Variational Monte Carlo—bridging concepts of machine learning and high-dimensional partial differential equations

Martin Eigel · Reinhold Schneider · Philipp Trunschke · Sebastian Wolf

Received: 4 October 2018 / Accepted: 21 August 2019 / Published online: 5 October 2019
© Springer Science+Business Media, LLC, part of Springer Nature 2019

Abstract
A statistical learning approach for high-dimensional parametric PDEs related to uncertainty quantification is derived. The method is based on the minimization of an empirical risk on a selected model class, and it is shown to be applicable to a broad range of problems. A general unified convergence analysis is derived, which takes into account the approximation and the statistical errors. By this, a combination of theoretical results from numerical analysis and statistics is obtained. Numerical experiments illustrate the performance of the method with the model class of hierarchical tensors.

Keywords Machine learning · Uncertainty quantification · Partial differential equations · Statistical learning · Tree tensor networks

Mathematics Subject Classification (2010) 68Q32 · 65D15 · 62J02 · 15A69 · 41A63 · 65N30 · 35R60 · 65C20 · 65N22

Communicated by: Anthony Nouy

Philipp Trunschke
ptrunschke@mail.tu-berlin.de

Martin Eigel
martin.eigel@wias-berlin.de

Reinhold Schneider
schneidr@math.tu-berlin.de

Sebastian Wolf
mail@haatschii.de

1 Weierstrass Institute, Mohrenstrasse 39, 10117 Berlin, Germany
2 TU Berlin, Straße des 17. Juni 136, 10623 Berlin, Germany
1 Introduction

In this article, we explore connections between two very active research areas, namely machine learning (ML) and uncertainty quantification (UQ) with high-dimensional partial differential equations (PDEs) like the backward Kolmogorov and Fokker-Planck equations. A central goal is to illustrate how ideas from statistical learning can be exploited for the solution of high-dimensional and possibly non-linear parametric deterministic problems. We generalize the concept of empirical risk minimization (ERM) to approximate the solution of these PDEs in non-linear model classes. While the treatment of regression problems is an important example, the framework can be applied to a large variety of problems, which do not necessarily have to be based on PDEs. We provide such an example in Section 5.2. In fact, most of the previous research using machine learning for the solution of PDEs is concerned with the application of regression techniques. In contrast to statistical problems, which are based on a fixed set of measured data points with statistical errors, the measurements we consider in this work are fundamentally different since we assume that samples can be generated arbitrarily by simulation of an explicit model. Apart from numerical approximation errors, these samples do not exhibit any statistical errors. Moreover, the underlying probability density is often known or can be chosen appropriately. Although we employ hierarchical tensor networks (as described, e.g., in [1]) in our experiments, the presented approach is sufficiently general to also cover more complicated model classes such as deep neural networks (DNNs) [2].

The term variational Monte Carlo method, which we use for the presented approach, has its origins in ground state computation in quantum physics. In large parts (in particular for linear models), the notion coincides with our method [3].

The application focus of this work is a class of computationally demanding problems, which play an important role in UQ [4, 5]. There, the uncertainty of model data is commonly described by random fields, leading to high-dimensional parametrized PDEs. These may either be solved by Monte Carlo sampling, allowing for the computation of quantities of interest (i.e., functionals) of the solution, or by spectral methods leading to a functional approximation of the solution [6, 7]. The usually faster convergence and more detailed solution information gained by the latter approach comes at the cost of a much higher computational complexity, in particular when using a stochastic (Galerkin) projection [7–10]. With the present work, we strive to combine function space approximations (in our case in a hierarchical tensor representation) and efficient solution sampling by means of a learning method, i.e., the functional solution is learned from generated sampling data. The solution approximation \( \Phi \) is determined by minimizing an objective functional \( J(\Phi) = \int_{\Omega} \ell(\Phi; x) \, d\rho(x) \) subject to some loss function \( \ell \), which, e.g., yields a least squares optimization. Since \( J \) cannot be determined exactly in many applications such as non-linear problems, one has to resort to an empirical minimization where the computation is based on (quasi) random samples constituting the empirical risk \( J_N(\Phi) = \frac{1}{N} \sum_{i=1}^{N} \ell(\Phi; x^i) \).

As with other numerical techniques, a convergence analysis and an a posteriori control of the occurring errors is of crucial interest. These errors can be split into
a deterministic and a stochastic part, which makes it possible to combine results from numerical analysis and probability theory. Since empirical (i.e., random) quantities are involved, one does in general not obtain worst-case error estimates for the stochastic error. We hence pursue the concept of convergence in probability. This results in error estimates which hold either with high probability or with a certain confidence, which can be improved exponentially fast by increasing the number of samples. The underlying theory has been developed in statistics and ML for regression and classification problems [11] and carries over with slight modifications. However, in addition to the mentioned qualitative difference of the used samples, while in statistics, the probability distribution of the data is unknown and its determination can be seen as part of the task; in our case, it is known and may be exploited in the method [12–15]. Another distinction is that we are primarily interested in the accuracy of the approximate solution of the PDE problem rather than computing the minimal risk.

When solving PDEs, the problem can often be cast into minimizing a specific integral like the error, the residual or the Dirichlet energy. For high-dimensional problems, due to the exponentially growing computational complexity (known as the curse of dimensionality), these integrals only become feasible with an empirical approach. In many situations, our method is equivalent to the solution of a regression problem, and we are not the first to apply regression techniques for solving PDEs (see, e.g., [16]). Nevertheless, it is our intention to present a unified and general theoretical foundation in the chosen framework.

It should be noted that the considered parametric PDEs are well understood in terms of regularity and sparsity [17–21]. As such, in our opinion, they represent a valuable and fruitful class of benchmark problems for ML algorithms, in particular since numerical methods from UQ are available as a reference. Recent ML approaches for (parametric) PDEs with DNNs can, e.g., be found in [22, 23]. The application of ML techniques to problems of scientific computing (in particular differential equations) was coined scientific machine learning (SciML) [24], and the presented VMC method contributes to this novel and growing class of methods.

Fundamental convergence results in statistical learning theory have been developed starting with the pioneering work of Vapnik and Chervonenkis [25–27] and Vailant [28]. We also refer to the works of Hauser [29] and Bartlett [30]. A modern treatment can be found in the recent monograph [31]. This theory is motivated by the binary classification problem and the inherent complexity is typically measured by the Vapnik-Chervonenkis (VC) dimension.

In contrast to that, a statistical learning theory where the complexity is measured in terms of the covering number is developed in [32, 33]. Since the covering number is a fundamental complexity measure in the approximation theory [34], we find this approach more amenable for our approach, and hence pursue this notion. Another view on regression problems in this framework can be found in [35]. While following the treatment of [32, 33], as a generalization, we also consider non-convex model classes. A comprehensive overview of this theory in the context of kernel methods including the theoretical background (e.g., covering numbers and Kolmogorov entropies) can be found in [25]. Note that a setting similar to this paper was considered in [36] for DNNs.
As discussed at the end of this paper, the theoretical results, so far, are not optimal, at least for linear models, which is illustrated by the numerical experiments in Section 3. The derived error bounds seem to be too pessimistic and certainly can be improved for a wide class of models. A recent example of this is provided in [13] and is briefly discussed in the outlook.

The structure of the paper is as follows: In the next section, we introduce the general framework of empirical risk minimization. In Section 3, we discuss typical choices of model classes and cost functionals. Section 4 is used to derive error bounds for deterministic and stochastic error components. In Section 5, we present an application of the theory in the context of uncertainty quantification, in particular with high-dimensional PDEs. Numerical experiments illustrate the performance of the approach in Section 6. Finally, we assess our results and point in directions for future research in Section 7.

2 Variational setting

Let $\mathcal{V}$ be a Hilbert space and $(\Omega, \Sigma, \rho)$ a measure space with finite measure $\rho$. We assume a given loss function $\ell : \mathcal{V} \times \Omega \to \mathbb{R}$ such that $\ell(\cdot; x)$ is continuous for all $x \in \Omega$ and $\ell(\Phi; \cdot)$ is integrable with respect to the measure $\rho$ for every $\Phi \in \mathcal{V}$. The objective is to find a minimizer as follows:

$$\Phi^* \in \arg \min_{\Phi \in \mathcal{V}} \mathcal{J}(\Phi)$$

of the cost functional

$$\mathcal{J}(\Phi) := \int_{\Omega} \ell(\Phi; x) \, d\rho(x) .$$

In applications in the numerical analysis, the space $\mathcal{V}$ is often infinite dimensional and one hence has to confine the minimization to a discrete model or hypothesis class $\mathcal{M} \subseteq \mathcal{V}$. To ensure the existence of the optimum, we further assume compactness of $\mathcal{M}$. The solution of the corresponding minimization problem is denoted by the following:

$$\Phi^*(\mathcal{M}) \in \arg \min_{\Phi \in \mathcal{M}} \mathcal{J}(\Phi) .$$

Since $\rho$ is a finite measure, we can interpret the cost functional as the expectation as follows:

$$\mathcal{J}(\Phi) = \int_{\Omega} \ell(\Phi; x) \, d\rho(x) = \mathbb{E}_{\rho}[\ell(\Phi; \cdot)] .$$

We assume that independent samples $\{x^i\}_{i \leq N}$, distributed according to $\rho$, can be generated. Instead of computing $\mathcal{J}$, one can then resort to computing the empirical cost functional as follows:

$$\mathcal{J}_N(\Phi) := \mathbb{E}[\ell(\Phi; \cdot); N] = \frac{1}{N} \sum_{i=1}^{N} \ell(\Phi; x^i) .$$
This Monte Carlo integral provides a surrogate functional that can be minimized to obtain the following:
\[ \Phi^*(M,N) \in \arg \min_{\Phi \in M} \mathcal{J}_N(\Phi). \]
We henceforth assume that \( \Phi^* \) indeed exists. The existence of the other two minimizers is guaranteed since \( M \) is compact and \( \ell \) is continuous in its first argument.

The central topic of this paper is to analyze the errors that are introduced by restricting the optimization from \( V \) to \( M \) and by substituting \( J \) by the Monte Carlo surrogate \( \mathcal{J}_N \). We aim to present examples that illustrate the versatility of this approach and to provide a rigorous error analysis for this general framework. The algorithm that is used to solve the minimization problem numerically can be chosen freely, and we consider neither its error analysis nor its complexity.

### 3 Cost functionals and model classes

This section is devoted to examples for cost functionals and model classes in our setting. For this, we choose \( V \) as a subspace of \( L^2(D) \) on a given Lipschitz domain \( D \) and consider the elliptic operator equation as follows:
\[ L\Phi^* = f \]
with a \( V \)-elliptic bounded linear operator \( L : V \to V' \) and \( f \in V' \). Common choices for \( L \) are second-order differential operators like the Laplace operator, the identity operator \( L\Phi(x) = \Phi(x) \), or a multiplication operator \( L\Phi(x) = a(x)\Phi(x) \) for some \( a : D \to \mathbb{R} \).

