Abstract. This paper develops a comprehensive probabilistic setup to compute approximating functions in active subspaces. Constantine et al. proposed the active subspace method in [8] to reduce the dimension of computational problems. It can be seen as an attempt to approximate a high-dimensional function of interest $f$ by a low-dimensional one. To do this, a common approach is to integrate $f$ over the inactive, i.e. non-dominant, directions with a suitable conditional density function. In practice, this can be done with a finite Monte Carlo sum, making not only the resulting approximation random in the inactive variable for each fixed input from the active subspace, but also its expectation, i.e. the integral of the low-dimensional function weighted with a probability measure on the active variable. In this regard we develop a fully probabilistic framework extending results from [8, 10]. The results are supported by a simple numerical example.

1. Introduction

The notion of active subspaces refers to a recent and emerging set of tools for dimension reduction [8]. Reducing dimensions is one natural approach to simplify computational problems suffering from the curse of dimensionality, a phenomenon that results in an exponential growth in computational cost with increasing dimension. What is regarded as a high dimension is dictated by the
actual problem considered. By "high", we mean a number of dimensions that leads to excessive computational times, the need of large memory, or even questions of feasibility of the computation.

There exist different approaches besides active subspaces to reduce computational effort, especially in the context of Uncertainty Quantification (UQ) and Bayesian inversion [22]. For example, in [4, 13, 21] the authors consider low-rank approximations for the prior-preconditioned Hessian of the data misfit function to approximate the posterior covariance in computationally intensive linear Bayesian inverse problems. An extension for the nonlinear setting was proposed in [18]. A drawback of these methods is that they still require work in the full, high-dimensional space. A promising way of dimension reduction was proposed in [11], where the authors seek dominant directions in the parameter space that drive the update from the prior to the posterior distribution. These directions span the so-called likelihood-informed subspace (LIS) and are computed using the posterior expectation of the prior-preconditioned Hessian. The authors of [25] propose a new methodology that constructs a controlled ridge approximation [20] of the data misfit such that an upper bound on the KL divergence between the posterior and the corresponding approximation falls under a given threshold. The bound is obtained via logarithmic Sobolev inequalities [14]. The paper also contains a comparison to likelihood-informed and active subspaces. Most of the methods work only for scalar-valued functions. In [24], the authors perform gradient-based dimension reduction for functions in Hilbert spaces, i.e. also for vector-valued functions.

Active subspaces also aim to find a ridge approximation to a function of interest \( f \). However, it exploits structure of the function's gradient, more precisely, the (prior-)averaged outer product of the gradient with itself. The technique was already successfully applied for a wide range of complex problems of engineering or economical relevance, e.g. in hydrology [15], for a lithium ion battery model [7], or to an elastoplasticity model for methane hydrates [23].

Independently of the concrete methodology, each approach to reduce dimension aims at unfolding main and dominant information hidden in a low-dimensional structure. Active subspaces concentrate on directions in a computational subdomain in which \( f \) is more sensitive, on average, than in other (orthogonal) directions. For that, the eigenvalues and corresponding eigenvectors of an uncentered covariance-type matrix defined by the average of the outer product of the gradient \( \nabla f \) with itself are studied. The span of eigenvectors with corresponding large eigenvalues form the so-called active subspace. With the active subspace at hand, \( f \) can be approximated by a low-dimensional ridge function depending on fewer variables.

A common approximation of \( f \) uses a conditional expectation of \( f \) over the complement of the active subspace, the inactive subspace, conditioned on the active variable, which is a linear combination of the variables from the original domain [8]. In practice, the conditional expectation is often approximated by a finite Monte Carlo sum. For this type of approximation, only a few samples are generally necessary since the function \( f \) is, by construction, only mildly varying on the inactive subspace.

The idea of active subspaces was introduced in [8] and exploited for an accelerated Markov chain Monte Carlo algorithm [3] in [10]. Theoretical considerations therein ignore stochasticity in the inactive subspace. In this paper, we include this aspect and perform a complete and rigorous analysis of approximating functions in active subspaces. Eventually, we aim at providing a comprehensive probabilistic framework that generalizes the existing theoretical setting from [8, 10]. Our findings are supported by a simple test example.

The manuscript is structured as follows. Section 2 formulates the mentioned problem generally without the notion of an active subspace. In Section 3, we explain and derive the concept of an active subspace in detail and set up a probabilistic setting for treating randomness in the inactive
subspace. The main results on approximating functions in active subspaces via a Monte Carlo approximation of a conditional expectation are contained in Section 4 (see e.g. Theorem 4.3 and Theorem 4.6). Additionally, a simple numerical example is shown to support theoretical results. Section 5 is devoted to restate and extend a result from [10]. A summary and concluding comments are collected in Section 6.

2. Problem formulation

Suppose two random variables  \( Y \) and  \( Z \) follow a joint distribution with joint density  \( \rho_{YZ} \). Also, assume that the corresponding marginal and conditional densities are defined in the usual way [2, Section 20 and 33]. Define

\[
g(y) := \int f(y, z) \rho_{Z|Y}(z|y) \, dz
\]

for a function  \( f \) which is integrable w.r.t.  \( \rho_{Z|Y}(·|y) \) in its second argument for every  \( y \). Let us approximate  \( g \) by a finite Monte Carlo sum

\[
g_N(y) := \frac{1}{N} \sum_{j=1}^{N} f(y, Z_j^y), \quad Z_j^y \sim \mathbb{P}_{Z|Y}(·|y)
\]

where  \( \mathbb{P}_{Z|Y}(·|y) / d\lambda = \rho_{Z|Y}(·|y) \) and  \( N > 0 \) denotes the number of Monte Carlo samples used for each  \( y \). That means  \( g_N \) is a random variable for every  \( y \). Now, assume that a high-dimensional variable  \( x \) is divided into  \( y \) and  \( z \), i.e.  \( x \mapsto (y, z) \). For convenience, define a function

\[
g_N(x) := g_N(y)
\]

defined on the corresponding high-dimensional domain.

The first main point of this manuscript is to give a rigorous description, in the context of active subspaces, of why the expression

\[
\mathbb{E}[g_N(X)] = \int g_N(x) \rho_X(x) \, dx,
\]

where  \( \rho_X(x) = \rho_{Y,Z}(y,z) \), is in general again random. The second point deals with the consequences (of treating this expression as non-deterministic) that lie in expanding results from [8, 10] in the given probabilistic framework.

3. Active subspaces

Active subspaces, introduced in [5, 8, 10], try to find a ridge approximation [6, 20] to a function  \( f : \mathcal{X} \to \mathbb{R} \),  \( \mathcal{X} \subseteq \mathbb{R}^n \) open, i.e.  \( f(x) \approx g(A^Tx) \) for all  \( x \in \mathcal{X} \) with a function  \( g : \mathcal{Y} \to \mathbb{R} \),  \( \mathcal{Y} \subseteq \mathbb{R}^k \), and a matrix  \( A \in \mathbb{R}^{n \times k} \). Obviously, one hopes that  \( k \ll n \) to sufficiently reduce the dimension.  \( A \) is computed to hold the directions in which  \( f \) is more sensitive, on average, than in other directions. This means that  \( f \) is nearly insensitive, on average, for directions in the null space of  \( A^\top \) since

\[
f(x + w) \approx g(A^\top(x + w)) = g(A^\top x) \approx f(x)
\]

for each  \( w \in \mathcal{N}(A^\top) := \{ y \in \mathbb{R}^n \mid A^\top y = 0 \} \). The notion "on average" is crucial in the following and means that sensitivities are weighted with a probability density function  \( \rho_X \) defined on  \( \mathbb{R}^n \).

In the following, let  \( \mathcal{X} \) denote the set of all  \( x \)'s with a positive density value, i.e.

\[
\mathcal{X} := \{ x \in \mathbb{R}^n \mid \rho_X(x) > 0 \}.
\]

We assume that  \( \mathcal{X} \) is open and hence  \( \mathcal{X} \in \mathcal{B}(\mathbb{R}^n) \). Thus,  \( \rho_X \) is assumed to be zero on the boundary  \( \partial \mathcal{X} \). Also, suppose that  \( \mathcal{X} \) is a continuity set, i.e.  \( \lambda^n(\partial \mathcal{X}) = 0 \). We will often make use of the fact
that it is enough to integrate over $\mathcal{X}$ instead of $\mathbb{R}^n$ when weighting with $\rho_X$. In order to find the matrix $A$ for the ridge approximation, we assume that $f$ has partial derivatives that are square integrable w.r.t. $\rho_X$. Additionally, we assume that $\rho_X$ is bounded and continuous on $\mathcal{X}$.

