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Active subspaces for Bayesian inversion

Application to a methane hydrate model

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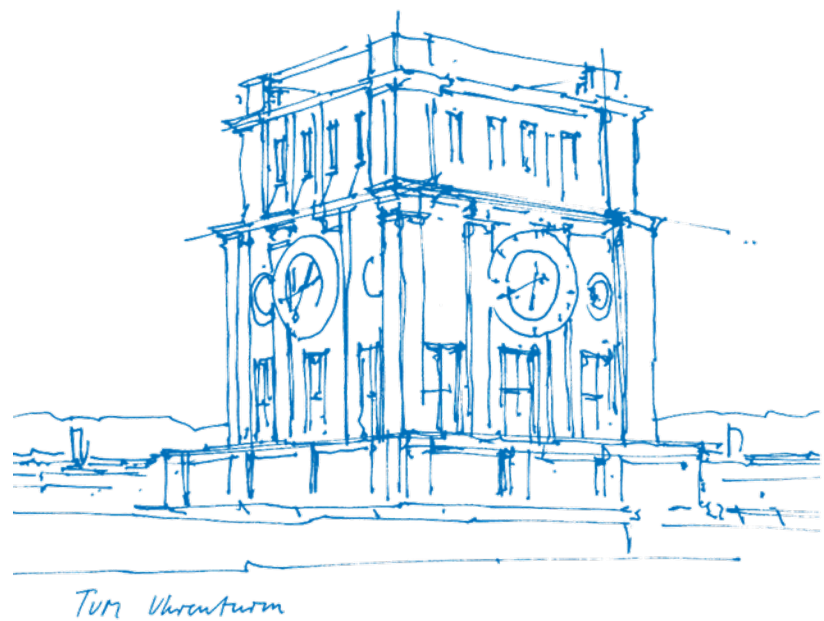

Outline

1. Bayesian inversion – Basics

2. Active subspaces – General

3. Active subspaces for Bayesian inversion

4. Application to a methane hydrate model

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Outline

Bayesian inversion

Uncertainties are modeled probabilistically.

Deterministic inverse problems are in general ill-posed.
$\rightarrow$ Regularization by a Bayesian problem formulation.

Task: Get a probabilistic description of model parameters $\mathbf{x}$ incorporating data $\mathbf{d}$.

$$\mathbf{d} = \mathscr{G}(\mathbf{x}^{\star}) + \eta \tag{1}$$

- $\mathbf{d}$ Data
- $\mathscr{G}$ Forward/Observable map
- $\mathbf{x}^{\star}$ “True“ parameter
- η Noise

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Using Bayes' theorem

Treat parameter **x** and data **d** as random variable. Assume $\eta \sim \mathscr{N}(0, \Gamma)$.

Task: "Get" posterior distribution on the parameter space.

$$\begin{aligned} \rho_{\text{post}}(\mathbf{x}|\mathbf{d}) &\propto \rho_{\text{like}}(\mathbf{d}|\mathbf{x})\rho_{\text{prior}}(\mathbf{x}) && (2) \\ &= \exp\left(-\frac{\|\mathbf{d}-\mathscr{G}(\mathbf{x})\|_\Gamma^2}{2}\right)\rho_{\text{prior}}(\mathbf{x}) && (3) \\ &= \exp\left(-f_{\mathbf{d}}(\mathbf{x})\right)\rho_{\text{prior}}(\mathbf{x}) && (4) \end{aligned}$$

- $\|\cdot\|_\Gamma := \|\Gamma^{-1/2}\cdot\|_2$
- ρ_{post} Posterior
- ρ_{like} Likelihood
- ρ_{prior} Prior
- $f_{\mathbf{d}}$ Data misfit function

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Sampling from the posterior

One way: ***M**arkov **c**hain **M**onte **C**arlo* (MCMC)

Construct a Markov chain s.t. its stationary distribution is the posterior.
$\rightarrow$ Metropolis(-Hastings) algorithm

Algorithm 1 Metropolis algorithm for the posterior.

Assume a symmetric proposal density function τ, an initial point $\mathbf{x}_1$, and a prior ρ_{prior} is given.
For $i = 1, 2, \ldots, N-1$

1. Draw a proposal $\tilde{\mathbf{x}}$ from τ centered at $\mathbf{x}_i$.
2. Calculate the acceptance ratio

$$\alpha(\tilde{\mathbf{x}}, \mathbf{x}_i) = \min\left(1, \frac{\exp(-f_{\mathbf{d}}(\tilde{\mathbf{x}}))\rho_{\text{prior}}(\tilde{\mathbf{x}})}{\exp(-f_{\mathbf{d}}(\mathbf{x}_i))\rho_{\text{prior}}(\mathbf{x}_i)}\right). \tag{5}$$

3. Draw $u \sim \mathscr{U}([0,1])$.
4. Set $\mathbf{x}_{i+1} = \tilde{\mathbf{x}}$ if $\alpha(\tilde{\mathbf{x}}, \mathbf{x}_i) \geq u$, otherwise set $\mathbf{x}_{i+1} = \mathbf{x}_i$.