Note that \( \Phi^* \) indeed exists and is unique in the Hilbert space \( (V, \langle \cdot, \cdot \rangle_V) \) equipped with the induced norm \( \| \cdot \|_V \). Since \( L \) is elliptic, an explicit restriction \( M \subseteq B_R(0) := \{ \Phi \in V | \| \Phi \|_V \leq R \} \) is not necessarily required. An upper bound \( R \) for \( \| \Phi^* \|_V \) is provided by the Lax-Milgram theorem. Given that \( 0 \in M \), we can find the upper bound \( \| \Phi^*(M) \|_V \leq \| \Phi^*(M) - \Phi^* \|_V + \| \Phi^* \|_V \leq 2\| \Phi^* \|_V \).

Note that even though this example is a linear problem, the presented approach also allows to solve non-linear equations.

#### 3.1 Model classes

The model class \( M \) for the optimization can be chosen quite liberally and some examples are given in the following:

(i) Let \( M = V \) be a finite element space.

(ii) Let \( M = V \) be the reproducing kernel Hilbert space (RKHS) corresponding to a kernel \( k : \mathcal{X}^2 \to \mathbb{R} \) with some Hilbert space \( \mathcal{X} \). Assume that the loss function has the form \( \ell(\Phi; x) = \tilde{\ell}(x, \Phi(x)) + g(\| \Phi \|_V) \) for a strictly increasing function \( g : \mathbb{R} \to \mathbb{R} \). This implies that \( \mathcal{J}(\Phi) = \mathbb{E}[\ell(\cdot, \Phi(\cdot))] + g(\| \Phi \|_V) \). Then, by the representer theorem, \( \Phi^*(M,N) = \Phi^*(V,N) \in \text{span}[k(\cdot, x_i)]_{i \leq N} \). This means that the optimization can be carried out in finite dimensions even though the solution space is indeed infinite. This is a popular choice in ML where the
additional summand \( g(\| \cdot \|_V) \) is often used to replace a constraint on the model class \( \mathcal{M} \subseteq \{ \Phi \in V : \| \Phi \|_V \leq R \} \). We refer to [37] for an exposition of this topic.

Both model classes are linear but the presented framework also allows for non-linear parametrizations of the minimizer.

(iii) \( \mathcal{M} \) may be a polynomial or a Gaussian mixture model.

(iv) \( \mathcal{M} \) may be a set of tensors in a given tensor format. This results in multilinear models which are built upon finite dimensional subspaces of univariate functions. We point out that recently introduced hierarchical tensor representations (HT and TT formats) exhibit striking mathematical properties. For instance, they form algebraic varieties (see, e.g., [1]) and have an exponential power of expressiveness [38].

(v) \( \mathcal{M} \) can be chosen to be multi-layer neural networks (NNs). Recent progress in ML demonstrates the superiority of deep neural networks over classical shallow architectures. Their theory however is rather incomplete as yet.

Further details about these model classes in the learning context can, e.g., be found in [2, 39, 40]. Classical finite element textbooks are [41, 42].

### 3.2 Cost functionals

The framework introduced in Section 2 is quite generic in the choice of the cost functional \( J \). Some possible choices are listed in the following.

(a) A *least squares approximation* of \( \Phi^* = L^{-1} f \) in \( \mathcal{M} \) is computed via the cost functional as follows:

\[
J(\Phi) = \int_{\Omega} |\Phi(x) - \Phi^*(x)|^2 \rho(x) \, dx.
\]

The respective loss is defined by \( \ell(\Phi; x) = |\Phi(x) - \Phi^*(x)|^2 \) and the probability space is \((\Omega, \mathcal{B}(\Omega), \rho)\) for any measure \( \rho \) that is absolutely continuous w.r.t. the Lebesgue measure. The empirical problem is equivalent to the statistical least squares regression problem with given data points \((x_i, \Phi^*(x_i))\).

(b) The *minimal residual problem* in \( L^2(\Omega) \) is solved by the following:

\[
J(\Phi) = \int_{\Omega} |L\Phi(x) - f(x)|^2 \rho(x) \, dx.
\]

The respective loss is defined by \( \ell(\Phi; x) = |L\Phi(x) - f(x)|^2 \) and the probability space can be chosen as above.

(c) If \( L \) is self-adjoint w.r.t., the \( L^2(\Omega, \rho) \) inner product, we can minimize the *Dirichlet energy* as follows:

\[
J(\Phi) := \frac{1}{2} (L\Phi, \Phi)_{L^2(\Omega, \rho)} - (f, \Phi)_{L^2(\Omega, \rho)}
= \frac{1}{2} \int_{\Omega} L\Phi(x)\Phi(x) \rho(x) \, dx - \int_{\Omega} f(x)\Phi(x) \rho(x) \, dx,
\]

\( \copyright \) Springer
Variational Monte Carlo—bridging concepts of machine learning...

with \( \ell(\Phi; x) := \frac{1}{2}L\Phi(x)\Phi(x) - f(x)\Phi(x) \) and the probability space again chosen as above. If \( L \) is positive definite as well, then there exists an operator \( B = L^{1/2} \) such that \( L \) can be written as \( L = B^*B \), and we can also consider the following:

\[
\mathcal{J}(\Phi) = \frac{1}{2} \int_{\Omega} B\Phi(x)B\Phi(x)\rho(x) \, dx - \int_{\Omega} f(x)\Phi(x)\rho(x) \, dx,
\]

where \( \ell(\Phi, x) := \frac{1}{2}B\Phi(x)B\Phi(x) - f(x)\Phi(x) \). A common example for this is given by \( B := \sqrt{\kappa(x)}\nabla_x \). Note that although both cost functionals are equal, the corresponding empirical functionals are quite different.

**Remark 3.1** For many examples the exact minimum \( \Phi^* \) is attained if \( 0 \leq \ell(\Phi^*, x) = 0 \) for almost all \( x \). In this case, the choice of \( \rho \) does not matter, and we can replace \( \rho \) by any density \( \tilde{\rho} \ll \rho \) that is absolutely continuous w.r.t. \( \rho \). The minimizers on the restricted model class \( \mathcal{M} \subseteq \mathcal{V} \) can however be different from the exact minimizers. In these cases, we have to keep in mind that the choice of \( \tilde{\rho} \) will influence the solution \( \Phi^*(\mathcal{M}) \). This can however be brought to bear by weighting the samples in the empirical functional and thereby reducing instabilities.

The preceding list is of course incomplete and is only intended to illustrate the use of surrogate functionals. Other examples like classification with softmax parametrization [2, 39] may prove to be interesting but are deferred to a forthcoming work.

### 4 Convergence analysis

This central section examines the convergence of the depicted framework in terms of the errors as follows:

\[
\mathcal{E}_{\text{cost}} := |\mathcal{J}(\Phi^*) - \mathcal{J}(\Phi^*(\mathcal{M},N))| \quad \text{and} \quad \mathcal{E}_{\text{norm}} := \|\Phi^* - \Phi^*(\mathcal{M},N)\|_{\mathcal{V}}.
\]

Here, \( \mathcal{E}_{\text{cost}} \) measures the error of the empirical approximation \( \Phi^*(\mathcal{M},N) \) with respect to the cost functional \( \mathcal{J} \) while \( \mathcal{E}_{\text{norm}} \) determines the approximation error of the minimizer in terms of a norm \( \| \cdot \|_{\mathcal{V}} \) related to the problem. For the further analysis, \( \mathcal{E}_{\text{cost}} \) is decomposed into two parts:

\[
\mathcal{E}_{\text{cost}} \leq \mathcal{E}_{\text{appr}} + \mathcal{E}_{\text{gen}} = |\mathcal{J}(\Phi^*) - \mathcal{J}(\Phi^*(\mathcal{M}))| + |\mathcal{J}(\Phi^*(\mathcal{M})) - \mathcal{J}(\Phi^*(\mathcal{M},N))|.
\]

The first term \( \mathcal{E}_{\text{appr}} \) is called the *approximation error*. It is a purely deterministic quantity due to the choice of the model class. The second term \( \mathcal{E}_{\text{gen}} \) is called the *generalization error* and is a result of the use of the empirical loss functional in the minimization. This splitting allows to use of the best bounds available for each part of the error and the problem at hand. In the following, we provide generic bounds for both \( \mathcal{E}_{\text{appr}} \) and \( \mathcal{E}_{\text{gen}} \).
In numerical applications, one is primarily interested in an upper bound of the norm error $E_{\text{norm}}$, which directly quantifies the approximation error. We derive such a bound in Section 4.3. In the subsequent analysis, certain assumptions are required, which are introduced upfront.

- Boundedness: There exists $C_1 > 0$ s.t. for all $\Phi \in \mathcal{M}$, it holds the following:
  \[ |\ell(\Phi; x)| \leq C_1 \text{ for almost all } x \in \Omega. \quad (A1) \]

- Lipschitz continuity on $\mathcal{M}$: There exists $C_2 > 0$ s.t. for all $\Phi_1, \Phi_2 \in \mathcal{M}$, it holds the following:
  \[ |\ell(\Phi_1; x) - \ell(\Phi_2; x)| \leq C_2 \|\Phi_1 - \Phi_2\|_V \text{ for almost all } x \in \Omega. \quad (A2) \]

- Global Lipschitz continuity: There exists $C_2 > 0$ s.t. for all $\Phi_1, \Phi_2 \in V$, it holds the following:
  \[ |J(\Phi_1) - J(\Phi_2)| \leq C_2 \|\Phi_1 - \Phi_2\|_V. \quad (A3') \]

- Bounded second derivative: $J$ is twice differentiable with bounded second derivatives, i.e.,
  \[ \Gamma = \sup_{\xi \in V} \|D^2 J(\xi)\|_{\mathcal{L}(V, V')} < \infty. \quad (A3'') \]

- Local strong convexity: $J$ is strongly convex in a neighbourhood $\mathcal{U}$ of $\Phi^*$. This means that for all $\Phi, \Psi \in \mathcal{U}$ and some $\gamma > 0$, it holds as the following:
  \[ J(\Phi) \geq J(\Psi) + D J(\Psi)(\Phi - \Psi) + \frac{\gamma}{2} \|\Phi - \Psi\|_V^2. \quad (A4) \]

Assumptions (A1) and (A2) are required for bounding the generalization error in Section 4.2. Either assumption (A3’) or (A3’’) is needed to provide bounds for the approximation error examined in Section 4.1. The last assumption (A4) is employed to bound the norm error $E_{\text{norm}}$.

It should be mentioned that, for most examples, the previous assumptions follow immediately from assuming that there exists $C > 0$ such as the following:
\[ \sup_{\Phi \in \mathcal{M}} \|\Phi\|_{L_\infty} \leq C, \]
bounding the (essential) supremum norm of $\Phi \in \mathcal{M}$. This can be a severe but essential restriction, e.g., when using tensor concepts.

