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Gradient-based dimension reduction of multivariate vector-valued functions

Olivier Zahm*, Paul Constantine†, Clémentine Prieur‡, and Youssef Marzouk§

Abstract. We propose a gradient-based method for detecting and exploiting low-dimensional input parameter dependence of multivariate functions. The methodology consists in minimizing an upper bound, obtained by Poincaré-type inequalities, on the approximation error. The resulting method can be used to approximate vector-valued functions (e.g., functions taking values in \mathbb{R}^n or functions taking values in function spaces) and generalizes the notion of *active subspaces* associated with scalar-valued functions. A comparison with the truncated Karhunen-Loève decomposition shows that using gradients of the function can yield more effective dimension reduction. Numerical examples reveal that the choice of norm on the codomain of the function can have a significant impact on the function’s low-dimensional approximation.

Key words. High-dimensional function approximation, dimension reduction, active subspace, ridge approximation, Karhunen-Loève decomposition, Poincaré inequality.

AMS subject classifications. 41A30, 41A63, 65D15

1. Introduction. Many problems that arise in uncertainty quantification—e.g., integrating or approximating multivariate functions—suffer from the curse of dimensionality: loosely, the cost of computing a sufficiently accurate approximation grows dramatically (typically exponentially) with the dimension of the input parameter space. One approach to alleviate this curse is to identify and exploit some notion of low-dimensional structure. For example, the function of interest might vary primarily along a few directions of the input parameter space. In this case, we can say that the problem has a *low intrinsic dimension*; algorithms for quantifying uncertainty can then focus on these important directions to reduce overall cost.

A common and rather simple approach to reducing a function’s input dimension is the truncated *Karhunen-Loève decomposition* [31], closely related to principal component analysis [19]. These techniques exploit the correlation structure of the function’s input space (specifically, decay in the spectrum of the covariance of the input measure). However more effective dimension reduction should be possible with techniques that exploit not only input correlations but also the structure of the input-output map itself. *Global sensitivity analysis* [29] seeks to rank the input coordinates’ importance relative to a particular output of interest. In practice, one may use this ranking to distinguish a subset of influential input variables; computations can proceed by fixing the uninfluential inputs and only varying the influential inputs. Limiting attention to subsets of input coordinates, however, may miss more general linear structure that is even lower-dimensional. *Active subspaces* [5, 7] are eigenspaces of the average outer product of the function’s gradient with itself. They capture directions along which the function “varies” the most—in the sense of its output responding most strongly to input perturbations, in expectation over the input measure. Active subspaces have been

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discovered and exploited in a wide range of science and engineering models [22, 6, 17]. Active subspaces are not necessarily coordinate-aligned, and in this sense they generalize coordinate-based global sensitivity analysis. Yet global sensitivity analysis and active subspaces have primarily been focused on scalar-valued functions (as in models with a single output quantity of interest). In the presence of multiple outputs of interest, as is the case in many practical applications, new approaches are needed. Generalized Sobol’ indices for multivariate or functional outputs have recently been introduced in [20], and further studied in [14, 13]. In the context of active subspaces, one could try to identify important input parameter directions for each output and then “combine” all those directions, as in [18]. But it is not clear how to interpret or even best perform such a combination step, particularly when seeking rigorous error guarantees.

In this paper, we develop a methodology for detecting and exploiting the low intrinsic dimension of vector-valued functions—for instance, functions with multiple real-valued outputs or functions taking values in function spaces. Our analysis extends the theoretical development of active subspaces to vector-valued outputs. We formulate the problem as seeking a particular kind of structure-exploiting approximation (a *ridge* function; see below) whose error is below a prescribed tolerance. To solve this problem, we use a Poincaré-type inequality to derive an upper bound on the error. This bound, defined by means of gradients of the function, admits a simple expression and can be easily (analytically) minimized. Then we construct an approximation of the vector-valued function such that the upper bound is below the prescribed tolerance. We argue that this methodology can yield more effective dimension reduction than the truncated Karhunen-Loève decomposition. The choice of norm on the codomain (output space) of the function, used to measure the approximation error, is of central importance. In this paper, we assume that the domain (input space) of the function is equipped with a Gaussian probability measure, and we use the corresponding weighted norm on the codomain to define a Hilbert space within which we seek approximations. The approximation we obtain thus depends on the input measure, the function to be approximated, and the norm on the output space. When choosing the latter norm according to some particular objective, we naturally obtain a *goal-oriented* approximation.

We demonstrate our results on several analytical examples and on a PDE model with a correlated random field input. In the latter case, we show how the low-dimensional structure and its associated approximation change as various vector-valued outputs—from the PDE solution at two points in the spatial domain to the entire PDE solution field—are considered. When no low-dimensional structure is present in the input-output map, the only possible dimension reduction comes from the correlation structure of the inputs.

The low-dimensional model we use to approximate the map from inputs to outputs is a *ridge function* [27]. Ridge functions and their approximation properties were extensively studied in the 1980s because of their connection to both projection pursuit regression and early neural networks [9, 15]. Recent work has exploited compressed sensing to recover a ridge function from point queries [11, 4]. In contrast, we are not recovering a true but unknown ridge function; instead, we approximate a given map by a ridge function up to a prescribed precision.

Finally, note also that input space dimension reduction arises in the statistical regression literature under the name *sufficient dimension reduction* [1, 8]. Similar to the ridge function

recovery problem, the goal is to identify linear combinations in the input space that are *statistically sufficient* to explain the regression response. Related ideas from regression include the well-known projection pursuit regression [12, 16], where the directions in the projection pursuit model are trained using given input/output pairs. In [30], gradient information is used to explore the underlying regression structure by means of *average derivative functionals*, estimated nonparametrically via kernels. Li *et al.* specifically studied vector-valued responses as *groupwise* dimension reduction [21]. Broadly, and in contrast with the approach proposed in this paper, these regression analyses are concerned with estimation from a given data set, and thus rely on statistical assessments of the error.

2. Dimension reduction of the input parameter space. Throughout the paper, the algebraic space \mathbb{R}^d refers to a parameter space of dimension $d \gg 1$. The Borel set of \mathbb{R}^d is denoted by $\mathcal{B}(\mathbb{R}^d)$ and we let $\mu = \mathcal{N}(m, \Sigma)$ be the Gaussian probability measure on \mathbb{R}^d with mean $m \in \mathbb{R}^d$ and covariance $\Sigma \in \mathbb{R}^{d \times d}$, which is assumed to be non-singular. We let V be a Hilbert space endowed with a scalar product $(\cdot, \cdot)_V$ and the associated norm $\|\cdot\|_V = (\cdot, \cdot)_V^{1/2}$. We denote by

$$\mathcal{H} = L^2(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \mu; V),$$

the Hilbert space which contains all the Borel-measurable functions $v : \mathbb{R}^d \rightarrow V$ such that $\|v\|_{\mathcal{H}} < \infty$, where $\|\cdot\|_{\mathcal{H}}$ is the norm associated with the scalar product $(\cdot, \cdot)_{\mathcal{H}}$ defined by

$$(u, v)_{\mathcal{H}} = \int (u(x), v(x))_V \mu(dx),$$

for any $u, v \in \mathcal{H}$.

We consider the problem of finding a *controlled approximation* of a function $f \in \mathcal{H}$ by a *ridge function* in \mathcal{H} of the form of

$$(1) \quad x \mapsto g(P_r x),$$

where $g : \mathbb{R}^d \rightarrow V$ is a Borel-measurable function and where $P_r \in \mathbb{R}^{d \times d}$ is a rank- r projector. Notice that $g(P_r x) = g(P_r y)$ whenever $x - y \in \text{Ker}(P_r)$, which means that the function (1) is constant along the kernel of the projector. In other words, $x \mapsto g(P_r x)$ is a function of at most r linear combinations of the input parameters. As in [24], the function g is called the *profile* of the ridge function. Given a prescribed tolerance $\varepsilon \geq 0$, the problem consists in finding the function g and the projector P_r , also seen as a (linear) function $P_r : \mathbb{R}^d \rightarrow \mathbb{R}^d$, such that

$$(2) \quad \|f - g \circ P_r\|_{\mathcal{H}} \leq \varepsilon.$$

The choice $P_r = I_d$ (the identity matrix) and $g = f$ in (1) yields a trivial solution. But in that case, the rank of P_r is equal to d and there is no dimension reduction. Thus, in order to make this problem meaningful, we want $r = \text{rank}(P_r)$ to be less than d , ideally $r \ll d$. We will say that f has a *low intrinsic dimension* if there exist g and P_r such that (2) holds with $r = r(\varepsilon) \ll d$.

Remark 2.1. An equivalent formulation of the problem is the following. Given a tolerance $\varepsilon > 0$, we want to find a Borel function $g : \mathbb{R}^d \rightarrow V$ and a low-rank projector $P_r \in \mathbb{R}^{d \times d}$ such that

$$\mathbb{E}(\|f(X) - g(P_r X)\|_V^2) \leq \varepsilon^2,$$

where $X \sim \mathcal{N}(m, \Sigma)$ is a random vector and where $\mathbb{E}(\cdot)$ denotes the mathematical expectation. If $\varepsilon^2 \ll \text{Var}(f(X)) = \mathbb{E}((f(X) - \mathbb{E}(f(X)))^2)$, the statistical interpretation is that the random variable $X_r = P_r X$ is an explanatory variable for $f(X)$, in the sense that most of the variance of $f(X)$ can be explained by X_r .

