A General Framework for Machine Learning based Optimization Under Uncertainty

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Abstract

We propose a general framework for machine learning based optimization under uncertainty. Our approach replaces the complex forward model by a surrogate, e.g., a neural network, which is learned simultaneously in a one-shot sense when solving the optimal control problem. Our approach relies on a reformulation of the problem as a penalized empirical risk minimization problem for which we provide a consistency analysis in terms of large data and increasing penalty parameter. To solve the resulting problem, we suggest a stochastic gradient method with adaptive control of the penalty parameter and prove convergence under suitable assumptions on the surrogate model. Numerical experiments illustrate the results for linear and nonlinear surrogate models.

Keywords: Surrogate Learning, Optimization under Uncertainty, Uncertainty Quantification, Stochastic Gradient Descent, PDE-constrained Risk Minimization

1. Introduction

Uncertainties have the potential to render worthless even highly sophisticated methods for large-scale inverse and optimal control problems, since their conclusions do not realize in practice due to imperfect knowledge about model correctness, data relevance, and numerous other factors that influence the resulting solutions. To quantify the uncertainty, we consider risk measures ensuring the robustness of the solutions, see (Kouri and Shapiro, 2018) and the references therein. For complex processes, the incorporation of these uncertainties typically results in high or even infinite dimensional problems in terms of the uncertain parameters as well as the optimization variables, which in many cases are not solvable with current state of the art methods. One promising potential remedy to this issue lies in the approximation of the forward problems using novel techniques arising in uncertainty quantification and machine learning. In this paper, we propose a general framework for incorporating surrogate models in optimization under uncertainty. The underlying optimal control problem is given by a partial differential equation (PDE) constrained optimization...
problem, where the uncertain input coefficients of the PDE are modeled as a random field. In general, we are interested in the situation, where a high resolution is needed for accurate approximations of the PDE. Hence, introducing an empirical approximation of the risk measure is attached with high computational costs as for each data point we need to solve the underlying PDE model.

Our framework is based on one-shot optimization approaches (Borzi and Schulz, 2012), where we reformulate the constrained optimization problem as an unconstrained one via a penalization method. In a recent work (Guth et al., 2020), we have introduced neural network based one-shot approach for inverse problems, where the starting point of the formulation has been mainly based on the all-at-once approach for inverse problems (Kaltenbacher, 2016, 2017) and physics-informed neural networks (Raissi et al., 2017a, b, 2019; Yang et al., 2020). We established the connection between the Bayesian approach and the one-shot formulation allowing to interpret the penalization parameter as the level of model error in the forward problem.

In the setting of this article, we consider the optimization w.r. to the control function and the corresponding optimal PDE solution in a one-shot fashion. In order to force the feasibility w.r. to the constraints, we include a penalty parameter allowing for more and more weight on the penalization term. From a Bayesian perspective, this parameter controls the model error, i.e., increasing the penalization parameter corresponds to vanishing model noise. This setting allows us to incorporate surrogate models straightforwardly. We replace the optimization w.r. to the infinite dimensional PDE solution by a parameterized family of functions, where the resulting optimization task is w.r. to the parameters describing the surrogate models. Examples of surrogate models include polynomial series representations, neural networks, Gaussian process approximations and low rank approximations. We discuss various choices in Section 3. However, please note that the suggested approach is not limited to the surrogates discussed here.

1.1 Literature Overview

Introducing uncertainties in optimization and control problems governed by PDEs leads to highly complex optimization tasks. The proper formulation, the well-posedness and the development of efficient algorithms have received increasing attention in the past (see e.g., Alexanderian et al., 2017; Ali et al., 2017; Alla et al., 2019; Borzi et al., 2010; Chen et al., 2019; Guth et al., 2021; Kouri et al., 2013; Kouri and Shapiro, 2018; Kouri and Surowiec, 2016, 2018; Milz and Ulbrich, 2020; Van Barel and Vandewalle, 2019). Despite the growing interest and recent advances in PDE-constrained optimization under uncertainty, including uncertainty in form of random parameters or fields is still not feasible for many PDE models due to the significant increase in the complexity of the resulting optimization or control problems. The use of surrogate models, i.e., the replacement of the expensive forward model by approximations which are usually cheap to evaluate, is a promising direction in order to reduce the overall computational effort. However, the surrogates need to be trained or calibrated in advance. In particular, in the optimization under uncertainty setting, a surrogate is needed for every feasible control. One promising remedy to this issue lies in one-shot approaches (see e.g., Borzi and Schulz, 2012; Guth et al., 2020; Schillings et al., 2011). In (Günther et al., 2020) one-shot ideas have been successfully generalized for the
training of residual neural networks. In addition, recent results on the convergence and error analysis of machine learning techniques for high-dimensional, complex systems open up the perspective to develop novel surrogates for optimization under uncertainty that admit a mathematically rigorous convergence analysis and are applicable to a large class of computationally intense, real-world problems. Neural networks (NN) have been successfully applied to various classes of PDEs (cp. e.g., Bhattacharya et al., 2021; Geist et al., 2021; Han et al., 2018; Kutyniok et al., 2021; Opschoor et al., 2019; Schwab and Zech, 2019; Yarotsky, 2017) and also as approximation to the underlying model (Dong et al., 2020; Lu et al., 2019). For parametric PDEs, generalized polynomial chaos expansion have been extensively studied, cp. (Cohen and DeVore, 2015) for an overview on approximation results. Recently, Gaussian processes have been suggested for solving general nonlinear PDEs (Chen et al., 2021). Here, we propose a general framework, which allows to include all different surrogate models in a one-shot approach.

1.2 Outline of the paper

In this paper, we are going to analyze the dependence of the optimization error on the number of data points as well as on the weight on the penalization. Furthermore, we propose a stochastic gradient descent method in order to implement the resulting empirical risk minimization problem efficiently. In this article, we make the following contributions:

- We formulate a penalized empirical risk minimization problem and provide a consistency result in terms of large data limit as well as increasing penalty parameters. To be more precise, we can split the error in an error term decreasing with number of data points independently of the penalty parameter as well in an error term decreasing in the strength of penalization independently of the number of data points.

- We formulate a stochastic gradient descent method in order to solve the penalized risk minimization problem where we allow an adaptive increase of the penalty parameter avoiding numerical instabilities due to high variance. Under suitable assumptions we prove convergence of the proposed stochastic gradient descent method. These assumptions can be verified for linear surrogate models.

- We test our proposed approach numerically, where we apply a linear as well as a nonlinear surrogate model. The linear surrogate model is based on a polynomial expansion, while the nonlinear surrogate model is described as a neural network.

The remainder of this article is structured as follows. In Section 2 we formulate the underlying setting of optimization under uncertainty in reduced and all-at-once formulation. In Section 3 we present a collection of surrogates for the parametric mapping. A detailed consistency analysis w.r. to number of data points and penalty weight is presented in Section 4. We formulate and analyse the penalized stochastic gradient descent method in Section 5. In Section 6 we illustrate numerically the performance of our proposed framework. We conclude the paper with brief summary and discussion about further directions of interest in Section 7.
2. PDE-constrained Optimization Under Uncertainty

We are interested in solving an optimal control problem in the presence of uncertainty by minimizing the averaged least square difference of the state \( u \) and a desired target state \( u_0 \). The state \( u \) is the solution of an elliptic PDE, steered by a control function, and having a random field as input coefficient. The random field is in principle infinite-dimensional, and in practice might need a large finite number of terms for accurate approximation.

Let \( D \subset \mathbb{R}^d \), \( d \in \{1, 2, 3\} \), denote a bounded domain with Lipschitz boundary \( \partial D \) and let \( U := [-1, 1]^N \) denote a space of parameters.