To study sensitivities, we regard an orthogonal eigendecomposition of the averaged outer product of the gradient $\nabla f : \mathcal{X} \to \mathbb{R}^n$ with itself, i.e.

$$C := \int_{\mathcal{X}} \nabla f(x) \nabla f(x)^\top \rho_X(x) \, dx = W \Lambda W^\top,$$

where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$ denotes the eigenvalue matrix with descending eigenvalues and $W = [w_1 \cdots w_n]$ consists of all corresponding normed eigenvectors. The fact that $C$ is real symmetric implies that the eigenvectors $w_i$ can be chosen to give an orthonormal basis (ONB) of $\mathbb{R}^n$. Since $C$ is additionally positive semi-definite, it holds that $\lambda_i \geq 0$, $i \in [n] := \{1, \ldots, n\}$. Note that the eigenvalues

$$\lambda_i = w_i^\top C w_i = \int_{\mathcal{X}} (w_i^\top \nabla f(x))^2 \rho_X(x) \, dx, \quad i \in [n],$$

reflect averaged sensitivities of $f$ in the direction of corresponding eigenvectors. That means that $f$ changes little, on average, in the directions of eigenvectors with small eigenvalues.

If it is possible to find a sufficiently large spectral gap, we can accordingly split $W = [W_1 \ W_2]$. That is, $W_1 \in \mathbb{R}^{n \times k}$, $k \in \{n-1\}$, holds the directions for which $f$ is more sensitive, on average, than for directions in $W_2 \in \mathbb{R}^{n \times (n-k)}$. Dimension $k$ denotes the number of eigenvalues before the spectral gap. The size of the gap is crucial for the approximation quality of the active subspace $5$.

After splitting $W$, we can get a new parametrization of $x$. We write

$$x = W W^\top x = W_1 W_1^\top x + W_2 W_2^\top x = W_1 y + W_2 z,$$

with $y := W_1^\top x$, $z := W_2^\top x$. The variable $y$ is called the active variable and the column space of $W_1$, $\mathcal{R}(W_1) := \{W_1 y \mid y \in \mathbb{R}^k\}$, the active subspace. 

**Notation.** Throughout the remainder, we use some notation to avoid uninformative text. According to the previous lines, define $[y, z] := [y, z]^\mathbb{R}_W := W_1 y + W_2 z$. This will shorten text in following equations. Also, for a compatible pair of a matrix $A$ and a set $\mathcal{V}$, we define $A \mathcal{V} := \{Av \mid v \in \mathcal{V}\}$. Additionally, for a set $\mathcal{V} \subseteq \mathbb{R}^n$, we set $\mathcal{V}_y := W_1^\top \mathcal{V}$, i.e. $\mathcal{V}_y$ is the set of $y$-coordinates of points in $\mathcal{V}$.

**Probabilistic setting.** Let $(\Omega, A, \mathbb{P})$ be an abstract probability space. The random variable $X : \Omega \to \mathbb{R}^n$ stands for $x \in \mathbb{R}^n$ viewed as a random element whose push-forward measure $\mathbb{P}_X := \mathbb{P} (X \in \cdot)$ has Lebesgue density $d\mathbb{P}_X/d\lambda = \rho_X$. The random variables $Y := W_1^\top X$ and $Z := W_2^\top X$ representing random elements in the active and inactive subspace also induce corresponding push-forward measures $\mathbb{P}_Y := \mathbb{P} (Y \in \cdot)$ and $\mathbb{P}_Z := \mathbb{P} (Z \in \cdot)$. It is possible to define a joint probability density function for the active and inactive variable with $\rho_X$, i.e.

$$\rho_X(x) = \rho_X([y, z]) =: \rho_{Y, Z}(y, z).$$

Note that $\rho_{Y, Z}$ inherits boundedness from $\rho_X$. The marginal densities are also defined in the usual way $2$ section 20 and 33, i.e.

$$\rho_Y(y) := \int_{\mathbb{R}^{n-k}} \rho_{Y, Z}(y, z) \, dz$$

and

$$\rho_Z(z) := \int_{\mathbb{R}^k} \rho_{Y, Z}(y, z) \, dy.$$
Note that
\[ \frac{dP_Y}{d\lambda} = \rho_Y \quad \text{and} \quad \frac{dP_Z}{d\lambda} = \rho_Z. \] (3.8)

For convenience, we define domains for the active and inactive variable, i.e.
\[ Y := W_1^T X \subseteq \mathbb{R}^k \quad \text{and} \quad Z := W_2^T X \subseteq \mathbb{R}^{n-k}. \] (3.9)

Note that \( Y \) will be the domain of the low-dimensional function \( g \) approximating \( f \).

The following lemma shows that \( Y \) and \( Z \) can be characterized as sets of vectors in the active and, respectively, inactive subspace with positive marginal density values. Let therefore
\[ Y^* := \{ y \in \mathbb{R}^k \mid \rho_Y(y) > 0 \} \quad \text{and} \quad Z^* := \{ z \in \mathbb{R}^{n-k} \mid \rho_Z(z) > 0 \}. \] (3.10)

We need the result for a proper definition of conditional densities.

**Lemma 3.1.** It holds that
\[ Y = Y^* \quad \text{and} \quad Z = Z^*. \] (3.11)

*Proof.* We only show the equality for \( Y \) since the proof follows the same arguments for \( Z \). Take arbitrary \( y \in Y \) and choose \( x \in X \) such that \( y = W_1^T x \). Set \( z' := W_2^T x \) and \( \rho := \rho_Y z(y, z') > 0 \).

By the openness of \( X \) and the continuity of \( \rho_X \) on \( X \), we can find a neighborhood \( Z_\epsilon \) of \( z' \) such that
\[ \rho_X([y, z_\epsilon]) \geq \frac{\epsilon}{2} \] (3.12)
for each \( z_\epsilon \in Z_\epsilon \). It follows that
\[ \rho_Y(y) = \int_{\mathbb{R}^{n-k}} \rho_{Y, Z}(y, z) \, dz \geq \int_{Z_\epsilon} \rho_{Y, Z}(y, z) \, dz \geq \frac{\epsilon}{2} \lambda^{n-k}(Z_\epsilon) > 0, \] (3.13)
and thus \( y \in Y^* \). Reversely, choose \( y^* \in Y^* \). Since \( \rho_Y(y^*) > 0 \), it exists a \( z^* \in \mathbb{R}^{n-k} \) such that \( x^* := [y^*, z^*] \in X \). Since \( y^* = W_1^T x^* \), it follows \( y^* \in Y \). \[ \square \]

**Corollary 3.2.** It holds that \( P_Y(Y) = 1 \) and \( P_Z(Z) = 1 \), i.e. \( Y \in Y \) a.s. and \( Z \in Z \) a.s.

**Lemma 3.3.** The sets \( Y \subseteq \mathbb{R}^k \) and \( Z \subseteq \mathbb{R}^{n-k} \) are open in respective topological spaces.

*Proof.* We only show the openness for \( Y \) since the proof follows the same arguments for \( Z \). Let \( y_0 \in Y \). By definition, there exists \( x_0 \in X \) with \( y_0 = W_1^T x_0 \). Since \( X \) is open, there exists a ball \( B(x_0) \subseteq X \). Since \( y_0 \in Y_{B(x_0)} \), it suffices to show that \( Y_{B(x_0)} \subseteq Y \).

Take \( y \in Y_{B(x_0)} \). We compute
\[ \rho_Y(y) = \int_{\mathbb{R}^{n-k}} \rho_{Y, Z}(y, z) \, dz \geq \int_{\mathbb{R}^{n-k}} \rho_{Y, Z}(y, z) \, dz > 0. \] (3.14)

Since \( W \) is orthogonal and hence causes only a rotation, the set \( \{ z \in Z \mid [y, z] \in B(x_0) \} \) has positive measure under \( \lambda^{n-k} \) which justifies the last equation above. The result follows by Lemma 3.1. \[ \square \]

In particular, the previous lemma implies that \( Y \in \mathcal{B}(\mathbb{R}^k) \) and \( Z \in \mathcal{B}(\mathbb{R}^{n-k}) \). Another auxiliary result shows that it is enough for the marginal densities to integrate over \( Y \) and \( Z \), respectively.