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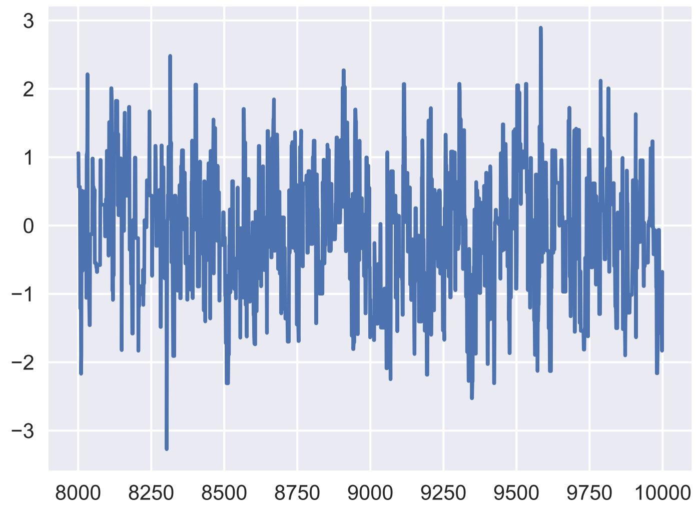
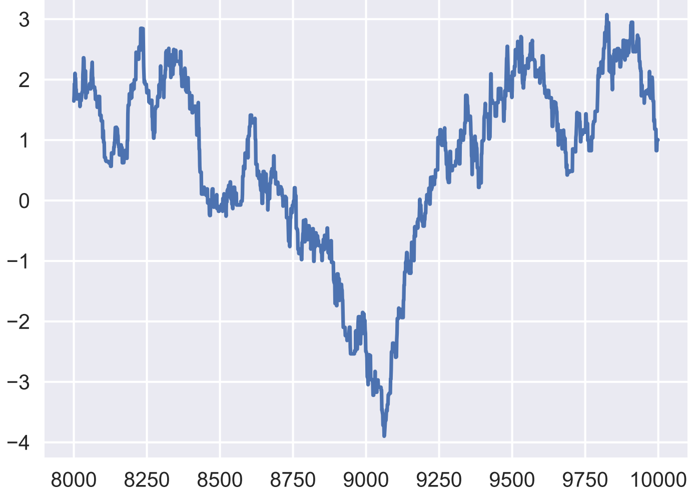
Mixing behavior



(a) Mixing in two dimensions.



(b) Mixing in 100 dimensions.

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Outline

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Active subspaces[1]

Goal: Approximate a function $f : \mathbb{R}^n \to \mathbb{R}$ by a function $g : \mathbb{R}^k \to \mathbb{R}$ ($k < n$), i.e. find $\mathbf{A} \in \mathbb{R}^{n \times k}$ and g s.t.

$$f(\mathbf{x}) \approx g(\mathbf{A}^\top \mathbf{x}). \tag{6}$$

(Also called *ridge approximation*.)

Note: $g(\mathbf{A}^\top \mathbf{x})$ constant along $\mathscr{N}(\mathbf{A}^\top)$. $\left[\nabla(g(\mathbf{A}^\top \mathbf{x})) = \nabla g(\mathbf{A}^\top \mathbf{x})\,\mathbf{A}^\top\right]$

[1] [Constantine et al., 2014, Constantine, 2015]

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Ridge approximation

Define

$$\mathbf{C} := \int_{\mathbb{R}^n} \nabla f \nabla f^\top \rho \, d\mathbf{x}. \tag{7}$$

$\mathbf{C}$ is symmetric and positive semi-definite.

$\rightarrow \mathbf{C} = \mathbf{W}\Lambda\mathbf{W}^\top$ for orthogonal $\mathbf{W} \in \mathbb{R}^{n\times n}$, $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$, $\lambda_i \geq 0$.

$$\lambda_i = \mathbf{w}_i^\top \mathbf{C} \mathbf{w}_i = \int_{\mathbb{R}^n} \left(\mathbf{w}_i^\top \nabla f\right)^2 \rho \, d\mathbf{x} \tag{8}$$

Ridge approximation

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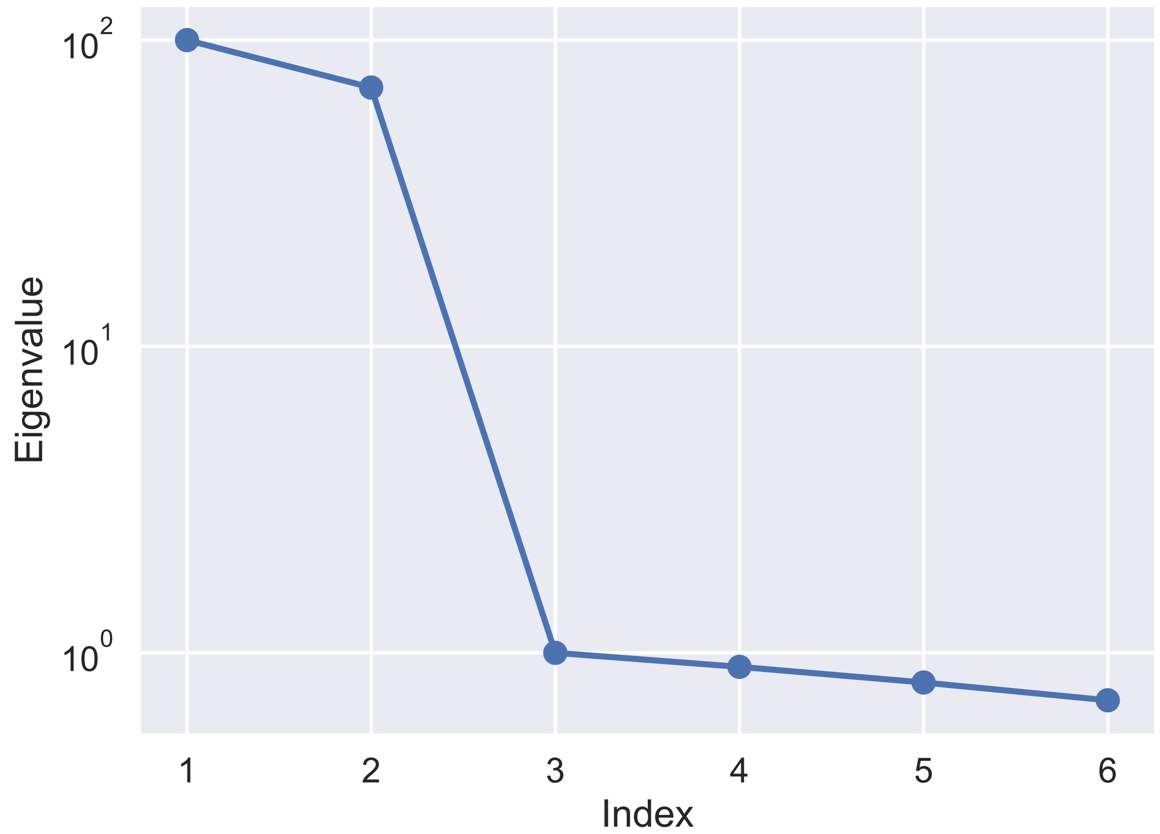
Eigenvalues