### 4.1 Approximation error

Define the best approximation error of $\Phi^*$ in $\mathcal{M}$ by the following:
\[ E_{\text{best}} := \inf_{\Phi \in \mathcal{M}} \|\Phi^* - \Phi\|_V. \quad (E_{\text{best}}) \]

An analysis for some classical model classes can be found in [32, 33, 43]. We can bound the approximation error in terms of the best approximation error in two ways.
Lemma 4.1 Let Assumption (A3') be satisfied. Then,
\[ \mathcal{E}_{\text{appr}} \leq C_2 \mathcal{E}_{\text{best}}. \]

Lemma 4.2 Let Assumption (A3'') be satisfied. Then,
\[ \mathcal{E}_{\text{appr}} \leq \frac{\Gamma^2}{2} \mathcal{E}_{\text{best}}. \]

Remark 4.3 It is worth noting the distinction between \( \mathcal{E}_{\text{appr}} \) and \( \mathcal{E}_{\text{best}} \). Both measure the minimal distance of elements \( \Phi \in \mathcal{M} \) in the model class to the global minimizer \( \Phi^* \). But \( \mathcal{E}_{\text{appr}} \) measures this distance in terms of the cost function, while \( \mathcal{E}_{\text{best}} \) measures it in the \( \mathcal{V} \)-norm.

Remark 4.4 The assumptions for both Lemmas are satisfied, for example, by linear and quadratic cost functionals on bounded model classes, which are quite common in numerical applications.

Proof of Lemma 4.1 Follows immediately.

Proof of Lemma 4.2 We can express the functional by a first order Taylor expansion of the form as follows:
\[ J(\Phi) = J(\Phi^*) + D J(\Phi^*)(\Phi - \Phi^*) + \frac{1}{2} D^2 J(\xi)(\Phi - \Phi^*)(\Phi - \Phi^*), \]
for some \( \xi \in \mathcal{V} \). Consequently, using \( \Gamma = \sup_{\xi \in \mathcal{V}} \| D^2 J(\xi) \|_{\mathcal{L}(\mathcal{V}, \mathcal{V}')} < \infty \) yields the following:
\[ |J(\Phi) - J(\Phi^*)| \leq \frac{\Gamma}{2} \| \Phi - \Phi^* \|^2_{\mathcal{V}}. \]
This implies the claim.

Remark 4.5Bounding \( \mathcal{E}_{\text{best}} \) is an issue of approximation theory and for many classical model classes sharp bounds are known. Moreover, approximation results for the popular DNNs, which could also be employed here, have been developed at a fast pace in recent years (see, e.g., [36, 44–47]). In [48–50], it was shown that DNNs are capable to alleviate the curse of dimensionality for specific SDEs.

4.2 Generalization error

Motivated by the arguments and conclusions of [32] and [51], the following analysis of the generalization error \( \mathcal{E}_{\text{gen}} \) relies on the concept of covering numbers, representing in a way the degree of compactness of the considered space. In our applications, this seems to be a more natural notion than, e.g., the classical VC dimension. For the sake of completeness, we provide full details of the derivations.

Definition 4.6 (covering number) The covering number \( \nu(\mathcal{M}, \varepsilon) \) of a subset \( \mathcal{M} \subseteq \mathcal{V} \) is defined as the minimal number of \( \| \cdot \|_{\mathcal{V}} \)-open balls of radius \( \varepsilon \) needed to cover \( \mathcal{M} \).
Example 4.7 Let \( M \) be a bounded subset of a finite dimensional linear space (e.g., a finite element space). The covering number of \( M \) can be estimated by the following:

\[
\nu(M, \varepsilon) \lesssim \text{vol}(B_1(0)) \left( \frac{R}{\varepsilon} \right)^{\dim(M)},
\]

where \( B_1(0) \) denotes the unit ball and \( R = \sup_{v \in M} \|v\| \) is the radius of the domain.

Example 4.8 Let \( M \) be a RKHS. As sketched above, the minimization can be performed in a finite dimensional subspace and the corresponding covering numbers are estimated in [33].

Example 4.9 Let \( M \) be a set of tensors in a given tensor format. Since \( M \) can be embedded into a finite dimensional linear space, we obtain the bound from example 4.7 as a crude upper bound. First sharper estimates for covering numbers for hierarchical tensors are provided by [52].

Example 4.10 For the currently extremely popular neural networks, estimates of the VC dimension (a quantity related to the covering number) are provided by [30] and recent results estimating the covering number are, e.g., derived in [36, 53, 54].

Remark 4.11 The concept of a covering number can be generalized to open balls with respect to a dissimilarity measure instead of the \( \| \cdot \|_V \) norm. This allows to apply the results of this section to more general loss functions \( \ell \).

The main convergence result for the generalization error is given in the following theorem.

Theorem 4.12 Under Assumptions (A1) and (A2), it holds for all \( \varepsilon > 0 \) that

\[
P[\epsilon_{gen} > \varepsilon] \leq 2\nu(M, \frac{\varepsilon}{8C_2}) \delta(\frac{\varepsilon}{4}, N),
\]

where \( \delta(\varepsilon, N) \) is an upper bound for \( P[|J(\Phi) - J_N(\Phi)| > \varepsilon] \).

Remark 4.13 Depending on \( \nu(M, \varepsilon) \) and the bound \( \delta(\varepsilon, N) \), Theorem 4.12 may provide a very pessimistic upper bound with a relatively large pre-asymptotic range and a “phase shift” that separates an area of almost absolute certainty from an area where failure is almost guaranteed. This happens for example in high-dimensional linear spaces and when using the Hoeffding bound for \( P[|J(\Phi) - J_N(\Phi)| > \varepsilon] \). Nevertheless, the bound still provides a proof of convergence and illustrates the relation
$N \in O(\varepsilon^{-2} \ln(\varepsilon))$. This is slightly worse than the classical Monte Carlo bound of $N \in O(\varepsilon^{-2})$ but is justified by the fact that we are not just evaluating integrals but are indeed optimizing a function $\Phi$ with respect to this integration. Moreover, we emphasize that the current analysis cannot explain the significantly faster convergence we see in practical experiments as illustrated in Section 6. Better bounds may indeed be provided by exploiting further properties (e.g., sparsity) of the problem. This is illustrated in [12] for the linear case.

We depict several lemmas in preparation of the proof of Theorem 4.12.

**Lemma 4.14** It holds,

$$E_{\text{gen}} \leq 2 \sup_{\Phi \in \mathcal{M}} |J(\Phi) - J_N(\Phi)|.$$

**Proof** Recall that $\Phi^*(\mathcal{M})$ denotes a minimizer of $J$ in the model class $\mathcal{M}$. We immediately derive the following:

$$E_{\text{gen}} = J(\Phi^*(\mathcal{M}, N)) - J(\Phi^*(\mathcal{M}))$$

$$= J(\Phi^*(\mathcal{M}, N)) - J_N(\Phi^*(\mathcal{M}, N)) + J_N(\Phi^*(\mathcal{M}, N)) - J(\Phi^*(\mathcal{M}))$$

$$\leq |J(\Phi^*(\mathcal{M}, N)) - J_N(\Phi^*(\mathcal{M}, N))| + J_N(\Phi^*(\mathcal{M})) - J(\Phi^*(\mathcal{M}))$$

$$\leq 2 \sup_{\Phi \in \mathcal{M}} |J(\Phi) - J_N(\Phi)|.$$  

**Lemma 4.15** Let $\varepsilon > 0$, $\nu := \nu(\mathcal{M}, \frac{\varepsilon}{8C_2^2})$ and $\{\Phi_j\}_{j \in [\nu]}$ the centers of the corresponding covering. Then, under Assumption (A2), it almost surely holds the following:

$$\sup_{\Phi \in \mathcal{M}} |J(\Phi) - J_N(\Phi)| < \frac{\varepsilon^4}{4} + \max_{1 \leq j \leq \nu} |J(\Phi_j) - J_N(\Phi_j)|.$$  

**Proof** Let $\Phi \in \mathcal{M}$ be given. By definition of the $\{\Phi_j\}_{j \in [\nu]}$ there exists some $\Phi_j$ with $\|\Phi - \Phi_j\|_\nu < \frac{\varepsilon}{8C_2^2}$. Assumption (A2) implies $|J(\Phi) - J(\Phi_j)| < \frac{\varepsilon^4}{4}$ and almost surely $|J_N(\Phi) - J_N(\Phi_j)| < \frac{\varepsilon^4}{4}$. Hence,

$$|J(\Phi) - J_N(\Phi)|$$

$$\leq |J(\Phi) - J_N(\Phi) - (J(\Phi_j) - J_N(\Phi_j))| + |J(\Phi_j) - J_N(\Phi_j)|$$

$$\leq |J(\Phi) - J(\Phi_j)| + |J_N(\Phi) - J_N(\Phi_j)| + |J(\Phi_j) - J_N(\Phi_j)|$$

$$< \frac{\varepsilon^4}{4} + |J(\Phi_j) - J_N(\Phi_j)|$$

$$< \frac{\varepsilon^4}{4} + \max_{1 \leq j \leq \nu} |J(\Phi_j) - J_N(\Phi_j)|$$

almost surely.  

**Lemma 4.16** Let $\varepsilon$, $\nu$, and $\{\Phi_j\}_{j \in [\nu]}$ be as in Lemma 4.15. Then,

$$\mathbb{P}[E_{\text{gen}} > \varepsilon] \leq \nu \max_{1 \leq j \leq \nu} \mathbb{P}[|J(\Phi_j) - J_N(\Phi_j)| > \varepsilon^4].$$
Proof With the preceding lemmas, we deduce the following:
\[
\begin{align*}
P[\mathcal{E}_{\text{gen}} > \varepsilon] & \leq P[\sup_{\Phi \in \mathcal{M}} |\mathcal{J}(\Phi) - \mathcal{J}_N(\Phi)| > \frac{\varepsilon}{2}] \quad \text{(Lemma 4.14)} \\
& \leq P[\max_{1 \leq j \leq \nu} |\mathcal{J}(\Phi_j) - \mathcal{J}_N(\Phi_j)| > \frac{\varepsilon}{4}] \quad \text{(Lemma 4.15)} \\
& \leq \sum_{1 \leq j \leq \nu} P[|\mathcal{J}(\Phi_j) - \mathcal{J}_N(\Phi_j)| > \frac{\varepsilon}{4}] \quad \text{(union bound)} \\
& \leq \nu \max_{1 \leq j \leq \nu} P[|\mathcal{J}(\Phi_j) - \mathcal{J}_N(\Phi_j)| > \frac{\varepsilon}{4}] \quad \text{(Lemma 4.15)} \hspace{1cm} \square
\end{align*}
\]

Using Lemma 4.16, the supremum can be factored out of the probability expression and then be bounded by means of classical concentration of measure arguments. This however comes at the price of the factor \(\nu\). Two well-known upper bounds for the probability \(P[|\mathcal{J}(\Phi_j) - \mathcal{J}_N(\Phi_j)| > \frac{\varepsilon}{4}]\) are given by the Hoeffding and the Bernstein inequalities.