2.1. Optimal profile for the ridge function. In this section, we assume that the projector P_r is given. We denote by

$$\mathcal{H}_{P_r} = L^2(\mathbb{R}^d, \sigma(P_r), \mu; V),$$

the space which contains all the $\sigma(P_r)$ -measurable functions $v : \mathbb{R}^d \rightarrow V$ such that $\|v\|_{\mathcal{H}} < \infty$. Here $\sigma(P_r)$ is the σ -algebra generated by P_r . By Doob-Dynkin's lemma, see for example Lemma 1.13 in [25], the set of all $\sigma(P_r)$ -measurable functions is exactly the set of the functions of the form $x \mapsto g(P_r x)$ for some Borel function g , so that

$$(3) \quad \mathcal{H}_{P_r} = \{g \circ P_r \mid g : \mathbb{R}^d \rightarrow V, \text{ Borel function}\} \cap \mathcal{H}.$$

Note that \mathcal{H}_{P_r} is a closed subspace in \mathcal{H} . Then, for any $f \in \mathcal{H}$, there exists a unique minimizer of $f_r \mapsto \|f - f_r\|_{\mathcal{H}}$ over \mathcal{H}_{P_r} . This minimizer corresponds to the orthogonal projection of $f \in \mathcal{H}$ onto \mathcal{H}_{P_r} and is denoted by $\mathbb{E}_{\mu}(f|\sigma(P_r))$. We can write

$$\|f - \mathbb{E}_{\mu}(f|\sigma(P_r))\|_{\mathcal{H}} = \min_{f_r \in \mathcal{H}_{P_r}} \|f - f_r\|_{\mathcal{H}} = \min_{\substack{g: \mathbb{R}^d \rightarrow V \\ \text{Borel function}}} \|f - g \circ P_r\|_{\mathcal{H}},$$

which means that $\mathbb{E}_{\mu}(f|\sigma(P_r))$ yields an optimal profile g . Note that $\mathbb{E}_{\mu}(f|\sigma(P_r)) \in \mathcal{H}_{P_r}$ can be uniquely characterized by the variational equation

$$(4) \quad \int (\mathbb{E}_{\mu}(f|\sigma(P_r)), h)_V \, d\mu = \int (f, h)_V \, d\mu,$$

for all $h \in \mathcal{H}_{P_r}$. In other words, $\mathbb{E}_{\mu}(f|\sigma(P_r))$ corresponds to the conditional expectation of f under the distribution μ given the σ -algebra $\sigma(P_r)$, which explains the choice of notation.

Proposition 2.2. Let P_r and Q_r be two projectors such that $\text{Ker}(P_r) = \text{Ker}(Q_r)$. Then we have

$$\mathcal{H}_{P_r} = \mathcal{H}_{Q_r}$$

Proof. Let $h \in \mathcal{H}_{P_r}$. By (3) we can write $h = g \circ P_r$ for some Borel function g . Since $\text{Ker}(Q_r) = \text{Ker}(P_r)$ we have $P_r x = P_r Q_r x = 0$ for all $x \in \text{Ker}(Q_r)$. Also for any $x \in \text{Im}(Q_r)$ we have $Q_r x = x$ and then $P_r x = P_r Q_r x$. Thus $P_r x = P_r Q_r x$ holds for any $x \in \mathbb{R}^d = \text{Ker}(Q_r) \oplus \text{Im}(Q_r)$ so that $P_r = P_r Q_r$. Then $h = g \circ P_r = (g \circ P_r) \circ Q_r$ which shows that $h \in \mathcal{H}_{Q_r}$. Then the inclusion $\mathcal{H}_{P_r} \subset \mathcal{H}_{Q_r}$ holds. By symmetry of the role of P_r and Q_r we obtain the result. ■

Let us recall that a projector is uniquely characterized by both its kernel and its image.¹ Proposition 2.2 shows that \mathcal{H}_{P_r} is invariant with respect to the image of P_r , and so is the conditional expectation $\mathbb{E}_\mu(f|\sigma(P_r))$. In particular, the error $P_r \mapsto \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$ depends only on the kernel of P_r . This means that, with regard to the initial dimension reduction problem (2), the goal is now to find a subspace where the function f does not vary significantly.

By Proposition 2.2 and without loss of generality, we can assume that P_r is an *orthogonal* projector with respect to an arbitrary norm on \mathbb{R}^d . In the present context, the natural norm to use is the one induced by the precision matrix Σ^{-1} associated with μ , meaning the norm $\|\cdot\|_{\Sigma^{-1}}$ defined by $\|x\|_{\Sigma^{-1}}^2 = x^T \Sigma^{-1} x$ for any $x \in \mathbb{R}^d$. Thus we will say that P_r is a Σ^{-1} -orthogonal projector iff

$$(5) \quad \|x\|_{\Sigma^{-1}}^2 = \|P_r x\|_{\Sigma^{-1}}^2 + \|(I_d - P_r)x\|_{\Sigma^{-1}}^2,$$

holds for all $x \in \mathbb{R}^d$. The following proposition gives a simple expression for the conditional expectation $\mathbb{E}_\mu(f|\sigma(P_r))$, provided P_r satisfies (5).

Proposition 2.3. *Let $\mu = \mathcal{N}(m, \Sigma)$ where $\Sigma \in \mathbb{R}^{d \times d}$ is a non-singular covariance matrix and $f \in \mathcal{H}$. Then for any Σ^{-1} -orthogonal projector P_r we have*

$$\mathbb{E}_\mu(f|\sigma(P_r)) : x \mapsto \mathbb{E}(f(P_r x + (I_d - P_r)Y)),$$

where the expectation is taken over the random vector $Y \sim \mu$.

Proof. Let $F : x \mapsto \int_{\mathbb{R}^d} f(P_r x + (I_d - P_r)y) \mu(dy)$ and $h \in \mathcal{H}_{P_r}$. By (3), h can be written as a $g \circ P_r$ for some Borel function g so that $h(x) = h(P_r x + (I_d - P_r)y)$ for all $x, y \in \mathbb{R}^d$. We can write

$$\begin{aligned} \int_{\mathbb{R}^d} (F(x), h(x))_V \mu(dx) &= \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} f(P_r x + (I_d - P_r)y) \mu(dy), h(x) \right)_V \mu(dx) \\ &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left(f(P_r x + (I_d - P_r)y), h(P_r x + (I_d - P_r)y) \right)_V \mu(dy) \mu(dx) \\ &= \mathbb{E}((f(Z), h(Z))_V), \end{aligned}$$

where the expectation is taken over the random vector $Z = P_r X + (I_d - P_r)Y$, where X and Y are two independent random vectors distributed as $\mu = \mathcal{N}(m, \Sigma)$. If $Z \sim \mu$ then the previous relation yields (4) for any $h \in \mathcal{H}_{P_r}$, which would conclude the proof.

It remains to show that $Z \sim \mu$. Note that Z is Gaussian with mean m and covariance

$$\text{Cov}(Z) = P_r \Sigma P_r^T + (I_d - P_r) \Sigma (I_d - P_r)^T = \Sigma - P_r \Sigma - \Sigma P_r^T + 2P_r \Sigma P_r^T.$$

Then $Z \sim \mu$ if and only if $P_r \Sigma + \Sigma P_r^T = 2P_r \Sigma P_r^T$. Since P_r is Σ^{-1} -orthogonal, relation (5) holds for any $x \in \mathbb{R}^d$ which is equivalent to

$$P_r^T \Sigma^{-1} + \Sigma^{-1} P_r = 2P_r^T \Sigma^{-1} P_r.$$

¹Of course an *orthogonal* projector (orthogonal with respect to any given norm) is uniquely characterized either by its kernel or by its image, since the other subspace can be uniquely defined as the orthogonal complement.

Multiplying by P_r^T to the left (resp. by P_r to the right) we get $P_r^T \Sigma^{-1} = P_r^T \Sigma^{-1} P_r$ (resp. $\Sigma^{-1} P_r = P_r^T \Sigma^{-1} P_r$) so that the relation $P_r^T \Sigma^{-1} = \Sigma^{-1} P_r$ holds and yields $\Sigma P_r^T = P_r \Sigma = P_r \Sigma P_r^T$. Therefore we have

$$P_r \Sigma + \Sigma P_r^T = 2P_r \Sigma P_r^T,$$

which concludes the proof. ■

2.2. Poincaré-based upper bound for the error. In this section we show how Poincaré-type inequalities can be used to derive an upper bound for $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$. This upper bound holds for any projector and is quadratic in P_r so that it can easily be minimized.

It is well known that the standard Gaussian distribution $\gamma = \mathcal{N}(0, I_d)$ satisfies the *Poincaré inequality*

$$(6) \quad \int (h - \mathbb{E}_\gamma(h))^2 d\gamma \leq \int \|\nabla h\|_2^2 d\gamma,$$

for any continuously differentiable function $h : \mathbb{R}^d \rightarrow \mathbb{R}$, where ∇h denotes the gradient of h (see for example Theorem 3.20 in [2]). Here $\mathbb{E}_\gamma(h) = \int h d\gamma$ and $\|\cdot\|_2 = \sqrt{(\cdot)^T(\cdot)}$ denotes the canonical norm of \mathbb{R}^d . As noticed in [3], non-standard Gaussian distributions also satisfy a Poincaré inequality. By replacing h by $x \mapsto h(\Sigma^{1/2}x + m)$ in (6), where $\Sigma^{1/2}$ is a symmetric square root of Σ , we have that $\gamma = \mathcal{N}(m, \Sigma)$ satisfies

$$(7) \quad \int (h - \mathbb{E}_\mu(h))^2 d\mu \leq \int \|\nabla h\|_\Sigma^2 d\mu,$$

for any continuously differentiable function $h : \mathbb{R}^d \rightarrow \mathbb{R}$, where $\|\cdot\|_\Sigma$ is the norm on \mathbb{R}^d such that $\|x\|_\Sigma^2 = x^T \Sigma x$ for all $x \in \mathbb{R}^d$. The next proposition shows that μ satisfies another Poincaré-type inequality which we call the *subspace Poincaré inequality*.

Proposition 2.4. *The probability distribution $\mu = \mathcal{N}(m, \Sigma)$ satisfies*

$$(8) \quad \int (h - \mathbb{E}_\mu(h|\sigma(P_r)))^2 d\mu \leq \int \|(I_d - P_r^T) \nabla h\|_\Sigma^2 d\mu,$$

for any continuously differentiable function $h : \mathbb{R}^d \rightarrow \mathbb{R}$ and for any projector P_r .