Subspaces

Decompose

$$\mathbf{W} = [\mathbf{W}_1 \;\; \mathbf{W}_2] \tag{9}$$

for $\mathbf{W}_1 \in \mathbb{R}^{n \times k}$, $\mathbf{W}_2 \in \mathbb{R}^{n \times (n-k)}$ and

$$\mathbf{x} = \mathbf{W}\mathbf{W}^\top \mathbf{x} = \mathbf{W}_1\mathbf{W}_1^\top \mathbf{x} + \mathbf{W}_2\mathbf{W}_2^\top \mathbf{x} \tag{10}$$

$$= \mathbf{W}_1 y + \mathbf{W}_2 z \tag{11}$$

for $y := \mathbf{W}_1^\top \mathbf{x}$, $z := \mathbf{W}_2^\top \mathbf{x}$.

$\mathbf{y}$ is called the *active*, $\mathbf{z}$ the *inactive* variable. $\mathscr{R}(\mathbf{W}_1)$ is the *active subspace*.

Approximation of f

(New) **Task**: If $\lambda_{k+1}, \dots, \lambda_n$ are small enough, approximate f by finding g s.t.

$$f(\mathbf{x}) \approx g(\mathbf{W}_1^\top \mathbf{x}). \tag{12}$$

Note: $\mathscr{N}(\mathbf{W}_1^\top) = \mathscr{R}(\mathbf{W}_2)$.

Algorithm 2 Computing the regression surface g in the active variable

---

Assume samples $\mathbf{x}_i$ $(i = 1, \dots, N)$ according to ρ and corresponding function values f_i $(i = 1, \dots, N)$ are given.

1. Compute samples $\mathbf{y}_i$ in the active subspace by

$$\mathbf{y}_i = \mathbf{W}_1^\top \mathbf{x}_i, \quad i = 1, \dots, N. \tag{13}$$

2. Find a regression surface g for pairs $(\mathbf{y}_i, f_i)$ such that

$$g(\mathbf{y}_i) \approx f_i, \quad i = 1, \dots, N. \tag{14}$$

Computing $\mathbf{C}^{[2]}$

Approximate

$$\mathbf{C} \approx \frac{1}{N} \sum_{i=1}^{N} \nabla f_i \nabla f_i^{\top} = \hat{\mathbf{W}} \hat{\Lambda} \hat{\mathbf{W}}^{\top} \tag{15}$$

with $\nabla f_i := \nabla f(\mathbf{x}_i)$ for samples $\mathbf{x}_i \sim \rho$.

Heuristic for N:

$$N = \alpha \times \ell \times \log(n) \tag{16}$$

- $\alpha \in [2, 10]$ oversampling factor
- ℓ number of eigenvalues to approximate
- n dimension of parameter space
- Basic tool: Eigenvalue Bernstein inequality for subexponential matrices

[2] [Constantine and Gleich, 2014]

Spectral gap – Theorem

Theorem

Let $\varepsilon > 0$ be "small enough" and choose $N = N(\varepsilon)$ "large enough". Then

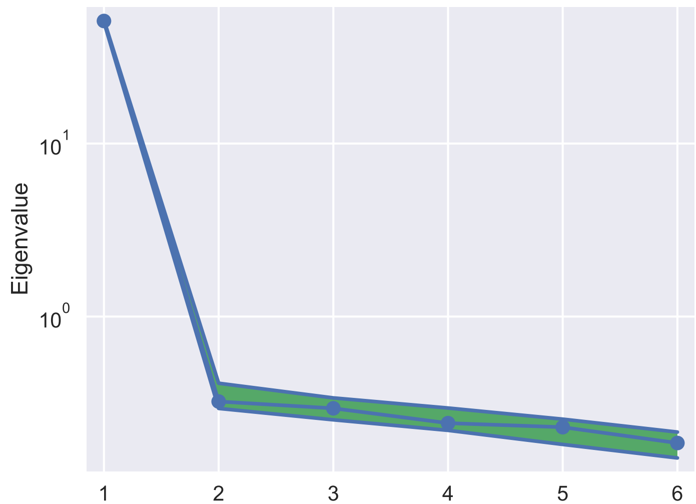
$$dist(\mathscr{R}(\mathbf{W}_1), \mathscr{R}(\hat{\mathbf{W}}_1)) \leq \frac{4\lambda_1\varepsilon}{\lambda_k - \lambda_{k+1}} \tag{17}$$

with "high probability".[3]

