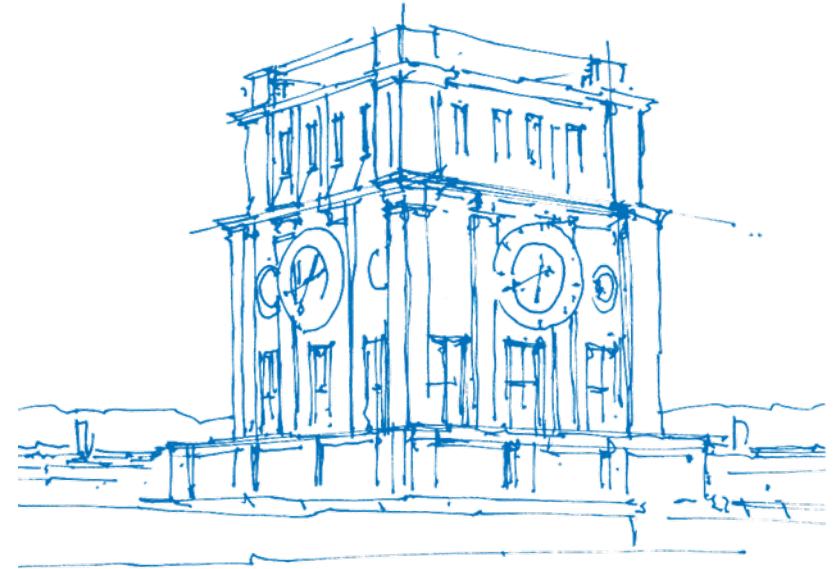


Active Subspaces in Bayesian Inverse Problems

Mario Teixeira Parente

Thesis Defense

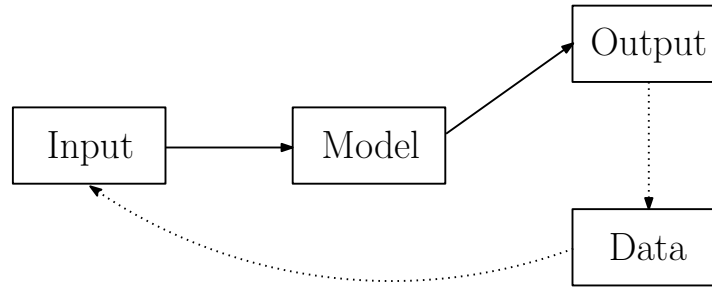
Garching, September 15, 2020



TUM Uhrenturm

Motivation

Statistical inference of model inputs



Computational challenges

- Performance of a single model run \Rightarrow efficient software, HPC, model reduction, ...
- Dimension of the input space ("curse of dimensionality") \Rightarrow **dimension reduction**.

The **Active Subspace Method** is a **gradient-based** technique for **subspace-based dimension reduction**.

Outline

Active Subspace Method (ASM)

- Motivation
- Setup
- Common bounds
- Generalized bounds
- Practical considerations

Bayesian Inverse Problems (BIPs)

- Motivation
- Setup
- Application of ASM

Case study

Iterative ASM for BIPs

- Idea
- Case study

Summary

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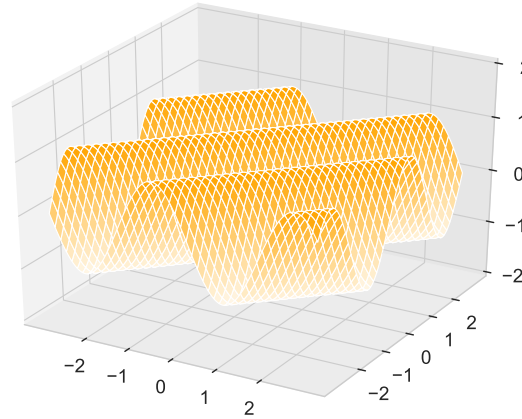
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Summary

ASM – Motivation



Ridge functions $f(\mathbf{x}) = g(A^\top \mathbf{x})$, for $g : \mathbf{R}^k \rightarrow \mathbf{R}$, $k \leq n$, and $A \in \mathbf{R}^{n \times k}$, are **constant** along the null space of A^\top since, for $\mathbf{v} \in \ker(A^\top)$,

$$f(\mathbf{x} + \mathbf{v}) = g(A^\top(\mathbf{x} + \mathbf{v})) = g(A^\top \mathbf{x}) = f(\mathbf{x}). \quad (1)$$

In the figure above, $f(\mathbf{x}) = \sin(-2x_1 + 2x_2)$.

ASM – Setup I (Constantine, Dow, and Wang, 2014)

- $(\Omega, \mathcal{A}, \mathbf{P})$ probability space.
- $\mathbf{X} \sim \mathbf{P}_{\mathbf{X}}$, $\mathbf{X} \in \mathbf{R}^n$, random vector (inputs, parameters).
- $\mathcal{X} := \text{supp}(\mathbf{P}_{\mathbf{X}}) \subseteq \mathbf{R}^n$ continuity set (i. e., $\mathbf{P}_{\mathbf{X}}(\partial \mathcal{X}) = 0$). In particular, $\mathbf{P}_{\mathbf{X}}(\mathcal{X}) = 1$.
- $f : \mathcal{X} \rightarrow \mathbf{R}$ such that $\nabla f \in L^2(\mathcal{X}, \mathbf{P}_{\mathbf{X}})$.

Goal: Approximate f by a **ridge function**, i. e., find g and $A \in \mathbf{R}^{n \times k}$, $k \leq n$, such that

$$f(\mathbf{x}) \approx g(A^{\top} \mathbf{x}) \tag{2}$$

for each $\mathbf{x} \in \mathcal{X}$.

ASM – Setup II

Define

$$\begin{aligned} C &:= \mathbf{E}[\nabla f(\mathbf{X})\nabla f(\mathbf{X})^\top] \\ &= \int_{\mathcal{X}} \nabla f(\mathbf{x})\nabla f(\mathbf{x})^\top \rho_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \\ &=: W\Lambda W^\top. \end{aligned} \tag{3}$$

Note that C is **symmetric** and **positive semi-definite**, i. e., we can choose

$$W = \begin{pmatrix} | & & | \\ \mathbf{w}_1 & \cdots & \mathbf{w}_n \\ | & & | \end{pmatrix} \in \mathbf{R}^{n \times n} \text{ to be } \mathbf{orthogonal} \text{ and } \Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} \in \mathbf{R}^{n \times n} \tag{4}$$

with

$$\lambda_1 \geq \cdots \geq \lambda_n \geq 0. \tag{5}$$

ASM – Setup III

Important:

$$\lambda_i = \mathbf{w}_i^\top C \mathbf{w}_i = \mathbf{E}[(\mathbf{w}_i^\top \nabla f(\mathbf{X}))^2]. \quad (6)$$

Question: What does λ_i small (or even zero) and λ_i large mean?

We hope that the eigenvalues λ_i are **decaying quickly** on a logarithmic scale. If so, for a certain $k \leq n$, split

$$W =: \begin{pmatrix} W_1 & W_2 \end{pmatrix} \quad (7)$$

for $W_1 \in \mathbf{R}^{n \times k}$ and $W_2 \in \mathbf{R}^{n \times (n-k)}$. The column space of W_1 (resp. W_2) is called the **active** (resp. **inactive**) **subspace of f** .