Proof. First we assume that P_r is a Σ^{-1} -orthogonal projector. Let $h : \mathbb{R}^d \rightarrow \mathbb{R}$ be a continuously differentiable function and define $g : x \mapsto h(P_r y + (I_d - P_r)x)$ for some $y \in \mathbb{R}^d$. For any $x \in \mathbb{R}^d$ we have $\nabla g(x) = (I_d - P_r)^T \nabla h(P_r y + (I_d - P_r)x)$. By Proposition 2.3 we have

$$\mathbb{E}_\mu(g) = \int_{\mathbb{R}^d} h(P_r y + (I_d - P_r)x') \mu(dx') = \mathbb{E}_\mu(h|\sigma(P_r))(y).$$

Notice that we can write $\mathbb{E}_\mu(h|\sigma(P_r))(y) = \mathbb{E}_\mu(h|\sigma(P_r))(P_r y + (I_d - P_r)x)$. Then the Poincaré inequality (7) applied with the function g yields

$$\begin{aligned} & \int_{\mathbb{R}^d} (h(P_r y + (I_d - P_r)x) - \mathbb{E}_\mu(h|\sigma(P_r))(P_r y + (I_d - P_r)x))^2 \mu(dx) \\ & \leq \int_{\mathbb{R}^d} \|(I_d - P_r)^T \nabla h(P_r y + (I_d - P_r)x)\|_\Sigma^2 \mu(dx). \end{aligned}$$

Recall that, since P_r is Σ^{-1} -orthogonal, we have $P_r Y + (I_d - P_r)X \sim \mu$ whenever $X \sim \mu$ and $Y \sim \mu$ are independent; see the proof of Proposition 2.3. Thus, replacing y by Y in the previous inequality and taking the expectation over Y yields (8).

It remains to show that (8) also holds for projectors that are not Σ^{-1} -orthogonal. Thus let P_r be any projector and define Q_r as the (unique) Σ^{-1} -orthogonal projector such that $\text{Ker}(Q_r) = \text{Ker}(P_r)$. Following the proof of Proposition 2.3, we have that Q_r satisfies $Q_r \Sigma + \Sigma Q_r^T = 2Q_r \Sigma Q_r^T$ which is equivalent to saying that the relation $\|x\|_\Sigma^2 = \|Q_r^T x\|_\Sigma^2 + \|(I_d - Q_r^T)x\|_\Sigma^2$ holds for any $x \in \mathbb{R}^d$. Then $\|x\|_\Sigma^2 \geq \|(I_d - Q_r^T)x\|_\Sigma^2$ for any $x \in \mathbb{R}^d$. Replacing x by $(I_d - P_r^T)x$ we get

$$\begin{aligned} \|(I_d - P_r^T)x\|_\Sigma^2 &\geq \|(I_d - Q_r^T)(I_d - P_r^T)x\|_\Sigma^2 \\ &= \|(I_d - Q_r^T - P_r^T + Q_r^T P_r^T)x\|_\Sigma^2 \\ (9) \quad &= \|(I_d - Q_r^T)x\|_\Sigma^2. \end{aligned}$$

For the last equality we used relation $P_r = P_r Q_r$, which holds true since $\text{Ker}(P_r) = \text{Ker}(Q_r)$. Finally, Proposition 2.2 allows writing $\mathbb{E}_\mu(h|\sigma(P_r)) = \mathbb{E}_\mu(h|\sigma(Q_r))$ so that

$$\begin{aligned} \int (h - \mathbb{E}_\mu(h|\sigma(P_r)))^2 d\mu &= \int (h - \mathbb{E}_\mu(h|\sigma(Q_r)))^2 d\mu \\ &\stackrel{(8)}{\leq} \int \|(I_d - Q_r^T)\nabla h\|_\Sigma^2 d\mu \stackrel{(9)}{\leq} \int \|(I_d - P_r^T)\nabla h\|_\Sigma^2 d\mu, \end{aligned}$$

which shows that (8) holds for any projector P_r . ■

The subspace Poincaré inequality stated in Proposition 2.4 allows us to derive an upper bound for the error $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$, as shown by the following proposition.

Proposition 2.5. *Let $\mu = \mathcal{N}(m, \Sigma)$ where $\Sigma \in \mathbb{R}^{d \times d}$ is a non-singular covariance matrix and let $f \in \mathcal{H} = L^2(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \mu; V)$ where V is a separable Hilbert space. Furthermore, assume that f is continuously differentiable. Then for any projector P_r we have*

$$(10) \quad \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}} \leq \sqrt{\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))},$$

where $H \in \mathbb{R}^{d \times d}$ is the matrix defined by

$$(11) \quad H = \int (\nabla f)^*(\nabla f) d\mu.$$

Here, $\nabla f(x) : \mathbb{R}^d \rightarrow V$ denotes the Jacobian of f at point x , which is the linear operator such that

$$(12) \quad f(x + \delta x) = f(x) + \nabla f(x)\delta x + o(\|\delta x\|_2),$$

for any $\delta x \in \mathbb{R}^d$. The linear operator $(\nabla f(x))^* : V \rightarrow \mathbb{R}^d$ is the adjoint of $\nabla f(x)$, defined by $y^T((\nabla f(x))^*v) = (\nabla f(x)y, v)_V$ for all $v \in V$ and for all $y \in \mathbb{R}^d$.

Proof. Denote by $\{e_i\}_{i \geq 1}$ an orthonormal basis of the separable Hilbert space V . The function $f \in \mathcal{H}$ can be represented as $x \mapsto \sum_{i \geq 1} f_i(x) e_i$ where, for all $i \geq 1$, the function $f_i : \mathbb{R}^d \rightarrow \mathbb{R}$ is defined by $f_i(x) = (f(x), e_i)_V$. By linearity of the conditional expectation and by orthogonality of the basis, we can write

$$(13) \quad \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 = \sum_{i \geq 1} \int (f_i - \mathbb{E}_\mu(f_i|\sigma(P_r)))^2 d\mu.$$

By assumption, f is continuously differentiable and so is f_i for all $i \geq 1$. Then the subspace Poincaré inequality (8) with $h = f_i$ allows writing

$$\begin{aligned} \int (f_i - \mathbb{E}_\mu(f_i|\sigma(P_r)))^2 d\mu &\leq \int \|(I_d - P_r^T) \nabla f_i\|_\Sigma^2 d\mu \\ &= \int \text{trace}(\Sigma(I_d - P_r^T)(\nabla f_i)(\nabla f_i)^T(I_d - P_r)) d\mu \\ &= \text{trace}(\Sigma(I_d - P_r^T) \left(\int (\nabla f_i)(\nabla f_i)^T d\mu \right) (I_d - P_r)), \end{aligned}$$

where $\nabla f_i(x) \in \mathbb{R}^d$ denotes the gradient of f_i at point $x \in \mathbb{R}^d$. Together with (13), the above relation yields (10) with

$$H = \int \sum_{i \geq 1} (\nabla f_i)(\nabla f_i)^T d\mu.$$

To conclude the proof, it remains to show that this definition of H matches the one in (11). It is sufficient to show $\sum_{i \geq 1} (\nabla f_i(x))(\nabla f_i(x))^T = (\nabla f(x))^*(\nabla f(x))$ for any $x \in \mathbb{R}^d$. Firstly, projecting (12) onto the basis vector e_i yields $f_i(x + \delta x) = f_i(x) + (\nabla f(x)\delta x, e_i)_V + o(\|\delta x\|_2)$ which allows identifying the gradient of f_i by $\nabla f_i(x)^T \delta x = (\nabla f(x)\delta x, e_i)_V$ for all $\delta x \in \mathbb{R}^d$. Then

$$\nabla f(x)\delta x = \sum_{i \geq 1} (\nabla f_i(x)^T \delta x) e_i.$$

Secondly, recall that the adjoint operator $\nabla f(x)^* : V \rightarrow \mathbb{R}^d$ is defined by $\delta y^T (\nabla f(x)^* v) = (\nabla f(x)\delta y, v)_V$ for all $v \in V$ and for all $\delta y \in \mathbb{R}^d$. Replacing v by $\nabla f(x)\delta x$ we get

$$\begin{aligned} \delta y^T \nabla f(x)^* \nabla f(x)\delta x &= (\nabla f(x)\delta y, \nabla f(x)\delta x)_V \\ &= \sum_{i,j \geq 1} (\nabla f_i(x)^T \delta y)(\nabla f_j(x)^T \delta x)(e_i, e_j)_V \\ &= \delta y^T \left(\sum_{i \geq 1} \nabla f_i(x) \nabla f_i(x)^T \right) \delta x, \end{aligned}$$

for any $\delta x, \delta y \in \mathbb{R}^d$ so that $\nabla f(x)^* \nabla f(x) = \sum_{i \geq 1} \nabla f_i(x) \nabla f_i(x)^T$. This concludes the proof. \blacksquare

We finish this section with an example. Assume $V = \mathbb{R}^m$ is an algebraic space endowed with the norm $\|\cdot\|_V$ defined by $\|v\|_V^2 = v^T M v$ for all $v \in V$, where $M \in \mathbb{R}^{m \times m}$ is a symmetric positive-definite matrix. The Jacobian of f at point $x \in \mathbb{R}^d$ is a m -by- d matrix defined by

$$(\nabla f(x))_{i,j} = \frac{\partial f_i}{\partial x_j}(x).$$

The adjoint of $\nabla f(x)$ is a d -by- m matrix given by $(\nabla f(x))^* = (\nabla f(x))^T M$ so that we can write the matrix H as follows

$$(14) \quad H = \int (\nabla f)^T M (\nabla f) d\mu.$$

Notice that H depends on the choice the norm $\|\cdot\|_V$ via the matrix M .