Our goal of computation is the following optimal control problem:

\[
\min_{z \in L^2(D)} J(u^y, z), \quad J(u, z) := \frac{1}{2} \int_U \int_D (u^y(x) - u_0(x))^2 \, dx \, dy + \frac{\alpha}{2} \int_D z(x)^2 \, dx, \tag{1}
\]

subject to the partial differential equation

\[
-\nabla \cdot (a^y(x) \nabla u^y(x)) = z(x) \quad x \in D, \quad y \in U, \tag{2}
\]

\[
u^y(x) = 0 \quad x \in \partial D, \quad y \in U, \tag{3}
\]

for \( \alpha > 0 \). To ensure wellposedness of (1)-(3) we make the following assumptions:

(A1) Let \( u_0 \in L^2(D) \).

(A2) Let the sequence of parameters \( y = (y_j)_{j \geq 1} \) be independently and identically distributed (i.i.d.) uniformly in \([-1, 1]\) for each \( j \in \mathbb{N} \), i.e., \( y \) is distributed on \( U \) with probability measure \( \mu \), where \( \mu(dy) = \otimes_{j \geq 1} \frac{dy_j}{2} = dy \).

(A3) Let the input uncertainty be described by the diffusion coefficient \( a^y(x) \) in (2), which is assumed to depend linearly on the parameters \( y_j \), i.e.

\[
a^y(x) := a_0(x) + \sum_{j \geq 1} y_j \psi_j(x), \quad x \in D, \quad y \in U. \tag{4}
\]

(A4) Let \( a_0(\cdot) \in L^\infty(D) \), \( \psi_j(\cdot) \in L^\infty(D) \) for all \( j \geq 1 \), and \( (\|\psi_j\|_{L^\infty})_{j \geq 1} \in \ell^1(\mathbb{N}) \).

(A5) Let the uniform ellipticity assumption hold, i.e.

\[
0 < a_{\min} \leq a^y(x) \leq a_{\max} < \infty, \quad x \in D, \quad y \in U, \tag{5}
\]

for some positive real numbers \( a_{\min} \) and \( a_{\max} \).

Assumptions (A2) and (A4) ensure that the random input field (4) is well-defined.

Our variational formulation of (2) and (3) is based on the Sobolev space \( V := H^1_D(D) \) and its dual space \( V' := H^{-1}(D) \) with the norm in \( V \) defined by

\[
\|v\|_V := \|\nabla v\|_{L^2(D)}. \tag{6}
\]

The duality between \( V \) and \( V' \) is understood to be with respect to the pivot space \( L^2(D) \), which we identify with its own dual. We denote by \( \langle \cdot, \cdot \rangle \) the \( L^2(D) \) inner product and
the duality pairing between $V$ and $V'$. We introduce the continuous embedding operators $E_1 : L^2(D) \to V'$ and $E_2 : V \to L^2(D)$, with the embedding constants $c_1, c_2 > 0$ for the norms

\begin{align}
\|v\|_{V'} &\leq c_1 \|v\|_{L^2(D)}, 
\|v\|_{L^2(D)} &\leq c_2 \|v\|_V. 
\end{align}

For fixed $y \in U$, define the parametric bilinear form $b^y(w, v)$ by

$$b^y(w, v) := \int_D a^y(x) \nabla w(x) \cdot \nabla v(x) \, dx \quad \forall w, v \in V,$n

allowing us to write the parameter-dependent variational form of the parametric PDE as

$$b^y(u^y, v) = \langle z, v \rangle \quad \forall v \in V.$$

By assumptions (A3), (A4), (A5) the parametric bilinear form (7) is continuous and coercive on $V \times V$, i.e., for all $y \in U$ and all $w, v \in V$ we have

$$b^y(v, v) \geq a_{\min} \|v\|_V^2 \quad \text{and} \quad |b^y(w, v)| \leq a_{\max} \|w\|_V \|v\|_V.$$

Then, by the lemma of Lax–Milgram, we know that for every $z \in V'$ and given $y \in U$, there exists a unique solution to the parametric weak problem: find $u^y(\cdot) \in V$ such that (8) holds. Hence, the following result holds, which can also be found, e.g., in (Cohen et al., 2010) and (Kuo et al., 2012).

**Theorem 1** For every $z \in V'$ and every $y \in U$, there exists a unique solution $u^y(\cdot) \in V$ of the parametric weak problem (8), which satisfies

$$\|u^y\|_V \leq \frac{\|z\|_{V'}}{a_{\min}}.$$

In particular, because of (5) and (6) it holds for $z \in L^2(D)$ that

$$\|u^y\|_{L^2(D)} \leq \frac{c_1 c_2}{a_{\min}} \|z\|_{L^2(D)}.$$

**2.1 Weak formulation in the parameter**

In this subsection we recall results from (Gittelson, 2011) and apply them to our specific problem. To this end we denote by $A^y \in \mathcal{L}(V, V')$ the bounded, linear operator that is associated with the parametric bilinear form in (8). The operator norms are bounded by the norm of the parametric bilinear form, i.e.

$$a_{\min} \leq \|A^y\|_{\mathcal{L}(V, V')} \leq a_{\max}$$

$$\frac{1}{a_{\max}} \leq \|(A^y)^{-1}\|_{\mathcal{L}(V', V)} \leq \frac{1}{a_{\min}}.$$
Note that $y \mapsto u^y$ is continuous because $y \mapsto z$ is constant and thus continuous. Let $C(U, V)$ denote the Banach space of continuous maps $U \to V$ with norm $\|v\|_{C(U, V)} := \sup_{y \in U} \|v\|_V$. Then, the operators

\[
A : C(U, V) \to C(U, V'), \quad v \mapsto [y \mapsto A^y v] \tag{12}
A^{-1} : C(U, V') \to C(U, V), \quad w \mapsto [y \mapsto (A^y)^{-1} w] \tag{13}
\]
are well-defined, inverse to each other and bounded by the same constants as $A^y$ and its inverse operator. This result can be extended to Lebesgue spaces of vector-valued functions.

**Theorem 2 (Theorem 1.1.6 in (Gittelson, 2011))** For all $1 \leq p < \infty$, the operator $A$ in (12) extends uniquely to a boundedly invertible operator on the Lebesgue–Bochner spaces $L^p_{\mu}(U, V)$. The norms of $A$ and $A^{-1}$ are bounded by $a_{\min}$ and $a_{\max}$ respectively.

As a Corollary to this result we get:

**Corollary 3** Let $1 \leq p < \infty$ and let $q$ be the Hölder conjugate of $p$. If $z \in L^p_{\mu}(U, V')$, then there is a unique $\tilde{u} \in L^p_{\mu}(U, V)$ such that

\[
\int_U \langle A^y \tilde{u}^y, w^y \rangle \, dy = \int_U \langle z, w^y \rangle \, dy, \quad \forall \, w^y \in L^q_{\mu}(U, V), \tag{15}
\]
where $\mu$ is defined in (A2). Moreover, the solution $u^y$ of (8) is a version of $\tilde{u}^y$.

We thus no longer distinguish between the solution $u^y$ of (8) and its equivalence class $\tilde{u}^y$.

Moreover, since $V$ is a separable Hilbert space, the Lebesgue–Bochner space $L^2_{\mu}(U; V)$ is isometrically isomorphic to the Hilbert tensor product $L^2_{\mu}(U) \otimes V$ by (Gittelson, 2011, Theorem A.3.2). Thus for $v^y(x) \in L^2_{\mu}(U) \otimes V$, we have $v^y(\cdot) \in V$ a.e. in $U$ and $v'(x) \in L^2(U)$ a.e. on $D$.

### 2.2 Reduced formulation

The discussion in Section 2 guarantees a unique solution operator of the parametric PDE for arbitrary $y \in U$. We denote this operator by $S^y : L^2(D) \to L^2(D)$, which for every $y \in U$ assigns to each $f \in L^2(D)$ the unique solution $g \in L^2(D)$ of the variational problem: find $g \in V$ such that $b^y(g, v) = \langle f, v \rangle \, \forall v \in V$. Note that $S^y$ is a self-adjoint operator for any $y$.