**Lemma 3.4.** It holds that
\[ \rho_Y(y) = \int_Z \rho_{Y, Z}(y, z) \, dz, \quad y \in \mathbb{R}^k, \quad \text{and} \quad \rho_Z(z) = \int_Y \rho_{Y, Z}(y, z) \, dy, \quad z \in \mathbb{R}^{n-k}. \] (3.16)
Proof. We only show the equality for \( \rho_Y \) since the proof follows the same arguments for \( \rho_Z \). Let \( y \in \mathbb{R}^k \). We write
\[
\rho_Y(y) = \int_Z \rho_{Y,Z}(y,z) \, dz + \int_{\mathbb{R}^n - Z} \rho_{Y,Z}(y,z) \, dz. \tag{3.17}
\]
For \( z \in \mathbb{R}^n - Z \), it holds that \([y,z] \notin \mathcal{X}\), since otherwise \( z \in Z \) which is contradictory. It follows that in (3.17)
\[
\int_{\mathbb{R}^n - Z} \rho_{Y,Z}(y,z) \, dz = \int_{\mathbb{R}^n - Z} \rho_X([y,z]) \, dz = 0 \tag{3.18}
\]
which implies the desired result.

As a consequence of Lemma 3.1, we are able to define a proper conditional density on \( \mathbb{R}^n - k \) given \( y \in \mathcal{Y} \), i.e.
\[
\rho_{Z|Y}(z|y) := \frac{\rho_{Y,Z}(y,z)}{\rho_Y(y)}, \quad z \in \mathbb{R}^n - k. \tag{3.19}
\]
Note that \( \rho_{Z|Y}(z|y) = 0 \) for \( z \notin Z \) and arbitrary \( y \in \mathcal{Y} \) as it was shown in the previous proof. It is possible to define a regular conditional probability distribution of \( Z \) given \( Y = y \) for \( y \in \mathcal{Y} \),
\[
\mathbb{P}_{Z|Y} := \mathbb{P}(Z \in \cdot | Y = y). \tag{3.20}
\]
For details of the construction, see e.g. [12]. It can be connected to the respective conditional density by
\[
\frac{d\mathbb{P}_{Z|Y}}{d\lambda} = \rho_{Z|Y}(.|y). \tag{3.21}
\]
for \( y \in \mathcal{Y} \). For \( y \notin \mathcal{Y} \), let us define \( \rho_{Z|Y}(z|y) = 0 \) for all \( z \in \mathbb{R}^n - k \). In the following, the random variable \( Z^Y \sim \mathbb{P}_{Z|Y}, y \in \mathcal{Y} \), is drawn from the conditional probability distribution defined in (3.20). However, it will be necessary to also regard \( Y \) as random which we denote by the random variable \( Y \). That is, the measure that \( Z^Y \) is drawn from is also random. An abstract framework to deal with in this context is the notion of a random measure (see e.g. [17]).

In order to apply Fubini’s theorem, which requires product measurability of the function to be integrated, in Theorem 4.3 and 4.6 we need to prove a measurability result for the map
\[
Z^Y : (\mathcal{Y} \times \Omega, \mathcal{B}(\mathcal{Y}) \otimes \mathcal{A}) \to (\mathbb{R}^n - k, \mathcal{B}(\mathbb{R}^n - k)), \tag{3.22}
\]
\[
(y, \omega_Z) \mapsto Z^Y(\omega_Z). \tag{3.23}
\]
It will be used in Lemma 4.1 to get a product measurable function. Note that we regard \( \mathcal{Y} \subseteq \mathbb{R}^k \) as a topological space equipped with the usual subspace topology denoted by \( \mathcal{B}(\mathcal{Y}) \).

Lemma 3.5. The map \((y, \omega_Z) \mapsto Z^Y(\omega_Z)\) is \( \mathcal{B}(\mathcal{Y}) \otimes \mathcal{A}\)-measurable.

Proof. Let \( y_0 \in \mathcal{Y} \).

For the moment, assume that \( Z \) is real-valued and change its notation to \( Z \). Let \( F_{Y^0} : \mathbb{R} \to [0,1] \) denote the cumulative distribution function of \( Z^y_0 \). Note that the map \( y \mapsto F_Y(t) \) is \( \mathcal{B}(\mathcal{Y})\)-measurable for each \( t \in \mathbb{R} \). Let \( t \in \mathbb{R} \). Indeed, for \( y \in \mathcal{Y} \), it holds that
\[
F_Y(t) = \int_{-\infty}^t \rho_{Y,Z}(y,z) \, dz. \tag{3.24}
\]
The measurability follows from the product measurability of \( \rho_{Y,Z} \). By the probability integral transform, we can write
\[
Z^y_0 = G_{Y^0}(U), \tag{3.25}
\]
where $U \sim \mathcal{U}([0, 1])$ and $G_{Y}^{\omega} : [0, 1] \to \mathbb{R}$ is the (generalized) inverse distribution function of $F_{Y}^{\omega}$. Hence, it suffices to show product measurability of $(y, u) \mapsto G_{Y}(u)$. It holds that
\[
\{(y, u) \in \mathcal{Y} \times [0, 1] \mid G_{Y}(u) \leq t\} = \{(y, u) \in \mathcal{Y} \times [0, 1] \mid u \leq F_{Y}(t)\} \in \mathcal{B}(\mathcal{Y} \times [0, 1]).
\] (3.26)
The last step follows from the measurability of $y \mapsto F_{Y}(t)$ and the fact that $h_{t}(y, u) := F_{Y}(t) - u$ is $\mathcal{B}(\mathcal{Y} \times [0, 1])$-measurable.

Now, let us assume that $Z$ is again $\mathbb{R}^{n-k}$-valued. Also, let $F_{i}^{Y_{0}}$ denote the cumulative distribution function of $Z_{i}^{Y_{0}}$, $i \in [n-k]$. Similarly to the one-dimensional case, the map $y \mapsto F_{i}^{Y}(t)$ is $\mathcal{B}(\mathcal{Y})$-measurable for each $t \in \mathbb{R}$, $i \in [n-k]$. Again, we can write
\[
Z_{i}^{Y_{0}} = G_{Y_{0}}^{i}(U),
\] (3.27)
where $U \sim C_{Z^{Y_{0}}}$ and
\[
G_{Y_{0}}^{i} : [0, 1]^{n-k} \to \mathbb{R}^{n-k}, \ u \mapsto \left( (F_{1}^{Y_{0}})^{-1}(u_{1}), \ldots, (F_{n-k}^{Y_{0}})^{-1}(u_{n-k}) \right).
\] (3.28)
$C_{Z^{Y_{0}}}$ is called a copula distribution of $Z_{i}^{Y_{0}}$ [19] and $(F_{i}^{Y_{0}})^{-1}$ denotes the (generalized) inverse distribution of $F_{i}^{Y_{0}}$, $i \in [n-k]$. Hence, it suffices to show product measurability of $(y, u) \mapsto G_{Y}(u)$. This follows by noting that the map $\pi_{i}(u) := u_{i}$ is measurable and by applying the steps from the one-dimensional case component-wise. It follows that $(y, \omega_{Z}) \mapsto Z_{i}^{Y}(\omega_{Z})$ is $\mathcal{B}(\mathcal{Y}) \otimes \mathcal{A}$-measurable. ■

**Notation.** It is important to clarify some notation that is used throughout the remainder. We will use three different expectations for the integration of random variables $X$, $Y$ and $Z$. The respective expectations will be denoted by $\mathbb{E}_{X}$, $\mathbb{E}_{Y}$ and $\mathbb{E}_{Z}$.

Also, often we will use a change of variables from $x$ to $(y, z)$ during integration. For that, a useful statement used frequently is proved in the subsequent lemma.