2.3. Minimizing the upper bound. The following proposition enables minimization of the upper bound in Proposition 2.5.

Proposition 2.6. *Let $\Sigma \in \mathbb{R}^{d \times d}$ be a symmetric positive-definite matrix and $H \in \mathbb{R}^{d \times d}$ a symmetric positive-semidefinite matrix. Denote by $(\lambda_i, v_i) \in \mathbb{R}_{\geq 0} \times \mathbb{R}^d$ the i -th generalized eigenpair of the matrix pair (H, Σ^{-1}) , meaning $Hv_i = \lambda_i \Sigma^{-1}v_i$ with $\|v_i\|_{\Sigma^{-1}} = 1$. For any $r \leq d$ we have*

$$(15) \quad \min_{\substack{P_r \in \mathbb{R}^{d \times d} \\ \text{rank-}r \text{ projector}}} \text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r)) = \sum_{i=r+1}^d \lambda_i.$$

Furthermore a solution to the above minimization problem is the Σ^{-1} -orthogonal projector defined by

$$(16) \quad P_r = \left(\sum_{i=1}^r v_i v_i^T \right) \Sigma^{-1}.$$

Proof. Let $H^{1/2}$ and $\Sigma^{1/2}$ be the symmetric positive square roots of H and Σ respectively. For any projector P_r we have

$$\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r)) = \|H^{1/2}(I_d - P_r)\Sigma^{1/2}\|_F^2 = \|A - X_r\|_F^2,$$

where $A = H^{1/2}\Sigma^{1/2}$ and $X_r = H^{1/2}P_r\Sigma^{1/2}$ and where $\|\cdot\|_F = \sqrt{\text{trace}(\cdot)^T(\cdot)}$ denotes the Frobenius norm. Consider the singular value decomposition of $A = UDV^T$ where $U, V \in \mathbb{R}^{d \times d}$ are two orthogonal matrices and $D = \text{diag}(a_1, \dots, a_d)$ with $a_1 \geq a_2 \geq \dots \geq 0$. The Eckart-Young theorem states that (i) the matrix $A_r = UD_rV^T$, with $D_r = \text{diag}(a_1, \dots, a_r, 0, \dots, 0)$, is a minimizer of $\|A - \tilde{A}_r\|_F^2$ over all matrices \tilde{A}_r with $\text{rank}(\tilde{A}_r) \leq r$ and (ii) that $\|A - A_r\|_F^2 = a_{r+1}^2 + \dots + a_d^2$. We now show that A_r can be written as $X_r = H^{1/2}P_r\Sigma^{1/2}$ for some rank- r projector P_r . Let $V_r \in \mathbb{R}^{d \times r}$ be the matrix containing the r first columns of V and let $P_r = \Sigma^{1/2}V_rV_r^T\Sigma^{-1/2}$. Since $V_r^TV_r = I_r$ we have $P_r^2 = P_r$ so that P_r is a rank- r projector. Also we have $X_r = H^{1/2}P_r\Sigma^{1/2} = AV_rV_r^T = A_r$. Then $\|A - X_r\|^2 = \|A - A_r\|^2 \leq \|A - \tilde{A}_r\|^2$ holds for any rank- r matrix \tilde{A}_r , in particular for the ones of the form of $\tilde{A}_r = H^{1/2}\tilde{P}_r\Sigma^{1/2}$ for any rank- r projector \tilde{P}_r . This shows that the minimum in (15) is reached by $P_r = \Sigma^{1/2}V_rV_r^T\Sigma^{-1/2}$. Furthermore it is easy to check that $P_r^T\Sigma^{-1} + \Sigma^{-1}P_r = 2P_r^T\Sigma^{-1}P_r$ holds so that, as we saw in the proof of Proposition 2.3, P_r is Σ^{-1} -orthogonal.

It remains to show that P_r can be written as in (16). Notice that $A^TA = \Sigma^{1/2}H\Sigma^{1/2} = VD^2V^T$ holds and yields $H\Sigma^{1/2}V = \Sigma^{-1/2}VD^2$. Denoting by v_i the i -th column of $\Sigma^{1/2}V$ (which is such that $\|v\|_{\Sigma^{-1}}^2 = 1$), the latter relation yields $Hv_i = a_i^2\Sigma^{-1}v_i$. This means that v_i

is the i -th generalized eigenvector of the matrix pair (H, Σ^{-1}) and the associated eigenvalue is $\lambda_i = a_i^2$. Therefore P_r satisfies $P_r = \Sigma^{1/2} V_r V_r^T \Sigma^{-1/2} = (\sum_{i=1}^r v_i v_i^T) \Sigma^{-1}$ as in (16) and $\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r)) = \|A - A_r\|_F^2 = \|U(D - D_r)V^T\|_F^2 = \lambda_{r+1} + \dots + \lambda_d$ as in (15). ■

Thanks to Propositions 2.5 and 2.6 we have that, for a sufficiently regular function $f \in \mathcal{H}$, the error $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$ can be controlled by means of the generalized eigenvalues $\lambda_1, \dots, \lambda_d$ of the matrix pair (H, Σ^{-1}) as follows

$$\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}} \leq \left(\sum_{i=r+1}^d \lambda_i \right)^{1/2},$$

where P_r is the projector defined as in (16) and $H = \int (\nabla f)^* (\nabla f) d\mu$. The matrix pair (H, Σ^{-1}) provides a test to reveal the low intrinsic dimension of the function f . Indeed, a fast decay in the spectrum of (H, Σ^{-1}) ensures that $\sum_{i=r+1}^d \lambda_i$ goes quickly to zero with r . In that case, given $\varepsilon > 0$, there exists $r(\varepsilon) \ll d$ and a projector P_r with rank $r(\varepsilon)$ such that $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}} \leq \varepsilon$. Notice, however, that a fast decay in the spectrum of (H, Σ^{-1}) is only a *sufficient* condition for the low intrinsic dimension: the absence of decay in the (λ_i) does not mean that f cannot be well approximated by $\mathbb{E}_\mu(f|\sigma(P_r))$ for some low-rank projector P_r .

3. Contrast with the truncated Karhunen-Loève decomposition. A simple yet powerful dimension reduction method is the truncated Karhunen-Loève (K-L) decomposition. In the finite-dimensional setting, it consists in reducing the parameter space to the subspace spanned by the leading eigenvectors of the covariance matrix of $\mu = \mathcal{N}(m, \Sigma)$. This approach is based on the observation that

$$(17) \quad \min_{\substack{P_r \in \mathbb{R}^{d \times d} \\ \text{rank-}r \text{ projector}}} \mathbb{E}(\|(X - m) - P_r(X - m)\|_2^2) = \sum_{i=r+1}^d \sigma_i^2,$$

where $X \sim \mu$ and where σ_i^2 is the i -th eigenvalue of Σ . If the left-hand side of (17) is small, then the random variable X can be well approximated (in the L^2 sense) by $m + P_r(X - m) = P_r X + (I_d - P_r)m$, where P_r is a solution² to (17). In that case, given a function $f \in \mathcal{H}$, we can hope that $f(P_r X + (I_d - P_r)m)$ is a good approximation of $f(X)$. In order to make a quantitative statement, we assume f is Lipschitz continuous, meaning that there exists a constant $L \geq 0$ such that

$$(18) \quad \|f(x) - f(y)\|_V \leq L \|x - y\|_2,$$

for all $x, y \in \mathbb{R}^d$. Letting $g : x \mapsto f(P_r x + (I_d - P_r)m)$, we can write

$$(19) \quad \begin{aligned} \|f - g \circ P_r\|_{\mathcal{H}} &= \mathbb{E}(\|f(X) - f(P_r X + (I_d - P_r)m)\|_V^2)^{1/2} \\ &\stackrel{(18)}{\leq} L \mathbb{E}(\|X - (P_r X + (I_d - P_r)m)\|_2^2)^{1/2} \stackrel{(17)}{=} L \left(\sum_{i=r+1}^d \sigma_i^2 \right)^{1/2}. \end{aligned}$$

²Consider the eigendecomposition of $\Sigma = \sum_{i=1}^d \sigma_i^2 u_i u_i^T$. Then the projector $P_r = \sum_{i=1}^r u_i u_i^T$ is a solution to (17).

This result shows that if the eigenvalues of Σ decay rapidly, then there exist a function g and a projector P_r such that $\|f - g \circ P_r\|_{\mathcal{H}} \leq \varepsilon$, where $\text{rank}(P_r) = r(\varepsilon) \ll d$. In other words, the low intrinsic dimension of a Lipschitz continuous function can be revealed by the spectrum of Σ . Approximations that exploit this type of low-dimensional structure have been used extensively in forward and inverse uncertainty quantification; see, e.g., [23].

Notice that the function $g : x \mapsto f(P_r x + (I_d - P_r)m)$ considered here does not satisfy $g \circ P_r = \mathbb{E}_\mu(f|\sigma(P_r))$ in general, and therefore is not the optimal choice of profile; see Section 2.1.

Proposition 3.1. *Let $f \in \mathcal{H} = L^2(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \mu; V)$ be a continuously differentiable function and let P_r be a minimizer of $P_r \mapsto \text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))$, where $H = \int (\nabla f)^* \nabla f d\mu$ and where Σ is the covariance matrix of $\mu = \mathcal{N}(m, \Sigma)$. If f is Lipschitz continuous such that (18) holds for some $L \geq 0$, we have*

$$\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}} \leq \left(\sum_{i=r+1}^d \lambda_i \right)^{1/2} \leq L \left(\sum_{i=r+1}^d \sigma_i^2 \right)^{1/2},$$

where σ_i^2 and λ_i are the i -th eigenvalues of Σ and of the matrix pair (H, Σ^{-1}) respectively.