**Lemma 4.17** (Hoeffding 1963) Let \(\{X_i\}_{i=1}^{N}\) be a sequence of i.i.d. bounded random variables \(|X_i| \leq M\) a.s. and define \(\overline{X} := \frac{1}{N} \sum_{i=1}^{N} X_i\). It then holds the following:
\[
P\left[|E[\overline{X}] - \overline{X}| \geq \varepsilon \right] \leq 2 \exp\left(-\frac{\varepsilon^2 N}{2M^2}\right).
\]

**Lemma 4.18** (Bernstein 1927) Let \(\{X_i\}_{i=1}^{N}\) be a sequence of i.i.d. bounded random variables \(|X_i| \leq M\) with bounded variance \(\text{Var}(X_i) \leq \sigma^2\) and define \(\overline{X} := \frac{1}{N} \sum_{i=1}^{N} X_i\). It then holds the following:
\[
P\left[|E[\overline{X}] - \overline{X}| \geq \varepsilon \right] \leq 2 \exp\left(-\frac{1}{2} \frac{\varepsilon^2 N}{\sigma^2 + \frac{1}{6} M \varepsilon}\right).
\]

**Corollary 4.19** If Assumptions (A1) holds, then Lemma 4.17 leads to the estimate as follows:
\[
\delta(\varepsilon, N) \leq 2e^{-2\varepsilon^2 N/C_1^2}.
\]

and Lemma 4.18 yields the bound as follows:
\[
\delta(\varepsilon, N) \leq 2e^{-\varepsilon^2 N^2/(2\sigma^2 + 2C_1 N \varepsilon/3)}.
\]

which reduces to the tighter bound \(\delta(\varepsilon, N) \leq 2e^{-3\varepsilon N/2C_1}\) if the variance \(\sigma^2\) of \(\ell(\Phi, \cdot)\) can be assumed to be negligible.

Proof Recall that the samples \(x^i\) are i.i.d. and therefore the \(\ell(\Phi, x^i)\) are i.i.d. for \(i = 1, \ldots, N\). Moreover, Eq. (A1) ensures that \(|\ell(\Phi, x^i)| \leq C_1\) holds almost surely for all \(i = 1, \ldots, N\). Hence, the assumptions for Lemma 4.17 are satisfied. Finally, Eq. (A1) also ensures that \(\text{Var}(\ell(\Phi, x^i)) \leq C_1^2\) holds for all \(i = 1, \ldots, N\). Therefore, Lemma 4.18 is applicable. \square

Theorem 4.12 now is a mere corollary of the preceding lemmas.
**Proof of Theorem 4.12.** Follows from Lemma 4.16 and Corollary 4.19.

### 4.3 Norm error

We aim at using the proposed framework in the numerical analysis of parametric PDEs as outlined in Section 5. Hence, we are primarily interested in the error of the empirical optimizer denoted by $\mathcal{E}_{\text{norm}} = \| \Phi^* - \Phi^*(\mathcal{M}, \mathcal{N}) \|_V$, i.e., the approximation error with respect to the exact optimizer. This section is devoted to the derivation of respective error bounds.

**Lemma 4.20** Let Assumption (A4) on local strong convexity be satisfied and assume that $\Phi^*(\mathcal{M}, \mathcal{N})$ lies in the strongly convex neighbourhood $\mathcal{U}$ of $\Phi^*$. Then,

$$
\mathcal{E}_{\text{norm}}^2 \leq \frac{2}{\gamma} \mathcal{E}_{\text{cost}}.
$$

**Proof** By the first-order optimality condition for $\Phi^*$, we show the following:

$$
D\mathcal{J}(\Phi^*)(\Phi - \Phi^*) = 0 \quad \text{for all } \Phi \in \mathcal{V}.
$$

Consequently, by Assumption (A4), we show the following:

$$
\mathcal{E}_{\text{norm}}^2 = \| \Phi^* - \Phi^*(\mathcal{M}, \mathcal{N}) \|^2 \leq \frac{2}{\gamma} \left( \mathcal{J}(\Phi^*(\mathcal{M}, \mathcal{N})) - \mathcal{J}(\Phi^*) - D\mathcal{J}(\Phi^*)(\Phi^*(\mathcal{M}, \mathcal{N}) - \Phi^*) \right)
$$

$$
= \frac{2}{\gamma} |\mathcal{J}(\Phi^*) - \mathcal{J}(\Phi^*(\mathcal{M}, \mathcal{N}))|.
$$

This proves the claim.

**Lemma 4.21** Let Assumptions (A3”) and (A4) be satisfied. Then,

$$
\mathcal{E}_{\text{norm}}^2 \leq \frac{\Gamma}{\gamma} \mathcal{E}_{\text{best}}^2 + \frac{2}{\gamma} \mathcal{E}_{\text{gen}}.
$$

An interpretation of this estimate is that $\mathcal{E}_{\text{gen}}$, in a way, measures the quality of the chosen cost functional. If the functional is chosen poorly, the minimum of the empirical functional $\Phi^*(\mathcal{M}, \mathcal{N})$ may deviate strongly from the minimum $\Phi^*(\mathcal{M})$ and may only converge with a slow rate.

**Proof of Lemma 4.21** By Lemma 4.20, the splitting of $\mathcal{E}_{\text{cost}}$ and Lemma 4.2 is shown in the following:

$$
\mathcal{E}_{\text{norm}}^2 \leq \frac{2}{\gamma} \mathcal{E}_{\text{cost}} \leq \frac{2}{\gamma} (\mathcal{E}_{\text{appr}} + \mathcal{E}_{\text{gen}}) \leq \frac{2}{\gamma} \left( \frac{\Gamma}{2} \mathcal{E}_{\text{best}}^2 + \mathcal{E}_{\text{gen}} \right).
$$

\(\square\)
Corollary 4.22 Let \( a > 0 \) and define the following:

\[
p(a, N) := \mathbb{P}[\mathcal{E}_{\text{gen}} \geq \frac{1}{2}a \Gamma \mathcal{E}_{\text{best}}^2].
\]

Then, with probability \( 1 - p(a, N) \), we sow the following:

\[
\mathcal{E}_{\text{best}}^2 \leq \mathcal{E}_{\text{norm}}^2 \leq (1 + a) \frac{\Gamma}{\gamma} \mathcal{E}_{\text{best}}^2.
\] (1)

Recall that the norm error \( \mathcal{E}_{\text{norm}} \) is the distance of the empirical solution \( \Phi^{*,(M,N)} \) to the exact solution \( \Phi^* \) and that the best approximation error \( \mathcal{E}_{\text{best}} \) is the smallest such distance that is obtainable in the given model class. Corollary 4.22 shows that in a “validity probability” the norm error is quasi-optimal in the sense that it is equivalent to the best approximation error. Using Lemma 4.12, we can bound \( p(a, N) \) in Corollary 4.22 and show that the probability \( 1 - p(a, N) \) of equivalence (1) tends to one with an exponential rate in the number of samples \( N \). This means that the convergence results hold with high probability, provided that \( N \) is sufficiently large.

Proof of Corollary 4.22 Lemma 4.21 implies the following:

\[
\mathbb{P}[\mathcal{E}_{\text{norm}}^2 \geq \varepsilon] \leq \mathbb{P}\left[ \frac{\Gamma}{\gamma} \mathcal{E}_{\text{best}}^2 + \frac{2}{\gamma} \mathcal{E}_{\text{gen}} \geq \varepsilon \right] \leq \mathbb{P}\left[ \mathcal{E}_{\text{gen}} \geq \frac{1}{2}(\gamma \varepsilon - \Gamma \mathcal{E}_{\text{best}}^2) \right].
\]

Choosing \( \varepsilon = \gamma^{-1}(1 + a)\Gamma \mathcal{E}_{\text{best}}^2 \) yields the assertion. \( \square \)

5 Problems in UQ

In this section, we discuss the intended application of the proposed method in the context of UQ. More specifically, consider the abstract problem as follows:

\[
\mathcal{D}(u; y) = 0,
\]

where \( \mathcal{D} \) encodes a (possibly non-linear) PDE model in a physical domain \( D \subset \mathbb{R}^d, d = 1, 2, 3 \), depending on parameters \( y \in \Gamma \subset \mathbb{R}^M \). The parameter vector \( y \) may be finite dimensional (\( M < \infty \)) or infinite dimensional (\( M = \infty \)). We assume that the parametric solution \( u(x, y) \) can be represented as \( u \in L^2(\Gamma, \rho; \mathcal{X}) \simeq \mathcal{X} \otimes \mathcal{Y} =: V \) with (typically) \( \mathcal{X} \subseteq H^1(D) \) and \( \mathcal{Y} \subseteq L^2(\Gamma, \rho) \) and \( \rho \) some probability measure on \( \Gamma \).

Further details of these problems can, e.g., be found in [6–8, 10, 20]. Moreover, adaptive Galerkin discretizations are for instance considered in [55–59], which is one of the UQ standard methods we have in mind.

5.1 Parametric PDEs

As a common benchmark example, we introduce a linear elliptic PDE with homogeneous Dirichlet boundary data where the solution \( u(x, y) \) solves the following:

\[
- \nabla \cdot (a(x, y) \nabla u(x, y)) = f(x), \quad u|_{\partial D} = 0.
\] (2)
This equation models the stationary density \( u(x, y) \) of a substance diffusing through a medium with permeability \( a(x, y) > 0 \). The parametric coefficient is assumed to be given either by an affine representation of the form as follows:

\[
a(x, y) = a_0(x) + \sum_{m=1}^{M} \sigma_m a_m(x) y_m \quad \text{with} \quad y \in \Gamma = [-1, 1]^M,
\]

or by the numerically more involved representation as follows:

\[
a(x, y) = \exp \left( a_0(x) + \sum_{m=1}^{M} \sigma_m a_m(x) y_m \right) \quad \text{with} \quad y \in \Gamma = \mathbb{R}^M.
\]

In both cases, \( \{a_0, a_1, \ldots, a_M\} \) is considered to be an orthonormal basis in \( L^2(D) \) and the coefficients \( \sigma_m > 0 \) are assumed to be positive. The parameter \( y \in \Gamma \) can be associated with a random variable \( y \sim \rho \) that determines uncertainty in the permeability of the medium. For the affine case (3), \( \rho \) is chosen to be a uniform distribution \( \rho = \mathcal{U}(\Gamma) \) while for the log-normal case (4), it is chosen to be standard Gaussian \( \rho = \mathcal{N}(0, 1) \). We assume the problem to be elliptic with high probability (uniform ellipticity assumption), i.e., for a small \( \varepsilon > 0 \), there exist constants \( \underline{a}, \overline{a} > 0 \) such as the following:

\[
P \left[ 0 < \underline{a} \leq a(x, y) \leq \overline{a} < \infty \right] > 1 - \varepsilon \quad (x, y) \in D \times \Gamma.
\]

We point out that for most random fields, choosing a finite parameter dimension \( M \) is a required simplifying restriction for the actual computation to become feasible. Adaptive a priori or a posteriori methods are available to sensibly control this parameter. For the stochastic Galerkin method, the affine setting is, e.g., examined in [55, 57, 60], and the first results with log-normal coefficients are shown in [58] for reliable residual-based error estimators. Other numerical methods such as stochastic collocation [61, 62] rely on a priori estimators or heuristic hierarchical indicators.