**Lemma 3.6.** For any real-valued function $h \in L^{1}(\Omega, \mathcal{A}, \mathbb{P})$, it holds that
\[
\mathbb{E}_{X} \left[ h(X) \right] = \mathbb{E}_{Y} \left[ \mathbb{E}_{Z} \left[ h([Y, Z]) \right] \right].
\] (3.29)

**Proof.** Define $\Phi(y, z) := [y, z] = x$. Note that $\nabla_{y,z}(\Phi(y, z)) = [W_{1} \ W_{2}] = W$. Integration by substitution for multiple variables gives
\[
\mathbb{E}_{X} \left[ h(X) \right] = \int_{\mathcal{Y}} \int_{\mathcal{Z}} h(\Phi(y, z)) \rho_{X}(x) \, dx \, dz \, dy
\] (3.30)
\[
= \int_{\mathcal{Y}} \int_{\mathcal{Z}} h(\Phi(y, z)) \rho_{X}(\Phi(y, z)) |\text{det}(W)| \, dz \, dy
\] (3.31)
\[
= \int_{\mathcal{Y}} \int_{\mathcal{Z}} h([y, z]) \rho_{Y,Z}(y, z) \, dz \, dy
\] (3.32)
\[
= \int_{\mathcal{Y}} \left( \int_{\mathcal{Z}} h([y, z]) \rho_{Z,Y}(z|y) \, dz \right) \rho_{Y}(y) \, dy
\] (3.33)
\[
= \int_{\mathcal{Y}} \left( \int_{\mathcal{Z}} h([y, z]) d\mathbb{P}_{Z|Y}(z) \right) d\mathbb{P}_{Y}(y)
\] (3.34)
\[
= \int_{\mathcal{Y}} \left( \int_{\mathcal{Z}} h([Y, Z]) d\mathbb{P}_{Z|Y}(z) \right) d\mathbb{P}(\omega_{Y})
\] (3.35)
\[
= \mathbb{E}_{Y} \left[ \mathbb{E}_{Z} \left[ h([Y, Z]) \right] \right].
\] (3.36)

In (3.32), we use that $\text{det}(W) = \pm 1$ for the orthogonal matrix $W$. ■
4. Approximating functions in the active subspace

Once the active subspace is computed, the function $f$ can be approximated by a function $g$ on a lower-dimensional domain. One way to define a suitable approximation is by a conditional expectation, i.e.

$$ g(y) := E_{X \mid Y = y} \left[ f(X) \right] $$

$$ := \int_{\mathbb{R}^{n-k}} f([y,z]) \, d\rho_{Z\mid Y}^y(z) $$

$$ = \int_{\mathbb{R}^{n-k}} f([y,z]) \rho_{Z\mid Y}^y(z|y) \, dz $$

$$ = \int_{Z} f([y,z]) \rho_{Z\mid Y}^y(z|y) \, dz $$

for $y \in \mathcal{Y}$. Note that the last line is justified by the fact that $\rho_{Z\mid Y}^y(z|y) = 0$ for $z \notin Z$ and arbitrary $y \in \mathcal{Y}$. The conditional expectation is known to be the best $L^2$ approximation of $f$ in the active subspace $\mathcal{Z}$.

To get a function on the same domain as $f$, i.e. $\mathcal{X}$, let us define

$$ f_g(x) := g(W_1^\top x). $$

In practice, the weighted integral in (4.4) can be approximated by a finite Monte Carlo sum with

$$ g_N(y, \cdot) := \frac{1}{N} \sum_{j=1}^{N} f([y,Z^\gamma_j(\cdot)]) , \quad Z^\gamma_j \sim \rho_{Y\mid Z}^y, \quad N > 0. $$

for $y \in \mathcal{Y}$. Note that $g_N(y, \cdot)$ is again random for every $y \in \mathcal{Y}$. Similar to (4.5), we define a suitable function on $\mathcal{X} \times \Omega$ by

$$ f_{g_N}(x, \cdot) := g_N(W_1^\top x, \cdot). $$

It is important to recognize the following relationship between the expectations of $f_{g_N}(X)$ and $g_N(Y)$. It holds that

$$ E_X \left[ f_{g_N}(X, \cdot) \right] = E_Y \left[ E_Z \left[ f_{g_N}(Y, Z^\gamma, \cdot) \right] \right] = E_Y \left[ E_Z \left[ g_N(Y, \cdot) \right] \right] = E_Y \left[ g_N(Y, \cdot) \right]. $$

This equation is a crucial point in this manuscript. It makes clear that both expressions $E \left[ f_{g_N}(X, \cdot) \right]$ and $E_Y \left[ g_N(Y, \cdot) \right]$ are random. More explicitly, this can be seen by the following equations. Let $\omega_Z \in \Omega$ be fixed. Then,

$$ E_X \left[ f_{g_N}(X, \omega_Z) \right] = \int_X f_{g_N}(x, \omega_Z) \rho_X(x) \, dx $$

$$ = \int_Y \left( \int_Z f_{g_N}([y,z], \omega_Z) \rho_{Z\mid Y}^y(z|y) \, dz \right) \rho_Y(y) \, dy $$

$$ = \int_Y \left( \int_Z g_N(y, \omega_Z) \rho_{Z\mid Y}^y(z|y) \, dz \right) \rho_Y(y) \, dy $$

$$ = \int_Y g_N(y, \omega_Z) \rho_Y(y) \, dy $$

$$ = E_Y \left[ g_N(Y, \omega_Z) \right]. $$

Note that in (4.11), the variable $z$, "belonging" to $x$, disappears such that the integral w.r.t. $z$ gets $\int_Z \rho_{Z\mid Y}(z|y) \, dz = 1$. The random variables $Z_j^\gamma$ within $g_N$ are not integrated by the integral over...
z, i.e. the variables $Z^y$ are not bound in terms of formal languages. This leads to the fact that $E_X[f_{gN}(X, \cdot)]$ is again random.

We can now regard expressions $E_Z[E_Y[g_N]]$ or $E_Y[E_Z[g_N]]$. We will show that both are equal and regard the first, i.e. $E_Z[E_Y[g_N]]$. In the proof of Theorem 4.3, we thus compute the expectation of the mean squared error between $f_g$ and $f_{gN}$ and have to change the order of integration w.r.t. $\omega_Y$ and $\omega_Z$, i.e. apply Fubini’s theorem. In order to do this properly, we need to show the measurability of $g_N$ in the product space $Y \times \Omega$.

**Lemma 4.1.** The function $g_N : Y \times Ω \to ℜ$ is $\mathcal{B}(Y) \otimes \mathcal{A}$-measurable.

**Proof.** Lemma 3.5 proves product measurability of $Z^y$, defined in (3.22). This implies the result. ■

One important result, already proved in [8, Theorem 3.1], gives an upper bound on the mean squared error of $f_g$ by the eigenvalues corresponding to the inactive subspace. For the sake of completeness, it is stated and also proved in our notational context.

**Theorem 4.2.** It holds that

$$E_X[(f(X) - f_g(X))^2] \leq C_{4.2}(\lambda_{k+1} + \cdots + \lambda_n), \quad (4.14)$$

where $C_{4.2} > 0$ is the Poincaré constant depending on $P_X$ and $\mathcal{X}$.

**Proof.** Note that

$$E_Z[f(\|y, Z^y\|) - g(y)] = 0 \quad (4.15)$$

for every $y \in Y$. It follows that

$$E_X[(f(X) - f_g(X))^2] = E_Y[E_Z[(f(\|Y, Z^Y\|) - g(Y))^2]] \quad (4.16)$$

$$\leq C_{4.2}E_Y[E_Z[\nabla_z f(\|Y, Z^Y\|)^\top \nabla_z f(\|Y, Z^Y\|)]] \quad (4.17)$$

$$= C_{4.2}E_X[\nabla_z f(X)^\top \nabla_z f(X)] \quad (4.18)$$

$$\leq C_{4.2}(\lambda_{k+1} + \cdots + \lambda_n). \quad (4.19)$$

In (4.16), we use Lemma 3.6 (4.17) uses a Poincaré inequality which is applicable due to (4.16) [1]. The last line follows from [8, Lemma 2.2]. ■

That means, if all eigenvalues corresponding to the inactive subspace are small or even zero, then the mean squared error of the conditional expectation is also small or zero. Contrarily, if the inactive subspace is spanned by too many eigenvectors with rather large corresponding eigenvalues, then the approximation might be poor.

Lemma 4.1 not only proves that $E_Y[g_N(Y, \cdot)]$ is indeed a random variable, i.e. a measurable map from $\Omega$ to $ℜ$. Additionally, we are ready to prove a crucial result with it. The main difference to [8, Theorem 3.2] is that the result is an upper bound on the expectation of the mean squared error of $f_{gN}$ to $f_g$.