Proof. The *trace duality* property allows writing $\text{trace}(AB) \leq \|A\| \text{trace}(B)$ for any symmetric positive-semidefinite matrices $A, B \in \mathbb{R}^{d \times d}$, where $\|A\| = \sup\{|x^T A x|, x \in \mathbb{R}^d \text{ s.t. } \|x\|_2 = 1\}$ denotes the spectral norm of A . With the choice $A = H$ and $B = (I_d - Q_r)\Sigma(I_d - Q_r)^T$ we can write

$$\begin{aligned} \text{trace}(\Sigma(I_d - Q_r)^T H(I_d - Q_r)) &= \text{trace}(H(I_d - Q_r)\Sigma(I_d - Q_r)^T) \\ &\leq \|H\| \text{trace}((I_d - Q_r)\Sigma(I_d - Q_r)^T) \\ &= \|H\| \mathbb{E}(\|(X - m) - Q_r(X - m)\|_2^2), \end{aligned}$$

for any projector Q_r . Let Q_r be a solution to (17) and P_r be a minimizer of $P_r \mapsto \text{trace}(\Sigma(I_d - P_r)^T H(I_d - P_r))$. By Propositions 2.5 and 2.6 we can write

$$\begin{aligned} \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 &\leq \sum_{i=r+1}^d \lambda_i = \text{trace}(\Sigma(I_d - P_r)^T H(I_d - P_r)) \\ &\leq \text{trace}(\Sigma(I_d - Q_r)^T H(I_d - Q_r)) \\ &\leq \|H\| \mathbb{E}(\|(X - m) - Q_r(X - m)\|_2^2) = \|H\| \sum_{i=r+1}^d \sigma_i^2. \end{aligned}$$

To conclude the proof, it remains to show that $\|H\| \leq L^2$. Since f is Lipschitz we can write

$$\begin{aligned} \|\nabla f(x)(ty)\|_V &= \|f(x + ty) - f(x) + o(\|ty\|_2)\|_V \\ &\leq \|f(x + ty) - f(x)\|_V + o(\|ty\|_2) \leq tL\|y\|_2 + o(t\|y\|_2), \end{aligned}$$

for any $x, y \in \mathbb{R}^d$ and $t > 0$. Dividing by t and letting $t \rightarrow 0$ we obtain $\|\nabla f(x)y\|_V \leq L\|y\|_2$. Thus we have

$$\|H\| = \sup_{y \in \mathbb{R}^d, \|y\|_2=1} |y^T H y| = \sup_{y \in \mathbb{R}^d, \|y\|_2=1} \int_{\mathbb{R}^d} \|\nabla f(x)y\|_V^2 \mu(dx) \leq \sup_{y \in \mathbb{R}^d, \|y\|_2=1} L^2 \|y\|_2^2 = L^2,$$

which concludes the proof. ■

Similar to the methodology proposed in this paper, the truncated K-L decomposition can be interpreted as a method that minimizes an upper bound of an approximation error; see equation (19). Proposition 3.1 shows that the minimum of the upper bound of the new method is always smaller or equal to that of the truncated K-L. Of course comparing upper bounds does not allow one to make any clear statement about which method performs better than the other. However, note that for the truncated K-L decomposition, the construction of the projector relies only on the covariance matrix Σ , whereas the proposed method also takes into account the function f (through the matrix H) in the construction of P_r . Thus we can expect the new approach to provide projectors that are better for the approximation of f .

4. Illustrations.

4.1. Analytical examples. We give here three analytical examples for which we can compute a closed-form expression for the error $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$. This allows us to find the projector that minimizes the true error. We then compare this projector with the one that minimizes the upper bound of $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$.

4.1.1. Linear functions. Assume $f \in \mathcal{H}$ is a linear function and let $P_r \in \mathbb{R}^{d \times d}$ be a Σ^{-1} -orthogonal projector. By Proposition 2.3 and by linearity of f we have

$$\mathbb{E}_\mu(f|\sigma(P_r))(x) = \mathbb{E}(f(P_r x + (I_d - P_r)Y)) = f(P_r x) + f((I_d - P_r)m),$$

for any $x \in \mathbb{R}^d$, where we recall that $m \in \mathbb{R}^d$ is the mean of $Y \sim \mu = \mathcal{N}(m, \Sigma)$. We can write

$$\begin{aligned} \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 &= \int_{\mathbb{R}^d} \|f(x) - f(P_r x) - f((I_d - P_r)m)\|_V^2 \mu(dx) \\ &= \int_{\mathbb{R}^d} \|f((I_d - P_r)(x - m))\|_V^2 \mu(dx) \\ &= \int_{\mathbb{R}^d} (x - m)^T (I_d - P_r)^T f^* f (I_d - P_r) (x - m) \mu(dx) \\ &= \text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r)), \end{aligned}$$

where, for the last equality, we used the relations $\Sigma = \int_{\mathbb{R}^d} (x - m)(x - m)^T \mu(dx)$ and $H = \int (\nabla f)^*(\nabla f) d\mu = f^* f$, which holds true since f is linear. Thus we have that equality is attained in (10) for any linear functions $f \in \mathcal{H}$ and for any Σ^{-1} -orthogonal projector P_r . Therefore minimizing the upper bound is the same as minimizing the true error $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$.

4.1.2. Quadratic forms. Assume $\mu = \mathcal{N}(0, I_d)$ is the standard normal distribution and let $f \in \mathcal{H}$ be a quadratic form defined by $f : x \mapsto \frac{1}{2}x^T A x$ for some symmetric matrix $A \in \mathbb{R}^{d \times d}$. It is a real-valued function so that $V = \mathbb{R}$ and $\|\cdot\|_V = |\cdot|$, the absolute value. Let P_r be an orthogonal projector with rank r so that $P_r^T = P_r$. One can easily check that the relation

$$f(P_r x + (I_d - P_r)Y) = f(P_r x) + Y^T (I_d - P_r) A P_r x + f((I_d - P_r)Y),$$

holds for all $x \in \mathbb{R}^d$ where $Y \sim \mu$. By taking the expectation with respect to Y , Proposition 2.3 allows writing

$$\mathbb{E}_\mu(f|\sigma(P_r))(x) = f(P_r x) + \mathbb{E}(f((I_d - P_r)Y)).$$

The function $f - \mathbb{E}_\mu(f|\sigma(P_r))$ is quadratic and can be written as $x \mapsto x^T \Lambda x + c$ where $\Lambda = \frac{1}{2}(A - P_r A P_r)$ and $c = -\mathbb{E}(Y^T \Lambda Y)$. We have

$$\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 = \mathbb{E}((Y^T \Lambda Y + c)^2) = \text{Var}(Y^T \Lambda Y).$$

Consider the eigendecomposition of $\Lambda = U \text{diag}(a_1, \dots, a_d) U^T$ and let $Z = U^T Y \sim \mathcal{N}(0, I_d)$. We have $Y^T \Lambda Y = \sum_{i=1}^d a_i Z_i^2$ so that

$$\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 = \sum_{i=1}^d a_i^2 \text{Var}(Z_i^2) = 2 \sum_{i=1}^d a_i^2 = 2 \text{trace}(\Lambda^2) = \frac{1}{2} \|A - P_r A P_r\|_F^2,$$

where $\|\cdot\|_F = \sqrt{\text{trace}(\cdot)^T(\cdot)}$ denotes the Frobenius norm. One can show that the rank- r projector which minimizes $P_r \mapsto \|A - P_r A P_r\|_F$ is the projector onto the leading eigenspace of A^2 . Denoting by α_i^2 the i -th largest eigenvalue of A^2 , we have

$$(20) \quad \min_{\substack{P_r \in \mathbb{R}^{d \times d} \\ \text{rank-}r \text{ orth. projector}}} \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}} = \frac{1}{\sqrt{2}} \left(\sum_{i=r+1}^d \alpha_i^2 \right)^{1/2}.$$

Now we consider the projector that minimizes the upper bound given by Proposition 2.5. We can write $\nabla f(x) = Ax$ so that $H = \int (\nabla f)(\nabla f)^T d\mu = A^2$. Therefore equation (10) yields

$$\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 \leq \text{trace}((I_r - P_r)A^2(I_r - P_r)) = \|A - P_r A\|_F^2,$$

for any orthogonal projector P_r with rank r . By Proposition 2.6, the rank- r orthogonal projector which minimizes the right-hand side in the above inequality is the projector onto the leading eigenspace of A^2 , which is the same as the solution to (20). In other words the minimizer of the upper bound of the error is, for the considered example, the same as the minimizer of the error itself. In addition, the upper bound evaluated at the optimal projector allows controlling the error $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$ by $(\sum_{i>r}^d \alpha_i^2)^{1/2}$ which is, up to a factor of $\sqrt{2}$, the same as the true error.

Remark 4.1. Notice that the same analysis can be carried out for centered normal distributions $\mu = \mathcal{N}(0, \Sigma)$ with any non-singular covariance Σ . To do so, it is sufficient to replace A by $\Sigma^{1/2} A \Sigma^{1/2}$ and to consider Σ^{-1} -orthogonal projectors P_r in the previous analysis.

4.1.3. Sum of sines. Let $\mu = \mathcal{N}(0, I_d)$ be a standard normal distribution. Consider the real-valued function $f \in \mathcal{H}$ such that

$$f : x \mapsto \sum_{i=1}^d a_i \sin(\omega_i x_i),$$

for any $x \in \mathbb{R}^d$, where $a \in \mathbb{R}^d$ and $\omega \in \mathbb{R}^d$ are two vectors. Let P_r be an orthogonal projector. For simplicity, we restrict our analysis to the case where P_r is a projector onto the span of r vectors from the canonical basis $\{e_1, \dots, e_d\}$ of \mathbb{R}^d , meaning

$$(21) \quad P_r = \sum_{i \in \Lambda_r} e_i e_i^T, \quad \text{where } \begin{cases} \Lambda_r \subset \{1, \dots, d\} \\ \#\Lambda_r = r \end{cases}$$

It is readily seen that $\mathbb{E}_\mu(f|\sigma(P_r))$ is the function $x \mapsto \sum_{i \in \Lambda_r} a_i \sin(\omega_i x_i)$. We can show that

$$\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 = \mathbb{E} \left(\left(\sum_{i \in \Lambda_r^c} a_i \sin(\omega_i X_i) \right)^2 \right) = \frac{1}{2} \sum_{i \in \Lambda_r^c} a_i^2 (1 - \exp(-2\omega_i^2)),$$

where Λ_r^c is the complementary set of Λ_r in $\{1, \dots, d\}$ and $X \sim \mu$. Therefore, the projector P_r of the form of (21) which minimizes the error $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$ is the one associated with the set Λ_r containing the indices of the r largest values of $a_i^2(1 - \exp(-2\omega_i^2))$.

