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Kernel-based Reconstructions for Parametric PDEs

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Abstract In uncertainty quantification, an unknown quantity has to be reconstructed which depends typically on the solution of a partial differential equation. This partial differential equation itself may depend on parameters, some of them may be deterministic and some are random. To approximate the unknown quantity one therefore has to solve the partial differential equation (usually numerically) for several instances of the parameters and then reconstruct the quantity from these simulations. As the number of parameters may be large, this becomes a high-dimensional reconstruction problem.

We will address the topic of reconstructing such unknown quantities using kernel-based reconstruction methods on sparse grids. First, we will introduce into the topic, then explain the reconstruction process and finally provide new error estimates.

1 Introduction

In modern applied sciences dynamic processes are often modeled by partial differential equations, whereby coefficient functions, representing certain material parameters, and forcing terms serve as input. Often, these are obtained by certain measurements or experiments and therefore are prone to being either inaccurate or incomplete and
consequently introduce an uncertainty to the model. For a general overview on the topic, see, for example, the recent books [8, 9, 10, 11].

To illustrate the general approach to such problems including randomness, we follow [5, 2, 1] and hence restrict ourselves to a Dirichlet-Poisson problem where the parametric diffusion coefficient is given by a function \( a : R_{N_p} \times D \to \mathbb{R} \). The set \( R_{N_p} \subset \mathbb{R}^{N_p} \) serves as a finite dimensional parameter space and is, for the sake of simplicity, the hyper-cube \( R_{N_p} := \bigtimes_{j=1}^{N_p} (-r_j, r_j) \subset (-1, 1)^{N_p} \). The number \( N_p \) determines the dimension of the parameter space and will be large but finite, i.e. \( 1 \ll N_p < \infty \), which is known in the literature as finite noise assumption.

The parametric partial differential equation is now given on a sufficiently regular domain \( D \subset \mathbb{R}^d \) and for \( G \in L^2(D) \) by

\[
-\nabla \cdot (a(y, x)\nabla u(y, x)) = G(x) \quad \text{in } R_{N_p} \times D, \\
u(y, x) = 0 \quad \text{in } R_{N_p} \times \partial D,
\]

giving rise to a solution \( u : R_{N_p} \times \overline{D} \to \mathbb{R} \). Obviously, the spatial derivatives are only taken with respect to the spatial variable \( x \).

Depending on the practical application, we are not interested in the solution \( u \) directly but rather in a derived quantity of interest, which will be modeled by a linear functional \( q \) acting on the solution space, i.e.

\[
Q(y) := q(\{u(y, \cdot)\}) \in \mathbb{R}, \quad y \in R_{N_p}.
\]

Hence, \( Q : R_{N_p} \to \mathbb{R} \) is a function operating only on the parameter space. The main task is now to reconstruct the map \( Q \) from sampled data \( \{Q(y_k)\} \) at specific parameter values \( y_k \in \mathcal{Y}_{N_S} := \{y_1, \ldots, y_{N_S}\} \subset R_{N_p}, \quad 1 \leq k \leq N_S \), where from now on we denote the number of sampling points by \( N_S \in \mathbb{N} \). To avoid any confusion, we note here that \( N_p \) and \( N_S \) are uncorrelated.

By inserting the sampling points \( y_k \in \mathcal{Y}_{N_S} \) into (1), solving the now deterministic Poisson-Dirichlet problem and applying the functional \( q \), we obtain the values \( \{Q(y_k)\} \). Except for only very few cases, these steps cannot be done analytically but only numerically. Hence, we introduce a finite dimensional finite element space \( \mathcal{V}_h \subset \mathcal{V} = H^1_0(D) \), over which we solve

\[
-\nabla \cdot (a(y_k, x)\nabla u_h(y_k, x)) = G(x) \quad \text{in } D, \\
u_h(y_k, x) = 0 \quad \text{on } \partial D,
\]

weakly, yielding an approximation \( u_h(y_k, \cdot) \in \mathcal{V}_h \) to the true solution \( u(y_k, \cdot) \in \mathcal{V} \) and consequently perturbed samples

\[
Q_h(y_k) = q(\{u_h(y_k, \cdot)\}) \approx Q(y_k) = q(\{u(y_k, \cdot)\}).
\]

Note, that we assume that we can compute \( q \) analytically. This assumption is made for simplicity and has no impact on the error estimates in Section 5.

Choosing a standard finite element method (FEM) for solving (3) weakly, yields well-known error estimates (see for example Brenner & Scott [3]) for the quantities
As mentioned above, we have to choose a discrete sampling set \( \mathcal{Y}_{NS} \) in the high-dimensional space \( \mathbb{R}^{NP} \). This set should on the one hand be dense enough to represent \( \mathbb{R}^{NP} \) well and to allow a good reproduction of \( Q \), but on the other hand, since we need to solve a partial differential equation for each element of \( \mathcal{Y}_{NS} \), has to be sparse enough for our method to be applicable. Hence, a natural choice for our set \( \mathcal{Y}_{NS} \) is a sparse grid \( \mathcal{Y}_{NS} := H(\ell, NP) \) of level \( \ell \) in \( NP \) dimensions.

The final task is then to reconstruct the high-dimensional function \( Q \) from the data \( \{(y_k, Q(y_k))\} \) which carry an intrinsic error. Thus, we do not want to use an interpolatory approach but rather a process from standard spline theory, called smoothing splines or penalised least-squares, see for example [12] and the references therein. The basic structure is a variational problem of the form

\[
\tilde{Q}_\lambda = \arg\min_{s \in \mathcal{H}_K} \sum_{k=1}^{NS} |Q_h(y_k) - s(y_k)|^2 + \lambda \|s\|^2_{\mathcal{H}_K},
\]

where \( \mathcal{H}_K \) denotes a reproducing kernel Hilbert space (RKHS) of real-valued functions with kernel \( K \) and where \( \lambda > 0 \) denotes a penalising parameter.