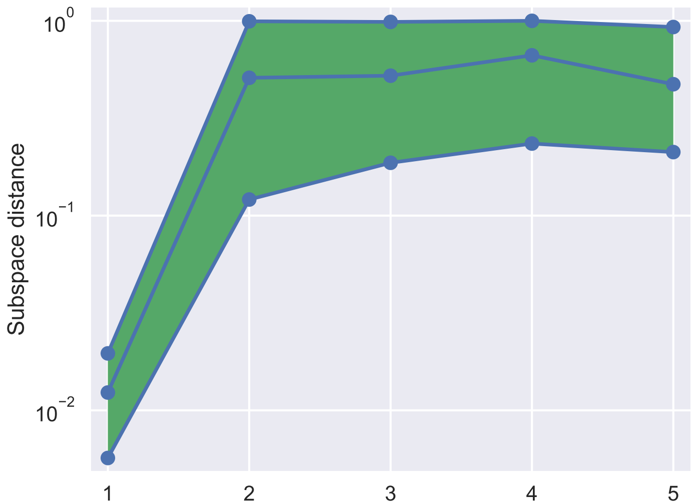
$$\left[\text{dist}(\mathscr{R}(\mathbf{W}_1), \mathscr{R}(\hat{\mathbf{W}}_1)) = \|\mathbf{W}_1\mathbf{W}_1^\top - \hat{\mathbf{W}}_1\hat{\mathbf{W}}_1^\top\|_2 = \|\mathbf{W}_1^\top\hat{\mathbf{W}}_2\|_2\right]$$

[3] [Constantine and Gleich, 2014]

Bootstrap intervals and subspace distances[4]



(a) Eigenvalues with bootstrap intervals.



(b) Subspace distances and bootstrap intervals.

- **Bootstrap**: Reuse samples to get a variance-like quantity
- Compute **subspace distances** and also bootstrap intervals

[4] [Constantine and Gleich, 2014]

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Outline

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Active subspaces for Bayesian inversion[5]

In the context of Bayesian inversion, we set

$$f(\mathbf{x}) = f_{\mathbf{d}}(\mathbf{x}) := \frac{\|\mathbf{d} - \mathscr{G}(\mathbf{x})\|_{\Gamma}^2}{2}. \tag{18}$$

Suppose we found a lower dimensional map $g_{\mathbf{d}}$ s.t. $f_{\mathbf{d}}(\mathbf{x}) \approx g_{\mathbf{d}}(\mathbf{W}_1^\top \mathbf{x}) = g_{\mathbf{d}}(\mathbf{y})$. Then

$$\begin{aligned}
\rho_{\text{post}}(\mathbf{x}|\mathbf{d}) &\propto \rho_{\text{like}}(\mathbf{d}|\mathbf{x})\rho_{\text{prior}}(\mathbf{x}) && (19)\\
&\propto \exp(-f_{\mathbf{d}}(\mathbf{x}))\rho_{\text{prior}}(\mathbf{x}) && (20)\\
&\approx \underbrace{\exp(-g_{\mathbf{d}}(\mathbf{y}))\rho_{\text{prior}}(\mathbf{y})}_{\propto \rho_{\text{post}}(\mathbf{y}|\mathbf{d})}\rho_{\text{prior}}(\mathbf{z}|\mathbf{y}) && (21)
\end{aligned}$$

$\rightarrow$ MCMC in the active subspace.

[5] [Constantine et al., 2016]

MCMC in the active subspace

Algorithm 3 Metropolis algorithm for the posterior in the active subspace

Assume a symmetric proposal density function τ, an initial point $\mathbf{y}_1$, and a kernel density estimate $\hat{\rho}$ for the prior on the active variable $\rho_{\text{prior}}(\mathbf{y})$ is given.

For $i = 1, 2, \ldots, N-1$

1. Draw a proposal $\tilde{\mathbf{y}}$ from τ centered at $\mathbf{y}_i$.
2. Calculate the acceptance ratio

$$\alpha(\tilde{\mathbf{y}}, \mathbf{y}_i) = \min\left(1, \frac{\exp(-g_{\mathbf{d}}(\tilde{\mathbf{y}}))\hat{\rho}(\tilde{\mathbf{y}})}{\exp(-g_{\mathbf{d}}(\mathbf{y}_i))\hat{\rho}(\mathbf{y}_i)}\right). \tag{22}$$

3. Draw $u \sim \mathscr{U}([0,1])$.
4. Set $\mathbf{y}_{i+1} = \tilde{\mathbf{y}}$ if $\alpha(\tilde{\mathbf{y}}, \mathbf{y}_i) \geq u$, otherwise set $\mathbf{y}_{i+1} = \mathbf{y}_i$.

MCMC in the active subspace gives *active samples* $\mathbf{y}$. Sample additionally from $\rho_{\text{prior}}(\mathbf{z}|\mathbf{y})$ to get

$$\mathbf{x} = \mathbf{W}_1\mathbf{y} + \mathbf{W}_2\mathbf{z}. \tag{23}$$

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Methane hydrates

- Crystalline solids formed when water molecules enclatharate methane molecules.
- Stable at low temperatures and high pressures.
- Occur in permafrost regions and marine off-shores.
- If warmed or depressurized, they destabilize and dissociate into water and gas.

  $\Rightarrow$ Energy content estimated to exceed the *combined* energy content of all other conventional fossil fuels[6].