Define (random) variables for the subspaces by an **orthogonal transformation**, i. e.,

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{z} \end{pmatrix} := W^\top \mathbf{x} = \begin{pmatrix} W_1^\top \mathbf{x} \\ W_2^\top \mathbf{x} \end{pmatrix}. \quad (8)$$

The variable $\mathbf{y} \in \mathbf{R}^k$ (resp. $\mathbf{z} \in \mathbf{R}^{n-k}$) is called the **active** (resp. **inactive**) **variable**.

ASM – Setup IV

Recall: The goal was to find g and $A \in \mathbf{R}^{n \times k}$ such that $f(\mathbf{x}) \approx g(A^\top \mathbf{x})$ for each $\mathbf{x} \in \mathcal{X}$.

The map $\mathbf{x} \mapsto g(A^\top \mathbf{x})$ was said to be constant along the null space of A^\top .

\Rightarrow We found $A = W_1$ since $\ker(W_1^\top) = \text{ran}(W_2)$ (by $\ker(W_1^\top) \perp \text{ran}(W_1)$ and orthogonality of W).

Next step: Find "best" function g .

It is well-known that, if $\mathbf{E}[f(\mathbf{X})^2] < \infty$, the conditional expectation of $f(\mathbf{X})$ given $\mathbf{Y} = W_1^\top \mathbf{X}$ minimizes the mean square error to f , i. e.,

$$\mathbf{E}[(f(\mathbf{X}) - \mathbf{E}[f(\mathbf{X}) | \mathbf{Y}])^2] \leq \mathbf{E}[(f(\mathbf{X}) - \mathbf{U})^2] \quad (9)$$

for any square-integrable random variable \mathbf{U} which is measurable w.r.t. the σ -algebra generated by \mathbf{Y} .

ASM – Setup V

Notation: We denote

$$\mathbf{x} = WW^\top \mathbf{x} = W_1 \mathbf{y} + W_2 \mathbf{z} =: \llbracket \mathbf{y}, \mathbf{z} \rrbracket_W = \llbracket \mathbf{y}, \mathbf{z} \rrbracket. \quad (10)$$

Hence, we define

$$\begin{aligned} g(\mathbf{y}) &:= \mathbf{E}[f(\llbracket \mathbf{Y}, \mathbf{Z} \rrbracket) \mid \mathbf{Y} = \mathbf{y}] \\ &= \int_{\mathbf{R}^{n-k}} f(\llbracket \mathbf{y}, \mathbf{z} \rrbracket) \rho_{\mathbf{Z}|\mathbf{Y}}(\mathbf{z}|\mathbf{y}) \, d\mathbf{z} \end{aligned} \quad (11)$$

and finally get the **approximating ridge function**

$$f_g(\mathbf{x}) := g(W_1^\top \mathbf{x}). \quad (12)$$

Question: How "good" is f_g in approximating f in terms of the neglected directions in W_2 ?

ASM – Common bounds

In Constantine et al. (2014), we have the following result.

Theorem

For each $\mathbf{P}_{\mathbf{X}}$, there exists a Poincaré constant $C_P = C_P(\mathbf{P}_{\mathbf{X}}) > 0$ such that

$$\mathbf{E}[(f(\mathbf{X}) - f_g(\mathbf{X}))^2] \leq C_P(\lambda_{k+1} + \dots + \lambda_n). \quad (13)$$

Proof

Main ingredient: Probabilistic Poincaré inequality.

[For a random variable $\mathbf{U} \sim \mathbf{P}_{\mathbf{U}}$ and a sufficiently regular function h , it holds that

$$\text{Var}(h(\mathbf{U})) \leq C_P \mathbf{E}[\|\nabla h(\mathbf{U})\|_2^2] \quad (14)$$

for some Poincaré constant $C_P = C_P(\mathbf{P}_{\mathbf{U}}) > 0$.]

The main step is to compute

$$\begin{aligned} \mathbf{E}[(f(\mathbf{X}) - f_g(\mathbf{X}))^2] &= \mathbf{E}[(f(\llbracket \mathbf{Y}, \mathbf{Z} \rrbracket) - g(\mathbf{Y}))^2] \\ &\leq C_P \mathbf{E}[\|\nabla^{\mathbf{Z}} f(\mathbf{X})\|_2^2]. \end{aligned} \quad (15)$$

Note: The Poincaré constant C_P was taken w.r.t. $\mathbf{P}_{\mathbf{X}}$ which is **not correct in general**. ■

ASM – Generalized bounds I (Teixeira Parente, Wallin, and Wohlmuth, 2020)

A correct application of the probabilistic Poincaré inequality gives

$$\begin{aligned} \mathbf{E}[(f(\mathbf{X}) - f_g(\mathbf{X}))^2] &= \mathbf{E}[\mathbf{E}[(f(\mathbf{Y}, \mathbf{Z}) - g(\mathbf{Y}))^2 | \mathbf{Y}]] \\ &\leq \mathbf{E}[C_{\mathbf{Y}} \cdot \mathbf{E}[\|\nabla^{\mathbf{Z}} f(\mathbf{Y}, \mathbf{Z})\|_2^2 | \mathbf{Y}]], \end{aligned} \tag{16}$$

where $C_{\mathbf{Y}} > 0$ is the Poincaré constant of $\mathbf{P}_{\mathbf{Z}|\mathbf{Y}}$ and hence **randomly depending** on \mathbf{Y} .

The constant $C_{\mathbf{Y}}$ is known to be **uniform** in \mathbf{Y} for, e. g., **compactly supported** and so-called **α -uniformly log-concave** ($\alpha > 0$) distributions $\mathbf{P}_{\mathbf{X}}$.

Question: Can we find a counterexample, i. e., a distribution $\mathbf{P}_{\mathbf{X}}$ and a transformation W such that the corresponding $C_{\mathbf{Y}}$ is unbounded in \mathbf{Y} /not compactly supported?

ASM – Generalized bounds II

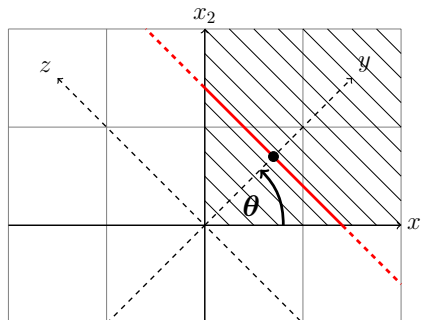
Answer: Yes.

Idea: We need to find a distribution that has heavier tails than any α -uniformly log-concave distribution but is still applicable for a Poincaré inequality. Look at the edge case when $\alpha \rightarrow 0$. \Rightarrow **General log-concave distributions**.

Example: Exponential distribution with unit rates in two dimensions; rotation by 45° .

Use **lower bound** for C_Y of **Bobkov (1999)**:

$$C_Y \geq \text{Var}(|Z| | Y = y) = y^2/12. \quad (17)$$



ASM – Generalized bounds III

Question: Can we derive **weaker bounds** for general log-concave distributions?

Answer: Yes. Use Hölder's inequality with a **weaker pair of conjugates** to get

$$\mathbf{E}[(f(\mathbf{X}) - f_g(\mathbf{X}))^2] \leq C_{P,\varepsilon,W} (\lambda_{k+1} + \dots + \lambda_n)^{1/(1+\varepsilon)} \quad (18)$$

for $\varepsilon > 0$ and a constant $C_{P,\varepsilon,W} > 0$.