With this set-up we are able to base our error analysis on a new sampling inequality developed by Wendland and Rieger [6]. The main contribution of this paper, after choosing a specific RKHS \( \mathcal{H}_{K_e} \), is the error estimate

\[
\|Q - \tilde{Q}_\lambda\|_{L^\infty(\mathbb{R}^{NP})} \leq C \left( f_{NP,k}(NS) + \sqrt{\lambda} g_{NP}(NS) \right) \|Q\|_{\mathcal{H}_{K_e}} \\
+ C \left( \frac{1}{\lambda} f_{NP,k}(NS) + g_{NP}(NS) \right) NS h^t \max_{1 \leq k \leq NS} |u(y_k, \cdot)|_{H^{t+1}(\mathcal{D})}
\]

where \( C > 0 \) is a constant, \( \tilde{Q}_\lambda \) is given in (6), \( Q \in \mathcal{H}_{K_e} \) is the function from (2) defined by applying the functional \( q \) to the exact solution \( u \) of (1), \( h \) is the discretisation parameter of the finite element mesh, \( t \geq 1 \) and \( f_{NP,k} \) and \( g_{NP} \) are known functions which have known asymptotic behaviour for \( NS \to \infty \). Furthermore, we derive conditions for \( \lambda \) and \( h \) such that

\[
\|Q - \tilde{Q}_\lambda\|_{L^\infty(\mathbb{R}^{NP})} \to 0, \quad NS \to \infty,
\]

with the order of \( f_{NP,k} \) and by further sharpening the estimate we even get nearly spectral convergence of the error.

As mentioned above, the setup described above closely follows in particular Griebel and Rieger [5]. However, there are two significant differences to their approach. On the one hand, we use a sparse grid as the sampling set \( \mathcal{Y}_{NS} \subset \mathbb{R}^{NP} \), instead of a quasi-uniform data set as it is done in [5]. In the given, particular setting this is of significance as we deal with a high-dimensional problem and choosing a sparse grid helps to reduce the effect of the curse of dimensionality. On the other hand, we use a penalised least-squares approach for reconstructing the function \( Q \) instead of
a support vector machine with Vapnik’s loss function, as it has been done in [5]. However, the analysis carried out here for the penalised least-squares problem can easily be replaced by a similar analysis for a support vector machine.

This paper is organised as follows. In Section 2 we will review the existence, uniqueness and regularity of the solution of parametric partial differential equations of type (1). In Section 3 we will briefly review the theory of reproducing kernel Hilbert spaces (RKHSs), introduce the kernel and associated Hilbert space which we will use throughout this paper and discuss the advantages of the penalised least-squares reconstruction process. A justification for choosing sparse grids as our sampling space will be given in Section 4. Finally, in Section 5, we will state our main result, the above mentioned error estimate on the reconstruction process, which will be based upon a recently introduced sampling inequality for sparse grids.

We will use the following notation. We denote multi-indices by small, bold Greek letters, e.g. \( \nu \in \mathbb{N}_0^d \), and set \( \nu! = \prod_{j=1}^d \nu_j! \) and \( \nu^\alpha = \prod_{j=1}^d \nu_j^{\alpha_j} \) for \( \alpha \in \mathbb{N}_0^d \). Furthermore, we use the notation \( \| \nu \|_1 = \nu_1 + \cdots + \nu_d \) for \( \nu \in \mathbb{N}_0^d \).

Additionally, we will use two kinds of Sobolev spaces over domains \( \Omega \subseteq \mathbb{R}^d \) of the form \( \Omega = \Omega_1 \times \cdots \times \Omega_d \) with \( \Omega_j = (-1, 1) \) or \( \Omega_j = (-r_j, r_j) \subset (-1, 1) \). On the one hand we will employ the classical Sobolev space

\[
W^{k, 2}_1(\Omega) := \left\{ f \in L^2(\Omega) : D^\alpha f \in L^2(\Omega), \| \alpha \|_1 \leq k \right\}
\]

equipped with norm

\[
\| f \|_{W^{k, 2}_1(\Omega)}^2 := \sum_{\| \alpha \|_1 \leq k} \| D^\alpha f \|_{L^2(\Omega)}^2.
\]

On the other hand, we will use the tensor product Sobolev space defined by

\[
W^{k, 2}_\infty(\Omega) := \bigotimes_{j=1}^d W^{k, 2}_1(\Omega_j)
= \left\{ f \in L^2(\Omega) : D^\alpha f \in L^2(\Omega), \| \alpha \|_\infty \leq k \right\}
\]

together with the norm

\[
\| f \|_{W^{k, 2}_\infty(\Omega)}^2 := \sum_{\| \alpha \|_\infty \leq k} \| D^\alpha f \|_{L^2(\Omega)}^2.
\]

2 Parametric Partial Differential Equations

In this section, we will give an introduction to the theory of parametric partial differential equations by looking at existence and uniqueness of the solutions of the model problem (1). To this end, we need two domains. On the one hand we require a high-dimensional parameter domain. In our case this will be the anisotropic
hyper-cube
\[ R_{N_P} := \prod_{j=1}^{N_P} (-r_j, r_j) \subset (-1, 1)^{N_P}, \]  
(7)

where \( 1 \ll N_P < \infty \).