Substituting $u^y = S^y z$ we can write the problem (1)-(3) as a quadratic problem in $L^2(D)$, the so-called reduced form of the problem:

\[
\min_{z \in L^2(D)} J(z), \quad J(z) := \frac{1}{2} \int_D \int_U (S^y z(x) - u_0(x))^2 \, dy \, dx + \frac{\alpha}{2} \int_D z(x)^2 \, dx. \tag{16}
\]

**Theorem 4** There exists a unique optimal solution $z^*$ of the problem (16).
Proof See, e.g., (Guth et al., 2021).

From standard optimization theory for convex $J$, we know that $z^*$ solves (16) if and only if the gradient of $J$ at $z^*$ vanishes. The gradient of $J(z)$ is given by

$$J'(z) = \int_U q^y \, dy + \alpha z,$$

with the adjoint state $q^y := S^y(z^* - u_0)$. Note that $q^y \in L^2(D)$ is obtained as the unique solution of the adjoint parametric variational problem: find $q^y \in V$ such that

$$b^y(q^y, w) = \langle u^y - u_0, w \rangle \quad \forall \, w \in V,$$

where $u^y$ is the unique solution of

$$b^y(u^y, v) = \langle z, v \rangle \quad \forall \, v \in V.$$

We obtain the following KKT-system for the problem (16).

Theorem 5 A control $z^* \in L^2(D)$ is the unique minimizer of (16) if and only if it holds for all $y \in U$ that

$$u^y = S^y z^*$$

and

$$q^y = S^y(u^y - u_0)$$

and

$$\int_U q^y \, dy + \alpha z^* = 0.$$

One can use a (full) gradient descent (see Guth et al., 2021) or a stochastic gradient descent (see Geiersbach and Pflug, 2019; Martin et al., 2021) to solve (19)-(21).

2.3 All-at-once formulation

Black-box methods are based on the reduced formulation (16) assuming that the forward problem can be solved exactly in each iteration, i.e., an existing algorithm for the solution of the state equation is embedded into an optimization loop. Thereby it is usually preferable to compute the gradient using a sensitivity or adjoint approach, cp. (17). However, the main drawback of black-box approaches is that they require the repeated costly solution of the (possibly nonlinear) state equation, even in the initial stages when the design variables are still far from their optimal value. This drawback can be partially overcome by carrying out the early optimization steps with a coarsely discretized PDE and/or only few samples from the space of parameters $U$.

In this section, we will follow a different approach, which solves the optimization problem and the forward problem simultaneously by treating both, the design and the state variables, as optimization variables. Various names for the simultaneous solution of the design and state equation exist: all-at-once, one-shot method, piggy-back iterations etc. The state and
the design variables are coupled through the PDE constraint, which is kept explicitly as a side constraint during the optimization.

Recall that the PDE constraint (8) can be written as

\[ b_y(u^y, v) = \langle A_y u^y, v \rangle = \langle (S^y)^{-1} u^y, v \rangle = \langle z, v \rangle, \quad \forall v \in V. \]

Hence, we can write the PDE constraint (8) as

\[ e(u^y, z) = 0, \]

where \( e(u^y, z) : L^2(D) \times L^2(D) \rightarrow L^2(D) \) is defined by \( e(u^y, z) := (S^y)^{-1} u^y - z \).

### 2.3.1 Penalty methods

A penalty method solves an constrained optimization problem by solving a sequence of unconstrained problems. Using for instance a quadratic penalty method in the present context, one aims to find a sequence of minimizers \((z_k, u^y_k)\), given by

\[
(z_k, u^y_k) = \arg \min_{z_k, u^y_k} \left( J(u_k, z_k) + \frac{\lambda_k}{2} \int_U \| e(u^y_k, z_k) \|^2_{L^2(D)} \, dy \right),
\]

that converges to the minimizer \((z^*, u^y(z^*))\) of the constrained problem (16). The disadvantage of penalty methods is that the penalty parameter \(\lambda_k\) needs to be sent to infinity which renders the resulting \(k\)-th problem increasingly ill-conditioned.

### 3. Surrogates

In many applications in the field of uncertainty quantification the forward model is computationally expensive to evaluate. Consequently, replacing the solution of the forward model by a surrogate, that is cheap to evaluate, can be a tremendous advantage. In the next sections we will analyze the optimization problem in which the parametric mapping is replaced by a surrogate, i.e., the mapping

\[ u^y : U \rightarrow V \]

is replaced by a surrogate

\[ u(\theta, y) : \Theta \times U \rightarrow V \]

where the \(\theta\) are the parameters of the surrogate. To do so we introduce the following notation: a multiindex is denoted by \(\nu = (\nu_j)_{j \in \mathbb{N}} \in \mathbb{N}^\mathbb{N}_0\). We denote the set of all indices with finite support by \(\mathcal{F} := \{ \nu \in \mathbb{N}_0^\mathbb{N} : \sum_{j \in \mathbb{N}} \nu_j < \infty \}\) and follow the conventions \(\nu! := \prod_{j \in \mathbb{N}} \nu_j^{-1}\) and \(0! := 1\). Moreover, for a sequence \(y = (y_j)_{j \in \mathbb{N}}\) and a multiindex \(\nu \in \mathcal{F}\) we write \(y^n := \prod_{j \in \mathbb{N}} y^{\nu_j}_j\), using the convention \(0^0 := 1\). By \(|\Lambda|\) we denote the finite cardinality of a set \(\Lambda\). For a real Banach space \(V\), its complexification is the space \(V_C := V + iV\) with the Taylor norm \(\|v + iw\|_{V_C} := \sup_{t \in [0,2\pi]} \|\cos(t)v - \sin(t)w\|_V\) for all \(v, w \in V\) and \(i\) denoting the imaginary unit. Possible surrogates include for instance...
• a power series of the form
\[ u(\theta, y) = \sum_{\nu \in \mathcal{F}} \theta_{\nu} y^{\nu} \]  
\[ (23) \]

• an orthogonal series of the form
\[ u(\theta, y) = \sum_{\nu \in \mathcal{F}} \theta_{\nu} P_{\nu} , \quad P_{\nu} := \prod_{j \geq 1} P_{\nu_j}(y_j) , \]  
\[ (24) \]
where \( P_k \) is the Legendre polynomial of degree \( k \) defined on \([-1, 1]\) and normalized with respect to the uniform measure, i.e., such that \( \int_{-1}^{1} |P_k(t)|^2 \, dt = 1 \).

• a neural network \( u(\theta, y) : \Theta \times U \to V, (\theta, y) \mapsto u(\theta, y) \) with \( L \in \mathbb{N} \) layers, defined by the recursion
\[ x_0 := y , \]
\[ x_\ell := \sigma(W_\ell x_{\ell-1} + b_\ell) , \quad \text{for } \ell = 1, \ldots, L - 1 , \]
\[ u(\theta, y) := W_L x_{L-1} + b_L . \]  
\[ (25) \]
Here the parameters \( \theta \in \Theta := \times_{\ell=1}^{L} (\mathbb{R}^{N_\ell \times N_{\ell-1} \times \mathbb{R}^{N_\ell}}) \) are a sequence of matrix-vector tuples
\[ \theta = ((W_\ell, b_\ell))_{\ell=1}^{L} = (W_1, b_1), (W_2, b_2), \ldots, (W_L, b_L) , \]
and the activation function \( \sigma \) is applied component-wise to vector-valued inputs.

• Gaussian process or kernel based approximations. Recently, a general framework for the approximation of solution of nonlinear pdes has been proposed in (Chen et al., 2021). The authors demonstrate the efficiency of Gaussian processes for nonlinear problems and derive a rigorous convergence analysis. We refer to (Chen et al., 2021) for more details, in particular also to the references therein.