**Theorem 4.3.** It holds that

$$E_Z[E_X[(f_g(X) - f_{gN}(X, \cdot))^2]] = E_Z[E_Y[(g(Y) - g_N(Y, \cdot))^2]] \leq \frac{C_{4.3}}{N}(\lambda_{k+1} + \cdots + \lambda_n). \quad (4.20)$$

**Proof.** For fixed $\omega_Z \in Ω,$

$$E_X[(f_g(X) - f_{gN}(X, \omega_Z))^2] = E_X[(g(W^\top_1 X) - g_N(W^\top_1 X, \omega_Z))^2] \quad (4.21)$$
\[ = \mathbb{E}_Y \left[ (g(Y) - g_N(Y, \omega_Z))^2 \right]. \] (4.22)

The last line is an application of Lemma \[3.6\]. Note that for fixed \( y \in \mathcal{Y} \) (and variable \( \omega_Z \in \Omega \)) it holds that
\[
\mathbb{E}_Z [g_N(y, \cdot)] = \int_\Omega \frac{1}{N} \sum_{j=1}^N f(\|y, Z_j^Y(\omega_Z)\|) \, d\mathbb{P}(\omega_Z)
\]
(4.23)
\[
= \int_\Omega f(\|y, Z_j^Y\|) \, d\mathbb{P}(\omega_Z)
\]
(4.24)
\[
= \int_Z f(\|y, z\|) \, d\mathbb{P}_{Z_j^Y}(z)
\]
(4.25)
\[
= g(y).
\]
(4.26)

In (4.24), we used that \( Z_j^Y, j \in [n] \), are independent and identically distributed. Taking expectations w.r.t. \( \omega_Z \) for the expression in (4.22) gives
\[
\mathbb{E}_Z \left[ \mathbb{E}_Y \left[ (g(Y) - g_N(Y, \cdot))^2 \right] \right] = \mathbb{E}_Y \left[ \mathbb{E}_Z \left[ (g(Y) - g_N(Y, \cdot))^2 \right] \right] \] (4.27)
\[
= \mathbb{E}_Y \left[ \text{Var}_Z (g_N(Y, \cdot)) \right] \] (4.28)
\[
= \frac{1}{N} \sum_{j=1}^N \mathbb{E}_Y \left[ \text{Var}_Z \left( f(\|Y, Z_j^Y\|) \right) \right] \] (4.29)
\[
= \frac{1}{N} \mathbb{E}_Y \left[ \text{Var}_Z \left( f(\|Y, Z_j^Y\|) \right) \right] \] (4.30)
\[
= \frac{1}{N} \mathbb{E}_Y \left[ \mathbb{E}_Z \left( (f(\|Y, Z_j^Y\|) - g(Y))^2 \right) \right] \] (4.31)
\[
= \frac{1}{N} \mathbb{E}_X \left[ (f(X) - g(W_1^T X))^2 \right] \] (4.32)
\[
= \frac{1}{N} \mathbb{E}_X \left[ (f(X) - f_g(X))^2 \right] \] (4.33)
\[
\leq \frac{C_2}{N} \left( \lambda_{k+1} + \cdots + \lambda_n \right). \] (4.34)

\[4.27\] applies Fubini’s theorem which is applicable since \( g_N \) is product measurable due to Lemma \[4.1\].

The result of (4.26) justifies (4.28). In (4.30), we use again that \( Z_j^Y, j \in [n] \), are independent and identically distributed for fixed \( y \in \mathcal{Y} \). Lemma \[3.6 \] with \( h(x) := (f(x) - g(W_1^T x))^2 \) gives (4.32).

The last equation in (4.34) follows from Lemma \[4.2\].

The number of samples \( N > 0 \) in the approximating sum shows up in the bound’s denominator which is common for Monte Carlo type approximations (the root mean squared error is \( O \left( N^{-1/2} \right) \)).

**Stability.** In practice, the matrix \( C \) in (3.2) and its eigendecomposition giving the active subspace are only approximately available. A well-investigated way to get an approximation is by using a finite Monte Carlo sum [5]. Independently of the concrete type of approximation, we only have a perturbed representation of the active and inactive subspace available that we denote here by
\[
\hat{W} = [\hat{W}_1 \hat{W}_2].
\]
(4.35)

This subsection is dedicated to discuss MSE analysis for perturbations. We repeat the behavior of active subspaces with respect to perturbations from [8] and extend theorems where necessary.
In the following, we will denote perturbed terms with a hat (\( \hat{\cdot} \)). For the sake of clarity, let us recall the definitions of the approximating function and its Monte Carlo version for the context of perturbed quantities. Analogously to the context without perturbations, the domain of \( \hat{g} \) is denoted by \( \hat{Y} := \hat{W}_1^\top \mathcal{X} \). Define

\[
\hat{g}(\hat{Y}) := \int_{\mathbb{R}^{n-k}} f([\hat{Y}, \hat{Z}]) \rho_{Z|Y}(\hat{Z}|\hat{Y}) \, d\hat{Z}, \quad f_\hat{g}(x) := \hat{g}(\hat{W}_1^\top x)
\]

and

\[
\hat{g}_N(\hat{Y}, \cdot) := \frac{1}{N} \sum_{j=1}^N f([\hat{Y}, \hat{Z}_j^\hat{Y}(\cdot)]) \|\hat{W}\|, \quad \hat{Z}_j^\hat{Y} \sim \mathbb{P}_{Z|Y}, \quad f_{\hat{g}_N}(x, \cdot) := \hat{g}_N(\hat{W}_1^\top x, \cdot)
\]

for \( y \in \hat{Y} \) and \( x \in \mathcal{X} \). Note that it is actually enough to integrate over \( \hat{Z} := \hat{W}_2^\top \mathcal{X} \) in (4.36). Let \( \|\cdot\| \) denote the Euclidean norm throughout the rest of the manuscript and assume that

\[
\|\hat{W}_1 - \hat{W}\| \leq \varepsilon
\]

for some \( \varepsilon > 0 \).

For subsequent statements, we need a small helping lemma. It is already stated in [\( 8, \text{Lemma } 3.4 \)], however our proof is only slightly different (there appears a \( \leq \) in (4.41) instead of \( = \)).

**Lemma 4.4.** Under the assumption in (4.38), it holds that

\[
\|\hat{W}_2 \hat{W}_2\| \leq 1, \quad \|\hat{W}_1 \hat{W}_2\| \leq \varepsilon, \quad \text{and} \quad \|\hat{W}_2^\top \hat{W}_1\| \leq \varepsilon.
\]

**Proof.** By orthogonality of the columns of \( \hat{W}_2 \) and \( \hat{W}_1 \), it holds that

\[
\|\hat{W}_2^\top \hat{W}_2\| \leq \|\hat{W}_2^\top\|\|\hat{W}_2\| = 1.
\]

Additionally,

\[
\|\hat{W}_2\| = \|\hat{W}_1^\top (W_2 - \hat{W}_2)\| \leq \|\hat{W}_1^\top\|\|\hat{W}_2 - \hat{W}_2\| = \|\hat{W}_2 - \hat{W}_2\| \leq \varepsilon.
\]

The last result follows similarly. \( \blacksquare \)

For the sake of completeness, a similar result as in Lemma 4.2, but in the context of perturbations, is stated next. It is taken from [\( 8, \text{Theorem } 3.5 \)].

**Theorem 4.5.** It holds that

\[
E_X \left[ (f(X) - f_\hat{g}(X))^2 \right] \leq C_{12} \left( \varepsilon (\lambda_1 + \cdots + \lambda_k)^{1/2} + (\lambda_{k+1} + \cdots + \lambda_n)^{1/2} \right)^2.
\]

**Proof.** The proof is from [\( 8, \text{Theorem } 3.5 \)]. It uses the chain rule for calculating \( \nabla_\hat{Z} f = \hat{W}_1^\top \hat{W}_2 \nabla_Y f + \hat{W}_2^\top \hat{W}_2 \nabla_\hat{Z} f \) and the result of Lemma 4.4. \( \blacksquare \)

In this bound, also the (large) eigenvalues of the active subspace play some role. Fortunately, they show up with the factor \( \varepsilon > 0 \) being itself a bound on the Euclidean norm of \( \hat{W}_1 - \hat{W} \). If this deviation of \( W \) and \( \hat{W} \) is sufficiently small, then the impact of the larger eigenvalues becomes rather small, and the bound is dominated by the eigenvalues corresponding to the inactive subspace.