On the other hand we need a spatial domain \( D \subset \mathbb{R}^d \), where usually \( d = 2, 3 \). We will assume \( D \) to be a bounded, convex and polygonal domain. If \( G \in L^2(D) \) then the usual elliptic regularity theory holds for the weak formulation of (1), which is, with the usual energy space \( V := H^1_0(D) \), given by
\[
\int_D a(y, x) \nabla u(y, x) \cdot \nabla v(x) \, dx = \int_D G(x)v(x) \, dx, \quad v \in V, y \in R_{N_P}.
\]  
(8)

In this paper, we assume the coefficient function \( a \) to have the form
\[
a(y, x) = a_0(x) + \sum_{k=1}^{N_P} \phi_k(x)y_k
\]  
(9)

with given \( \phi_k \in L^\infty(D) \), \( k \in \mathbb{N} \). In general, the sum in (9) will not be finite, so that the restriction to the first \( N_P \) terms introduces an additional error, which we will ignore throughout this paper.

We now follow [4] and extend the usual Lax-Milgram theory to complex valued coefficient functions \( \tilde{a} : R_{N_P} \times D \to \mathbb{C} \). To this end, we introduce the so-called uniform (complex) ellipticity assumption which requires the existence of two constants \( R \geq r > 0 \) such that
\[
0 < r \leq \mathfrak{R}(\tilde{a}(y, x)) \leq |\tilde{a}(y, x)| \leq R \quad x \in D, y \in R_{N_P}.
\]  
(10)

Here, \( \mathfrak{R}(\cdot) \) denotes the real part of a complex number. By rearranging, we see that (10) is satisfied for the function \( a \) from (9) if the bounds
\[
\sum_{k=1}^{N_P} |\phi_k(x)| \leq \sum_{k=1}^{\infty} |\phi_k(x)| \leq \mathfrak{R}(\min(a_0(x) - r, R - a_0(x)))
\]

hold. Here, we have used that \( y \in R_{N_P} \subset (-1, 1)^{N_P} \). While this assumption already leads to solutions \( u(y, x) \), which are analytic as functions of \( y \), we need one additional assumption to also bound the coefficients of a Taylor expansion of the function \( y \mapsto u(y, x) \). Following [4] again, we will call a sequence \((\rho_k)\) of positive numbers \( \delta \)-admissible for the sequence \((\phi_k)\) if
\[
\sum_{k=1}^{\infty} \rho_k |\phi_k(x)| \leq \mathfrak{R}(a_0(x)) - \delta,
\]  
(11)

For \( \delta \leq r \), one can even have \( \rho_k \geq 1 \) for all \( k \in \mathbb{N} \), see [4]. With this, we have the following result from [4, Theorem 1.2, Lemma 2.4].
**Proposition 1.** Suppose that the uniform (complex) ellipticity assumption \((10)\) holds with parameters \(0 < r \leq R < \infty\). Then, the solution of \((8)\) has the form

\[
u(y, \cdot) = \sum_{\nu \in \mathbb{N}_0^N} u_{\nu}(\cdot)y^\nu. \tag{12}\]

for \(u_{\nu} \in V\), where convergence of the infinite series is understood with respect to the \(\| \cdot \|_V\)-norm. Furthermore, if \((\rho_k)\) is a \(\delta\)-admissible sequence, then

\[
\| u_{\nu}(y, \cdot) \|_V \leq \frac{\|G\|_{V^*}}{\delta} \prod_{k=1}^{N_0^N} \rho_k^{-\nu_k}, \quad y \in R_{N_0^N}.
\]

We now want to derive a parametric representation of the quantity of interest \((2)\). To this end, we introduce the notation \(R(\lambda) \in V\) for the Riesz representer of a linear functional \(\lambda \in V^*\). Then we have, by \((12)\),

\[
Q(y) = q(u(y, \cdot)) = \left( \sum_{\nu \in \mathbb{N}_0^N} u_{\nu}(\cdot)y^\nu, R(q) \right)_V = \sum_{\nu \in \mathbb{N}_0^N} \langle u_{\nu}, R(q) \rangle_V y^\nu,
\]

which shows that the function \(Q\), under certain assumption on the functional \(q\), is also analytic. Later on, this representation of \(Q\) will guarantee that \(Q\) is indeed an element of the reproducing kernel Hilbert space of our specific choice.

### 3 Reproducing Kernel Hilbert Spaces

The reproduction problem \((6)\) is at first sight an optimisation problem over an infinite dimensional function space. However, basic linear algebra shows that the solution must be contained in the span of the Riesz representers of the point evaluation functionals \(\delta_{y_k}\). These Riesz representers become particularly simple if the underlying Hilbert space \(H_K\) is a *Hilbert space with a reproducing kernel*. The Hilbert space \(H_K\) is a reproducing kernel Hilbert space with kernel \(K: \Omega \times \Omega \to \mathbb{R}\) if \(K\) satisfies \(K(\cdot, y) \in H_K\) and \(f(y) = \langle f, K(\cdot, y) \rangle_{H_K}\) for all \(y \in \Omega\) and all \(f \in H_K\). Details on such spaces can be found, for example, in [13].

#### 3.1 Taylor Spaces and Power Series Kernels

In this paper, we are interested in a particular reproducing kernel Hilbert space, which consists of analytic functions and which was introduced in [14] and further investigated in [15]. The results below are taken from [5].