We employ the variational formulation of problem (2) with respect to a test function \( v \in \mathcal{V} \), cf. [55, 57]. It reads as follows:

\[
A(u, v) := \int_{\Gamma} \int_D a(x, y) \nabla u(x, y) \cdot \nabla v(x, y) \rho(y) \, dx \, dy
\]

\[
= \int_{\Gamma} \int_D f(x, y) v(x, y) \rho(y) \, dx \, dy.
\]

Since \( \mathcal{V} = \mathcal{X} \otimes \mathcal{Y} := H^1_0(D) \otimes L^2(\Gamma, \rho) \) is a Hilbert space, this variational problem can be treated directly by means of the presented variational Monte Carlo approach by defining the energy norm \( \| v \|_A^2 := A(v, v) \) and considering the optimization problem as follows:

\[
u = \arg \min_{\Phi \in \mathcal{V}} \frac{1}{2} \| \Phi - u \|^2_A.
\]

This means that the solution \( u \in \mathcal{V} \) can be obtained by minimizing the following:

\[
\mathcal{J}(\Phi) := \frac{1}{2} \int_{\Gamma} \| \Phi(y) - u(y) \|^2_{B(y)} \rho(y) \, dy,
\]
with the bilinear form $B(y): \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ defined by the following:

$$B(y)(u, v) := \int_D a(x, y) \nabla u(x) \nabla v(x) \, dx ,$$

and $\|v\|_{B(y)}^2 := B(y)(v, v)$.

To find an appropriate finite dimensional model class, recall that $\mathcal{Y} = \mathcal{X} \otimes \mathcal{Y} := H^1_0(D) \otimes L^2(\Gamma, \rho)$. We first choose finite dimensional subspaces as follows:

$$\mathcal{X}_{\text{FEM}} \subseteq \mathcal{X} \quad \text{and} \quad \mathcal{Y}_\mathcal{I} \subseteq \mathcal{Y} ,$$

and consider the discrete solution subspace

$$\mathcal{V}_\mathcal{I} = \mathcal{X}_{\text{FEM}} \otimes \mathcal{Y}_\mathcal{I} \subseteq \mathcal{V} ,$$

generated explicitly by the $S$-dimensional conforming FE space $\mathcal{X}_{\text{FEM}} = \text{span}\{\varphi_j\}_{j=1}^S$ with respect to a regular triangulation of the domain $D$. Since $\mathcal{Y} = L^2(\Gamma, \rho)$ exhibits a (countable) product structure, we can choose $\mathcal{Y}_\mathcal{I}$ as the vector space generated by a tensor product basis of multivariate polynomials with $\alpha \in \mathcal{I}$ given by the following:

$$P_\alpha(y) = \bigotimes_{m=1}^M P_{\alpha_m}(y_m) .$$

Here, the $P_{\alpha_m}$ are orthogonal w.r.t., the marginal distribution $\rho_m$, and $\mathcal{I}$ is a finite subset of $\prod_{m=1}^M [q_m]$ for given $q_m \in \mathbb{N}$. Hence, every $\Phi \in \mathcal{V}_\mathcal{I}$ can be written as follows:

$$\Phi(x, y) = \Phi_W(x, y) = \sum_{j=1}^S \sum_{\alpha \in \mathcal{I}} W(j, \alpha) \varphi_j(x) P_\alpha(y) ,$$

with coefficient tensor $W \in \mathbb{R}^{S \times q_1 \times \cdots \times q_M}$. As described in [1, 57, 63–65], we can represent $W$ by the following:

$$W(j, \alpha) = U_0(j) U_1(\alpha_1) \cdots U_M(\alpha_M) ,$$

with

$$U_0(j) \in \mathbb{R}^{r_0} , \quad U_1(\alpha_1) \in \mathbb{R}^{r_1-1 \times r_1} , \quad U_M(\alpha_M) \in \mathbb{R}^{r_M-1} ,$$

for some ranks $r_0, \ldots, r_{M-1} \in \mathbb{N}$. The set of all coefficient tensors $W$ with prescribed ranks $\vec{r} = (r_0, \ldots, r_{M-1})$ is denoted by $\mathcal{M}_{\leq \vec{r}}$. We now define the model class by the following:

$$\mathcal{M} = \{ \Phi_W \in \mathcal{V}_\mathcal{I} : W \in \mathcal{M}_{\leq \vec{r}} \} .$$

Denote by $u_h(y)$ the FE solution of $B(y)u_h(y) = f(y)$ in $\mathcal{X}_{\text{FEM}}$ where $B(y) \in \mathcal{L}(\mathcal{X}, \mathcal{X}')$ is the bounded linear operator $B(y)u := B(y)(u, \cdot)$. Then, by Galerkin orthogonality, it holds that for all $\Phi \in \mathcal{M}$, it is shown in the following:

$$\mathcal{J}(\Phi) = \int_\Gamma \|\Phi(y) - u(y)\|_{B(y)}^2 \rho(y) \, dy$$

$$= \int_\Gamma \|\Phi(y) - u_h(y)\|_{B(y)}^2 \rho(y) \, dy .$$
Due to the uniform ellipticity assumption, the norms \( \| \cdot \|_{B(y)} \) and \( \| \cdot \|_{H^1_0(D)} \) are equivalent with high probability, i.e.,
\[
\tilde{a} \| \cdot \|_{H^1_0(D)} \leq \| \cdot \|_{B(y)} \leq \overline{a} \| \cdot \|_{H^1_0(D)}.
\]
We thus can introduce the functional as follows:
\[
\mathcal{J}(\Phi) = \int_{\Gamma} \overline{a}^2 \| \Phi(y) - u_h(y) \|_{H^1_0(D)}^2 \rho(y) \, dy,
\]
which is numerically much easier to handle than \( J(\Phi) \). The corresponding minimum \( \tilde{\Phi} \in \mathcal{M} \) is quasi-optimal by the equivalence of the norms, namely
\[
\int_{\Gamma} \| \tilde{\Phi}(y) - u(y) \|_{B(y)}^2 \rho(y) \, dy \leq \int_{\Gamma} \overline{a}^2 \| \Phi(y) - u(y) \|_{H^1_0(D)}^2 \rho(y) \, dy \leq \int_{\Gamma} \overline{a}^2 \| \Phi^*(\mathcal{M})(y) - u(y) \|_{H^1_0(D)}^2 \rho(y) \, dy \leq \int_{\Gamma} \overline{a}^2 \| \Phi^*(\mathcal{M})(y) - u(y) \|_{B(y)}^2 \rho(y) \, dy.
\]
Consequently, it follows with high probability as follows:
\[
\| \tilde{\Phi} - u \|_V \leq \frac{\overline{a}}{\tilde{a}} \| \Phi^*(\mathcal{M}) - u \|_V \quad \text{and} \quad \| \tilde{\Phi} - u \|_A \leq \frac{\overline{a}}{\tilde{a}} \| \Phi^*(\mathcal{M}) - u \|_A.
\]
Finally, in accordance with the proposed framework, this is formulated as an empirical functional as follows:
\[
\mathcal{J}_N(\Phi) := \frac{1}{N} \sum_{i=1}^{N} \| \Phi(y^i) - u_h(y^i) \|_{H^1_0(D)}^2,
\]  
with \( y^i \) sampled according to the density \( \rho \). The approximations \( u_h(y^i) \) can be obtained numerically by standard FE methods.

In the present setting, \( a(\cdot, y) \) and \( y \) are in a one-to-one relation. Thus, the central notion of this scheme is to learn the solution operator \( y \mapsto a(\cdot, y) \mapsto u(\cdot, y) \) from generated data \( u(\cdot, y^i) \). The computation of the data \( u(\cdot, y^i) \) is completely non-intrusive, meaning that standard FE solvers can be employed to compute \( u(\cdot, y^i) \) and perform the optimization of the mean squared errors in a standard tensor recovery algorithm as described in [66].

**Remark 5.1** For numerical reasons, it is beneficial to represent the samples in a basis \( \Psi \) that is orthogonal w.r.t. the \( H^1_0(D) \) scalar product. If \( \Phi \) denotes the vector of standard FE basis functions, every function \( u \in \mathcal{X}_{\text{FEM}} \) can be represented by the following:
\[
u(x) = \pi^T \Phi(x) = \underline{u}^T \Psi(x),
\]
where \( \pi \) and \( \underline{u} \) denote the coefficient vectors. Using the stiffness matrix \( S \), the \( H^1_0(D) \) scalar product can then be computed via as following:
\[
(u, v)_{H^1_0(D)} = \pi^T S \underline{v} = \underline{u}^T \underline{v}.
\]
This makes obvious that any decomposition $S = X^T X$ provides a basis transform $X$ from $\Phi$ to a basis $\Psi = X^{-T} \Phi$ satisfying the orthogonality condition. In fact, this allows for the computation of the $H^1_0(D)$ norm of functions in the FE space more efficiently and provides numerical stability to the minimization problem (5). Note also that one can use a standard tensor reconstruction algorithm as in [66] since $\|u\|_{H^1_0(D)} = \|u\|_{L^2(\Omega)}$. However, the resulting tensor represents the solution w.r.t. the orthogonal basis $\Psi$, and another basis transformation after optimization is thus required. Moreover, the price for the described efficiency and numerical stability is a costly and numerically unstable Cholesky factorization of the ill-conditioned stiffness matrix $S$.

Remark 5.2 For the considered problem class, the best approximation error ($E_{\text{best}}$) in (chaos) polynomials was, e.g., analyzed in [17, 18, 67].

5.2 Backward Kolmogorov and Fokker-Planck equations

As another viable application of our variational Monte Carlo method, we derive a suitable formulation of the backward Kolmogorov and Fokker-Planck equations, which are high-dimensional elliptic PDEs derived from stochastic processes. Let us consider a Langevin dynamic driven by a gradient field with a confining potential $V : \mathbb{R}^d \to \mathbb{R}$, $V \in C^2(\mathbb{R}^d)$, such that $V(x) \to \infty$ for $|x| \to \infty$ and $x \mapsto e^{-V(x)} \in L^1(\mathbb{R}^d)$. We then define the following stochastic differential equations subject to a stochastic process $\{X_t\}_{t \geq 0}$ with a $d$-dimensional random variable $X_t$,

$$dX_t = -\nabla V(X_t) \, dt + \sigma \, dW_t,$$

where $\sigma > 0$ constant and $\{W_t\}_{t \geq 0}$ is a standard $d$-dimensional Wiener process [68]. The probability density $p$ of finding a particle at position $x$ and time $t$ is governed by the Fokker-Planck (FP) equation as follows:

$$\frac{\partial}{\partial t} p = L^\dagger p := \text{div}((\nabla V) p) + \frac{\sigma^2}{2} \Delta p.$$

The formal adjoint of the Fokker-Planck operator leads to the backward Kolmogorov equation as follows:

$$\frac{\partial}{\partial t} u = Lu := -\nabla V \cdot \nabla u + \frac{\sigma^2}{2} \Delta u.$$

The presented approach can be used to solve an implicit Euler step for the backward Kolmogorov equation of the form as follows:

$$(I - hL)u_{k+1} = u_k,$$

with $u_k(x) := u(t_k, x)$ and $t_k := hk$.