• reduced basis or low rank approaches, which haven been demonstrated to efficiently approximate the solution of the forward problem even in high- or infinite dimensional settings (see e.g., Bachmayr et al., 2017; Rozza et al., 2008).

There has been a lot of research towards efficient surrogates, in particular in the case of parametric PDEs and the above list is by far not exhaustive. We provide in the following a general framework to train surrogates simultaneously with the optimization step and illustrate the ansatz for polynomial chaos and neural network approximations.

Based on the smoothness of the underlying function, approximation results of the above surrogates can be stated. To quantify the smoothness of the underlying function we will first recall the \((b, \epsilon)\)-holomorphy of a function, which is a sufficient criterion for many approximation results, see (Schwab and Zech, 2019) and the references therein. Given a monotonically decreasing sequence \( b = (b_j)_{j \in \mathbb{N}} \) of positive real numbers that satisfies \( b \in \)]
\( \ell^p(\mathbb{N}) \) for some \( p \in (0, 1] \), a continuous function \( u^y : U \to V \) is called \((b, \epsilon)\)-holomorphic if for any sequence \( \rho := (\rho_j)_{j \geq 1} \in [1, \infty)^N \), satisfying
\[
\sum_{j \geq 1} (\rho_j - 1) b_j \leq \epsilon,
\]
for some \( \epsilon > 0 \), there exists a complex extension \( \tilde{u} : B_\rho \to V_C \) of \( u \), where \( B_\rho := \times_{j \in \mathbb{N}} B_{\rho_j} \), with \( \tilde{u}(y) = u(y) \) for all \( y \in U \), such that \( w \mapsto \tilde{u}(w) : B_\rho \to V_C \) is holomorphic as a function in each variable \( z_j \in B_{\rho_j} \), \( j \in \mathbb{N} \) with uniform bound
\[
\sup_{w \in B_\rho} \| u(w) \|_{V_C} \leq C.
\]

From (Cohen and DeVore, 2015, Corollary 3.11) we know that a \((b, \epsilon)\)-holomorphic function admits an unconditionally convergent Taylor gpc expansion, i.e., the series in (23) with coefficients \( \theta_\nu := \frac{1}{\nu!} \partial^\nu u^y |_{y=0} \) converges unconditionally towards \( u^y \) in \( L^\infty(U, V) \). Moreover, let \( \Lambda_s \) be the set of indices that correspond to the \( s \) largest \( \| \theta_\nu \|_V \), then we have
\[
\sup_{y \in U} \| u^y - \sum_{\nu \in \Lambda_s} \theta_\nu y^\nu \|_V \leq C(s + 1)^{-\frac{1}{p} + \frac{1}{2}},
\]
with \( C = \| (\| \theta_\nu \|_V)_{\nu \in \mathcal{F}} \|_\ell^p < \infty \).

Furthermore, we known from (Cohen and DeVore, 2015, Corollary 3.10) that a \((b, \epsilon)\)-holomorphic function admits an unconditionally convergent Legendre series expansion, i.e., the series in (24) with coefficients \( \theta_\nu := \int_U u^y L_\nu(y) \, dy \) converges unconditionally towards \( u^y \) in \( L^2_{\mu}(U, V) \) with
\[
\| u - \sum_{\nu \in \Lambda_s} \theta_\nu P_\nu \|_{L^2_{\mu}(U, V)} \leq C(s + 1)^{-\frac{1}{p} + \frac{1}{2}},
\]
where \( C = \| (\| \theta_\nu \|_V)_{\nu \in \mathcal{F}} \|_\ell^p < \infty \) and \( \Lambda_s \) denotes the indices with the \( s \) largest \( \| \theta_\nu \|_V \).

More recent results (Schwab and Zech, 2019) show that \((b, \epsilon)\)-holomorphic functions, i.e., the parametric solution manifold \( U \ni y \mapsto u^y \in V \), can be expressed by a neural network of finite size. Therefore, let \( 0 < q_\nu \leq q_X < 2 \) and denote \( p_\nu := (1/q_\nu + 1/2)^{-1} \in (0, 1) \) and \( p_X := (1/q_X + 1/2)^{-1} \in (0, 1) \). Let \( \beta_\nu := (\beta_{\nu,j})_{j \in \mathbb{N}} \in (0, 1)^N \) and \( \beta_X := (\beta_{X,j})_{j \in \mathbb{N}} \in (0, 1)^N \) be monotonically decreasing sequences such that \( \beta_\nu \in \ell^{q_\nu}(\mathbb{N}) \) and \( \beta_X \in \ell^{q_X}(\mathbb{N}) \) and such that
\[
\left\| \sum_{j \in \mathbb{N}} \frac{\beta_{\nu,j}^{-1}|\psi_j(\cdot)|}{a_0(\cdot)} \right\|_{L^\infty(D)} < 1, \quad \left\| \sum_{j \in \mathbb{N}} \frac{\beta_{X,j}^{-1}|\psi_j(\cdot)|}{a_0(\cdot)} \right\|_{L^\infty(D)} < 1, \quad \left\| \sum_{j \in \mathbb{N}} \frac{\beta_{X,j}^{-1}|\psi_j'(\cdot)|}{L^\infty(D)} < \infty.
\]

Then (see Schwab and Zech, 2019, Theorem 4.8) there is a constant \( C > 0 \) such that for every \( s \in \mathbb{N} \), there exists a ReLU neural network (i.e., a neural network (25) with activation function \( \sigma(x) = \max(0, x) \)) denoted by \( u(\theta, y) \) with \( s + 1 \) input units and for a number \( \mathcal{N} \geq s \) with \( r = \min(1, (1 + p_\nu^{-1})(1 + p_X^{-1} + p_\nu^{-1})) \), it holds
\[
\sup_{y \in U} \| u^y - u(\theta, y) \|_V \leq CN^{-r}.
\]
Furthermore, for any \( s \in \mathbb{N} \) the size and depth of the neural network can be bounded by

\[
\begin{align*}
\text{size}(u(\theta, y)) & \leq C(1 + N \log (N) \log (\log (N))) \\
\text{depth}(u(\theta, y)) & \leq C(1 + \log (N) \log (\log (N))) ,
\end{align*}
\]

where the size of neural network is defined as the total number of nodes plus the total number of nonzero weights \( \text{size}(u(\theta, y)) := |\{(i, j, \ell) : (W_{i,j})_{\ell} \neq 0\}| + \sum_{\ell=0}^{L} N_{\ell} \) and the depth of a neural network \( \text{depth}(u(\theta, y)) = L - 1 \) is the number of hidden layers. Setting \( b := (\|\psi_{j}\|_{L^{\infty}(D)})_{j \in \mathbb{N}} \) and assuming in addition to (A2)-(A5) that \( b \in \ell^{p}(\mathbb{N}) \) for some \( p \in (0, 1) \), the parametric solution \( u_{y} \) of the uniformly elliptic problem (8) is \((b, \epsilon)-holomorphic\) (see e.g., Cohen and DeVore, 2015; Schwab and Zech, 2019). We conclude that the convergence results of the polynomial expansions and the approximation result of the neural network apply to the PDE problem at hand. We note also that the series expansions (23) and (24) are linear in its parameters \( \theta \), whereas the neural network is nonlinear in its parameters due to the nonlinear activation function \( \sigma \).

4. Consistency analysis

For the analysis in the following we assume that all spaces are finite dimensional. More precisely we make the following assumptions

- We discretize the spatial part of our problem using piecewise linear finite element basis functions on a regular, simplicial mesh of the domain \( D \). We denote the state space, spanned by the finite element basis functions, \( V_{h} \subset V \). For simplicity, we assume here and in the following that the finite dimensional state space \( V_{h} \) and the space of the controls \( V_{h}^{\prime} \subset V^{\prime} \) have the same dimension, which is of order \( h^{-d} \) and \( d \) is the dimension of \( D \).