Let \(y \in \mathbb{N}_0^{N_0^N}\) be a multi-index and \((w_\nu)\) be a sequence of positive numbers such that the summability condition \(\sum_{\nu \in \mathbb{N}_0^{N_0^N}} \frac{w_\nu}{\nu!} < \infty\) holds. Under these assumptions, a
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power series kernel $K : (-1, 1)^{NP} \times (-1, 1)^{NP} \to \mathbb{R}$, which is a kernel of the form

$$K(x, y) := \sum_{\nu \in \mathbb{N}^N} \frac{w_{\nu}}{\nu!^2} x^\nu y^\nu, \quad x, y \in (-1, 1)^{NP}, \quad (13)$$

is well-defined and analytic in each variable. The so-defined kernel $K$ is the reproducing kernel of the Hilbert space $\mathcal{H}_K$ of functions

$$\mathcal{H}_K := \left\{ f : (-1, 1)^{NP} \to \mathbb{R} : f(x) = \sum_{\nu \in \mathbb{N}^N} f_{\nu} x^\nu \text{ with } \|f\|_{\mathcal{H}_K} < \infty \right\}. \quad (14)$$

where the norm is defined by the inner product

$$\langle f, g \rangle_{\mathcal{H}_K} := \sum_{\nu \in \mathbb{N}^N} \frac{1}{w_{\nu}} D^\nu f(0) D^\nu g(0) = \sum_{\nu \in \mathbb{N}^N} \frac{\nu!^2}{w_{\nu}} f_{\nu} g_{\nu}. \quad (15)$$

see [14]. The next two results are taken from [5] and illustrate the reason for using such Taylor spaces $\mathcal{H}_K$ in this context.

First, we consider the embedding constant of the embedding of $\mathcal{H}_K$ into either of both Sobolev spaces, the classical isotropic space $W^{k,2}$ and the tensor product space $W^{k,\infty}$, i.e. we investigate the norm of the injection

$$W^s(k) : \mathcal{H}_K \hookrightarrow W^s_k(R_{NP}), \quad (16)$$

for $s \in \{1, \infty\}$, which is given in the next lemma.

**Lemma 1.** Let $R_{NP}$ be defined by (7) Let $s \in \{1, \infty\}$. Suppose that there is a constant $\hat{c} \in (0, 1)$ such that the weights $w_{\nu}$ satisfy $w_{\nu} \leq \hat{c}^{\nu!} \nu!^2$ for all $\nu \in \mathbb{N}^N_0$. Then, there is a constant $C > 0$ such that the norm of the embedding operator (16) can be bounded by

$$\|W^s_k(k)\| \leq \exp \left( \frac{C}{2} k \right) k!.$$

The second result which we require from [5] states that the function $Q$ which we want to reconstruct indeed belongs to a Taylor space $\mathcal{H}_K$ if the weights $w_{\nu}$ are chosen appropriately.

**Lemma 2.** Suppose that the uniform (complex) ellipticity assumption (10) holds with parameters $0 < r \leq R < \infty$. Furthermore, let $(\rho_k)_{k}$ be a $\delta$-admissible sequence with $0 < \delta < r$ and $\rho_k > 1$ for all $k$. Let $\ell \in \mathbb{R}^{NP}$ have components $c_j$ with $c_j \in (\rho_j^{-1}, 1)$, $1 \leq j \leq NP$. Let $K = K_{c}$ be defined by (13) with weights $w_{\nu} = c^{\nu} \nu!^2$. Then we have $Q \in \mathcal{H}_{K_{c}}$.

The space $\mathcal{H}_{K_{c}}$ is a special case of $\mathcal{H}_K$. With the given, specific weights, the inner product becomes
\[ \langle f, g \rangle_{\mathcal{H}_K} = \sum_{v \in \mathbb{N}_0^p} \frac{1}{e^v y^2} D^v f(0) D^v g(0) = \sum_{v \in \mathbb{N}_0^p} \frac{1}{e^v} f_v g_v. \]

Furthermore, it is easy to see that this specific choice of weights leads to an explicit, analytic form of the reproducing kernel \( K_c \) given by
\[ K_c(x, y) = \sum_{\nu \in \mathbb{N}_0^p} e^\nu x^\nu y^\nu = \prod_{k=1}^{N_p} \frac{1}{1 - c_k x_k y_k}. \] (17)

### 3.2 Penalised Least Squares

A typical application of reproducing kernel Hilbert spaces \( \mathcal{H}_K \) are reconstruction processes of the form
\[ \min_{s \in \mathcal{H}_K} \left( \sum_{k=1}^{N} |f(x_k) - s(x_k)|^2 + \lambda \|s\|_{\mathcal{H}_K}^2 \right), \] (18)

where the data \( \{ (x_k, f(x_k)) \}_{k=1}^{N} \), \( f \in \mathcal{H}_K \) is given. The parameter \( \lambda > 0 \) serves as a moderator between the fit to the data and the smoothness of the reconstruction \( \tilde{s}_\lambda \). In the RKHS setting, we have, by the well-known representer theorem, that the solution of the minimisation \( \tilde{s}_\lambda \) lies in the finite-dimensional space spanned by \( K(\cdot, x_k) \), \( 1 \leq k \leq N \), i.e. we have the representation
\[ \tilde{s}_\lambda = \sum_{k=0}^{N} \alpha_k K(\cdot, x_k). \]

Furthermore, the coefficients \( \alpha = (\alpha_1, \ldots, \alpha_N)^T \) can be computed by solving the linear system
\[ (K + \lambda I) \alpha = f, \]
where \( K_{ij} = K(x_i, x_j), f_i = f(x_i) \) and \( I \) is the identity matrix. It is well-known that this system has a positive definite system matrix and hence a unique solution. This also means that the least-squares problem (18) has a unique solution. Hence, in our situation, when employing the kernel \( K = K_c \) in (6), these general considerations give us a unique approximation \( \tilde{Q}_d \) to \( Q \) derived from the noisy data \( Q_h(y_k), 1 \leq k \leq N_S \).