ASM – Practical considerations (Constantine, 2015)

In practice, we **approximate** the matrix $C = \mathbf{E}[\nabla f(\mathbf{X})\nabla f(\mathbf{X})^\top]$ by a **finite Monte Carlo sum**, i. e., by

$$\tilde{C} := \frac{1}{N_{\tilde{C}}} \sum_{j=1}^{N_{\tilde{C}}} \nabla f(\mathbf{x}_j) \nabla f(\mathbf{x}_j)^\top \quad (19)$$

for $N_{\tilde{C}} > 0$ and $\mathbf{x}_j \stackrel{\text{i.i.d.}}{\sim} \mathbf{P}_{\mathbf{x}}, j = 1, \dots, N_{\tilde{C}}$.

It is well-known by an eigenvalue Bernstein inequality that $N_{\tilde{C}} = O(\log n)$ samples are enough to approximate "the first eigenvalues of C sufficiently accurate."

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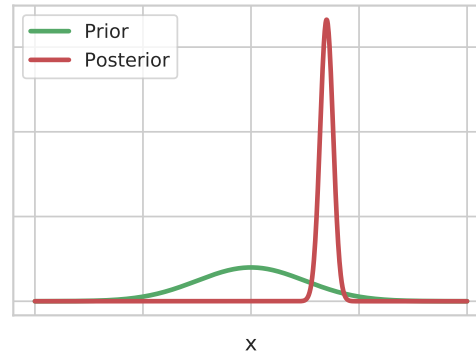
Iterative ASM for BIPs

- Idea
- Case study

Summary

BIPs – Motivation

Bayesian inverse problems exploit **observational data** to update a **prior distribution** on model parameters to a **posterior distribution**.



In view of **Uncertainty Quantification**, the posterior distribution quantifies the updated, remaining **uncertainty** on model parameters.

BIPs – Setup I (Stuart, 2010; Dashti and Stuart, 2016)

Parameters are denoted by $\mathbf{X} \sim \mathbf{P}_{\mathbf{X}}$ or \mathbf{x} , both in \mathbf{R}^n .

The forward model $\mathcal{G} : \mathcal{X} \rightarrow \mathbf{R}^{n_d}$ maps a parameter to a corresponding value for the Quantity of Interest (QoI).

The observational data $\mathbf{d} \in \mathbf{R}^{n_d}$ are assumed to be noisy realizations of a model evaluation, i. e.,

$$\mathbf{D} = \mathcal{G}(\mathbf{X}) + \eta, \tag{20}$$

where noise $\eta \sim \mathcal{N}(0, \Gamma)$ is assumed to be Gaussian with mean zero and covariance matrix $\Gamma \in \mathbf{R}^{n_d \times n_d}$.

BIPs – Setup II

For observed data $\mathbf{d} \in \mathbf{R}^{n_d}$, the **posterior distribution** $\mu^{\mathbf{d}}$ is the conditional distribution of parameters \mathbf{X} given that $\mathbf{D} = \mathbf{d}$, i. e.,

$$\mu^{\mathbf{d}} := \mathbf{P}_{\mathbf{X}|\mathbf{D}}(\cdot|\mathbf{d}) = \mathbf{P}(\mathbf{X} \in \cdot | \mathbf{D} = \mathbf{d}). \quad (21)$$

The corresponding **posterior density** $\rho^{\mathbf{d}}$ is proportional to the **likelihood** and the **prior density** $\rho_0 := \rho_{\mathbf{X}}$, i. e.,

$$\rho^{\mathbf{d}}(\mathbf{x}) := \rho_{\mathbf{X}|\mathbf{D}}(\mathbf{x}|\mathbf{d}) \propto \exp(-f^{\mathbf{d}}(\mathbf{x})) \cdot \rho_0(\mathbf{x}) \quad (22)$$

for the **data misfit function** (or negative log-likelihood)

$$f^{\mathbf{d}}(\mathbf{x}) = \frac{1}{2} \|\mathbf{d} - \mathcal{G}(\mathbf{x})\|_{\Gamma}^2, \quad (23)$$

where $\|\cdot\|_{\Gamma} := \|\Gamma^{-1/2} \cdot\|_2$.

BIPs – Application of ASM (Constantine, Kent, and Bui-Thanh, 2016)

In the setting of ASM, we set

$$f = f^{\mathbf{d}} \tag{24}$$

and thus compute the **active subspace of the data misfit function** to obtain a ridge approximation

$$f^{\mathbf{d}}(\mathbf{x}) \approx g^{\mathbf{d}}(W_1^{\top} \mathbf{x}). \tag{25}$$

Consequently, we can find a **low-dimensional approximation of the posterior density**, i. e., for $\mathbf{x} = [\mathbf{y}, \mathbf{z}]$,

$$\begin{aligned} \rho^{\mathbf{d}}(\mathbf{x}) &\propto \exp(-f^{\mathbf{d}}(\mathbf{x})) \cdot \rho_0(\mathbf{x}) \\ &\approx \exp(-g^{\mathbf{d}}(W_1^{\top} \mathbf{x})) \cdot \rho_0(\mathbf{x}) \\ &= \underbrace{\exp(-g^{\mathbf{d}}(\mathbf{y})) \cdot \rho_{\mathbf{y}}(\mathbf{y})}_{\propto: \rho_{g, \mathbf{y}}^{\mathbf{d}}(\mathbf{y})} \cdot \rho_{\mathbf{z}|\mathbf{y}}(\mathbf{z}|\mathbf{y}). \end{aligned} \tag{26}$$

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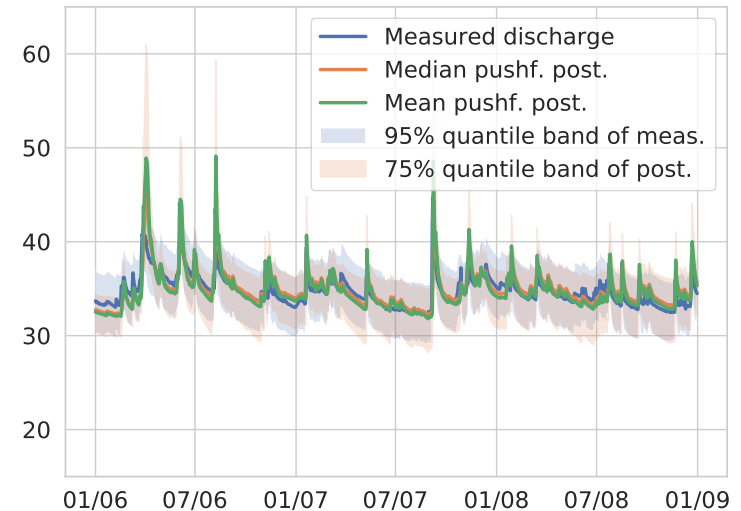
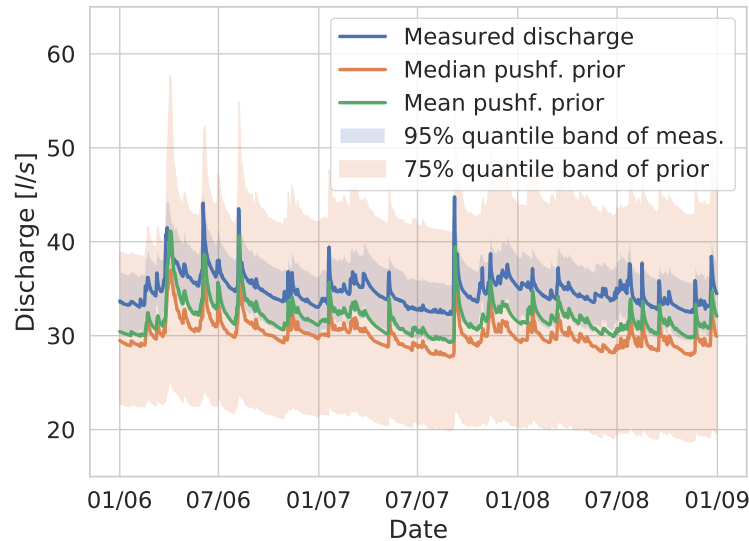
Iterative ASM for BIPs