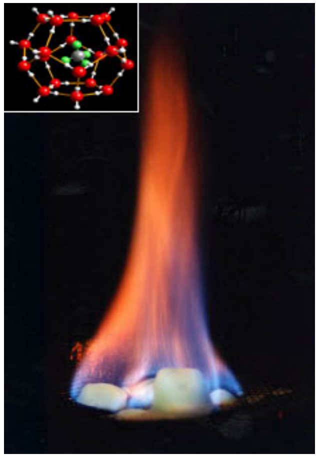

Figure : Burning hydrate (source: *United States Geological Survey*)

[6] [Piñero et al., 2013]

Methane hydrates model

- Interested in hydrates' reaction under forces/loading
  $\rightarrow$ Elastoplasticity model
- Linear relationship of *stress* σ and *elastic strain* ε^e through Hooke's law

$$\sigma = \mathbf{C} : \varepsilon^e,$$

  where $\mathbf{C}$ is a symmetric, positive definite, fourth order elastic stiffness tensor depending on the material (Lamé coefficients, Young's modulus, Poisson's ratio, ...).
- More details in e.g. [Gupta et al., 2015]

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Inference for model parameters[8]

Goal: Match *stress-strain curves* of the elastoplasticity model for methane hydrates and quantify uncertainties in parameters.

- Data for *gas-saturated* sediments from laboratory experiments[7]
- 8 parameters controlling evolution of curves (peak stress, hardening and softening slopes)
- Uniform prior on $[-1, 1]^8$
- 2% noise level (Γ is diagonal)

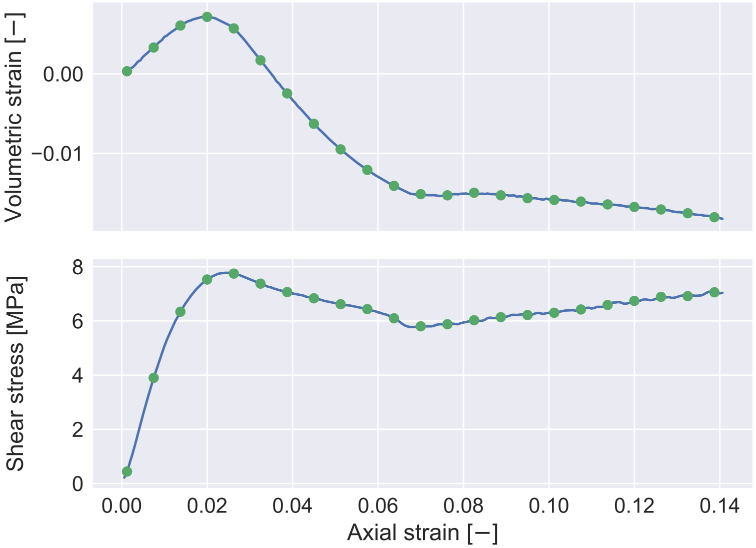

Figure : $n_{\mathbf{d}} = 46$ data points on stress and strain curves.

[7] [Deusner et al., 2012]

[8] [Teixeira Parente et al., 2018]

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Computational costs

Costs lie in computing the gradient

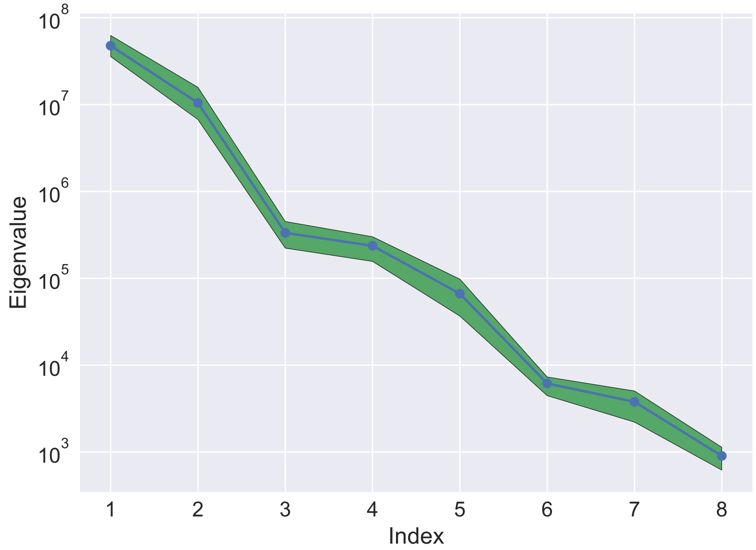
$$\nabla f_{\mathbf{d}}(\mathbf{x}) = \nabla \mathscr{G}(\mathbf{x})^\top \Gamma^{-1}(\mathscr{G}(\mathbf{x}) - \mathbf{d}) \tag{24}$$

with $\nabla \mathscr{G} : \mathbb{R}^n \to \mathbb{R}^{n_{\mathbf{d}} \times n}$, $\mathbf{d} \in \mathbb{R}^{n_{\mathbf{d}}}$.

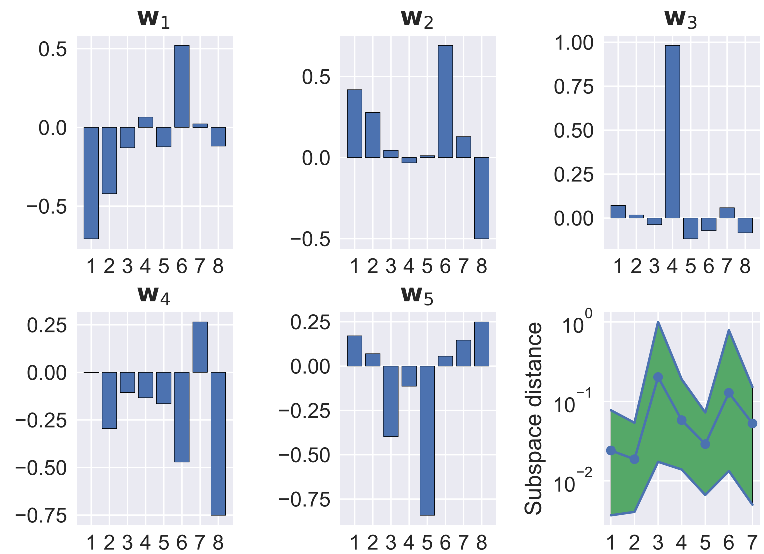
We apply (central) finite differences. $\to$ 17 forward runs

Number of gradient samples was $N = 250$ (trivially parallelizable).