- We assume finite-dimensional noise in our problem. More precisely, we assume that the sequence \( y \in U \) is now a \( s \)-dimensional vector in the \( s \)-dimensional space \( U_{s} := [-1,1]^{s} \). Consequently, the series in (4) becomes a sum, i.e., is truncated after \( s < \infty \) terms and the expected values in the following are integrals over the \( s \)-dimensional domain \( U_{s} \), i.e., \( \mathbb{E}[\cdot] := \int_{U_{s}} (\cdot) dy \).

- We use a \( N \)-point Monte Carlo approximation of the integral over the parametric domain \( U_{s} \).

Discretizing the problem in this way, we can state a convergence result for the reduced formulation (16) of the problem.

**Theorem 6** Let \( z^{\ast} \) be the solution of (16) and \( z_{s,h,N}^{\ast} \) the solution of the discretized problem. Then

\[
\|z^{\ast} - z_{s,h,N}^{\ast}\|_{L^{2}(D)} \leq C \alpha \left( \|z^{\ast}\|_{L^{2}(D)} + \|u_{0}\|_{L^{2}(D)} \right) \left( s^{-\frac{2}{p}+1} + h^{2} + N^{\frac{1}{2}} \right) ,
\]

where \( C > 0 \) is independent of \( s, h, N \) and \( y \in U \).
The result follows immediately from (Guth et al., 2021, Theorem 5.10) by replacing Quasi-Monte Carlo points with Monte Carlo points. The existence and uniqueness of the minimizer $z^*_{s,h,N}$ of the discretized problem follows from the fact that the convexity structure of the original problem is retained by the Monte Carlo approximation.

**Remark 7** In the following we think of elements $v_h \in V_h$, such as $z_{s,h,n}$, as a vectors containing the coefficients of the finite element discretization. By $\| \cdot \|$ we denote the Euclidean norm or the Euclidean norm weighted by the mass matrix in the corresponding finite-dimensional spaces. We will remark extensions to infinite-dimensional spaces in the following analysis where possible.

In our consistency analysis, we are going to analyse the proposed penalty method, see Section 2.3.1, w.r. to the penalty parameter $\lambda_k$ and the number of i.i.d. data point $N$, denoted as $(y^i)_{i=1}^N$, which are used to approximate the expected values w.r. to $y$. Here, we assume that $u_k^y$ has been parametrized by $u(\theta, y)$ and the penalty parameters $(\lambda_k)_{k \in \mathbb{N}}$ are monotonically increasing to infinity. In particular, we try to connect the following optimization problems:

1. The original constrained risk minimization (cRM) problem

$$\min_{z, \theta} \mathbb{E}_y [\| u(\theta, y) - u_0 \|^2] + \frac{\alpha}{2} \| z \|^2$$

subjected to

$$\mathbb{E}_y [\| e(u(\theta, y), z) \|^2] = 0.$$  

We assume there exists a unique solution of this problem, which we will denote by $(z^*_\infty, \theta^*_\infty)$.

2. The penalized risk minimization (pRM) problem

$$\min_{z, \theta} \mathbb{E}_y [\| u(\theta, y) - u_0 \|^2] + \frac{\alpha}{2} \| z \|^2 + \frac{\lambda_k}{2} \mathbb{E}_y [\| e(u(\theta, y), z) \|^2].$$  

(26)

We assume there exists a unique solution denoted by $(z^k_\infty, \theta^k_\infty)$.

3. The penalized empirical risk minimization (pERM) problem

$$\min_{z, \theta} \frac{1}{N} \sum_{i=1}^N \| u(\theta, y^i) - u_0 \|^2 + \frac{\alpha}{2} \| z \|^2 + \frac{\lambda_k}{2} \frac{1}{N} \sum_{i=1}^N \| e(u(\theta, y^i), z) \|^2.$$  

(27)

We assume there exists a unique solution denoted by $(z^k_\infty, \theta^k_\infty)$.

For simplicity, in the following we denote $x = (z, \theta) \in \mathcal{X} : = \mathbb{R}^n \times \mathbb{R}^d$ and define the functions

$$f : \mathcal{X} \times U \to \mathbb{R}_+, \quad \text{with} \quad f(x, y) = \| u(\theta, y) - u_0 \|^2 + \frac{\alpha}{2} \| z \|^2,$$

$$g : \mathcal{X} \times U \to \mathbb{R}_+, \quad \text{with} \quad g(x, y) = \| e(u(\theta, y), z) \|^2.$$
4.1 Convergence of pRM to cRM

We start with the error dependence on the penalty parameter $\lambda_k$. The following is a long known result (see e.g., Polyak, 1971, Theorem 1) providing unique existence of solutions as well as convergence towards the unconstrained problem for increasing penalty parameter $\lambda_k$.

**Theorem 8** Let $H_1$ and $H_2$ be two Hilbert spaces and let $f(x)$ be a functional on $H_1$ and the constraint $h(x)$ be an operator from $H_1$ into $H_2$. Moreover, suppose

- there exists a unique global minimizer $x^* \in \mathcal{X}$ of the problem
  $$\min_{x \in \mathcal{X}} f(x) \quad \text{s.t.} \quad h(x) = 0 \text{ in } H_2.$$

- that $\nabla_x f(x), \nabla_x^2 f(x)$ and $\nabla_x h(x), \nabla_x^2 h(x)$ exist with
  $$\|\nabla_x^2 f(x) - \nabla_x^2 f(y)\|_{L(H_1, L(H_1, \mathbb{R}))} \leq L_1 \|x - y\|_{H_1}$$
  and
  $$\|\nabla_x^2 h(x) - \nabla_x^2 h(y)\|_{L(H_1, L(H_1, H_2))} \leq L_2 \|x - y\|_{H_1}.$$

- the linear operator $\nabla_x h(x^*)$ is non-degenerate, i.e., $\|(\nabla_x h(x^*))^* y\|_{H_2} \geq c \|y\|_{H_2}$ for $c > 0$ and for all $y \in H_2$.

- the self-adjoint operator $\nabla_x^2 L(x^*, y^*)$ is positive definite, i.e., $\langle \nabla_x^2 L(x^*, y^*) \tilde{x}, \tilde{x} \rangle \geq m \|\tilde{x}\|_{H_1}^2$ for $m > 0$ and all $\tilde{x} \in H_1$. Here, the functional $L$ denotes the Lagrangian and the Lagrange multiplier rule is applicable because of the first three assumptions.

Then, for sufficiently large $\lambda_k > 0$, there exists a unique minimizer $x_k^*$ of the problem

$$\min_{x \in H_1} f(x) + \frac{\lambda_k}{2} \|h(x)\|_{H_2}^2$$

which satisfies

$$\|x_k^* - x^*\|_{H_1} \leq \frac{C}{2\lambda_k} \|y^*\|_{H_2} \quad \text{and} \quad \|\lambda_k h(x_k^*) - y^*\|_{H_1} \leq \frac{C}{2\lambda_k} \|y^*\|_{H_2}.$$ 

This theorem holds in infinite-dimensional Hilbert spaces $H_1$ and $H_2$, in that case the derivatives w.r. to $x \in H_1$ in the theorem are Fréchet derivatives. For the discretized problem at hand with $x = (\theta, z) \in \mathcal{X}$ the assumptions need to be satisfied for $f(x) := E[\|u(\theta, y) - u_0\|^2] + \frac{\rho}{2} \|z\|^2$, $h(x) = e(u(\theta, y, z))$ and $g(x) := \|h(x)\|^2$ based on the spaces $H_1 = \mathcal{X}$ and $H_2 = L^2(U, V_h)$. In this case the $H_1$-norm is just the Euclidean norm and the $H_2$-norm is $\| \cdot \|_{L^2(U, V_h)} := (\int_U \| \cdot \|^2 dy)^{1/2}$. The derivatives w.r. to $x \in H_1 = \mathcal{X}$ in the above theorem, then simplify to gradients and Hessian matrices.