Remark 5.3 The solution of the corresponding Fokker-Planck equation is given by $p(t, x) = \rho(x)u(t, x)$, and can thus be computed indirectly by the variational Monte Carlo method.
Under suitable conditions [69], to solve (6), we consider the equation in a weighted $L^2$ space. The weight is chosen as the equilibrium density as follows:

$$\rho(x) := \frac{1}{Z} e^{-\frac{2}{\sigma^2} V(x)} , \ x \in \mathbb{R}^d ,$$

with the normalization constant $Z = \int_{\mathbb{R}^d} e^{-\frac{2}{\sigma^2} V(x)} dx$ which satisfies the stationary equation $L^\dagger \rho = 0$. The backward Kolmogorov operator $L : H^1(\mathbb{R}^d, \rho^{1/2}) \to (H^1(\mathbb{R}^d, \rho^{1/2}))^*$ is considered as acting on the weighted Sobolev space as follows:

$$H^1(\mathbb{R}^d, \rho) := \{ u \in L^2(\mathbb{R}^d, \rho) : \nabla u \in L^2(\mathbb{R}^d, \rho) \},$$

with the inner product

$$a(u, v) := \langle \nabla u, \nabla v \rangle_{L^2(\mathbb{R}^d, \rho)} + \langle u, v \rangle_{L^2(\mathbb{R}^d, \rho)} .$$

It is straightforward to verify that in this weighted space the backward Kolmogorov operator $L$ becomes symmetric [69] and that solving (6) is equivalent to the minimization of the cost functional as follows:

$$\mathcal{J}(v) := \frac{1}{2} \langle v, v \rangle_{L^2(\mathbb{R}^d, \rho)} + h \sigma^2 \langle \nabla v, \nabla v \rangle_{L^2(\mathbb{R}^d, \rho)} - \langle u_k, v \rangle_{L^2(\mathbb{R}^d, \rho)} . \quad (7)$$

**Theorem 5.4** For all $u, v \in H^1_0(\mathbb{R}^d, \rho)$ it holds the following:

$$\langle u, Lv \rangle_{L^2(\mathbb{R}^d, \rho)} = -\sigma^2 \langle \nabla u, \nabla v \rangle_{L^2(\mathbb{R}^d, \rho)} .$$

As a consequence, $L$ is a symmetric w.r.t., the prescribed weighted $L^2$ inner product.

**Proof** In the following, we denote by $\langle \cdot, \cdot \rangle$ the $L^2$ inner product and by $\langle \cdot, \cdot \rangle_\rho$ the weighted $L^2$ inner product w.r.t., the weight $\rho$. Integration by parts and the product rule yield the following:

$$\langle u, Lv \rangle_\rho = \frac{\sigma^2}{2} \langle u, \Delta v \rangle_\rho - \langle u, (\nabla V) \cdot (\nabla v) \rangle_\rho$$

$$= -\frac{\sigma^2}{2} \langle \nabla (u \rho), \nabla v \rangle - \langle u, (\nabla V) \cdot (\nabla v) \rangle_\rho$$

$$= -\frac{\sigma^2}{2} \langle \nabla u, \nabla v \rangle_\rho - \frac{\sigma^2}{2} \langle u \nabla \rho, \nabla v \rangle - \langle u, (\nabla V) \cdot (\nabla v) \rangle_\rho .$$

Now observe that by definition of $\rho$, we show the following:

$$\nabla \rho = -\frac{2}{\sigma^2} (\nabla V) \rho .$$

Substitution concludes the proof. 

Clearly, we can use the variational Monte Carlo framework to minimize the cost functional (7). This provides a further striking example for the proposed methodology. The solution of the eigenvalue problem for the backward Kolmogorov operators including more details about the operators is considered in a forthcoming paper, which will also contain numerical verifications of the suggested approach. Another
way to obtain a solution of the backward Kolmogorov equation by deep neural networks is considered in a recent publication [70].

6 Numerical experiments

This section is concerned with illustrating the performance of the proposed variational Monte Carlo approach for a set of benchmark problems with parametric PDEs. To assess the quality of the resulting approximation of the parametric solution, the error of the expectation and the variance with respect to a quasi-Monte Carlo (QMC) reference solution from $10^6$ Sobol samples is depicted.

The used model classes and cost functionals are defined analogously to Section 5. In the resulting tensor representation, the high-dimensional integrals (quantities of interest such as the expectation) can be evaluated efficiently and exactly. The computation of the FE solution samples is carried out with a standard conforming P1-Galerkin method on the domain $D = (0, 1)^2$ using the open source FEniCS software package [71]. For the tensor reconstructions, the Block-ASD optimization algorithm described in [66] is employed. A complete implementation is contained in the open source C++ library xerus [72], which is interfaced in the open source Python framework ALEA [73]. For the reconstruction, a maximal polynomial degree of 12 (affine) and 4 (log-normal) is allowed for each polynomial basis in the stochastic dimensions. We plot the error progression with respect to the number of reconstruction samples. The rank is chosen adaptively with an allowed maximum of 40, which for most problems does not impose a restriction. We prevent excessive rank increases by allowing each rank to increase only once every 10 iterations. For the experiments, we follow and extend our previous work [66] and use the same optimization algorithm for the tensor reconstruction. A broader overview of tensor representations can be found in [21, 65, 74].

6.1 Parametric PDEs

We consider parametric second-order PDEs in the context of UQ as described in Section 5. The model for the coefficient $a(x, y)$ is given by the following:

$$a(x, y) := a_0(x) + \sum_{m=1}^{M} \sigma_m a_m(x) y_m.$$ 

Here, $a_0$ determines the mean field, which is set to 1 if not stated otherwise, and $a_m(x) \propto m^{-2} \sin(\lfloor \frac{m+2}{2} \rfloor \pi x_1) \sin(\lceil \frac{m+2}{2} \rceil \pi x_2)$. This choice corresponds to the slow decay experiments, e.g., in [55, 56] but with a larger scaling factor of the modes.

The examined examples are defined by the following PDEs with homogeneous Dirichlet boundary conditions and $a(x, y)$ expanded in $M = 20$ terms.\(^1\) The relative

\(^1\)Note that the parameter vector $y$ is the image of a random variable, and hence is associated to a probability distribution but (despite the inaccurate notation) not actually a random quantity.
errors for the expectation value and variance obtained by the reconstruction are compared to Monte Carlo and quasi-Monte Carlo simulations in Figs. 1, 2, 3, and 4.

(I) Diffusion (affine)

$$-\nabla \cdot (a(x, y) \nabla u(x, y)) = 1 \quad \text{with} \quad y \sim \mathcal{U}([-1, 1]^M)$$

(II) Diffusion (log-normal, \(a_0 \equiv 0\))

$$-\nabla \cdot (\exp(a(x, y)) \nabla u(x, y)) = 1 \quad \text{with} \quad y \sim \mathcal{N}(0, I_M)$$

(III) Non-linear Diffusion (affine)

$$-\nabla \cdot \left( \left( \frac{a(x, y)}{10} + u(x, y) \right)^2 \nabla u(x, y) \right) = 1 \quad \text{with} \quad y \sim \mathcal{U}([-1, 1]^M)$$
(IV) Convection-diffusion (affine, SUPG-stabilized FEM)

\[-\nabla \cdot (\kappa \nabla u(x, y)) + \beta \cdot \nabla u(x, y) = 1,\]

with \( \kappa = 10^{-2} \) and \( \beta = (1 - a(x, y) 1 - |a(x, y)|)\top. \)

The examples demonstrate that the suggested approach can be successfully applied to linear and non-linear PDE problems alike. In Figs. 1, 2, 3, and 4, the relative errors for the expectation and variance obtained by the tensor reconstruction are compared to Monte Carlo simulations. We emphasize again that the tensor reconstruction in fact represents the entire stochastic parametric solution \( u(x, y) \in \mathcal{V} \) from which the first two moments are evaluation in order to compare the approximation quality with classical methods, which only allow for an evaluation of functionals. As a consequence, in principle arbitrary statistical quantities can be obtained globally and locally from the tensor representation of \( u(x, y) \) (e.g., pointwise densities).
In all cases, we observe that the presented approach provides significantly better results for the expectation than Monte Carlo sampling. It is striking that for the Darcy examples, this even holds when compared with the QMC simulations. The log-normal case (II) is considered as rather involved and the observed results are quite encouraging. We note that the pointwise error ("Error"), which represents the approximation quality of the actual parametric solution (not just a functional), is also small.

Due to the comparatively mild influence of the stochastic diffusion coefficient in the non-linear case (III), the reconstruction outperforms the sampling by at least an order of magnitude. We note that all error graphs of the reconstruction eventually stagnate and attribute the stagnation of the relative error at about $N = 5000$ to the approximation error. The earlier stagnation of the MC errors at about $N = 3800$, however, is evidence of the fact that the reconstructed estimates are more accurate than the reference values obtained by QMC.

For the complicated non-linear setting (IV), the QMC results are slightly better for the first two moments when compared to the tensor reconstruction. Nevertheless, the relative errors are of the same order of magnitude. A good indication for the large variance of the solution manifold is the now larger pointwise "Error." However, it should be noted that this is still quite accurate for the types of problems considered here. It can be expected that a sensible increase of the tensor ranks, the polynomial degree, and the number of samples used for the reconstruction would lead to even better results.

### 6.2 Cookie problems

In this section, in order to examine a different type of setup with inherently finite dimensional noise, we consider two so-called “cookie problems.” With these, circular inclusions of fixed or random size and with different random diffusion coefficients are prescribed.

(V) **Diffusion (fixed radii)** Let 9 subdomains of $D$ be given by discs $D_k$ ($k = 1, \ldots, 9$) with fixed radius $r = 1/8$ and centers $c = (i/6, j/6)^T$ for $i, j \in \{1, 3, 5\}$. The considered problem depends on $y = (y_1 \ldots y_9)^T$ with $y_k \sim \mathcal{U}(-1, 1)$, has homogeneous Dirichlet boundary conditions, and is given by the following:

$$-\nabla \cdot (\kappa(x, y) \nabla u(x, y)) = 1,$$

where $\kappa|_{D \setminus \bigcup_{k=1,\ldots,4} D_k} = 1$ and $\kappa|_{D_k} = y_k + 10^{-3}$.