Now we find the projector of the form (21) that minimizes the upper bound of the error given by Proposition 2.5. Recall that $H = \int (\nabla f)(\nabla f)^T d\mu$, so we can write

$$\begin{aligned} \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 &\stackrel{(10)}{\leq} \text{trace}((I_d - P_r)^T H (I_d - P_r)) \\ &\stackrel{(21)}{=} \sum_{i \in \Lambda_r^c} e_i^T H e_i = \sum_{i \in \Lambda_r^c} \int \left(\frac{\partial f}{\partial x_i} \right)^2 d\mu \\ &= \sum_{i \in \Lambda_r^c} \mathbb{E}((a_i \omega_i \cos(\omega_i X_i))^2) \\ &= \frac{1}{2} \sum_{i \in \Lambda_r^c} a_i^2 \omega_i^2 (1 + \exp(-2\omega_i^2)). \end{aligned}$$

The projector (21) which minimizes the above upper bound is the one associated with the set Λ_r containing the indices of the r largest values of $a_i^2 \omega_i^2 (1 + \exp(-2\omega_i^2))$.

Let us consider the case where $\omega_i = \omega$ for all $i \leq d$. The index sets corresponding to the largest $a_i^2 \omega^2 (1 + \exp(-2\omega^2))$ and $a_i^2 (1 - \exp(-2\omega^2))$ are the same, and therefore the projector that minimizes the upper bound is the same as the minimizer of the true error. Notice, however, that when $\omega \rightarrow \infty$ the true error tends to $\frac{1}{2} \sum_{i \in \Lambda_r^c} a_i^2$, whereas the upper bound tends to infinity. This shows that the upper bound is a poor estimator for the error, even if its minimization allows recovering the optimal projector.

Suppose now that $\omega_i = a_i^{-2} \geq 1$ for all $i \leq d$. Then the index set corresponding to the largest $a_i^2 \omega_i^2 (1 + \exp(-2\omega_i^2)) = \omega_i (1 + \exp(-2\omega_i^2)) =: h_1(\omega_i)$ is the same as the index set of the smallest $a_i^2 (1 - \exp(-2\omega_i^2)) = \omega_i^{-1} (1 - \exp(-2\omega_i^2)) =: h_2(\omega_i)$. Indeed h_1 is increasing on $(1, \infty)$ whereas h_2 is decreasing. Hence, for this particular example, minimizing the upper bound yields the worst possible projector, i.e., the one that maximizes the true error.

4.2. Elliptic PDE. Consider the diffusion equation on the square-shaped domain $\Omega = [0, 1]^2$, which consists in finding $u \in H^1(\Omega)$ such that

$$(22) \quad \begin{cases} \nabla_s(\kappa \nabla_s u) &= 0 & \text{in } \Omega, \\ u &= s_1 + s_2 & \text{on } \partial\Omega. \end{cases}$$

Here $s = (s_1, s_2) \in \Omega$ denotes the spatial coordinates and ∇_s refers to the gradient in the spatial variable s . The diffusion coefficient κ is a random field and follows a log-normal distribution such that $\log(\kappa)$ is a Gaussian process on Ω with zero mean and with a covariance function $c : \Omega \times \Omega \rightarrow \mathbb{R}$ defined by $c(s, t) = \exp(-\|s - t\|_2^2 / (0.15)^2)$ for all $s, t \in \Omega$. A numerical approximation of (22) is obtained with the finite element method (FEM); see, for example, [10]. The diffusion field κ is approximated by the piecewise constant random field

$$(23) \quad \kappa(x) : s \mapsto \exp\left(\sum_{i=1}^d x_i \mathbf{1}_i(s)\right),$$

where $\mathbf{1}_i$ denotes the indicator function associated with the i th element of the mesh represented in Figure 1a. Here $d = 3252$ corresponds to the number of elements, and $x \sim \mu = \mathcal{N}(0, \Sigma)$ with

$$\Sigma_{i,j} = c(s_i, s_j), \quad 1 \leq i, j \leq d,$$

and s_i being the center of the i th element. With a slight abuse of notation, we denote by $u(x)$ the Galerkin projection of the solution to (22) onto the space of continuous piecewise affine functions associated with the mesh in Figure 1a. We consider the following scenarios, where the function $f : \mathbb{R}^d \rightarrow V$ is defined by three different post-solution treatments of $u(x)$:

1. $f : x \mapsto u(x)$, which means that f is the solution map from the parameter x to the FEM solution to (22). In that case V is the FEM approximation space with dimension $\dim(V) = 1691$, the number of nodes in the mesh. Since $V \subset H^1(\Omega)$, the natural choice for the norm $\|\cdot\|_V$ is

$$\|v\|_V^2 = \int_{\Omega} (v(s))^2 ds + \int_{\Omega} \|\nabla_s v(s)\|_2^2 ds.$$

2. $f : x \mapsto u|_{\Omega_s}(x)$, where $\Omega_s = [0.35, 0.65]^2 \subset \Omega$. In other words, $f(x)$ corresponds to the restriction of $u(x)$ to a subdomain Ω_s of Ω . For this scenario, $V \subset H^1(\Omega_s)$ is of dimension 168 (the number of nodes in the mesh) and is endowed with the norm $\|\cdot\|_V$ given by

$$\|v\|_V^2 = \int_{\Omega_s} (v(s))^2 ds + \int_{\Omega_s} \|\nabla_s v(s)\|_2^2 ds.$$

3. $f : x \mapsto (u|_{s_a}(x), u|_{s_b}(x))$, where $s_a = (0.2, 0.8) \in \Omega$ and $s_b = (0.8, 0.2) \in \Omega$. In this scenario, we are interested in the evaluation of the solution $u(x)$ at two different spatial locations s_a and s_b . There are two scalar-valued outputs so that $V = \mathbb{R}^2$ is an algebraic space. Consider the weighted norm $\|\cdot\|_V$ defined by

$$\|v\|_V^2 = \alpha v_1^2 + \beta v_2^2,$$

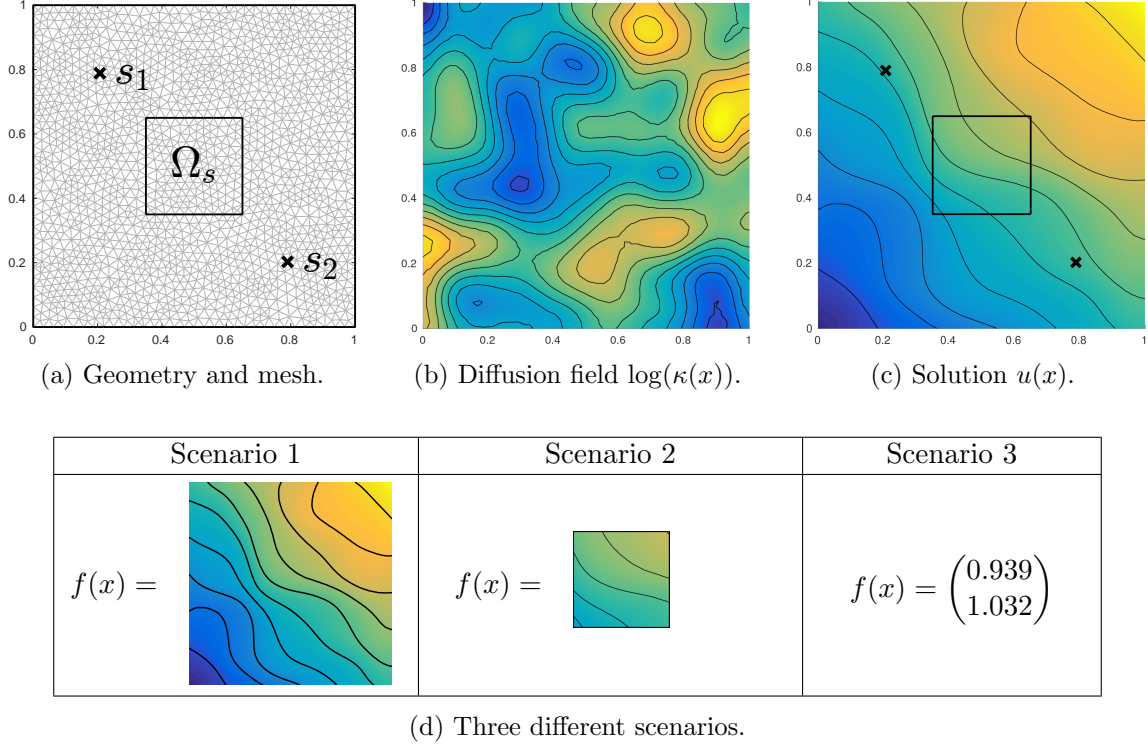


Figure 1: Illustration of the Elliptic PDE problem: geometry and mesh (Figure 1a), representation of the diffusion field associated with a parameter $x \in \mathbb{R}^d$ drawn randomly from μ (Figure 1b), corresponding solution (Figure 1c) and representation of $f(x)$ for the three different scenarios given this particular x (Figure 1d).

where $\alpha, \beta > 0$ are two positive weights to be specified. For example the choice $\alpha = 2\beta$ will put twice the weight on the error associated with the first output compared to the second. This is a way to model the fact that, for the final purpose of the simulation, one output is more important than the other.

4.2.1. Computational aspects. We consider the problem of computing the matrix $H = \int (\nabla f)^* (\nabla f) d\mu$. Since $H = \mathbb{E}((\nabla f(X))^* (\nabla f(X)))$, with $X \sim \mu$, H can be approximated by the K -sample Monte-Carlo estimate

$$(24) \quad \hat{H} = \frac{1}{K} \sum_{i=1}^K (\nabla f(X_i))^* (\nabla f(X_i)),$$

where X_1, \dots, X_K are independent copies of X . To numerically compute a realization of \hat{H} , one needs to evaluate the Jacobian of the function f K times. To do so, we employ the *adjoint method*; see for example [28]. Then, to construct the projector, instead of minimizing

$\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))$ we consider a projector \hat{P}_r such that

$$(25) \quad \hat{P}_r \in \arg \min_{\substack{P_r \in \mathbb{R}^{d \times d} \\ \text{rank-}r \text{ projector}}} \text{trace}(\Sigma(I_d - P_r^T)\hat{H}(I_d - P_r)).$$

By construction, \hat{P}_r depends upon \hat{H} , and thus it is random. Recall that such a projector can be obtained by computing the generalized eigendecomposition of the matrix pair (\hat{H}, Σ^{-1}) ; see Proposition 2.6.