If a surrogate satisfies the assumptions of the preceding theorem, the convergence of the minimizers of the (pRM) problem to the minimizer of the (cRM) problem is guaranteed.

**Lemma 9** Suppose that $f$ and $g$ satisfy the assumptions of Theorem 8. Then the solution of the pRM problem converges to the solution of the cRM problem, in the sense that there exists $C_1 > 0$ independent of $N$ such that

$$\| (z_k^\infty, \theta_k^\infty) - (z^\infty, \theta^\infty) \|^2 \leq \frac{C_1}{\lambda_k^2}.$$
4.2 Convergence of pERM to pRM

The following result describes the error arising due to the empirical approximation of the risk function uniformly in the penalization.

**Lemma 10** Suppose that \( f \) is convex and \( g \) is strongly convex in the sense that \( \nabla^2 x g(x, y) > m \cdot \text{id} \) for all \( x \in L^2(D) \times \mathbb{R}^d \) and \( y \in U \). Let \( \lambda_0 = 1 \) and assume that

\[
\text{Tr}(\text{Cov}_y (\nabla x (f(x, y)) + \frac{\lambda_0}{2} g(x, y))) < \infty.
\]

Then the solution of the pERM problem converges uniformly in \( \lambda_k \) to the solution of the pRM problem, in the sense that there exists \( C_2 > 0 \) independent of \( \lambda_k \) such that

\[
\mathbb{E}_y [\| (z_{\lambda N}^k, \theta_{\lambda N}^k) - (z_{\lambda \infty}^k, \theta_{\lambda \infty}^k) \|^2] \leq \frac{C_2}{N}.
\]

**Proof**

Under the above assumption the objective function in (27) is strongly convex. The unique solution \( x_{\lambda N}^k \) satisfies

\[
\frac{1}{N} \sum_{i=1}^{N} \nabla_x f(x_{\lambda N}^k, y^i) + \lambda_k \frac{1}{2} \frac{1}{N} \sum_{i=1}^{N} \nabla_x g(x_{\lambda N}^k, y^i) = 0.
\]

Similarly, the unique minimizer of (26) is characterized by

\[
\nabla_x \mathbb{E}_y [f(x_{\lambda \infty}^k, y)] + \lambda_k \frac{1}{2} \nabla_x \mathbb{E}_y [g(x_{\lambda \infty}^k, y)] = 0.
\]

We are now interested in the discrepancy of \( x_{\lambda N}^k \) and \( x_{\lambda \infty}^k \). We define the functions

\[
\Psi^k(x) = \mathbb{E}_y [f(x, y)] + \frac{\lambda_k}{2} \mathbb{E}_y [g(x, y)]
\]

and its empirical approximation

\[
\Psi_N^k(x) = \frac{1}{N} \sum_{i=1}^{N} f(x, y^i) + \frac{\lambda_k}{2} \frac{1}{N} \sum_{i=1}^{N} g(x, y^i).
\]

By the strong convexity of \( \Psi_N^k \), it follows that

\[
\| x_{\lambda N}^k - x_{\lambda \infty}^k \|^2 \leq \frac{1}{m \cdot \lambda_k} \langle x_{\lambda N}^k - x_{\lambda \infty}^k, \nabla_x \Psi_{\lambda N}^k(x_{\lambda N}^k) - \nabla_x \Psi_{\lambda N}^k(x_{\lambda \infty}^k) \rangle
\]

\[
= \frac{1}{m \cdot \lambda_k} \langle x_{\lambda N}^k - x_{\lambda \infty}^k, \nabla_x \Psi^k(x_{\lambda \infty}^k) - \nabla \Psi_{\lambda N}^k(x_{\lambda \infty}^k) \rangle
\]

using the stationarity of the minimizers. Applying the Cauchy–Schwarz inequality leads to

\[
\| x_{\lambda N}^k - x_{\lambda \infty}^k \| \leq \frac{1}{m \cdot \lambda_k} \| \nabla \Psi_{\lambda N}^k(x_{\lambda \infty}^k) - \nabla \Psi^k(x_{\lambda \infty}^k) \|.
\]
Next, we note that for \( \psi^k(x) := f(x, y) + \frac{\lambda_k}{2} g(x, y) \)
\[
\| \nabla \Psi_N^k(x_\infty) - \nabla_x \Psi_N^k(x_\infty) \|^2
\]
\[
= \text{Tr} \left( \left( \frac{1}{N} \sum_{i=1}^{N} \psi^k(x_\infty, y^i) - \mathbb{E}_y[\psi^k(x_\infty, y)] \right) \cdot \left( \frac{1}{N} \sum_{i=1}^{N} \psi^k(x_\infty, y^i) - \mathbb{E}_y[\psi^k(x_\infty, y)] \right) \right)^{\top}
\]
and by taking the expectation
\[
\mathbb{E}[\| \nabla \Psi_N^k(x_\infty) - \nabla_x \Psi_N^k(x_\infty) \|^2] = \frac{1}{N} \text{Tr}(\text{Cov}(\nabla_x \psi^k(x_\infty, y))).
\]
It holds that
\[
\text{Tr}(\text{Cov}(\nabla_x \psi^k(x, y))) = \text{Tr}(\text{Cov}(\nabla_x f(x, y) + \frac{\lambda_k}{2} \nabla_x g(x, y)))
\]
\[
= \text{Tr}(\text{Cov}(\nabla_x f(x, y) + \frac{\lambda_k}{2} \text{Cov}(\nabla_x f(x, y), \nabla_x g(x, y)))
\]
\[
+ \frac{\lambda_k}{2} \text{Cov}(\nabla_x g(x, y), \nabla_x f(x, y)) + \frac{\lambda_k^2}{4} \text{Cov}(\nabla_x g(x, y)))
\]
\[
\leq \text{Tr}(\max\{1, \frac{\lambda_k^2}{4}\}(\text{Cov}(\nabla_x f(x, y))) + \text{Cov}(\nabla_x f(x, y), \nabla_x g(x, y))
\]
\[
+ \text{Cov}(\nabla_x g(x, y), \nabla_x f(x, y)) + \text{Cov}(\nabla_x g(x, y)))
\]
\[
= \max\{1, \frac{\lambda_k^2}{4}\} \text{Tr}(\text{Cov}(\nabla_x \psi^0(x, y)))
\]
with \( \lambda_0 = 1 \). Finally, we obtain the bound
\[
\mathbb{E}[\| x_N^k - x_\infty^k \|^2] \leq C_{m, \lambda_k} \frac{1}{N} \text{Tr}(\text{Cov}(\nabla_x \psi^0(x, y))),
\]
where
\[
C_{m, \lambda_k} := \frac{1}{m^2} \max\{1, \frac{\lambda_k^2}{4}\} \leq \frac{1}{m^2}.
\]

### 4.3 Convergence of pERM to cRM

Finally, we are ready to prove consistency in the sense that solutions of the pERM converge to solutions of the original cRM. We can use Lemma 10 and Lemma 9 by applying
\[
\mathbb{E}[\| (z_N^k, \theta_N^k) - (z_\infty^k, \theta_\infty^k) \|^2] \leq 2 \mathbb{E}[\| (z_N^k, \theta_N^k) - (z_N^k, \theta_\infty^k) \|^2] + 2 \| (z_\infty^k, \theta_\infty^k) - (z_\infty^k, \theta_\infty^k) \|^2.
\]