### 4 Sparse Grids

In this section, we demonstrate how we construct the sparse grid \( H(\ell, d) \) of level \( \ell \) and dimension \( d \). Here, we follow mainly Wendland and Rieger [6].
To obtain the $d$-dimensional grid, we start with univariate sets of Chebyshev points. To do so we define a sequence of numbers $(m_i)$ by
\[
    m_1 = 1, \quad m_i = 2^{i-1} + 1, \quad i > 1.
\]
Then, we define the Chebyshev point sets $X^{(i)}$ to be
\[
    X^{(1)} := X_{m_1} = \{0\},
    X^{(i)} := X_{m_i} = \left\{ x_j^{(i)} = -\cos \left( \frac{\pi (j-1)}{m_i-1} \right) : 1 \leq j \leq m_i \right\}, \quad i > 1.
\]
With these univariate point sets, we now define the sparse grid $\tilde{H}(\ell, d)$ of level $\ell$ and dimension $d$, $\ell \geq d$, by
\[
    \tilde{H}(\ell, d) = \bigcup_{\|i\| = \ell} X^{(i_1)} \times \cdots \times X^{(i_d)}.
\]
As mentioned in Section 1, we choose the sampling space $\mathcal{Y}_{NS}$ to be a sparse grid. As, by construction, $\tilde{H}(\ell, NP) \subset [-1, 1]^N$ is not a subset of $\mathbb{R}^N$, we simply scale its points with a component-wise factor $r_j(1-\mu)$, $0 < \mu \ll 1$, $1 \leq j \leq NP$ and receive the scaled sparse grid
\[
    H(\ell, NP) := \left\{ (r_1(1-\mu)x_1, \ldots, r_{NP}(1-\mu)x_{NP}) : x \in \tilde{H}(\ell, NP) \right\}.
\]
Now, we choose $\mathcal{Y}_{NS} := H(\ell, NP) \subset R_{NP}$, where $\ell$ is a degree of freedom. For statements on the error of the reconstruction process we need to know the number of sampling points $NS$. Unfortunately, the exact number is a priori unknown and there exist only lower and upper bounds, provided in [6],
\[
    2^{\ell-2NP+1} \leq NS \leq 2^{\ell-NP+1} \frac{\ell^{NP-1}}{(NP-1)!}.
\]
Fortunately, as soon as we have created the sparse grid, we know exactly how many points it contains. A selection is given in Table 1. Clearly, we can control the number $NS$ for a given dimension $NP$ by choosing the level $\ell$ appropriately.

5 Error Estimates

We use this section to state the main results of this paper concerning error estimates for the optimisation problem (6), whose definition we recall here. We use the reproducing kernel Hilbert space $\mathcal{H}_{K_{\ell}}$ introduced in (14) with the power series kernel $K_{\ell}(x, y) = \prod_{j=1}^{NP} \frac{1}{1-x_j y_j}$ of (17). Next, we define $J_{Q_{\ell},t} : \mathcal{H}_{K_{\ell}} \to \mathbb{R}$, where
Table 1 Number of points $N_S$ of the grid $H(\ell, d)$ for various space dimensions $d$ and $\ell \geq d$.

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$$J_{Q_h, A}(s) := \sum_{k=1}^{N_P} |Q_h(y_k) - s(y_k)|^2 + \lambda \|s\|^2_{H_{Kc}}, \quad s \in H_{Kc},$$

and set

$$\tilde{Q}_A := \arg \min_{s \in H_{Kc}} J_{Q_h, A}(s).$$

The main objective is now to reconstruct the function $Q : R_{N_P} \to \mathbb{R}$ from perturbed samples $Q_h(y_k) = q(u_h(y_k, \cdot))$, $1 \leq k \leq N_S$, where the $y_k \in H(\ell, N_P)$ and $u_h(y_k, \cdot) \in V_h$ is a FEM approximation of the exact solution.

As the data we have are corrupted by numerical error, we cannot directly employ the classic error estimates for penalised least-squares used in [6] since we cannot assume the function $Q_h$ to be in the Hilbert space $H_{Kc}$. Nonetheless, we can assess this error. To do so we use the quantity

$$\varepsilon_k = Q_h(y_k) - Q(y_k) = q(u_h(y_k, \cdot)) - q(u(y_k, \cdot)) = q(u_h(y_k, \cdot) - u(y_k, \cdot)).$$

Hence we have the estimate

$$|\varepsilon_k| \leq \|q\| \|u_h(y_k, \cdot) - u(y_k, \cdot)\|,$$

which means that $|\varepsilon_k|$ is bounded by the numerical error, which occurs in the solution of equation (3). This error enjoys well-known bounds depending on the smoothness of the solution. For example, we have from Brenner & Scott [3] the following estimate.