Plots of eigenpairs



(a) Eigenvalues with spectral gaps after λ_2 and λ_5.



(b) First 5 eigenvectors and subspaces distances.

$\rightarrow$ Comparison between $2D$ and $5D$ subspace.

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2D summary plot of $f_{\mathbf{d}}$

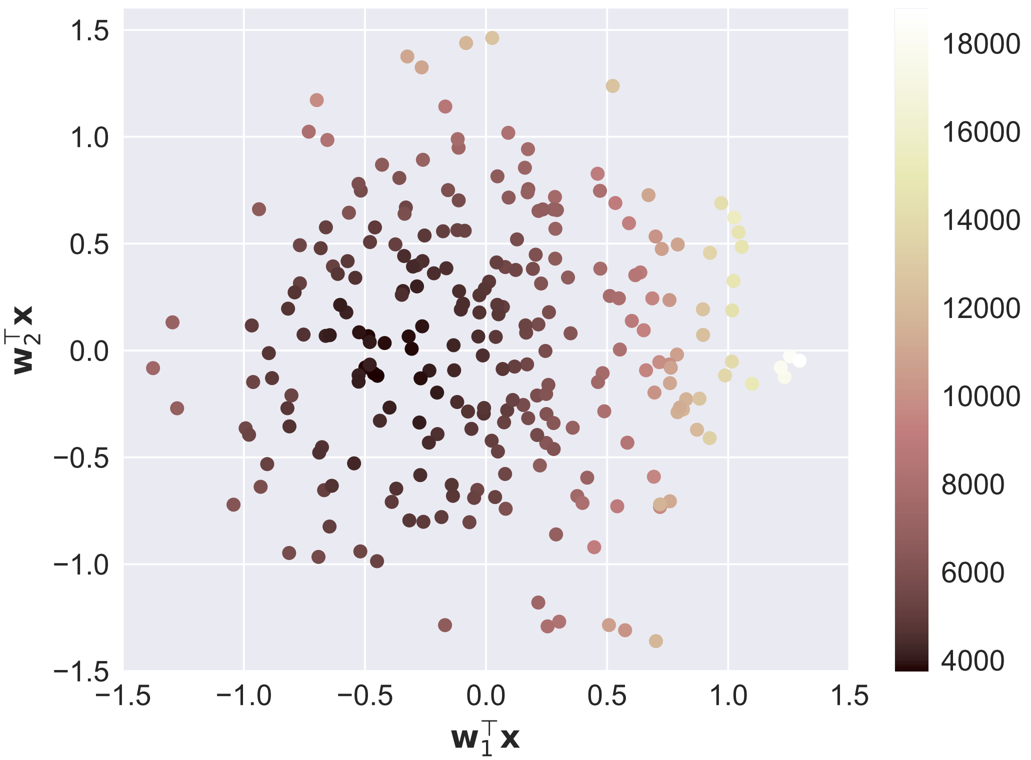

Figure : r^2 scores: 0.9776 ($2D$), 0.9824 ($5D$)

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Prior/posterior on the active variable