(VI) **Diffusion (random radii)** The setting is the same as before. However, the problem depends on additional parameters $y^* = (y^*_1 \ldots y^*_9)^T$ with $y^*_j \sim \mathcal{U}(-1, 1)$ determining the radii $r_j = (1 + y^*_j / 3) / 3$ of the inclusions $j = 10, \ldots, 18$.

The relative errors for the expectation value and variance obtained by the reconstruction are compared to (quasi) Monte Carlo simulations in Figs. 5 and 6. As before, the tensor reconstruction yields significantly more accurate results (fixed radii) or at least errors comparable to the QMC simulations. This is especially noteworthy since
setting (VI) clearly exhibits no tensor structure. When compared to the simpler PDE setting (V), all depicted results apparently indicate a much more difficult problem.

7 Assessment and outlook

The analysis in this paper is based on known results from statistical learning, which we scrutinize from the perspective of UQ and high-dimensional PDEs. Central references for our exposition are [32, 33] with additional relations to the theory of Chervonenkis and Vapnik. We consider the presented treatise as an initial step in this direction with rigorous error estimates but with many remaining open questions. Numerical experiments show that the pursued strategy provides a promising approach for solving high-dimensional PDEs and problems in UQ. A notable observation is that the achieved accuracy often is significantly better than what could be expected.

Fig. 5 PDE setting (V): TT reconstruction error of the first two moments (M1) and (M2) compared to MC and QMC estimations (left). Additionally the average relative error for a random set of 1000 samples not used for the reconstruction is shown (right).

Fig. 6 PDE setting (VI): TT reconstruction error of the first two moments (M1) and (M2) compared to MC and QMC estimations (left). Additionally the average relative error for a random set of 1000 samples not used for the reconstruction is shown (right).
from the theoretical estimates. This raises the question if there are ways to improve the derivations for the problems under consideration. In particular, we have shown that for model classes in finite dimensional vector spaces the generalization error behaves like $N \in \mathcal{O}(\varepsilon^{-2} \ln \varepsilon)$. In fact, in the presence of noise in the input data, we should not expect major improvements. However, in the present setting, we are mainly interested in the noise-free case,\(^2\) since the samples are only used to approximate an integral. In a series of recent publications [13, 75], it was shown that in this case, one can achieve the (almost) best approximation rate in $\ell^\infty$ with high probability for the approximation of problems like in this work. The authors considered linear model classes of (orthogonal) polynomials in $\mathbb{R}^d$ and the least squares loss function. Convergence is guaranteed by bounding the condition number of the Gram matrices. Using recent results of Chern'ov type, it can be shown that this holds for different types of polynomials high probability. A related analysis in the context of regression with sparse grids can be found in [35].

When compared to the works of Cucker et al., the analytical approach of Cohen et al. is in line with the fundamental theory of numerical methods for elliptic partial differential equation, manifested, e.g., in finite elements [76] and projection methods [77]. Broadly speaking, convergence follows from stability together with consistency. Therefore, the approach of these authors is rooted mathematically in numerical analysis and based on a stability result, which in principle is an inf-sup condition [78], but limited to linear models.

We believe that this is an intriguing ansatz, which could also be adopted to non-linear model classes and empirical functionals, allowing for an explanation of our empirical observations. A way to extend the present results may be to formulate a corresponding RIP (restricted isometry property) condition for non-linear model classes due to which stability would follow immediately. This is, e.g., common in the area of compressed sensing. From this perspective, we conjecture that under the assumption of a RIP condition, the solution can be reconstructed exactly for a rather general set of model classes. This then allows for better estimates of the total error than what is achieved with the techniques used in this work. We defer an extended treatment of these ideas to forthcoming work. Nevertheless, the presented theory already provides a robust and versatile framework which guarantees convergence and is not restricted to linear models classes although the results appear to be too pessimistic for data with small noise.

We would like to point out that the condition $|\ell(\Phi; x)| \leq C$ a.e. $\forall \Phi \in \mathcal{M}$ also asserts a certain kind of stability. However, in many cases, it not easy to immediately show that this condition holds. In the case of RKHS $\mathcal{V}$, this estimate is guaranteed by the assumption $\|\Phi\|_{\mathcal{V}} \leq R$ (see). If no regularization of a similar kind is invoked, it is not even clear for linear models that this condition holds. For example, this assumption can be violated in finite dimensional spaces if the dimension is larger than the number of samples.

In this article, we neglect the optimization task, which otherwise raises many further question like the convergence to a global minimum and the complexity of the

\(^2\)In other words,”noise” in the samples is only due the numerical approximation.
employed algorithm. Both aspects are of major importance for our PDE setting since the best approximation problem on tensor manifolds exhibits many local minima and is delicate with respect to computational complexity by its high-dimensional nature. In a high-dimensional empirical risk minimization, variance-reduced stochastic gradient methods [79–81] are established as a standard, but an efficient adaptation to tensor networks is not straightforward. In the implementations, it is also of interest to explore the possibility of importance sampling techniques (that may also be used to adaptively modify the sampling density) [14, 15] and of size adaptive sampling strategies [82, 83]. Moreover, recent experiences in the deep learning setting indicate that for highly non-convex models, stochastic gradient updates have an advantageous effect on the generalization error. This important issue is not understood yet and it is not clear how it impacts solving high-dimensional PDEs where the noise level is relatively low and the required accuracy is relatively high.

In order to render the presented approach more relevant for practical applications, adaptive strategies will have to be devised, which automatically steer the discretization parameters depending on the considered problem. Since the derived a priori bounds are quite pessimistic, they are inappropriate to yield an indication of the required sample number $N$. Moreover, in initial iterations, one does not need a very good approximation of the functional, which leaves some freedom to numerical methods.

To sketch some first ideas, recall that for given $\Phi \in \mathcal{M}$ it holds $\mathbb{E}[|J(\Phi) - J_N(\Phi)|] \leq \frac{C_4}{N^4}$. This provides a crude bound for the error of the approximation of the cost functional. Since optimizing $J_N$ becomes more difficult with every sample and numerical (non-convex) optimization is bound to errors, we argue that we can start with a relatively small set of samples and increase the sample size dynamically. This conjecture is confirmed in numerical experiments in Section 6. The reasoning is that if the optimization algorithm converges with order $O(k^{-1})$ on $J$, we want the error $|\mathcal{J} - J_N|$ to be at least of the same order in some sense.\(^3\) However, this bound for $\mathbb{E}[\mathcal{E}(\Phi)]$ cannot be used to choose $N$ since the constants are unknown. To still use this a posteriori bound, one could assume a minimization algorithm which converges with rate $k^{-1}$ (where $k$ is the iteration number). One can then choose a sequence $N_k$ s.t. the error in the approximation $\mathbb{E}[\mathcal{E}(\Phi)(N_k)] \in O(k^{-1})$ vanishes as quickly as the error of the optimization.

Additionally, with the employed FE solution samples, an a posteriori error control of the approximation error can be achieved easily. If the approximation error is defined as the expectation of the energy error, an averaging of pathwise standard FE error estimators yields a sensible a.s. reliable error estimation for an adaptive mesh refinement procedure. The efficacy of this approach was presented in [84] for goal-oriented error control.

Acknowledgments R. Schneider was supported by the DFG project ERA Chemistry and through MATHEON by the Einstein Foundation Berlin. M. Eigel was supported by the DFG SPP1886.

\(^3\)Such as with respect to the expectation as derived above.
Funding information Research of S. Wolf was funded in part by the DFG MATHEON project SE10. P. Trunschke acknowledges support by the Berlin International Graduate School in Model and Simulation based Research (BIMoS).