**Lemma 3.** Let the finite element space be made up of elements up to order $t$ with mesh width $h$. Assume that $u(y_k, \cdot) \in H^{s+1}(\Omega)$, for all $1 \leq s \leq t$ and all $1 \leq k \leq N_P$. Then, there is a constant $c > 0$ such that

$$\|u_h(y_k, \cdot) - u(y_k, \cdot)\| \leq c h^s \|u(y_k, \cdot)\|_{H^{s+1}(\Omega)}, \quad 1 \leq k \leq N_P. \quad (21)$$
We mainly follow the ideas employed in [5] with appropriate modifications. We start by deriving two estimates for \( f_{NP,k}(NS) \) and \( g_{NP}(NS) \), where \( \tilde{c} \) is a modified constant, depending additionally on \( \mu \) and \( r \).

As we can embed \( H_{K_{\mu}} \) into \( W^{k,2}_{\infty}(R_{NP}) \), see Lemma 1, (25) above holds particularly for functions \( b \in H_{K_{\mu}} \).

With these tools we are now able to estimate the error \( Q - \tilde{Q}_I \) in the \( L^\infty \)-norm. We mainly follow the ideas employed in [5] with appropriate modifications. We start by deriving two estimates for \( \tilde{Q}_I \). The first one is based upon the bound

\[
\left| Q_h(y_k) - \tilde{Q}_I(y_k) \right|^2 \leq \sum_{i=1}^{N_S} \left| Q_h(y_i) - \tilde{Q}_I(y_i) \right|^2 + \lambda \left\| Q_h \right\|_{H_{K_{\mu}}}^2
\]

\[
= J_{Q_h,I} \left( \tilde{Q}_I \right) \leq J_{Q_h,I}(Q).
\]
where we introduced positive summands and used that \( \tilde{Q}_\lambda \) is the minimiser of the functional \( J_{Q_h,\lambda} \). This leads to

\[
|Q_h(y_k) - \tilde{Q}_\lambda(y_k)| \leq \sum_{i=1}^{N_S} |Q_h(y_i) - Q(y_i)| + \sqrt{\lambda} \|Q\|_{H_{K_e}} .
\] (26)

Here, we used that for any \( a, b \geq 0 \) the estimate \((a + b)^{1/2} \leq a^{1/2} + b^{1/2}\) holds.

Next, we can estimate the consistency error, i.e. the point-wise error at the sampling nodes. We have by applying the triangle inequality

\[
|Q(y_k) - \tilde{Q}_\lambda(y_k)| \leq |Q_h(y_k) - Q(y_k)| + |Q_h(y_k) - \tilde{Q}_\lambda(y_k)| ,
\]

which, together with (26), leads to our first crucial estimate

\[
|Q(y_k) - \tilde{Q}_\lambda(y_k)| \leq |Q_h(y_k) - Q(y_k)| + \sum_{i=1}^{N_S} |Q_h(y_i) - Q(y_i)| + \sqrt{\lambda} \|Q\|_{H_{K_e}} .
\]

The second estimate on \( \tilde{Q}_\lambda \) follows from

\[
\lambda \|\tilde{Q}_\lambda\|_{H_{K_e}}^2 \leq J_{Q_h,\lambda}(\tilde{Q}_\lambda) \leq J_{Q_h,\lambda}(Q) \leq \sum_{k=1}^{N_S} (Q_h(y_k) - Q(y_k))^2 + \lambda \|Q\|_{H_{K_e}}^2
\]

and leads to

\[
\|\tilde{Q}_\lambda\|_{H_{K_e}}^2 \leq \frac{1}{\lambda} \sum_{k=1}^{N_S} (Q_h(y_k) - Q(y_k))^2 + \|Q\|_{H_{K_e}}^2 .
\]

We collect these results in the following lemma.

**Lemma 4.** The reconstruction \( \tilde{Q}_\lambda \) from (6) of the function \( Q \) satisfies the bounds

\[
|Q(y_k) - \tilde{Q}_\lambda(y_k)| \leq |Q_h(y_k) - Q(y_k)| + \sum_{i=1}^{N_S} |Q_h(y_i) - Q(y_i)| + \sqrt{\lambda} \|Q\|_{H_{K_e}} ,
\]

\[
\|\tilde{Q}_\lambda\|_{H_{K_e}}^2 \leq \frac{1}{\lambda} \sum_{i=1}^{N_S} (Q_h(y_i) - Q(y_i))^2 + \|Q\|_{H_{K_e}}^2 .
\]

With these results we arrive at the following error estimate.

**Theorem 2.** Let \( H(\ell, N_P) \) with \( \ell \geq N_P \) be the scaled sparse grid from (20) with \( N_S \) points. Assume that \( Q \in H_{K_e} \), where \( H_{K_e} \) is as in (14) with \( K = K_e \) from (17) satisfying the assumptions of Lemma 2. Then, there is a constant \( c > 0 \) such that for \( \tilde{Q}_\lambda = \arg \min_{s \in H_{K_e}} J_{Q_h,\lambda}(s) \) the error estimate
\[ \left\| Q - \tilde{Q}_t \right\|_{L^\infty(R_{N_p})} \leq c \left( f_{N_p,k}(N_S) + \sqrt{1} g_{N_p}(N_S) \right) \left\| Q \right\|_{\mathcal{H}_{Ke}} \\
+ c \left( \frac{1}{\sqrt{t}} f_{N_p,k}(N_S) + g_{N_p}(N_S) \right) \sum_{i=1}^{N_S} |Q_h(y_i) - Q(y_i)| \]

holds, where \( f_{N_p,k} \) and \( g_{N_p} \) are from (23) and (24).