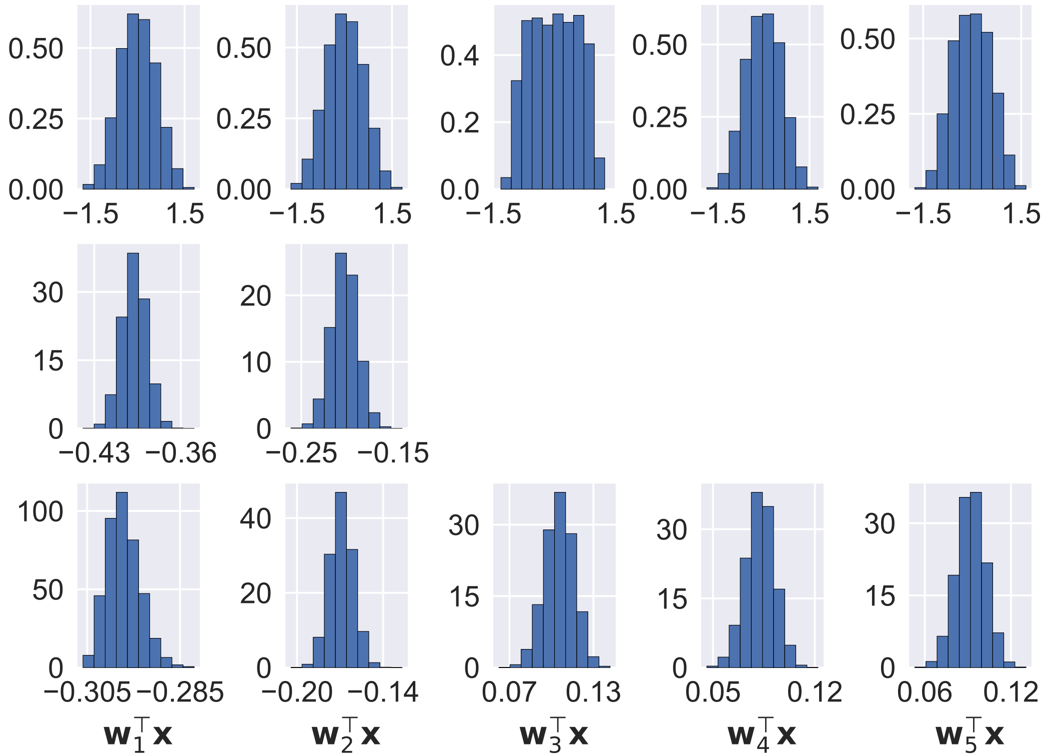

Figure : Top row: prior on the active variable(s); middle row: posterior on the $2D$ active variable; bottom row: posterior on the $5D$ active variable

Posterior in $2D$

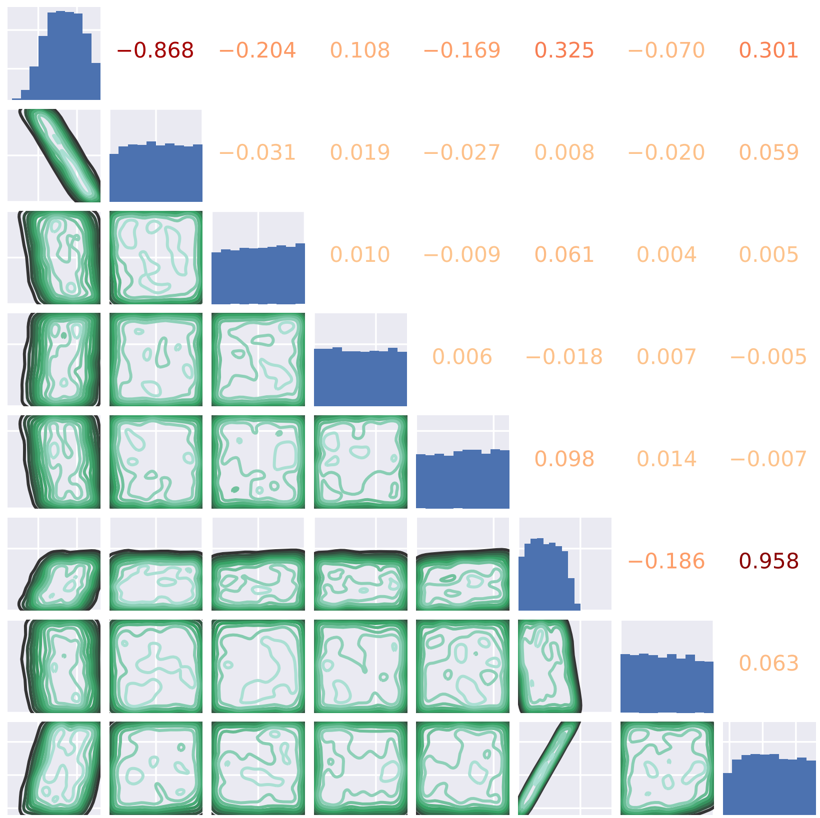

Figure : Uni- and bivariate marginals of $2D$ posterior. Colored numbers display the absolute value of correlation coefficients.