To approximate the conditional expectation $\mathbb{E}_\mu(f|\sigma(\hat{P}_r))$, we consider the random function

$$(26) \quad \hat{F}_r : x \mapsto \frac{1}{M} \sum_{i=1}^M f(\hat{P}_r x + (I_d - \hat{P}_r)Y_i),$$

where Y_1, \dots, Y_M are independent copies of $Y \sim \mu$. Given a realization of the projector \hat{P}_r , a realization of \hat{F}_r can be obtained by drawing M samples of Y and by using those samples to evaluate \hat{F}_r using (26). Notice that the samples are *not* redrawn for each new evaluation point x of \hat{F}_r . By Proposition 2.3 and for any $x \in \mathbb{R}^d$, $\hat{F}_r(x)$ can be interpreted as an M -sample Monte Carlo approximation of $\mathbb{E}_\mu(f|\sigma(\hat{P}_r))(x)$. Finally, notice that if $M = 1$ and $Y_1 = 0$ (i.e., the mean of Y), then our approximation of f reduces to the form used in Section 3 when truncating a K-L decomposition, albeit for a different projector; see relation (19) with $m = 0$ and $P_r = \hat{P}_r$.

4.2.2. Modes and influence of the norm $\|\cdot\|_V$. For each scenario, an approximation \hat{H} of H is computed with a large number of samples, $K = 10^4$. This approximation is considered sufficiently accurate and will be used in place of H unless specified otherwise. Figure 2 illustrates the leading generalized eigenvectors of the matrix pair (H, Σ^{-1}) as well as the leading eigenvectors of Σ , meaning the K-L modes; see Section 3. Since they do not depend upon f , the K-L modes do not have any particular relation to the elliptic PDE solution other than some symmetry properties related to the shape of the domain Ω . In contrast, the modes associated with the three scenarios present specific features which depend on the function f . For example with scenario 2, we observe that the modes in the parameter space somehow represent more information *local* to the region of interest Ω_s .

The choice of the norm $\|\cdot\|_V$ also impacts the generalized eigenvectors of (H, Σ^{-1}) through the matrix H . For instance, with scenario 3, relation (14) with $M = \text{diag}(\alpha, \beta)$ allows us to write

$$H = \alpha H_1 + \beta H_2, \quad \text{with} \quad H_i = \int (\nabla f_i)^T (\nabla f_i) dx.$$

With the choice $\alpha = \beta = 1$, the modes in Figure 2 suggest that the two points of interest s_a and s_b are considered equally important, whereas the choice $\alpha = 10$ and $\beta = 1$ leads to significantly more patterns around point s_a (on the top-left of Ω) than around point s_b .

4.2.3. Approximating the conditional expectation and comparison with K-L. Assume the matrix H is known (again, an approximation \hat{H} with $K = 10^4$ samples is used in place of H) and let P_r be the rank- r projector which minimizes $\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))$. We consider the approximation \hat{F}_r of the conditional expectation $\mathbb{E}_\mu(f|\sigma(P_r))$ given by (26) with

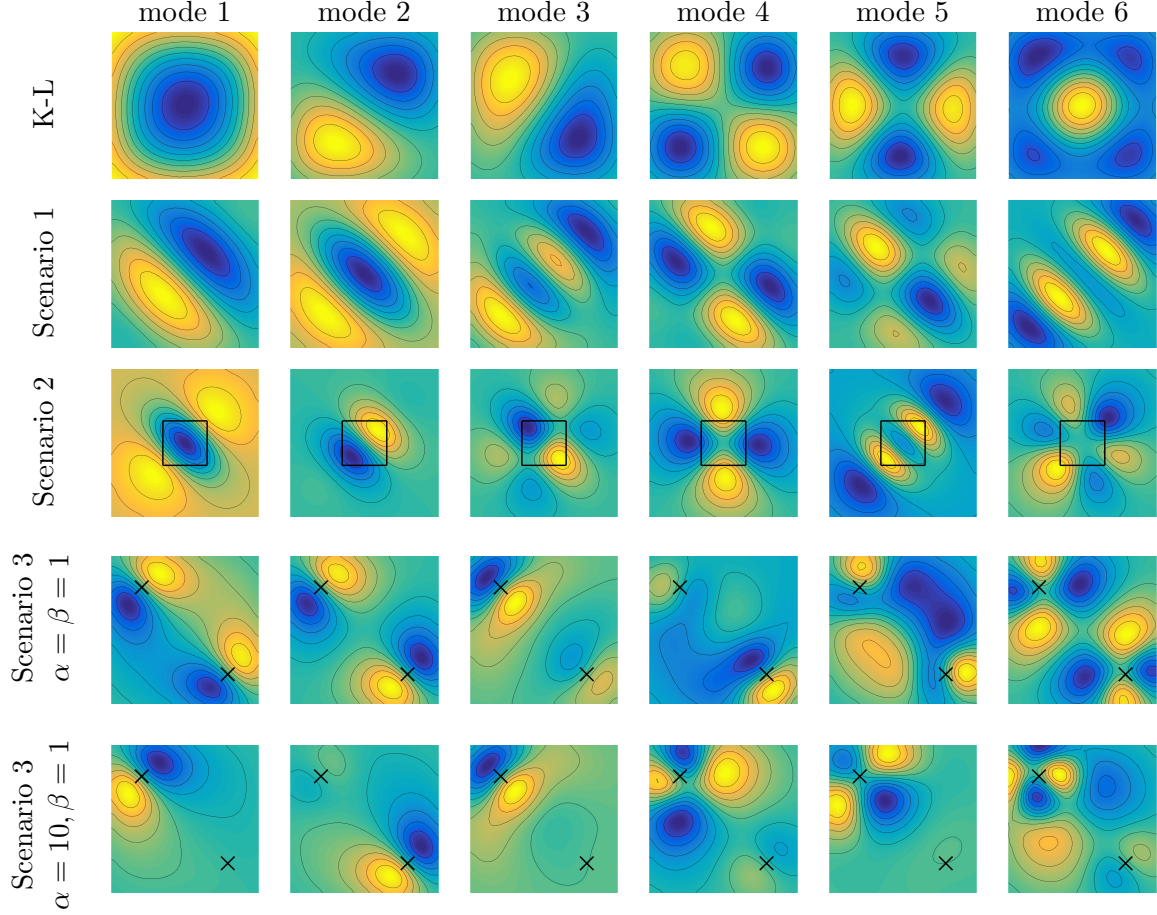


Figure 2: Parameter modes: each figure represents the function $s \mapsto \sum_{i=1}^d v_i \mathbf{1}_i(s)$ for different $v \in \mathbb{R}^d$, where $\mathbf{1}_i$ is the indicator function of the i -th element of the mesh. In the first row (K-L) v is the i -th eigenvector of Σ , which corresponds to the Karhunen-Loève modes. In the four other rows, v is the i -th generalized eigenvector of the matrix pair (H, Σ^{-1}) , for different H depending on the scenario.

$\hat{P}_r = P_r$. Figure 3 shows the error $\|f - \hat{F}_r\|_{\mathcal{H}}$ as a function of the rank r of the projector. For each scenario, one realization of \hat{F}_r is computed with either $M = 1$, $M = 5$, or $M = 20$ samples. We first note that, since we do not exactly compute the conditional expectation, the errors (dotted curves) are sometimes above the upper bound (solid red curves). In this inexact setting, $\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))^{1/2}$ is no longer a certified upper bound for the error. However we observe it can still be used as a good error indicator.

The three scenarios do not have the same convergence rate with r : the first scenario has the slowest and the third the fastest. Even though they are different post-solution treatments of the same solution map $x \mapsto u(x)$, the functions f associated with each scenario do not have the same complexity in terms of intrinsic dimension.

Interestingly, increasing M does not lead to significant improvements of the approximation. This phenomenon can be explained by the following relation,

$$\begin{aligned} \mathbb{E}(\|f - \widehat{F}_r\|_{\mathcal{H}}^2) &\stackrel{(4)}{=} \mathbb{E}(\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 + \|\widehat{F}_r - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2) \\ &\stackrel{(26)}{=} \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 + \frac{1}{M} \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2 \\ &= \left(1 + \frac{1}{M}\right) \|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2, \end{aligned}$$

where the expectation is taken over the samples Y_1, \dots, Y_M (the projector P_r being fixed here). This result shows that even with small M , one can still hope to obtain a good approximation \widehat{F}_r of f provided P_r is chosen such that $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$ is sufficiently small. In other words a crude approximation of the conditional expectation yields at most a factor of two (when $M = 1$) in the expected error squared, so that it remains of the same order of magnitude as $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}^2$; see also Theorem 3.2 from [7].

We now compare with the truncated Karhunen-Loève decomposition, for which P_r is defined as the rank- r orthogonal projector onto the leading eigenspace of the covariance matrix Σ . The black dash-dotted curves in Figure 3 represent the upper bound $\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))^{1/2}$ for this choice of P_r , as a function of r . (The true error $\|f - \mathbb{E}_\mu(f|\sigma(P_r))\|_{\mathcal{H}}$ is substantially the same as its upper bound, so we decided not to plot it.) It is interesting to see that in the first scenario, the K-L projector is essentially as effective as the projector obtained by minimizing the upper bound. As shown in Figure 4, the spectrum of H is flat, which means that H is close to a rescaled identity matrix. Then, minimizing $\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))$ is nearly the same as minimizing $\text{trace}((I_d - P_r)\Sigma(I_d - P_r^T)) = \mathbb{E}(\|X - P_r X\|_2^2)$, where $X \sim \mathcal{N}(0, \Sigma)$, and yields the same projector as the truncated K-L method; see (17). However, this reasoning does not apply to scenarios 2 and 3, where the spectrum of H decays rapidly. For these scenarios we observe in Figure 3 that the new method outperforms the truncated K-L method. For instance, in scenario 2 the new method reaches an error of 10^{-4} with only $r = 150$ whereas the truncated K-L method requires $r = 300$.