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- Case study

Summary

Case study (Teixeira Parente, Bittner, Mattis, Chiogna, and Wohlmuth, 2019)

Groundwater karst model for a **discharge time series** of the Kerschbaum spring recharge area in Waidhofen a.d. Ybbs (Austria).



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Case study

Iterative ASM for BIPs

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- Case study

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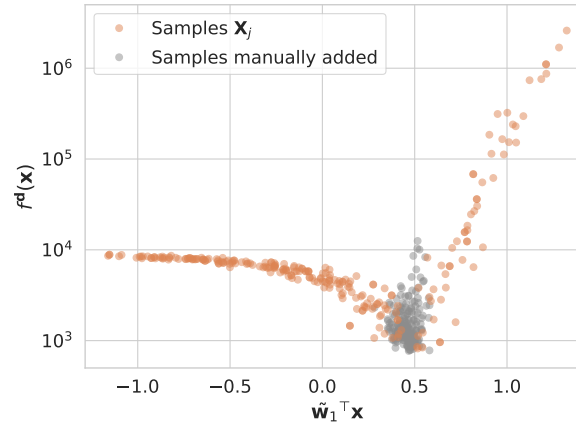
Iterative ASM – Idea I (Section 7 in dissertation)

Problem: Since sensitivities are computed w.r.t. the **prior**, i. e.,

$$C_0 = \int_{\mathcal{X}} \nabla f^d(\mathbf{x}) \nabla f^d(\mathbf{x})^\top \rho_0(\mathbf{x}) d\mathbf{x}, \quad (27)$$

a "bad prior" may cause a **misleading active subspace**.

Example:

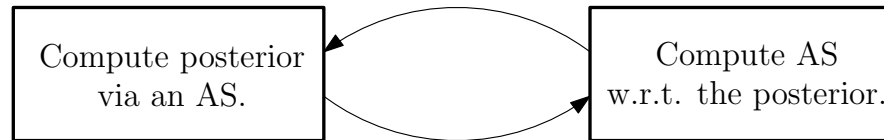


Iterative ASM – Idea II

Actual goal: Compute sensitivities w.r.t. the **posterior**, i. e.,

$$C^{\mathbf{d}} := \int_{\mathcal{X}} \nabla f^{\mathbf{d}}(\mathbf{x}) \nabla f^{\mathbf{d}}(\mathbf{x})^{\top} \rho^{\mathbf{d}}(\mathbf{x}) d\mathbf{x}. \quad (28)$$

Problem:



⇒ **Iterative** scheme.

Iterative ASM – Idea III

Compute a **sequence of distributions** $\mu^{(\ell)}$ approaching $\mu^{\mathbf{d}}$ starting from the prior $\mu^{(0)} = \mu_0$.

Ideal algorithm: Set $\mu^{(0)} := \mu_0$. In the ℓ -th step, $\mathbf{X}^{(\ell)} \sim \mu^{(\ell)}$ and the main steps are:

- Compute

$$\mathbf{C}^{(\ell)} := \mathbf{E}[\nabla f^{\mathbf{d}}(\mathbf{X}^{(\ell)}) \nabla f^{\mathbf{d}}(\mathbf{X}^{(\ell)})^{\top}] = \mathbf{W}^{(\ell)} \mathbf{\Lambda}^{(\ell)} \mathbf{W}^{(\ell)\top}. \quad (29)$$

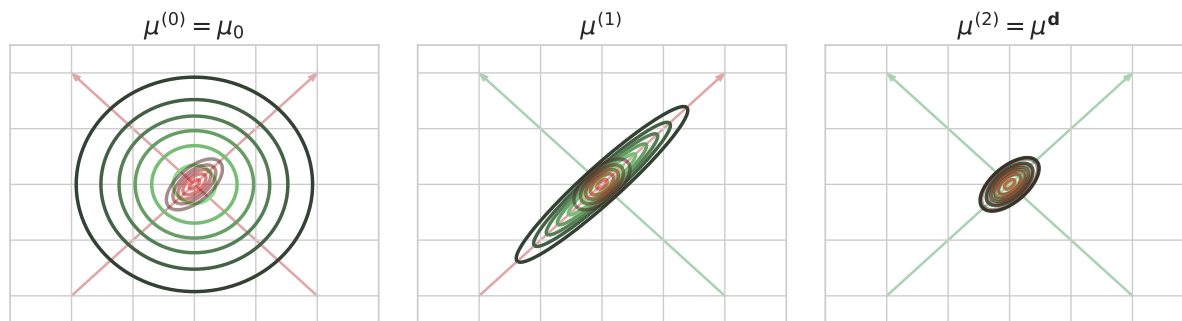
- Decide for an active subspace, i. e., for $\mathbf{W}_1^{(\ell)}$, and compute

$$\mathbf{g}^{(\ell)}(\mathbf{y}) := \mathbf{E}[f^{\mathbf{d}}(\llbracket \mathbf{Y}^{(\ell)}, \mathbf{Z}^{(\ell)} \rrbracket_{\mathbf{W}^{(\ell)}}) \mid \mathbf{Y}^{(\ell)} = \mathbf{y}]. \quad (30)$$

- Compute samples $\mathbf{X}^{(\ell+1)} \sim \mu^{(\ell+1)}$ using $\mathbf{g}^{(\ell)}$.