As a consequence of our framework, also a perturbed version of Theorem 4.3 can be proved. We will stay with the previous notations, \( E_Y \) and \( E_Z \), to denote expectations involving the perturbed random variables \( \hat{Y} \) and \( \hat{Z} \), respectively.
Theorem 4.6. It holds that
\[\mathbb{E}_Z \mathbb{E}_X \left[ (f_{\hat{g}}(X) - f_{\hat{g}N}(X, \cdot))^2 \right] = \mathbb{E}_Z \left[ \mathbb{E}_Y \left[ \left( \hat{g}(\hat{Y}) - \hat{g}_N(\hat{Y}, \cdot) \right)^2 \right] \right] \]
\[\leq \frac{C_4}{N^2} \left( \varepsilon (\lambda_1 + \cdots + \lambda_k)^{1/2} + (\lambda_{k+1} + \cdots + \lambda_n)^{1/2} \right)^2. \quad (4.43)\]

Proof. The result is proven in a similar way as in the proof of Theorem 4.3. In the last step, it uses Theorem 4.5 instead. ■

Eventually, according to Theorem 3.6 in [8] (see also [9]), we can give an upper bound on the expectation of the mean squared error between \(f\) and \(f_{\hat{g}N}\).

Theorem 4.7. It holds that
\[\mathbb{E}_Z \mathbb{E}_X \left[ (f(X) - f_{\hat{g}N}(X, \cdot))^2 \right] \leq C_4 \left( 1 + N^{-1/2} \right)^2 \left( \varepsilon (\lambda_1 + \cdots + \lambda_k)^{1/2} + (\lambda_{k+1} + \cdots + \lambda_n)^{1/2} \right)^2. \quad (4.44)\]

The bound shows that the number of samples \(N > 0\) for the Monte Carlo approximation has little influence on the approximation quality of \(f_{\hat{g}N}\). The eigenvalues corresponding to the inactive subspace are more crucial.

Numerical experiment. We want to verify previous statements numerically with a simple example that is computationally cheap to analyze. Let us consider a quadratic function of interest
\[f : \mathcal{X} \to \mathbb{R}, \quad x \mapsto \frac{1}{2} x^\top A x\] (4.46)
in \(n = 10\) variables for a symmetric matrix \(A \in \mathbb{R}^{n \times n}\). Additionally, we assume a standard normal distribution on the domain of \(f\), i.e. \(\mathbb{P}_X := \mathcal{N}(0, I)\), and thus \(\mathcal{X} = \mathbb{R}^n\). To calculate the active subspace of this function, we need the gradient of \(f\) which is
\[\nabla f(x) = Ax, \quad x \in \mathcal{X}.\] (4.47)

Now, we can compute
\[C = \int_{\mathcal{X}} \nabla f(x) \nabla f(x)^\top \rho_X(x) \, dx\] (4.48)
\[= A \left( \int_{\mathcal{X}} xx^\top \rho_X(x) \, dx \right) A^\top\] (4.49)
\[= A^2.\] (4.50)

In order to get a good test example, let us choose
\[A := W \Lambda^{1/2} W^\top,\] (4.51)
where \(W \in \mathbb{R}^{n \times n}\) is an arbitrary orthogonal matrix and \(\Lambda \in \mathbb{R}^{n \times n}\) a diagonal matrix containing descending eigenvalues having a spectral gap of almost two orders of magnitude after the second eigenvalue, i.e.
\[\Lambda := \text{diag}(10^4, 10^{3.8}, 10^2, 10^{1.75}, \ldots, 10^{0.25})\] (4.52)
\[= \left( \Lambda_1, \Lambda_2 \right).\] (4.53)

The diagonal submatrices \(\Lambda_1 \in \mathbb{R}^{k \times k}\), \(k = 2\), and \(\Lambda_2 \in \mathbb{R}^{(n-k) \times (n-k)}\) contain eigenvalues from the active and inactive subspace, respectively. The eigenvalues are plotted in Figure 1. The function
Figure 1. Decay of eigenvalues occurring in the numerical experiment.

\[ f, \text{ in terms of the active variable } y \in \mathbb{R}^k \text{ and the inactive variable } z \in \mathbb{R}^{n-k}, \text{ can be computed explicitly to} \]

\[ f([y, z]) = \frac{1}{2} [y, z]^T A [y, z] \]

\[ = \frac{1}{2} (y^T W_1^T W A^{1/2} W^T W_1 y + z^T W_2^T W A^{1/2} W^T W_2 y) \]

\[ + y^T W_1^T W A^{1/2} W^T W_2 z + z^T W_2^T W A^{1/2} W^T W_2 z) \]  \hspace{1cm} (4.54)

\[ = \frac{1}{2} \left( y^T [I \ 0] A^{1/2} [I \ 0] y + z^T [0 \ I] A^{1/2} [0 \ I] z \right) \]

\[ + y^T [I \ 0] A^{1/2} [I \ 0] z + z^T [0 \ I] A^{1/2} [0 \ I] z) \]  \hspace{1cm} (4.55)

\[ = \frac{1}{2} \left( y^T A_1^{1/2} y + z^T A_2^{1/2} z \right). \]  \hspace{1cm} (4.56)

It follows that \( g \), defined in (4.4), can be written as

\[ g(y) = \frac{1}{2} y^T A_1^{1/2} y + \frac{1}{2} \int_{\mathbb{R}^n} z^T A_2^{1/2} z \rho_{Z|Y}(z|y) dz \]  \hspace{1cm} (4.57)

\[ = \frac{1}{2} y^T A_1^{1/2} y + \frac{1}{2} \sum_{i=1}^{n-k} \lambda_i^{1/2} \int_{\mathbb{R}^n} z_i^2 \rho_{Z|Y}(z|y) dz \]  \hspace{1cm} (4.58)

\[ = \frac{1}{2} y^T A_1^{1/2} y + \frac{1}{2} \text{tr}(A_2^{1/2}) \]  \hspace{1cm} (4.59)

for \( y \in \mathcal{Y} \). The last line uses the fact that \( \rho_{Z|Y} \) is again a standard normal density since \( \rho_X \) is rotationally symmetric and \( x \mapsto (y, z) \) is an orthogonal mapping. Note that \( g(y) \) depends only on eigenvalues corresponding to the active subspace if eigenvalues in \( A_2 \) are all zero. Similarly, the
Monte Carlo approximation of $g$, $g_N$, defined in (4.6), is

$$g_N(y) = \frac{1}{2} y_{\top}\Lambda_1^{1/2} y + \frac{1}{2N} \sum_{j=1}^{N} (Z_j')_{\top}\Lambda_2^{1/2} Z_j$$

(4.63)

for $y \in \mathcal{Y}$, where $Z_j' \sim P_{Z|Y} = \mathcal{N}(0, I)$. First, we want to examine the convergence behavior of the mean squared error $\text{MSE}_{f,g_N} := \mathbb{E}_X [(f(X) - f_{g_N}(X, \cdot))^2]$ between $f$ and $f_{g_N}$, in the number of samples $N$ used for the approximation of $f_{g_N}$. For fixed $N > 0$, we approximate the mean squared error by

$$\text{MSE}_{f,g_N} \approx \frac{1}{N_x} \sum_{i=1}^{N_x} (f_g(X_i) - f_{g_N}(X_i, \cdot))^2,$$

(4.64)

where $X_i \sim P_X$, $i \in [N_x]$, are $N_x > 0$ random values in the domain of $f$. We choose $N_x = 10^4$ to get a sufficiently accurate approximation. Since the mean squared error is random, we compute $N_x = 10^3$ realizations of it to approximate

$$\mathbb{E}_Z \left[ \text{MSE}_{f,g_{1N}} \right]$$

(4.65)

which is the quantity we found a bound for in Theorem 4.3. Additionally, we investigate the coefficient of variation, denoted by $\text{CV}_Z$, of $\text{MSE}_{f,g_{1N}}$ defined by

$$\text{CV}_Z \left( \text{MSE}_{f,g_{1N}} \right) := \frac{\text{Std}_Z \left( \text{MSE}_{f,g_{1N}} \right)}{\mathbb{E}_Z \left[ \text{MSE}_{f,g_{1N}} \right]},$$

(4.66)

where Std denotes the standard deviation. We run the experiment for $N = 2, 5, 10, 20, 50, 100$ samples. We follow the same steps to investigate the random variable $\text{MSE}_{f,g_{1N}} := \mathbb{E}_X [(f(X) - f_{g_N}(X, \cdot))^2]$. Theorem 4.7 provides an upper bound on its expectation value. The computational results are plotted in Figure 2. They verify the first order behavior in $N$ of $\mathbb{E}_Z[\text{MSE}_{f,g_{1N}}]$ and show furthermore that the variation of the random variables $\text{MSE}_{f,g_{1N}}$ and $\text{MSE}_{f,g_{5N}}$ is nearly constant w.r.t. $N$. This information is valuable since it means that the consequences of regarding $\text{MSE}_{f,g_{1N}}$ and $\text{MSE}_{f,g_{5N}}$ as deterministic are limited. Additionally, the left plot confirms the fact that an increasing number of samples has a decreasing effect on the (expectation of the) mean squared error between $f$ and $f_{g_N}$.