4.2.4. Quality of the projector. In this section we assess the quality of a projector \widehat{P}_r defined by (25), where \widehat{H} is the K -sample Monte Carlo approximation of H given by (24). In the present context, an *optimal* projector would be a minimizer of $P_r \mapsto \text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))^{1/2}$ so that the only relevant criteria for the quality of \widehat{P}_r is how close $\text{trace}(\Sigma(I_d - \widehat{P}_r^T)H(I_d - \widehat{P}_r))^{1/2}$ is to the minimum of the upper bound. Figure 5 contains two sets of curves: the solid curves represent the error bound $\text{trace}(\Sigma(I_d - \widehat{P}_r^T)H(I_d - \widehat{P}_r))^{1/2}$ as a function of the rank of \widehat{P}_r , whereas the dotted curves correspond to the *approximate* error bound $\text{trace}(\Sigma(I_d - \widehat{P}_r^T)\widehat{H}(I_d - \widehat{P}_r))^{1/2}$. This approximate error bound is the quantity we would use in place of the error bound when the matrix H is not known. For each scenario we observe that for small K , the approximate error bound underestimates the true error bound. This means that $\text{trace}(\Sigma(I_d - \widehat{P}_r^T)\widehat{H}(I_d - \widehat{P}_r))^{1/2}$ can be used as an error estimator only if K is sufficient large.

Observe in Figure 5 that scenarios 1 and 2 need fewer samples to obtain a good projector (say around $K = 30$ samples) compared to the last scenario (at least $K = 400$ samples). To understand this result, let us note that if r is larger than the rank of \widehat{H} , the projector \widehat{P}_r is not

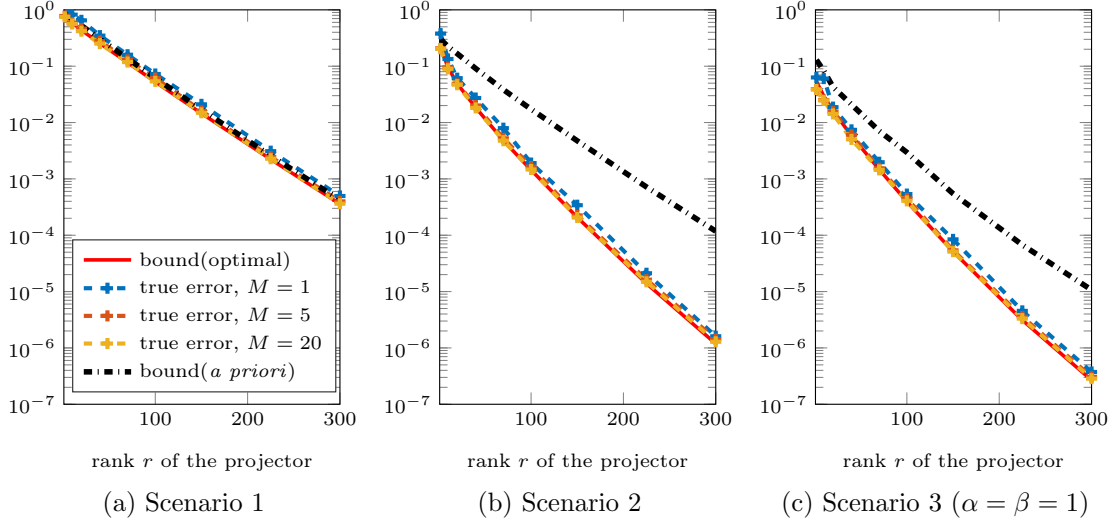


Figure 3: Error $\|f - \hat{F}_r\|_{\mathcal{H}}$ as a function of the rank of P_r . The error $\|f - \hat{F}_r\|_{\mathcal{H}} = \mathbb{E}(\|f(X) - \hat{F}_r(X)\|_V^2)^{1/2}$, $X \sim \mu$, is estimated via Monte Carlo with 300 samples for X . The red (solid) and black (dash-dot) lines represent the upper bound $\text{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))^{1/2}$ with P_r defined either as the minimizer of the upper bound (red lines) or as the projector onto the leading eigenspace of Σ (black lines).

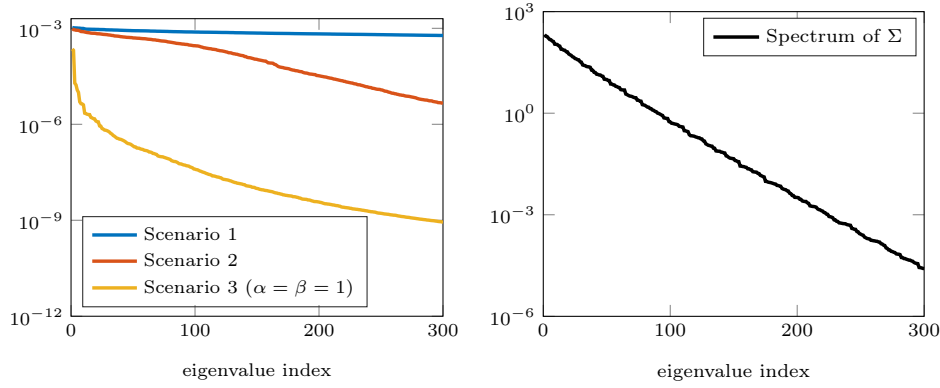


Figure 4: Spectrum of H for the three scenarios (left) and spectrum of Σ (right).

uniquely determined: any \hat{P}_r such that $\text{Im}(\hat{H}) \subset \text{Im}(\hat{P}_r)$ is a solution to (25). Therefore the rank of \hat{P}_r should not exceed that of \hat{H} which, thanks to (24), satisfies the following relation

$$\text{rank}(\hat{H}) \leq K \text{rank}\left((\nabla f(X))^*(\nabla f(X))\right) \leq K \dim(V).$$

With scenario 3 we have $\dim(V) = 2$ so that the rank of \hat{P}_r should not exceed $2K$. This limitation is represented by the vertical lines on Figure 5c. With scenarios 1 and 2 we have

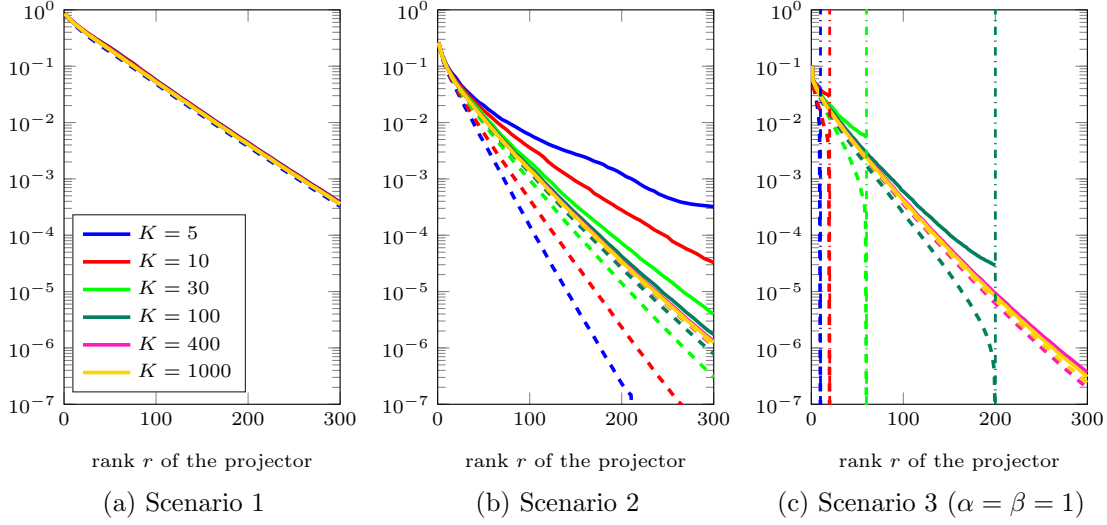


Figure 5: Error bound $\text{trace}(\Sigma(I_d - \hat{P}_r^T)H(I_d - \hat{P}_r))^{1/2}$ (solid curves) and approximate error bound $\text{trace}(\Sigma(I_d - \hat{P}_r^T)\hat{H}(I_d - \hat{P}_r))^{1/2}$ (dotted curves) as a function of the rank of \hat{P}_r . For each scenario, the curves correspond to one realization of \hat{H} and \hat{P}_r defined by (24) and (25) for different values of K . In Figure 5c, the vertical lines correspond to $r = 2K$.

$\dim(V) = 1691$ and $\dim(V) = 168$ so that this limit is not attained within the range of the plots. The conclusion is that when the dimension of V is large, one needs fewer samples from $\nabla f(X)$ to obtain a suitable projector, because each sample is a matrix with potentially a large rank.

5. Conclusions. We have addressed the problem of approximating multivariate functions taking values in a vector space. We approximate such functions by means of *ridge functions* that depend only on a few linear combinations of the input parameters. Our approach exploits structure in the original function, in the (Gaussian) measure on the domain, and in the chosen norm on the codomain. Rather than seeking an optimal approximation, we build a *controlled* approximation: we develop an upper bound on the approximation error and minimize this upper bound.

Our analytical and numerical examples demonstrate good performance of the method, and also illustrate conditions under which it might not work well. For example, we show cases where minimizing the upper bound leads to an optimal approximation, and contrasting cases where the error bound is not tight. Numerical demonstrations on an elliptic PDE also illustrate various computational issues: sampling to compute both the projector (yielding the important directions) and the conditional expectation (yielding the ridge profile). We also contrast our new approach with the K-L expansion: our approach is in general more efficient, but when the function itself provides little low-dimensional structure, we essentially revert to the dimension reduction provided by a low-rank approximation of the input covariance.

Future work may explore several natural extensions of the proposed methodology. First

is the extension to non-Gaussian input measures, e.g., uniform measure on bounded domains in \mathbb{R}^d . Second is the extension to infinite-dimensional input spaces: for example, letting the domain of f be a function space endowed with Gaussian measure or Besov measure. Finally, it may be possible to develop sharper error bounds based on higher-order derivatives, e.g., Hessians of f . For the last two points, we may be able to use recent results on higher-order Poincaré inequalities [26]. Another open issue is the existence of a best approximation, i.e., a ridge function that minimizes the L^2 error. To our knowledge, this problem has not been fully addressed.

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