**Proof.** The modified sampling inequality (25) with \( b = Q - \tilde{Q}_t \) and Lemma 1 show

\[
\left\| Q - \tilde{Q}_t \right\|_{L^\infty(R_{N_p})} \leq c f_{N_p,k}(N_S) \left\| Q - \tilde{Q}_t \right\|_{W^{0,2}_{\infty}(R_{N_p})} \\
+ c g_{N_p}(N_S) \left\| Q - \tilde{Q}_t \right\|_{\ell^\infty(H(\ell,N_p))} \\
\leq c f_{N_p,k}(N_S) \left\| Q - \tilde{Q}_t \right\|_{\mathcal{H}_{Ke}} \\
+ c g_{N_p}(N_S) \left\| Q - \tilde{Q}_t \right\|_{\ell^\infty(H(\ell,N_p))},
\]

Next, Lemma 4 allows us to bound the terms \( \left\| Q - \tilde{Q}_t \right\|_{\ell^\infty(H(\ell,N_p))} \) and \( \left\| Q - \tilde{Q}_t \right\|_{\mathcal{H}_{Ke}} \) separately. We have

\[
\left\| Q - \tilde{Q}_t \right\|_{\ell^\infty(H(\ell,N_p))} \\
\leq \max_{k=1,...,N_S} |Q_h(y_k) - Q(y_k)| + \sum_{i=1}^{N_S} |Q_h(y_i) - Q(y_i)| + \sqrt{1} \left\| Q \right\|_{\mathcal{H}_{Ke}} \\
\leq 2 \sum_{i=1}^{N_S} |Q_h(y_i) - Q(y_i)| + \sqrt{1} \left\| Q \right\|_{\mathcal{H}_{Ke}}
\]

and

\[
\left\| Q - \tilde{Q}_t \right\|_{\mathcal{H}_{Ke}} \leq \left\| Q \right\|_{\mathcal{H}_{Ke}} + \left\| \tilde{Q}_t \right\|_{\mathcal{H}_{Ke}} \\
\leq 2 \left\| Q \right\|_{\mathcal{H}_{Ke}} + \frac{1}{\sqrt{1}} \sum_{i=1}^{N_S} |Q_h(y_i) - Q(y_i)|.
\]

Inserting these bounds into the above bound on \( \left\| Q - \tilde{Q}_t \right\|_{L^\infty(R_{N_p})} \) concludes the proof. □

Taking also the error bound (21) of the finite element approximation into account yields the following corollary.

**Corollary 1.** Let the assumptions of Theorem 2 hold. Assume further that \( u(y_k, \cdot) \in H^{\ell+1}(\mathcal{D}), \ t \in \mathbb{N}, \) for every \( y_k \in H(\ell,N_p), \ 1 \leq k \leq N_S. \) Then the error estimate

\[
\left\| Q - \tilde{Q}_t \right\|_{L^\infty(R_{N_p})} \leq c \left( f_{N_p,k}(N_S) + \sqrt{1} g_{N_p}(N_S) \right) \left\| Q \right\|_{\mathcal{H}_{Ke}} \\
+ c \left( \frac{1}{\sqrt{1}} f_{N_p,k}(N_S) + g_{N_p}(N_S) \right) N_S h^t \max_{1 \leq k \leq N_S} \left| u(y_k, \cdot) \right|_{H^{\ell+1}(\mathcal{D})}
\]
holds. The functions $f_{N,p,k}$ and $g_{N,p}$ are from (23) and (24).

Next, we want to discuss the convergence behaviour of the estimate above. As it is, this result is problematic since for $N_S \to \infty$ the function $g_{N,p}$ tends to infinity. Hence, to achieve convergence, we have to couple the penalisation parameter $\lambda$ and the mesh width $h$ of the finite element grid to the number of points $N_S$ in our sparse grid appropriately.

We start with the first term on the right-hand side of the bound in Corollary 1. Its behaviour is determined by

$$f_{N,p,k}(N_S) + \sqrt{\lambda} g_{N,p}(N_S).$$

To have this term to behave like $f_{N,p,k}(N_S)$, which converges to zero for $N_S \to \infty$, we must choose $\sqrt{\lambda}$ sufficiently small. However, as we have a $1/\sqrt{\lambda}$ in the second term of the bound of Corollary 1, we cannot choose it too small. Hence, we choose a proportional constant $c_p > 0$ and let

$$\lambda = c_p \left( \frac{f_{N,p,k}(N_S)}{g_{N,p}(N_S)} \right)^2. \quad (27)$$

With this choice, the bound in Corollary 1 becomes

$$\left\| Q - \tilde{Q}_\lambda \right\|_{L^\infty(\mathbb{R}^n_{N,p})} \leq c \left( f_{N,p,k}(N_S) \|Q\|_{H^k} + g_{N,p}(N_S) N_S h^t \max_{1 \leq k \leq N_S} |u(y_k, \cdot)|_{H^{t+1}(D)} \right).$$

Hence, in order to have convergence, we need to ensure that the factor $g_{N,p}(N_S)N_S h^t$ in the second summand also tends to zero. If we want to keep the convergence order of size $f_{N,p,k}(N_S)$ then we have to choose $h$ to satisfy

$$h \leq \left( \frac{f_{N,p,k}(N_S)}{N_S g_{N,p}(N_S)} \right)^{1/t}. \quad (28)$$

We summarise these results in the next corollary.

**Corollary 2.** Under the assumptions of Corollary 1 and with the choices (27) for the smoothing parameter and (28) for the finite element mesh size, the reconstruction error satisfies

$$\left\| Q - \tilde{Q}_\lambda \right\|_{L^\infty(\mathbb{R}^n_{N,p})} \leq c f_{N,p,k}(N_S) = c N_S^{-k+\frac{1}{2}} \log(N_S) N_p(k+\frac{1}{2})^{-k+\frac{1}{2}}$$

with a constant $c = c(Q, u, k)$ depending only on $Q$, $u$ and $k$.