Iterative ASM – Idea IV

Illustrative example:

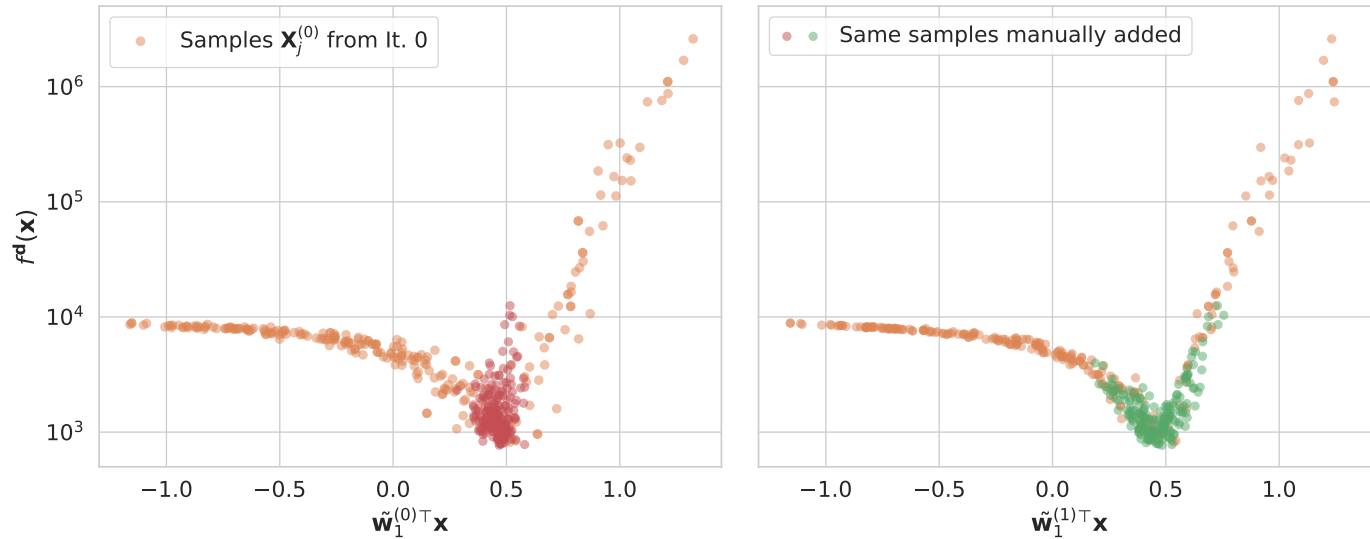


Remark I: Convergence and consistency of the ideal algorithm are formally well-understood for a linear Gaussian BIP.

Remark II: In practice, we do not aim to converge to the posterior since the exact quantities used in the algorithm are not available. But we can use the algorithm with approximate quantities as a "preconditioner" for BIPs with bad prior distributions.

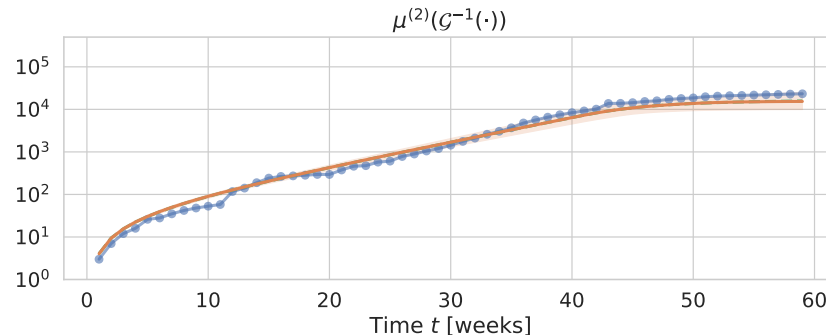
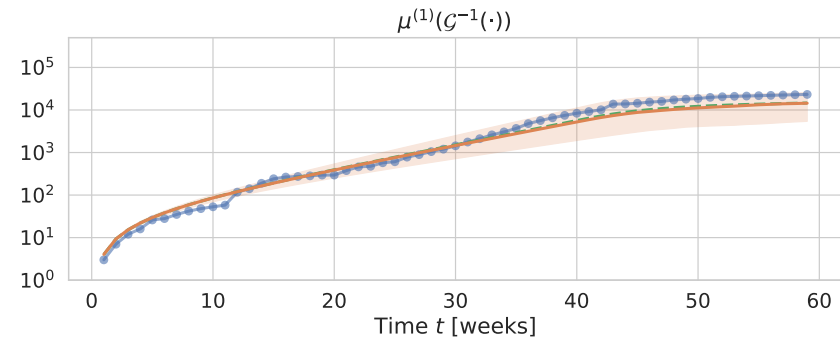
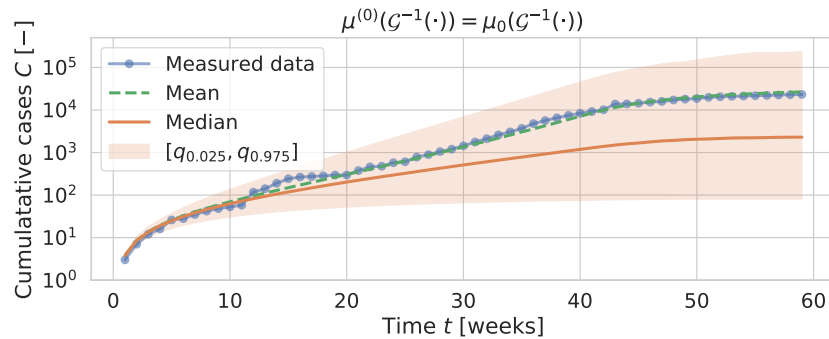
Iterative ASM – Case study I

Compartmental model for 2014 Ebola outbreak in West Africa (Barbarossa et al., 2015).



Iterative ASM – Case study II

The following figures show the evolution of the push-forward distribution of $\mu^{(\ell)}$, $\ell = 0, 1, 2$.



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Summary

We presented a **counterexample** to existing **Active Subspace** theory and provided a solution by **generalized bounds**.

A case study involving a **complex high-dimensional hydrological model** demonstrated that ASM can substantially **reduce the dimension and computational expenses** of **Bayesian inverse problems**.

For BIPs with "bad priors", we suggested an **iterative scheme** to find a better active subspace by **computing sensitivities in regions of low data misfit**. This was demonstrated on a model for the 2014 Ebola outbreak in West Africa.

Thank you!

I would like to **sincerely thank**

- the **audience** for their attention,
- my **supervisor** Prof. Barbara Wohlmuth for stimulating discussions during the last 4 years,
- my **collaborators** (sorted by surname):

GEOMAR Helmholtz Centre for Ocean Research Kiel: Christian Deusner, Shubhangi Gupta

Lund University, Department of Statistics: Prof. Krzysztof Podgórski, Jonas Wallin

TUM Chair of Hydrology and River Basin Management: Daniel Bittner, Prof. Gabriele Chiogna

- the **TUM M2 unit** for their support,
- the **TUM International Graduate School for Science and Engineering** (IGSSE) for financial support, GSC 81,
- and the **chair of the examination board** Prof. Christina Kuttler for organizing my defense.



Publications

Teixeira Parente, M., Wallin, J., & Wohlmuth, B., Generalized Bounds for Active Subspaces, *Electronic Journal of Statistics*, 14(1):917–943, 2020

Bittner, D., **Teixeira Parente, M.**, Mattis, S., Wohlmuth, B., & Chiogna, G., Identifying Relevant Hydrological and Catchment Properties in Active Subspaces: An Inference Study of a Lumped Karst Aquifer Model. *Advances in Water Resources*, 135, 103472, 2020.

Teixeira Parente, M., Bittner, D., Mattis, S., Chiogna, G., & Wohlmuth, B., Bayesian Calibration and Sensitivity Analysis for a Karst Aquifer Model using Active Subspaces, *Water Resources Research*, 55(8):7086–7107, 2019

Teixeira Parente, M., Mattis, S., Gupta, S., Deusner, C., & Wohlmuth, B., Efficient Parameter Estimation for a Methane Hydrate Model with Active Subspaces, *Computational Geosciences*, 23(2):355–372, 2019

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- M. Teixeira Parente, D. Bittner, S. A. Mattis, G. Chiogna, and B. Wohlmuth. Bayesian Calibration and Sensitivity Analysis for a Karst Aquifer Model using Active Subspaces. *Water Resources Research*, 55(8):7086–7107, 2019.

