, u=1$ on top, $u=0$ on bottom.
- The Qol $s(u(\boldsymbol{p}))=100 \int_{[0,0.1]^{2}} u(\boldsymbol{p}) d x$.
- $N_{t}=1000$, uniform mesh of $65 \times 65$.

Ex 1. heat conduction in thermal blocks

$$
\begin{gathered}
\kappa(p)=\sum_{k=1}^{K} k^{-\beta} \chi_{D_{k}}(x) p_{k}, \quad \beta=1 \\
p \sim \mathcal{U}\left([-\sqrt{3}, \sqrt{3}]^{K}\right)
\end{gathered}
$$



$K=16^{2}=256$

## RB errors POD vs Greedy for solution



## RB errors POD vs Greedy for Qol



## RB errors random vs Hessian for solution



## RB errors random vs Hessian for Qol



## RB errors with different \# Hessian modes for solution



## RB errors with different \# Hessian modes for Qol



## Decay of the eigenvalues of Hessian at mean



## Comparison of different Hessians for solution



## Comparison of different Hessians for Qol



## Subsurface flow in porous medium

- Let $V$ denote a Hilbert space with dual $V^{\prime}$. Given $\boldsymbol{p} \in P, \mu$-a.e., find $u \in V$ such that

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

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


$$
a(u, v ; \boldsymbol{p})=\int_{D} \kappa(\boldsymbol{p}) \nabla u \cdot \nabla v d x
$$

- $f=0, u=1$ on top, $u=0$ on bottom.
- The Qol $s(u(\boldsymbol{p}))=100 \int_{[0,0.1]^{2}} u(\boldsymbol{p}) d x$.
- $N_{t}=1000$, uniform mesh of $129 \times 129$.

Ex 2. subsurface flow in a porous medium

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

log-normal diffusion with

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



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

## RB errors random vs Hessian for solution



## RB errors random vs Hessian for Qol



## Decay of eigenvalues of Hessian $\mathbb{H}_{\bar{p}}$ and covariance $\mathbb{C}$



## Comparison of different Hessians for Qol



## Summary

- Even the solution manifold is high-dimensional, the manifold of the Qol 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 .

## Parametrization


\# pixels $K=64^{2}$

\# modes $K=64$