**Theorem 11** Suppose \( f \) and \( g \) satisfy the assumptions of Lemma 9 and Lemma 10. Then the solution \((z_N^k, \theta_N^k)\) is consistent in the sense that there exists \( C_1, C_2 > 0 \) such that
\[
\mathbb{E}[\| (z_N^k, \theta_N^k) - (z_\infty^k, \theta_\infty^k) \|^2] \leq \frac{C_1}{\lambda_k^2} + \frac{C_2}{N}.
\]
For a surrogate that is linear in its parameters, i.e., \( u(\theta, z) = By\theta \), the first assumption of Theorem 8 (and thus Lemma 9) follows from the strong convexity of \( f \). The second assumption is clearly satisfied since for a linear surrogate, the constraint \( h \) is linear and hence the objective \( f \) is quadratic. The third assumption is true if we have for all \( y \in L^2_\mu(U, V_h) \) that

\[
\mathbb{E}[\| (\nabla_{(\theta,z)} h(\theta^*, z^*))^* y \|_X^2] \geq c \| y \|_{L^2_\mu(U, V_h)}^2.
\]

In the finite-dimensional setting the operator \((\nabla_{(\theta,z)} h(\theta^*, z^*))^* : L^2_\mu(U, V_h) \rightarrow \mathcal{X}\) simplifies to \((A^T B y, -\text{id})^T\), such that we have \(\mathbb{E}[\|((A^T B y, -\text{id})^T y\|^2_X] = \mathbb{E}[\|((B y)^T (A^T y)]^2_{\mathbb{R}^d} + \|y\|_{\mathbb{R}^n}^2] \geq \mathbb{E}[a^2_{\min} \sigma_{\min}(B y (B y)^T) + 1]\|y\|^2]. \) Hence, the third assumption is satisfied. Furthermore, from the linearity of the constraint follows that the Hessian of the Lagrangian simplifies to the Hessian of the objective function \(\nabla_x^2 f(\theta, z) = \text{diag}(\mathbb{E}[(B y)^T B y])\). The fourth condition is thus satisfied if \(\alpha > 0\) and \(\sigma_{\min}(\mathbb{E}[(B y)^T B y]) \geq M\) for some \(M > 0\).

5. Stochastic gradient descent for pRM problems

In order to solve the pRM problem we propose to apply the stochastic gradient descent (SGD) method. This means, instead of solving the pERM problem offline for large but fixed number of data \(N\), we solve the pRM online. Therefore, we further propose to adaptively increase the penalty parameter \(\lambda_k\) within the SGD.

We firstly formulate a general convergence result for the penalized SGD method, which we then apply in order to verify the convergence in the setting of our PDE-constrained optimization problem given by the cRM problem.

**Algorithm 1** Penalized stochastic gradient descent method with adaptive penalty parameter.

**Require:** \(x_0, \beta = (\beta_k)_{k=1}^n, (\lambda_k)_{k=1}^n, \) i.i.d. sample \((y^k)_{k=1}^n \sim y\).

1: for \(k = 0, 1, \ldots, n-1\) do
2: \(x_{k+1} = x_k - \beta_k \nabla_x [f(x_k, y^k) + \lambda_k g(x_k, y^k)]\)
3: end for

The sequence of step sizes \(\beta\) is assumed to satisfy the Robbins-Monro condition

\[
\sum_{j=1}^{\infty} \beta_k = \infty, \quad \sum_{j=1}^{\infty} \beta_k^2 < \infty,
\]

which means that \(\beta_k\) converges to zero, but not too fast (Robbins and Monro, 1951). In the following theorem we present sufficient conditions under which the resulting estimate \(x_n\) from Algorithm 1 converges to the solution of the pRM with penalty parameter choice \(\lambda \gg 0\), i.e., to

\[
x^* \in \arg \min_{x \in \mathbb{R}^n \times \mathbb{R}^d} \Psi_\lambda(x), \quad \Psi_\lambda(x) := \mathbb{E}_y[f(x, y) + \frac{\lambda}{2} g(x, y)].
\]
Theorem 12 We assume that the objective function satisfies
\[(x - x^*)^T (\nabla_x \Psi(x)) > c||x - x^*||^2 \tag{28}\]
for all \(x \in \mathbb{R}^n \times \mathbb{R}^d\) and some \(c > 0\) and that for each \(\lambda_k\) we have
\[\mathbb{E}_y[|\nabla_x[f(x, y) + \lambda_k g(x, y)]|^2] < a_k + b_k||x - x^*||^2, \tag{29}\]
where \((a_k)\) and \((b_k)\) are monotonically increasing with \(a_0, b_0 > 0\) and \(a_k \leq a, \ b_k \leq b\). Furthermore, we assume that in a compact subset \(M \subset \mathbb{R}^n \times \mathbb{R}^d\) with \(x^* \in M\) the discrepancy of the penalized stochastic gradients can be bounded by
\[\inf_{x \in M} \|\mathbb{E}_y[(\lambda_k - \bar{\lambda})\nabla_x g(x, y)]\|^2 \leq \kappa_1 |\lambda_k - \bar{\lambda}|^2, \tag{30}\]
for some \(\kappa_1 > 0\). Suppose that \(|\lambda_k - \bar{\lambda}|^2\) is monotonically decreasing and \(\beta_k \leq c/b_k\), then it holds true that
\[\mathbb{E}[\mathbb{I}_M(x_k)||x_k - x^*||^2] \leq \left(\mathbb{E}[||x_0 - x^*||^2 + 2\bar{a} \sum_{j=1}^{\infty} \beta_j^2] C_n + \frac{2\kappa_1 c^2}{\bar{c}^2} |\lambda_0 - \bar{\lambda}|^2,\right) \tag{31}\]
with
\[C_n := \min_{k \leq n} \max_{j \leq k+1} \{ \prod_{j=k+1}^{n} \left(1 - c\beta_j\right), \frac{\bar{a}}{\bar{c}} \beta_k \}\]
converging to zero for \(n \to \infty\). Further, for an adaptive choice of the penalty parameter \(\lambda_k\) such that \(\frac{2\kappa_1}{\bar{c}^2} |\lambda_k - \bar{\lambda}|^2 \leq D\beta_k\) we obtain
\[\mathbb{E}[\mathbb{I}_M(x_k)||x_k - x^*||^2] \leq \left(\mathbb{E}[||x_0 - x^*||^2 + 2(\bar{a} + \frac{D}{\bar{c}}) \sum_{j=1}^{\infty} \beta_j^2] C_n.\right) \tag{32}\]

Proof The basic idea of the proof is similar to the proof of Proposition 3.3 in (Chada et al. 2021). We denote \(\Delta_k = x_k - x^*\) and write the SGD update step as
\[\Delta_{k+1} = \Delta_k - \beta_k \nabla_x \Psi(\lambda_k(x_k)) + \beta_k \delta_k + \beta_k \xi_k\]
with
\[\delta_k = \nabla_x \Psi(x_k) - \nabla_x \Psi_{\lambda_k}(x_k), \quad \xi_k = \nabla_x \Psi_{\lambda_k}(x_k) - \nabla_x (f(x_k, y^k) + \lambda_k g(x_k, y^k)).\]
We note that
\[||- \nabla_x \Psi(x_k) + \delta_k ||^2 + \mathbb{E}[||\xi_k||^2 | \mathcal{F}_k] = \mathbb{E}[||\nabla_x (f(x_k, y) + \lambda_k g(x_k, y))||^2].\]
with \(\mathcal{F}_k = \sigma(y^m, m \leq k)\). Introducing the notation \(1^k_M := 1_M(x_k)\), we can bound the increments by
\[
\mathbb{E}[1^k_M||\Delta_{k+1}||^2 | \mathcal{F}_k] \leq 1^k_M \left(||\Delta_k||^2 - 2\beta_k \langle \Delta_k, \nabla_x \Psi_{\lambda_k}(x_k) - \delta_k \rangle + \beta_k \|\nabla \Psi_{\lambda_k}(x_k) + \delta_k \|^2 + \beta_k^2 \mathbb{E}[||\xi_k||^2 | \mathcal{F}_k]\right)
\leq 1^k_M \left(||\Delta_k||^2 - 2\beta_k c ||\Delta_k||^2 + 2\beta_k ||\Delta_k|| ||\delta_k|| + \beta_k^2 \mathbb{E}[||\nabla_x (f(x_k, y^k) + \lambda_k g(x_k, y^k))||^2]\right),
\]
where we have used the convexity assumption (28) and the Cauchy-Schwarz inequality. Using the variance bound (29) and applying Young’s inequality of the form $a \cdot b \leq \varepsilon/2a^2 + 2/\varepsilon b^2$ with $\varepsilon > 0$ leads to