Supplementary Material

ASM – Generalized bounds IV

Theorem

Let $\varepsilon > 0$. If $\|\nabla f(\mathbf{X})\|_2^2 \leq L$ \mathbf{P} -a.s. for some constant $L > 0$, then

$$\mathbf{E}[(f(\mathbf{X}) - f_g(\mathbf{X}))^2] \leq C_{P,\varepsilon,W} (\lambda_{k+1} + \dots + \lambda_n)^{1/(1+\varepsilon)}, \quad (31)$$

where

$$C_{P,\varepsilon,W} = C_{P,\varepsilon,W}(\varepsilon, n, k, L, W, \mathbf{P}_X) := L^{\varepsilon/(1+\varepsilon)} \mathbf{E}[C_Y^{(1+\varepsilon)/\varepsilon}]^{\varepsilon/(1+\varepsilon)}. \quad (32)$$

Proof

Main ingredient: Hölder's inequality for $\mathbf{E}[C_Y \cdot \mathbf{E}[\|\nabla^2 f(\llbracket \mathbf{Y}, \mathbf{Z} \rrbracket)\|_2^2 | \mathbf{Y}]]$ with a **weaker pair of conjugates**

$$(p, q) = ((1 + \varepsilon)/\varepsilon, 1 + \varepsilon) \quad (33)$$

instead of $(p, q) = (+\infty, 1)$. ■

Remark: For exponential distributions, the constant $C_{P,\varepsilon,W}$ can be **bounded uniformly in W** by **an analytical expression**.

ASM – Practical considerations II

Approximation of eigenvalues of C

Theorem (Constantine (2015, Thm. 3.3))

Assume that $\|\nabla f(\mathbf{x})\|_2 \leq L$ for some $L > 0$ and all $\mathbf{x} \in \mathcal{X}$. For $\varepsilon \in (0, 1]$, it holds that

$$\mathbf{P}\left(\tilde{\lambda}_\ell \geq (1 + \varepsilon)\lambda_\ell\right) \leq (n - \ell + 1) \exp\left(-\frac{N_{\tilde{C}}\lambda_\ell^2\varepsilon^2}{4L^2}\right) \quad (34)$$

and

$$\mathbf{P}\left(\tilde{\lambda}_\ell \leq (1 - \varepsilon)\lambda_\ell\right) \leq \ell \exp\left(-\frac{N_{\tilde{C}}\lambda_\ell^2\varepsilon^2}{4\lambda_1 L^2}\right) \quad (35)$$

for $\ell = 1, \dots, n$.

Proof

Main ingredient: **Eigenvalue Bernstein inequality** for a finite sum of random, independent, and symmetric matrices satisfying a subexponential growth condition. ■

ASM – Practical considerations III

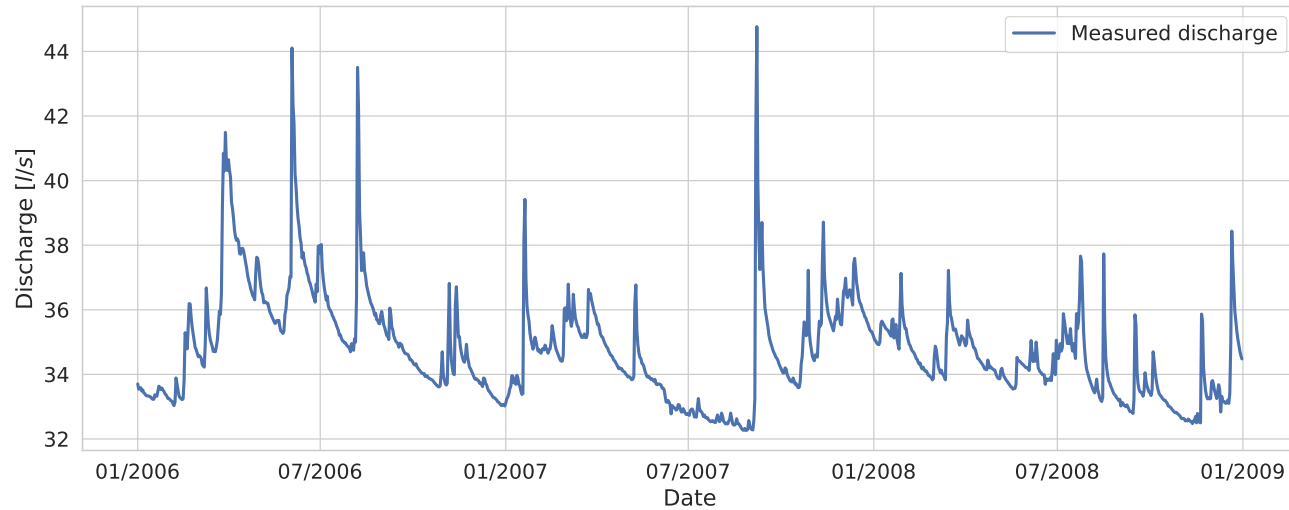
The function $g(\mathbf{y}) = \mathbf{E}[f(\llbracket \mathbf{Y}, \mathbf{Z} \rrbracket) \mid \mathbf{Y} = \mathbf{y}]$ is also approximated by a **finite Monte Carlo sum**, i. e., by

$$g_N(\mathbf{y}) := \frac{1}{N} \sum_{j=1}^N f(\llbracket \mathbf{y}, \mathbf{z}_j^{\mathbf{y}} \rrbracket) \quad (36)$$

for $N > 0$ and $\mathbf{z}_j^{\mathbf{y}} \stackrel{\text{i.i.d.}}{\sim} \mathbf{P}_{\mathbf{Z}|\mathbf{Y}}(\cdot | \mathbf{y})$, $j = 1, \dots, N$.

Case study II

Measured discharge data



Case study III

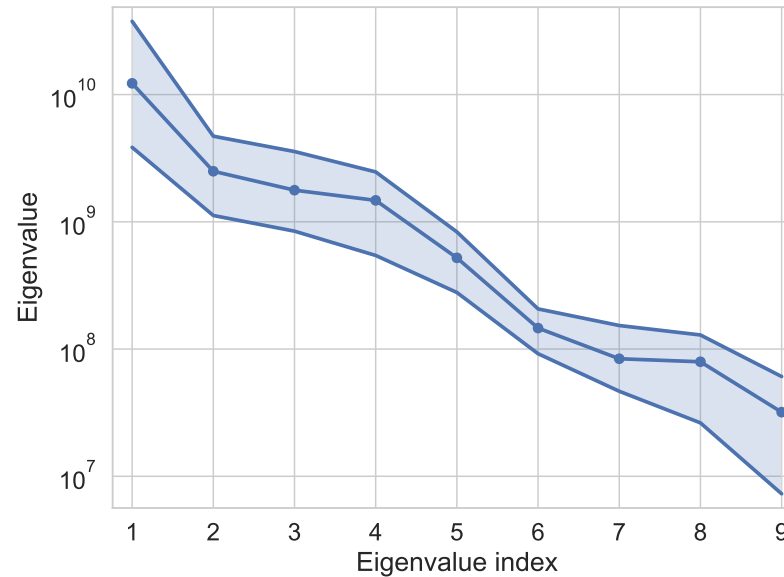
Problem characteristics:

- Parameter space is $n = 21$ -dimensional.
- Data consists of $n_d = 1096$ discharge values.
- We assume a 5% noise level on the measured data.
- The prior distribution is chosen to be uniform on intervals predefined by hydrologists.
- A single model run needs about 2.5 seconds.