5. BAYESIAN INVERSION IN THE ACTIVE SUBSPACE

In [10], the authors were able to accelerate the mixing in a Metropolis-Hastings algorithm that produces samples of a posterior distribution from a Bayesian setting. Let us first define the setup in the context of Bayesian inversion before we come to the more interesting and critical point relevant to the current framework.

In Bayesian inversion, one tries to infer parameters $x \in \mathbb{R}^n$ of a model $\mathcal{G}: \mathcal{X} \rightarrow \mathbb{R}^n$ in a statistical setting [16]. The theory is not restricted to the parameter and data space we use here for simplicity, but can be extended to a much more general setting [22]. For example, the outcome of $\mathcal{G}$ can be the solution of a PDE applied to a linear functional called the Quantity of Interest (QoI). The parameters are regarded as random variables and are thus able to model uncertainty. First, we assume a prior probability distribution, induced by a density function $p_{\text{prior}}$, on the space of parameters. The prior is updated to the posterior distribution $p_{\text{post}}$ by incorporating data $d \in \mathbb{R}^n$ which is also treated as a random variable. We model data by $d = \mathcal{G}(X) + \eta$, where $\eta \sim \mathcal{N}(0, \Gamma)$.
is additive Gaussian noise modeling measurement error with a covariance matrix $\Gamma \in \mathbb{R}^{n_d \times n_d}$. The update is formulated by Bayes’ Theorem which makes a statement about the conditional probability of $X$ given $d$. That is,

$$
\rho_{\text{post}}(x|d) := \frac{\rho_{\text{like}}(d|x)\rho_{\text{prior}}(x)}{\int_{\mathbb{R}^n} \rho_{\text{like}}(d|x')\rho_{\text{prior}}(x') \, dx'}
$$

(5.1)

for $x \in \mathcal{X}$. The concrete expression of the likelihood $\rho_{\text{like}}$ is determined by the model for the measurement error. In our case, i.e. assuming additive Gaussian noise for the measurement error, it holds that for $x \in \mathcal{X}$$$
\rho_{\text{like}}(x|d) \propto \exp \left( -\frac{1}{2} \|d - G(x)\|^2_{\Gamma} \right) =: \exp \left( -f_d(x) \right).
$$

(5.2)

The function $f_d(x) := \frac{1}{2} \|d - G(x)\|^2_{\Gamma} := \frac{1}{2} \|\Gamma^{-1/2}(d - G(x))\|^2$, $x \in \mathcal{X}$, is called the data misfit function.

Markov chain Monte Carlo (MCMC) \[3\] methods are a well-known technique to interrogate the posterior distribution. MCMC constructs a Markov chain such that its stationary distribution is the one we want to sample from, i.e. the posterior in this case. One popular MCMC algorithm is the Metropolis-Hastings algorithm \[3\] which is also used in \[10\].

Metropolis-Hastings can be computationally inefficient in high-dimensional parameter spaces. One opportunity to increase efficiency that is presented in \[10\] is dimension reduction by active subspaces. That is, our function of interest $f$ from the active subspace context is chosen to be the data misfit function $f_d$ from the Bayesian setting, i.e. $f(x) := f_d(x)$, $x \in \mathcal{X}$. Intuitively, the active subspace of $f_d$ contains directions in the parameter space that are informed by data $d$ very well.

The prior plays the role of the given density function used for weighting the gradients in (3.2), i.e. $\rho_X := \rho_{\text{prior}}$. Hence, the posterior on the whole space is given by

$$
\rho_{\text{post}}(x) = \frac{\exp(-f(x))\rho_X(x)}{Z}
$$

(5.3)
for $\mathbf{x} \in \mathcal{X}$, where $Z := \int_{\mathcal{X}} \exp(-f(\mathbf{x}')) \rho(\mathbf{x}') d\mathbf{x}'$ is a normalizing constant necessary in order to get a proper probability density function with unit mass. We remove conditioning on $\mathbf{d}$ explicitly to keep notation clear. Respective versions for approximate posteriors using approximations $f_g$ and $f_{gN}$ are defined through

$$
\rho_{\text{post, } g}(\mathbf{x}) := \frac{\exp(-f_g(\mathbf{x})) \rho(\mathbf{x})}{Z_g} \quad \text{and} \quad \rho_{\text{post, } gN}(\mathbf{x}, \cdot) := \frac{\exp(-f_{gN}(\mathbf{x}, \cdot)) \rho(\mathbf{x})}{Z_{gN}(\cdot)}.
$$  \hspace{1cm} (5.4)

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

Consequently, we also want to regard results involving perturbed versions of the posterior which we define by

$$
\rho_{\text{post, } \hat{g}}(\mathbf{x}) := \frac{\exp(-f_{\hat{g}}(\mathbf{x})) \rho(\mathbf{x})}{Z_{\hat{g}}} \quad \text{and} \quad \rho_{\text{post, } \hat{g}N}(\mathbf{x}, \cdot) := \frac{\exp(-f_{\hat{g}N}(\mathbf{x}, \cdot)) \rho(\mathbf{x})}{Z_{\hat{g}N}(\cdot)}
$$  \hspace{1cm} (5.5)

for $\mathbf{x} \in \mathcal{X}$. Note that $\rho_{\text{post, } gN}(\mathbf{x}, \cdot)$ and $\rho_{\text{post, } \hat{g}N}(\mathbf{x}, \cdot)$ are random variables for each $\mathbf{x} \in \mathcal{X}$, as well as the normalizing constants $Z_g(\cdot)$ and $Z_{\hat{g}N}(\cdot)$.

The result that we want to restate here gives an upper bound on the (expected) Hellinger distance between the true posterior and its approximation via $\hat{g}_N$. First, let us investigate a bound involving the approximation with $\hat{g}$, i.e. the perturbed version of $g$ but without randomness. The following theorem is taken from [10, Theorem 3.1]. Its proof is attached in Appendix A for the sake of completeness and uses results from Section 4.

**Theorem 5.1.** It holds that

$$
d_{H}(\rho_{\text{post, } g}, \rho_{\text{post, } \hat{g}}) \leq \sqrt{C_{\mathbf{L}} L} \left( \varepsilon (\lambda_1 + \cdots + \lambda_k)^{1/2} + (\lambda_{k+1} + \cdots + \lambda_n)^{1/2} \right),
$$  \hspace{1cm} (5.6)

where

$$
L^2 := \frac{1}{8} \left( Z \exp \left( -\int_{\mathcal{X}} f(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x} \right) \right)^{-1/2} > 0.
$$  \hspace{1cm} (5.7)

Note that, contrary to [10, Theorem 3.1], the Poincaré constant appears as a square root $\sqrt{C_{\mathbf{L}}}$ (instead of $C_{\mathbf{L}}$). This is a similar result as in Theorem 4.5 saying that the Hellinger distance between the true posterior and the one approximated with $\hat{g}$ is dominated by the eigenvalues from the inactive subspace if the Euclidean norm of $\mathbf{W} - \mathbf{W}$ is small. That is, the smaller these eigenvalues are, the better is the approximation of the posterior with perturbed $\hat{g}$, on average.

For the approximation with random $\hat{g}_N$, note that the Hellinger distance $d_{H}(\rho_{\text{post, } g}, \rho_{\text{post, } \hat{g}_N}(\cdot))$ is also a random variable, i.e. we can, for example, make statements on its expectation $\mathbb{E}_{\mathbb{Z}}$. A corresponding statement is given next.

**Theorem 5.2.** It holds that

$$
\mathbb{E}_{\mathbb{Z}} \left[ d_{H}(\rho_{\text{post, } \hat{g}}, \rho_{\text{post, } \hat{g}_N}) \right] \leq \sqrt{C_{\mathbf{L}} L} \left( \varepsilon (\lambda_1 + \cdots + \lambda_k)^{1/2} + (\lambda_{k+1} + \cdots + \lambda_n)^{1/2} \right),
$$  \hspace{1cm} (5.8)

where $L > 0$ is the same constant as in Theorem 5.1.