Comparing this result to the one obtained in [5] and by experience from classical RKHS results, see [13], one would, in light of the analyticity of the kernel, expect
spectral convergence of the reconstruction error, similar to [7]. And indeed, a more thorough analysis of the occurring constants leads to the following result.

**Corollary 3.** Under the assumptions of Corollary 1 and with the choices (27) for the smoothing parameter and (28) for the finite element mesh size, the reconstruction error satisfies for sufficiently large $N_S$ the bound

$$
\|Q - \tilde{Q}\|_{L^\infty(R_{N_P})} \leq c_1 N_S^2 e^{-c_2 N_S} \left( \|Q\|_{H_{K_e}} + \max_{1 \leq k \leq N_S} |u(y_k, \cdot)|_{H^{1+1}(\Omega)} \right),
$$

where $c_1, c_2 > 0$ are constants.

**Proof.** Corollary 2, together with the embedding constant from Lemma 1, gives the estimate

$$
\|Q - \tilde{Q}\|_{L^\infty(R_{N_P})} \leq c k! e^\xi c_k N_S^{-k+\frac{1}{2}} \log(N_S)^{N_P(k+\frac{1}{2})-(k+\frac{1}{2})} \left( \|Q\|_{H_{K_e}} + \max_{1 \leq k \leq N_S} |u(y_k, \cdot)|_{H^{1+1}(\Omega)} \right)
$$

Using Stirling’s estimate $k! \leq c k^{k+\frac{1}{2}} e^{-k}, k \geq 1$, and keeping in mind that the logarithmic term $\log(N_S)$ grows slower than any root of $N_S$, especially $N_S^{-\frac{N_P(k+\frac{1}{2})-(k+\frac{1}{2})}{2}}$, we obtain

$$
\|Q - \tilde{Q}\|_{L^\infty(R_{N_P})} \leq c k^{k+\frac{1}{2}} e^{-k} e^\xi c_k N_S^{-k+\frac{1}{2}} N_S \left( \|Q\|_{H_{K_e}} + \max_{1 \leq k \leq N_S} |u(y_k, \cdot)|_{H^{1+1}(\Omega)} \right)
$$

$$
= c \left( k N_S^3 \right)^{\frac{1}{2}} \left( e^{\xi} c_k \frac{N_S}{k} \right)^{-k} \left( \|Q\|_{H_{K_e}} + \max_{1 \leq k \leq N_S} |u(y_k, \cdot)|_{H^{1+1}(\Omega)} \right). \tag{29}
$$

Next, for sufficiently large $N_S$, we choose $k$ as $k = \frac{N_S}{\nu}$, where $\nu$ is a fixed constant such that $k \in \mathbb{N}$ and $e^{\xi - 1} < \nu \leq N_S$ holds. Inserting this particular choice of $k$ into (29) yields

$$
\|Q - \tilde{Q}\|_{L^\infty(R_{N_P})} \leq c \nu^{1/2} N_S^{-2} \left( e^{\xi - \frac{\xi}{2}} \right)^{-N_S} \left( \|Q\|_{H_{K_e}} + \max_{1 \leq k \leq N_S} |u(y_k, \cdot)|_{H^{1+1}(\Omega)} \right)
$$

$$
= c v^{-1/2} N_S^{-2} \left( e^{\frac{1}{2}(1 - \frac{\xi}{2} + \log \nu)} \right)^{-N_S} \left( \|Q\|_{H_{K_e}} + \max_{1 \leq k \leq N_S} |u(y_k, \cdot)|_{H^{1+1}(\Omega)} \right)
$$

$$
= c_1 N_S^2 e^{-c_2 N_S} \left( \|Q\|_{H_{K_e}} + \max_{1 \leq k \leq N_S} |u(y_k, \cdot)|_{H^{1+1}(\Omega)} \right),
$$

with $c_1 = c v^{-1/2} > 0$ and $c_2 = \frac{1}{2} \left( 1 - \frac{\xi}{2} + \log \nu \right) > 0$ for $\nu$ in the given range. \qed
6 Concluding Remarks and Future Work

We have recaptured the basics of the regularity theory of parametric elliptic partial differential equations. One important result was that the solution, as a function of the parameter, is analytic and hence so is the quantity of interest.

The analyticity of the function we wanted to reconstruct motivated the choice of the specific reproducing kernel Hilbert space, a Taylor space, whose kernel is a power series kernel and thus analytic itself. With these choices we employed a regularised reconstruction process for approximating the smooth function from data which are usually corrupted by a (numerical) error, which means that the data-giving function is not an element of the approximation space.

To alleviate the curse of dimensionality we employed sparse grids, and a new type of sampling inequality which is expressed in the number of points rather than the fill distance of the sampling set.

Finally, we used the two degrees of freedom at our disposal, namely the FEM mesh width and the penalty parameter of the reconstruction process, to derive an overall error estimate.

Unfortunately, numerical verification of the derived error estimate is difficult due to the lack of good examples and the high dimensionality of the parameter space. Nonetheless, this will be pursued in the future.

Additionally, the kernel we used is globally supported which will lead to dense system matrices which should be avoided in practical applications, especially if the number of sampling points, i.e. the dimension of the matrix, becomes large. Switching to compactly supported kernels is subject of ongoing research. However, due to the high-dimensional nature of the underlying domain, a compactly supported kernel might not “see” enough information unless various scales are employed.

References