Implementation: The computation of $N_{\tilde{C}} = 1000$ gradients needed about 4.3 hours using 7 CPU cores in parallel.

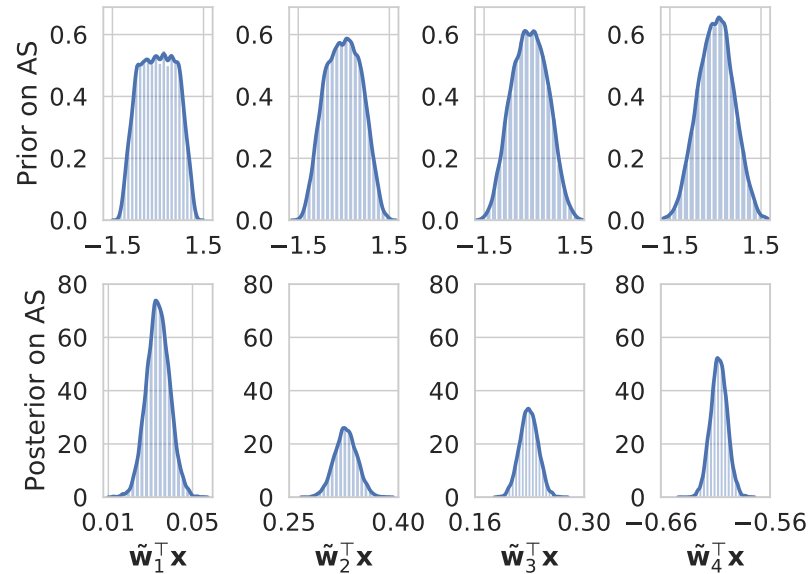
Case study IV

The following figure shows the **approximated eigenvalues** with an "uncertainty band" to reflect their random nature.



Case study V

The following figure shows the **prior** (top) and **posterior** (bottom) distribution on the active subspace.



Iterative ASM – Analysis

Proposition (Dissertation, Prop. 7.3.1)

Let $\mu_0 = \mathcal{N}(\mathbf{m}_0, I)$ with $\mathbf{m}_0 \in \mathbf{R}^n$. Suppose that $\mathcal{G}(\mathbf{x}) := A\mathbf{x}$ for $\mathbf{x} \in \mathcal{X}$ with $A \in \mathbf{R}^{n_d \times n}$, and $\eta \sim \mathcal{N}(0, \gamma^2 I)$ for $\gamma > 0$. Furthermore, assume that $\mathbf{d} = \mathcal{G}(\mathbf{m}_0)$.

Considering the ideal algorithm, set $\Lambda := \Lambda^{(0)}$ and $W := W^{(0)}$. Then, for every iteration $\ell \in \mathbf{N}_0$, it holds that

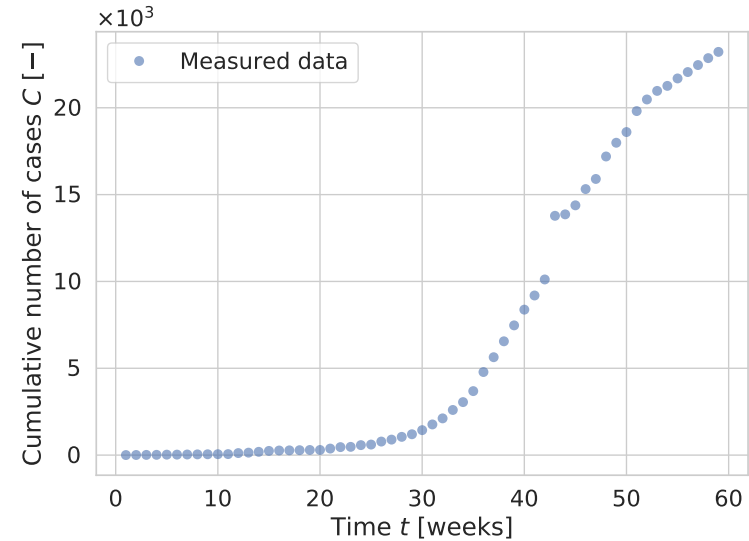
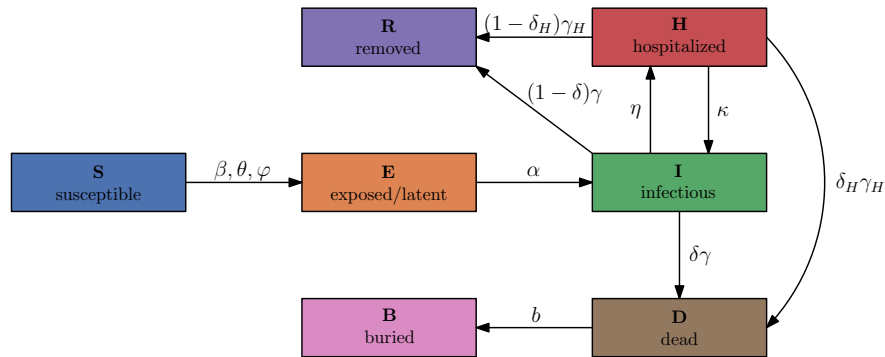
$$\mathbf{x}^{(\ell)} \sim \mathcal{N}(\mathbf{m}_0, \Sigma^{(\ell)}) \quad (37)$$

with

$$\Sigma^{(\ell)} = W \begin{pmatrix} (I + \Lambda_{1:K^{(\ell)}}^{1/2})^{-1} & 0 \\ 0 & I \end{pmatrix} W^\top \quad (38)$$