**Proof.** The proof is similar to the one in Theorem 5.1. The main difference is the usage of the Cauchy-Schwarz inequality and Theorem 4.6 in the last step instead. Specifically, the last step is

$$
\mathbb{E}_{\mathbb{Z}} \left[ d_{H}^{2}(\rho_{\text{post, } \hat{g}}, \rho_{\text{post, } \hat{g}_N}) \right] \leq \frac{1}{8} Z_{\hat{g}}^{-1/2} \mathbb{E}_{\mathbb{Z}} \left[ \left( Z_{\hat{g}_N}^{-1/2} \mathbb{E}_{\mathbb{X}} \left[ (f_{\hat{g}}(\mathbf{X}) - f_{\hat{g}_N}(\mathbf{X}, \cdot))^2 \right] \right)^{1/2} \right]^2
\leq \frac{1}{8} Z_{\hat{g}}^{-1/2} \mathbb{E}_{\mathbb{Z}} \left[ Z_{\hat{g}_N}^{-1/2} \mathbb{E}_{\mathbb{X}} \left[ (f_{\hat{g}}(\mathbf{X}) - f_{\hat{g}_N}(\mathbf{X}, \cdot))^2 \right] \right] (5.9)
$$  \hspace{1cm} (5.9)

$$
\leq \frac{1}{8} Z_{\hat{g}}^{-1/2} \mathbb{E}_{\mathbb{Z}} \left[ Z_{\hat{g}_N}^{-1/2} \mathbb{E}_{\mathbb{X}} \left[ (f_{\hat{g}}(\mathbf{X}) - f_{\hat{g}_N}(\mathbf{X}, \cdot))^2 \right] \right] (5.10)
$$  \hspace{1cm} (5.10)
\[
\leq \frac{C}{N} L_{g,\hat{g}N}^2 \left( \varepsilon (\lambda_1 + \cdots + \lambda_k)^{1/2} + (\lambda_{k+1} + \cdots + \lambda_n)^{1/2} \right)^2,
\]
(5.11)

where
\[
L_{g,\hat{g}N}^2 := \frac{1}{8} Z_g^{-1/2} E_Z \left[ Z_g^{-1/2} \right] > 0.
\]
(5.12)

The result follows by noting that
\[
E_Z \left[ Z_{\hat{g}N} \right] \geq \exp \left( - \int Y \ E_Z \left[ g_N (\hat{y}, \cdot) \right] \rho_{\hat{Y}} (\hat{y}) \ d\hat{y} \right)
= \exp \left( - \int Y \ g (\hat{y}) \ \rho_{\hat{Y}} (\hat{y}) \ d\hat{y} \right)
= \exp \left( - \int X \ f (x) \ \rho_X (x) \ dx \right).
\]
(5.13)

In (5.13), we changed integrals according to the result of Lemma 4.1 (for perturbed quantities).

According to Theorem 3.1 in [10], we can find an upper bound on the expectation of the Hellinger distance between the true posterior and \( \rho_{\text{post}, \hat{g}N} \) by using the triangle equality.

Theorem 5.3. It holds that
\[
E_Z \left[ d_H (\rho_{\text{post}}, \rho_{\text{post}, \hat{g}N}) \right] \leq \sqrt{C_{\text{TT}}} \left( 1 + N^{-1/2} \right) \left( \varepsilon (\lambda_1 + \cdots + \lambda_k)^{1/2} + (\lambda_{k+1} + \cdots + \lambda_n)^{1/2} \right),
\]
(5.16)

where \( L > 0 \) is the same constant as in Theorem 5.1.

Similar to Theorem 4.7, increasing the number of samples \( N \) to gain accuracy will not have a large effect if the eigenvalues of the inactive subspace are too large and hence dominating.

6. Summary

In this manuscript, we propose a comprehensive probabilistic setting for approximating functions in active subspaces. This was necessary in order to show that a certain expression for the mean squared error of a conditional expectation and its Monte Carlo approximation is again a random term, suggesting extensions of the analyses in [8, 10] to a truly probabilistic setting.

Section 2 formulate the problem in general and tried to motivate the reason for subsequent discussions. We introduce the notion of an active subspace in Section 3 and prove fundamental lemmas needed for rigorous reasoning about later details. In Section 4, we define the conditional expectation of a function of interest \( f \) over the inactive subspace and use it as an approximation to \( f \). The randomness of the mean squared error between the conditional expectation and its Monte Carlo approximation brought us to extend results from [8]. We also verify the results numerically with a simple test example. Figures support the presence of randomness and display statistical properties, e.g. expectations and coefficients of variation, of random terms. Section 5 is dedicated to applications of theorems from Section 4 to restate results from [10] in the context of Bayesian inversion. The Hellinger distance of an exact Bayesian posterior distribution and its approximation using active subspaces is bounded from above by eigenvalues from the inactive subspace. Since this expression, using a Monte Carlo approximation, is also random, we were able to use previous results and confirmed a similar bound from [10].
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Repeating the steps from [10, Theorem 3.1] gives

**Proof.** Repeating the steps from [10, Theorem 3.1] gives

\[
\begin{align*}
    d_\text{H}(\rho_{\text{post}}, \rho_{\text{post}, \hat{g}})^2 &= \frac{1}{2} \int_x \left[ \left( \frac{\exp(-f(x))}{Z_g} \right)^{1/2} - \left( \frac{\exp(-f_{\hat{g}}(x)) }{Z_{\hat{g}}} \right)^{1/2} \right] \, dx \\
    &= \frac{1}{2} \int_x \left[ \left( \frac{\exp(-f(x))}{Z} \right)^{1/2} - \left( \frac{\exp(-f_{\hat{g}}(x)) }{Z_{\hat{g}}} \right)^{1/2} \right] \, dx \\
    &= \frac{1}{2} \int_x \left[ \left( \frac{\exp(-f(x))}{Z} \right)^{1/2} - \left( \frac{\exp(-f_{\hat{g}}(x)) }{Z_{\hat{g}}} \right)^{1/2} \right]^2 \, dx \\
    &\leq \frac{1}{2} \left( \frac{Z}{Z_g} \right)^{1/2} \int_x \left[ \exp(-f(x))^{1/2} - \exp(-f_{\hat{g}}(x))^{1/2} \right]^2 \rho_x(x) \, dx \\
    &= \frac{1}{2} \left( \frac{Z}{Z_g} \right)^{1/2} \int_x \left[ \left( \frac{1}{2} (f(x) - f_{\hat{g}}(x)) \right)^2 \rho_x(x) \, dx \\
    &\leq \frac{1}{8} \left( \frac{Z}{Z_g} \right)^{1/2} \int_x (f(x) - f_{\hat{g}}(x))^2 \rho_x(x) \, dx \\
    &= \frac{1}{8} \left( \frac{Z}{Z_g} \right)^{1/2} \mathbb{E}_x \left[ (f(X) - f_{\hat{g}}(X))^2 \right] \\
    &\leq C_L^2 f_{\hat{g}}^2 \left( \varepsilon \lambda_1 + \cdots + \lambda_k^{1/2} + (\lambda_{k+1} + \cdots + \lambda_n)^{1/2} \right)^2 ,
\end{align*}
\]

where

\[
L_{f, \hat{g}}^2 := \frac{1}{8} \left( \frac{Z}{Z_g} \right)^{-1/2} .
\]

The last equation in (A.10) uses the result of Theorem 4.5. The result follows by noting that

\[
Z_g \geq \exp \left( - \int_x f_{\hat{g}}(x) \rho_x(x) \, dx \right) \\
= \exp \left( - \int_{\hat{g}(\hat{y})} \rho_{\hat{y}}(\hat{y}) \, d\hat{y} \right)
\]
\[
\begin{align*}
&= \exp \left( - \int_{\mathcal{Y}} \left( \int_{\mathcal{Z}} f(\mathbf{y}, \mathbf{z}) \rho_{\mathbf{Z}}(\mathbf{y}) \mathbf{d} \mathbf{z} \right) \rho_{\mathbf{Y}}(\mathbf{y}) \mathbf{d} \mathbf{y} \right) \\
&= \exp \left( - \int_{\mathcal{X}} f(\mathbf{x}) \rho_{\mathbf{X}}(\mathbf{x}) \mathbf{d} \mathbf{x} \right). 
\end{align*}
\]

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