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Posterior in $5D$

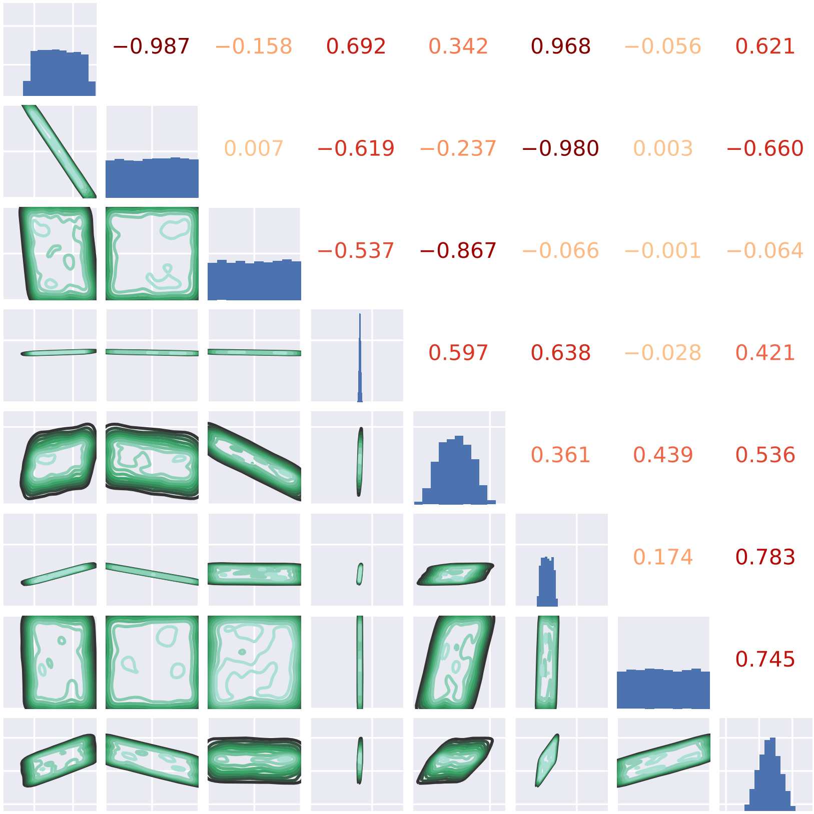
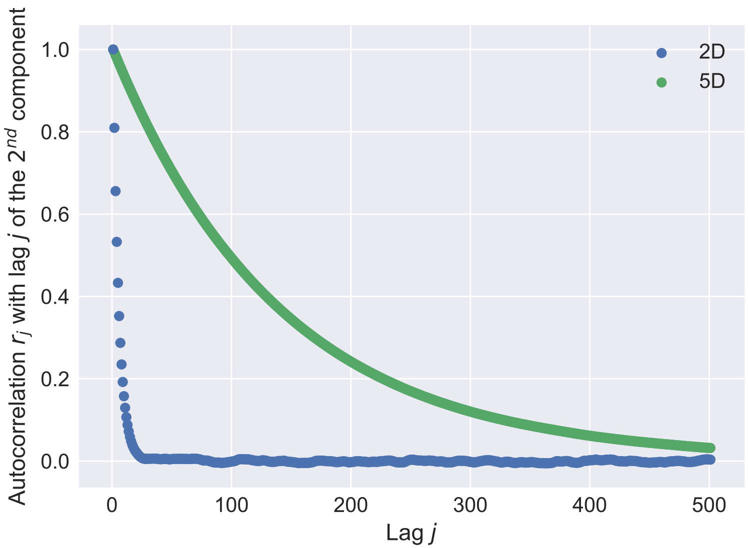
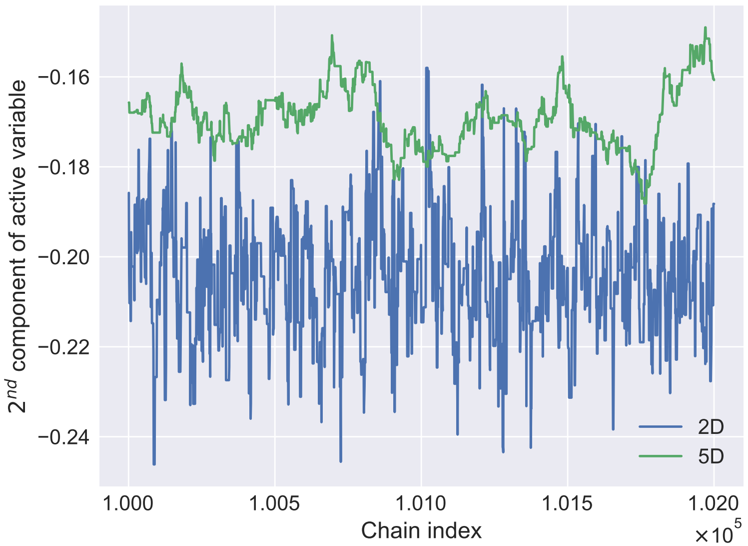


Figure : Uni- and bivariate marginals of $5D$ posterior. Colored numbers display the absolute value of correlation coefficients.

Autocorrelations + mixing



(a) Autocorrelations are much less in $2D$.



(b) Mixing is better in $2D$.

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Posterior means

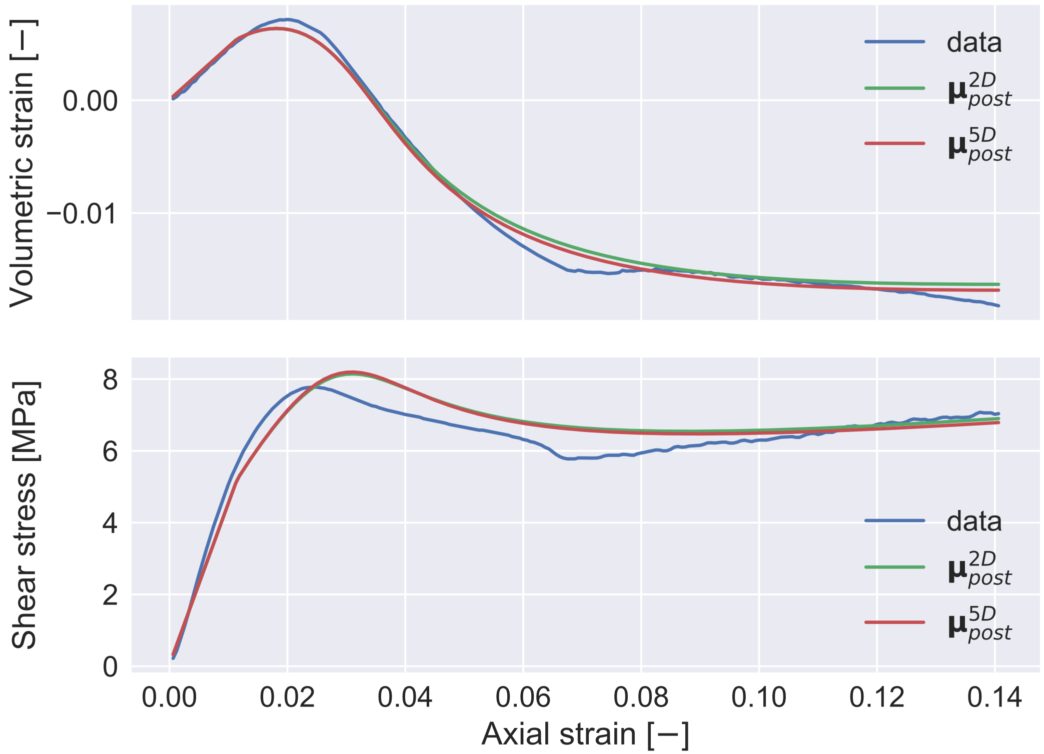

Figure : Forward evaluations with $2D$ and $5D$ posterior mean values.

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