References

1. Bachmayr, M., Schneider, R., Uschmajew, A.: Tensor networks and hierarchical tensors for the solution of high-dimensional partial differential equations. In: Foundations of Computational Mathematics, pp. 1–50 (2016)
2. Goodfellow, I., Bengio, Y., Courville, A.: Deep learning. http://www.deeplearningbook.org. MIT Press (2016)
3. Ceperley, D., Chester, G.V., Kalos, M.H.: Monte Carlo simulation of a many-fermion study, vol. 16, pp. 3081–3099 (1977)
4. Lord, G.J., Powell, C.E., Shardlow, T.: An introduction to computational stochastic PDEs. Cambridge Texts in Applied Mathematics, p. xii+503. Cambridge University Press, New York (2014)
5. Smith, R.C.: Uncertainty quantification: theory, implementation, and applications. vol. 12. Siam (2013)
6. Schwab, C., Gittelson, C.J.: Sparse tensor discretizations of high-dimensional parametric and stochastic PDEs. Acta Numer. 20, 291–467 (2011)
7. Le Maître, O., Knio, O.M.: Spectral methods for uncertainty quantification: with applications to computational fluid dynamics. Springer Science & Business Media (2010)
8. Matthies, H.G., Keese, A.: Galerkin methods for linear and nonlinear elliptic stochastic partial differential equations, vol. 194, pp. 1295–1331 (2005)
9. Deb, M.K., Babuška, I.M., Oden, J.T.: Solution of stochastic partial differential equations using Galerkin finite element techniques, vol. 190, pp. 6359–6372 (2001)
10. Ghanem, R.G., Spanos, P.D.: Stochastic finite elements: a spectral approach, p. x+214. Springer, New York (1991)
11. Friedman, J., Hastie, T., Tibshirani, R.: The elements of statistical learning. vol. 1. 10. Springer series in statistics. New York, NY, USA (2001)
12. Cohen, A., Davenport, M.A., Leviatan, D.: On the stability and accuracy of least squares approximations (2011)
13. Cohen, A., Migliorati, G.: Optimal weighted least-squares methods (2016)
14. Lepage, G.P.: Vegas - an adaptive multi-dimensional integration program
15. Ohl, T.: Vegas revisited: adaptive Monte Carlo integration beyond factorization. arXiv preprint arXiv:hep-ph/9806432 (1998)
16. Giraldi, L., Liu, D., Matthies, H.G., Nouy, A.: To be or not to be intrusive? the solution of parametric and stochastic equations—?proper generalized decomposition. SIAM J. Sci. Comput. 37(1), A347–A368 (2015)
17. Cohen, A., DeVore, R., Schwab, C.: Analytic regularity and polynomial approximation of parametric and stochastic elliptic PDE’s. Anal. Appl. (Singap.) 9(1), 11–47 (2011)
18. Cohen, A., DeVore, R., Schwab, C.: Convergence rates of best N-term Galerkin approximations for a class of elliptic sPDEs. Found. Comput. Math. 10(6), 615–646 (2010)
19. Cohen, A., DeVore, R., Schwab, C.: Analytic regularity and polynomial approximation of parametric and stochastic elliptic PDE’s. Anal. Appl. (Singap.) 9(1), 11–47 (2011)
20. Cohen, A., DeVore, R.: Approximation of high-dimensional parametric PDEs. Acta Numerica. 24, 1–159 (2015)
21. Bachmayr, M., Cohen, A., Dahmen, W.: Parametric PDEs: sparse or low-rank approximations?. arXiv preprint arXiv:1607.04444 (2016)
22. Raissi, M., Perdikaris, P., Karniadakis, G.E.: Physics informed deep learning (Part I): data-driven solutions of nonlinear partial differential equations. In: arXiv preprint arXiv:1711.10561 (2017)
23. Raissi, M., Perdikaris, P., Karniadakis, G.E.: Physics informed deep learning (Part II): data-driven discovery of nonlinear partial differential equations. In: arXiv preprint arXiv:1711.10566 (2017)
24. Lu, L., Meng, X., Mao, Z., Karniadakis, G.E.: DeepXDE: a deep learning library for solving differential equations. In: arXiv preprint arXiv:1907.04502 (2019)
25. Vapnik, V.: The nature of statistical learning theory. Springer science & business media (2013)
26. Chervonenkis, A., Vapnik, V.: Theory of uniform convergence of frequencies of events to their probabilities and problems of search for an optimal solution from empirical data (Average risk minimization based on empirical data, showing relationship of problem to uniform convergence of averages toward expectation value). Autom. Remote. Control. 32, 207–217 (1971)
27. Vapnik, V.N., Chervonenkis, A.Y.: Necessary and sufficient conditions for the uniform convergence of means to their expectations. Theory of Probability & Its Applications 26(3), 532–553 (1982)
28. Valiant, L.G.: A theory of the learnable. Commun. ACM 27(11), 1134–1142 (1984)
29. Haussler, D.: Decision theoretic generalizations of the PAC model for neural net and other learning applications. Inf. Comput. 100(1), 78–150 (1992)
30. Anthony, M., Bartlett, P.L.: Neural network learning: theoretical foundations. Cambridge University Press, Cambridge (2009)
31. Shalev-Shwartz, S.: Online learning and online convex optimization. Foundations and Trends® in Machine Learning 4(2), 107–194 (2011)
32. Cucker, F., Smale, S.: On the mathematical foundations of learning. Bull. Amer. Math. Soc. 39(01), 1–50 (2001)
33. Cucker, F., Zhou, D.X.: Learning theory: an approximation theory viewpoint. Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, Cambridge (2007)
34. Pinkus, A.: n-Widths in approximation theory. Springer, Berlin (1985)
35. Bohn, B., Griebel, M.: Error estimates for multivariate regression on discretized function spaces. SIAM J. Numer. Anal. 55(4), 1843–1866 (2017)
36. Berner, J., Grohs, P., Jentzen, A.: Analysis of the generalization error: empirical risk minimization over deep artificial neural networks overcomes the curse of dimensionality in the numerical approximation of Black-Scholes partial differential equations. In: arXiv preprint arXiv:1809.03062 (2018)
37. Schölkopf, B., Smola, A.J., et al.: Learning with kernels: support vector machines, regularization, optimization, and beyond. MIT press, Cambridge (2002)
38. Cohen, N., Shashua, A.: Convolutional rectifier networks as generalized tensor decompositions (2016)
39. Bishop, C.M.: Pattern recognition and machine learning. Springer, Berlin (2006)
40. James, G., Witten, D., Hastie, T., Tibshirani, R.: An introduction to statistical learning. Vol. 112. Springer, Berlin (2013)
41. Brenner, S., Scott, R.: The mathematical theory of finite element methods. Vol. 15. Springer Science & Business Media (2007)
42. Braess, D.: Finite elements: theory, fast solvers, and applications in solid mechanics. Cambridge University Press, Cambridge (2007)
43. Teymlyakov, V.: Approximation in learning theory. Constr. Approx. 27(1), 33–74 (2008)
44. Bölcskei, H., Grohs, P., Kutyniok, G., Petersen, P.: Optimal approximation with sparsely connected deep neural networks. In CoRR arXiv:1705.01714 (2017)
45. Henry-Labordere, P.: (Martingale) optimal transport and anomaly detection with neural networks: a primal-dual algorithm. In: arXiv e-prints arXiv:1904.04546 (2019)
46. Han, J., Jentzen, A., Weinan, E.: Solving high-dimensional partial differential equations using deep learning. Proc. Natl. Acad. Sci. 115(34), 8505–8510 (2018)
47. Weinan, E., Yu, B.: The deep Ritz method: a deep learning-based numerical algorithm for solving variational problems. Communications in Mathematics and Statistics 6, 1–12 (2018)
48. Jentzen, A., Salimova, D., Welti, T.: A proof that deep artificial neural networks overcome the curse of dimensionality in the numerical approximation of Kolmogorov partial differential equations with constant diffusion and nonlinear drift coefficients. In: arXiv e-prints arXiv:1809.07321 (2018)
49. Hutzenthaler, M., Jentzen, A., Kruse, T., Nguyen, T.A.: A proof that rectified deep neural networks overcome the curse of dimensionality in the numerical approximation of semilinear heat equations. In: arXiv e-prints arXiv:1901.10854 (2019)
50. Grohs, P., Hornung, F., Jentzen, A., von Wurstemberger, P.: A proof that artificial neural networks overcome the curse of dimensionality in the numerical approximation of Black-Scholes partial differential equations. In: arXiv e-prints arXiv:1809.02362 (2018)
51. Macdonald, J.L.: Image classification with wavelet and Shearlet based scattering transforms. MA thesis. Technische Universität Berlin (2017)
52. Rauhut, H., Schneider, R., Stojanac, Ž.: Low rank tensor recovery via iterative hard thresholding. Linear Algebra Appl. 523, 220–262 (2017)
Variational Monte Carlo—bridging concepts of machine learning...

53. Golowich, N., Rakhlin, A., Shamir, O.: Size-independent sample complexity of neural networks. In: arXiv preprint arXiv:1712.06541 (2017)

54. Barron, A.R., Klusowski, J.M.: Approximation and estimation for high-dimensional deep learning networks. In: arXiv preprint arXiv:1809.03090 (2018)

55. Eigel, M., Gittelson, C.J., Schwab, C., Zander, E.: Adaptive stochastic Galerkin FEM. Comput. Methods Appl. Mech. Engrg. 270, 247–269 (2014)

56. Eigel, M., Gittelson, C.J., Schwab, C., Zander, E.: A convergent adaptive stochastic Galerkin finite element method with quasi-optimal spatial meshes. ESAIM Mathematical Modelling and Numerical Analysis 49(5), 1367–1398 (2015)

57. Eigel, M., Pfeffer, M., Schneider, R.: Adaptive stochastic Galerkin FEM with hierarchical tensor representations. Numerische Mathematik 136(3), 765–803 (2017)

58. Eigel, M., Marschall, M., Pfeffer, M., Schneider, R.: Adaptive stochastic Galerkin FEM for lognormal coefficients in hierarchical tensor representations (2018)

59. Bespalov, A., Powell, C.E., Silvester, D.: Energy norm a posteriori error estimation for parametric operator equations. SIAM J. Sci. Comput. 36(2), A339–A363 (2014)

60. Eigel, M., Merdon, C.: Local equilibration error estimators for guaranteed error control in adaptive stochastic higher-order Galerkin FEM. In WIAS Preprint 1997 (2014)

61. Babuška, I., Nobile, F., Tempone, R.: A stochastic collocation method for elliptic partial differential equations with random input data. SIAM J. Numer. Anal. 45(3), 1005–1034 (2007)

62. Nobile, F., Tempone, R., Webster, C.G.: An anisotropic sparse grid stochastic collocation method for partial differential equations with random input data. SIAM J. Numer. Anal. 46(5), 2411–2442 (2008)

63. Oseledets, I.: Tensor-train decomposition. SIAM J. Sci. Comput. 33(5), 2295–2317 (2011)

64. Hackbusch, W., Kühn, S.: A new scheme for the tensor representation. English. J. Fourier Anal. Appl. 15(5), 706–722 (2009)

65. Hackbusch, W.: Tensor spaces and numerical tensor calculus. Vol. 42. Springer Science & Business Media (2012)

66. Eigel, M., Neumann, J., Schneider, R., Wolf, S.: Non-intrusive tensor reconstruction for high dimensional random PDEs

67. Hoang, V.H., Schwab, C.: N-term Wiener chaos approximation rate for elliptic PDEs with lognormal Gaussian random inputs. Math. Models Methods Appl. Sci. 24(4), 797–826 (2014)

68. Øksendal, B.: Stochastic differential equations. In: Stochastic differential equations. Springer, pp. 65–84 (2003)

69. Pavliotis, G.A.: Stochastic processes and applications: diffusion processes, the Fokker-Planck and Langevin equations. Vol. 60. Springer (2014)

70. Beck, C., Becker, S., Grohs, P., Jaafari, N., Jentzen, A.: Solving stochastic differential equations and Kolmogorov equations by means of deep learning. In: arXiv preprint arXiv:1806.00421 (2018)

71. FEniCS Project: automated solution of differential equations by the finite element method. fenicsproject.org

72. Huber, B., Wolf, S.: Xerus: a general purpose tensor library. libxerus.org

73. Eigel, M., Gruhlke, R., Marschall, M., Trunschke, P., Zander, E.: ALEA - a python framework for spectral methods and low-rank approximations in uncertainty quantification

74. Nouy, A.: Low-rank methods for high-dimensional approximation and model order reduction. Model Reduction and Approximation: Theory and Algorithms 15, 171 (2017)

75. Arras, B., Bachmayr, M., Cohen, A.: Sequential sampling for optimal weighted least squares approximations in hierarchical spaces. In: arXiv preprint arXiv:1805.10801 (2018)

76. Ciarlet, P.G., Kesavan, S., Ranjan, A., Vanninathan, M.: Lectures on the finite element method. Vol. 49. Tata Institute of fundamental research Bombay (1975)

77. Prössdorf, S., Silbermann, B.: Numerical analysis for integral and related operator equations. Operator Theory 52, 5–534 (1991)

78. Em, A., Guermond, J.-L.: Theory and practice of finite elements. Vol. 159. Springer Science & Business Media (2013)

79. Johnson, R., Zhang, T.: Accelerating stochastic gradient descent using predictive variance reduction. In: Burges, C.J.C., Bottou, L., Welling, M., Ghahramani, Z., Weinberger, K.Q. (eds.) Advances in Neural Information Processing Systems 26, pp. 315—323 (2013). Curran Associates, Inc.

80. Babanezhad, R., Ahmed, M.O., Virani, A., Schmidt, M., Konečný, J., Sallinen, S.: Stop wasting my gradients: practical SVRG (2015)

81. Zhang, S., Choromanska, A., LeCun, Y.: Deep learning with elastic averaging SGD (2014)
82. Mokhtari, A., Ribeiro, A.: First-order adaptive sample size methods to reduce complexity of empirical risk minimization (2017)
83. Daneshmand, H., Lucchi, A., Hofmann, T.: Starting small – learning with adaptive sample sizes (2016)
84. Eigel, M., Merdon, C., Neumann, J.: An adaptive multilevel Monte Carlo method with stochastic bounds for quantities of interest with uncertain data. SIAM/ASA Journal on Uncertainty Quantification 4(1), 1219–1245 (2016)

Publisher’s note  Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.