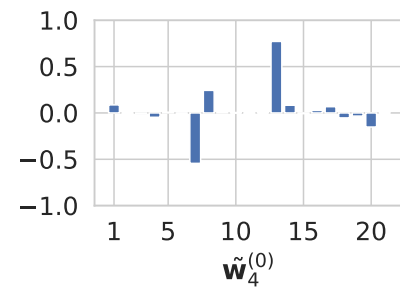
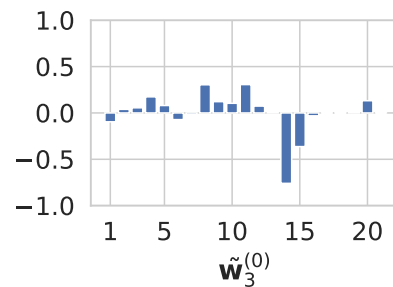
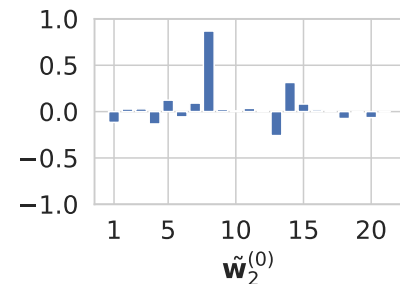
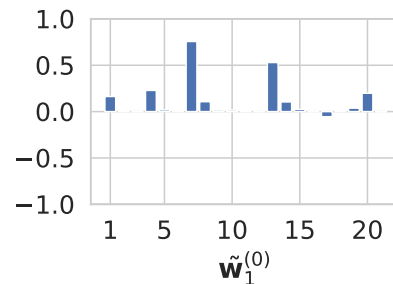
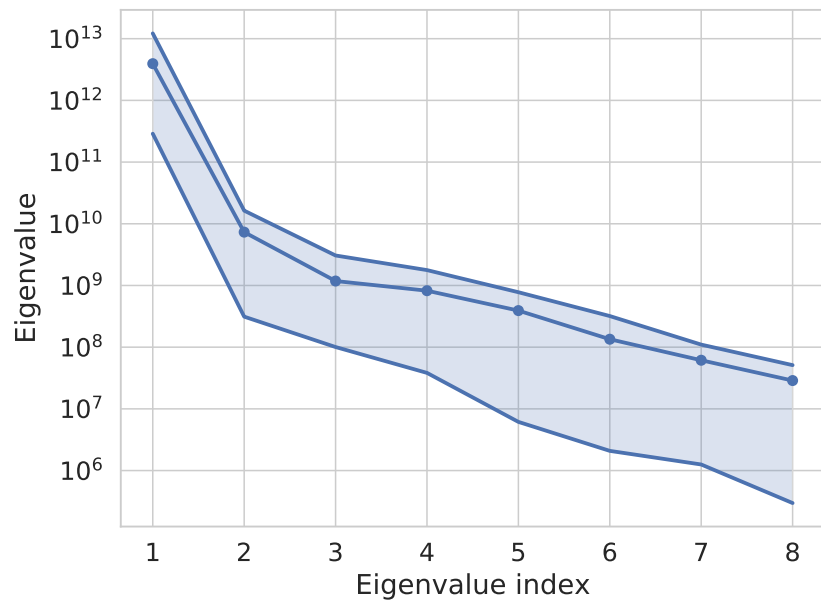
for some natural number $0 \leq K^{(\ell)} \leq n$.

Iterative ASM – Case study, Fig. I



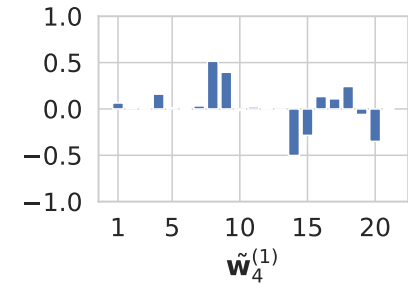
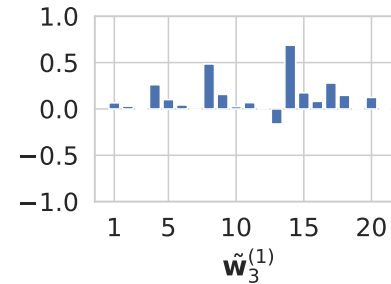
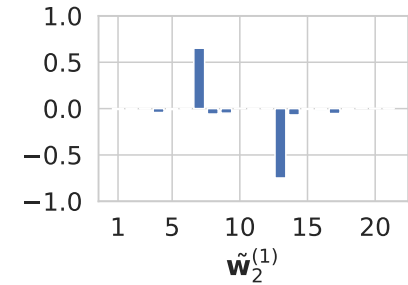
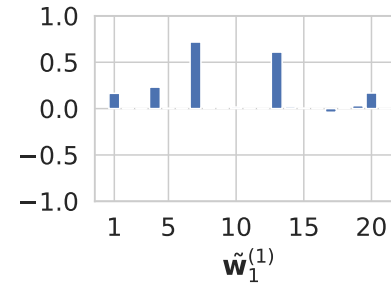
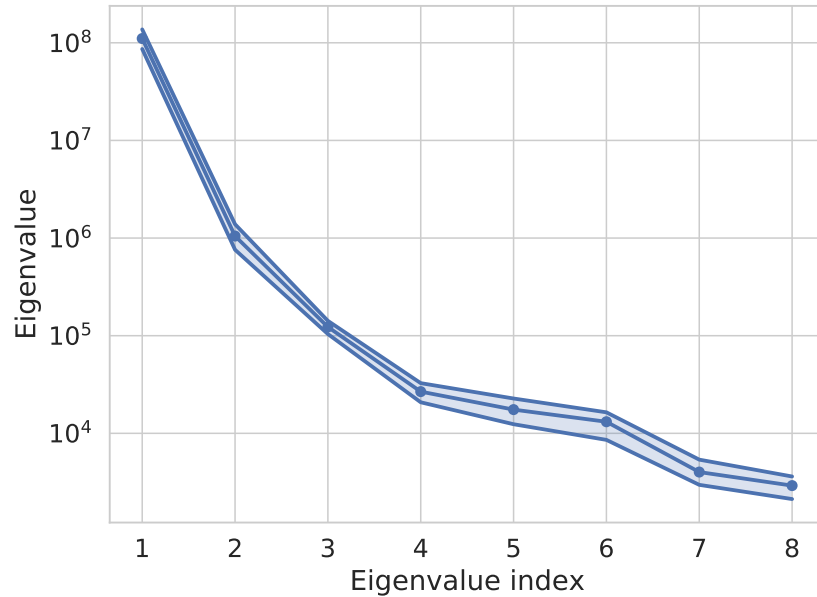
Iterative ASM – Case study, Fig. II

Eigendecomposition It. 0



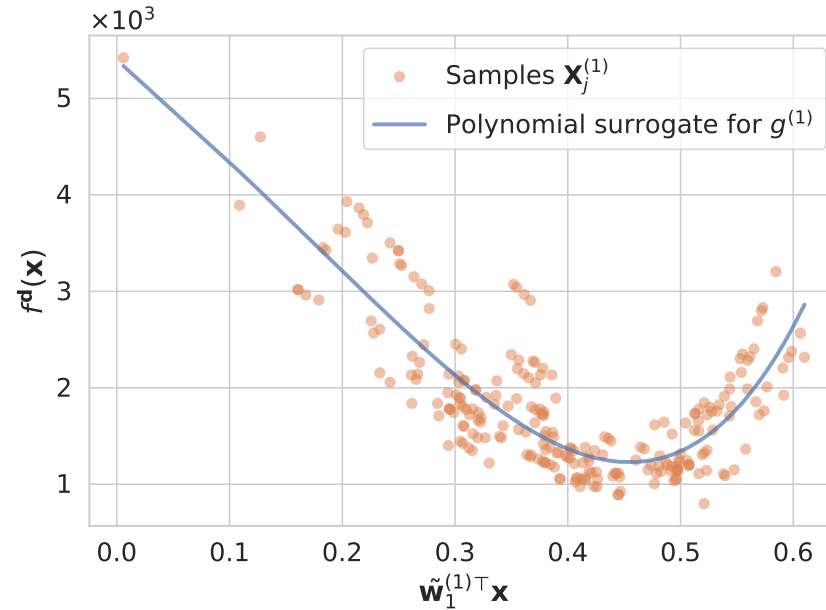
Iterative ASM – Case study, Fig. III

Eigendecomposition It. 1



Iterative ASM – Case study, Fig. IV

Surrogate for $g^{(1)}$



Iterative ASM – Case study, Fig. V

Subspace distances lt. 0 \leftrightarrow lt. 1 \leftrightarrow lt. 2