$$
\mathbb{E}[\mathbb{I}_{M}^{k+1}\|\Delta_{k+1}\|^2 \mid \mathcal{F}_k] \leq \mathbb{I}_{M}^{k} \left( \|\Delta_k\|^2 - 2\beta_k \varepsilon \|\Delta_k\|^2 + 2\beta_k \frac{\varepsilon}{2} \|\Delta_k\|^2 + \beta_k \frac{1}{\varepsilon} \|\delta_k\|^2 \right. \\
+ \beta_k^2 a_k + \beta_k^2 b_k \|\Delta_k\|^2 \\
\left. \leq \mathbb{I}_{M}^{k} \left( \|\Delta_k\|^2 (1 - 2\beta_k \varepsilon + 2\beta_k \frac{\varepsilon}{2} + \beta_k^2 b_k) + \beta_k (\frac{\kappa_1}{\varepsilon} \|\lambda_k - \bar{\lambda}\|^2 + \beta_k a_k) \right) \right)
$$

where we have used (30). We set $\varepsilon = \frac{\delta}{2}$ such that we obtain with $\beta_k \leq \frac{\delta}{2\delta_k}$

$$
\mathbb{E}[\mathbb{I}_{M}^{k+1}\|\Delta_{k+1}\|^2 \mid \mathcal{F}_k] \leq (1 - c\beta_k) \mathbb{I}_{M}^{k} \|\Delta_k\|^2 + \beta_k (\frac{2\kappa_1}{c} \|\lambda_k - \bar{\lambda}\|^2 + \beta_k a_k)
$$

We apply the discrete Gronwall’s inequality and obtain

$$
\mathbb{E}[\mathbb{I}_{M}^{n}\|\Delta_n\|^2] \leq \sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) a_k \beta_k^2 \right) \\
+ \frac{2\kappa_1}{c} \sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) \|\lambda_k - \bar{\lambda}\|^2 \beta_k \right) \\
+ \exp \left( -c \sum_{k=1}^{n} \beta_k \right) \mathbb{E}[\|\Delta_0\|^2].
$$

First note that $|\lambda_k - \bar{\lambda}|^2 \leq |\lambda_0 - \bar{\lambda}|^2$, then it holds true that

$$
\frac{2\kappa_1}{c} \sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) \|\lambda_k - \bar{\lambda}\|^2 \beta_k \right) \\
\leq \frac{2\kappa_1}{c^2} |\lambda_0 - \bar{\lambda}|^2 \sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k \right) \leq \frac{2\kappa_1}{c^2} |\lambda_0 - \bar{\lambda}|^2
$$

and with (31) we obtain

$$
\mathbb{E}[\mathbb{I}_{M}^{n}\|\Delta_n\|^2] \leq \bar{a} \sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k^2 \right) + \frac{2\kappa_1}{c^2} |\lambda_0 - \bar{\lambda}|^2 \\
+ \exp \left( -c \sum_{k=1}^{n} \beta_k \right) \mathbb{E}[\|\Delta_0\|^2].
$$

Similarly, assuming that $\frac{2\kappa_1}{c^2} |\lambda_k - \bar{\lambda}|^2 \leq D\beta_k$ gives

$$
\mathbb{E}[\mathbb{I}_{M}^{n}\|\Delta_n\|^2] \leq (\bar{a} + D/c) \sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k^2 \right) + \exp \left( -c \sum_{k=1}^{n} \beta_k \right) \mathbb{E}[\|\Delta_0\|^2].
$$
For the details of proving that
\[
\sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c_j \beta_j) \beta_k^2 \right) \leq \left( \sum_{k=1}^{\infty} \beta_k^2 \right) C_n, \quad \exp \left( -c \sum_{k=1}^{n} \beta_k \right) \leq C_n
\]
and the fact that \( C_n \) converges to 0 we refer the reader to the proof of Proposition 3.3 in (Chada et al., 2021).

\[\text{Remark 13} \quad \text{We note that the restriction on the compact subset } M \subset \mathbb{R}^n \times \mathbb{R}^d \text{ is a technical reason for the proof and can be forced through a projection onto } M \text{ by}
\]
\[\mathcal{P}_M : \mathbb{R}^n \times \mathbb{R}^d \to M, \quad \text{with} \quad \mathcal{P}_M(x) = \arg \min_{x' \in M} \|x - x'\|.
\]
The projected stochastic gradient descent method then evolves through the update
\[x_{k+1} = \mathcal{P}_M \left( x_k - \beta_k \nabla_x [f(x_k, y^k) + \lambda_k g(x_k, y^k)] \right).
\]
The above proof remains the same since the projection operator is nonexpansive in the sense that
\[\|x_{k+1} - x^*\| = \|\mathcal{P}_M \left( x_k - \beta_k \nabla_x [f(x_k, y^k) + \lambda_k g(x_k, y^k)] \right) - \mathcal{P}_M(x^*)\|^2
\]
\[\leq \|x_k - \beta_k \nabla_x [f(x_k, y^k) + \lambda_k g(x_k, y^k)] - x^*\|^2.
\]

\[\text{5.1 Application to linear surrogate models}
\]
In this section we verify that a surrogate, that is linear in its parameters, satisfies the assumptions of Theorem 12. Therefore, we assume in this section that the surrogate is of the following form:
\[u(\theta, y) := B^y \theta \quad \text{(32)}
\]
for surrogate parameters \( \theta \in \mathbb{R}^d \) and \( y \)-dependent matrices \( B^y \). The following two lemmas will help to prove this result:

\[\text{Lemma 14} \quad \text{Let } g(x, y) := \|e(u(\theta, y), z)\|^2, \text{ with } e(u(\theta, y), z) := A^y u(\theta, y) - z = A^y B^y \theta - z, \text{ where } x = (\theta, z), \text{ and with bounded largest eigenvalue } \sigma_{\text{max}}(A^y) \leq a_{\text{max}} \text{ for all } y \in U. \text{ Then it holds that}
\]
\[\|\nabla_x g(x, y)\|^2 \leq 4(a_{\text{max}}^2 \sigma_{\text{max}}(B^y(B^y)^\top) + 1) g(x, y).
\]

\[\text{Proof} \quad \text{We have}
\]
\[\|\nabla_x g(x, y)\|^2 = 2(A^y B^y)^\top (A^y B^y \theta - z))^2 + 2(z - A^y B^y \theta)^2
\]
\[= 4(a_{\text{max}}^2 \sigma_{\text{max}}(B^y(B^y)^\top) + 1) \|A^y B^y \theta - z\|^2
\]
\[= 4(a_{\text{max}}^2 \sigma_{\text{max}}(B^y(B^y)^\top) + 1) g(x, y).
\]
Lemma 15 Let \( g(x, y) := \|e(u(\theta, y), z)\|^{2} \), with \( e(u(\theta, y), z) := A^{y} u(\theta, y) - z = A^{y} B^{y} \theta - z \), where \( x = (\theta, z) \), and with bounded largest eigenvalue \( \sigma_{\max}(A^{y}) \leq a_\max \) for all \( y \in U \). Then it holds that
\[
g(x, y) \leq 2(a_\max^{2} \sigma_{\max}((B^{y})^{T} B^{y}) + 1)\|x\|^{2}.
\]

Proof
\[
g(x, y) = \|A^{y} B^{y} \theta - z\|^{2} \leq 2(\|A^{y} B^{y} \theta\|^{2} + \|z\|^{2})
\[
\leq 2(a_\max^{2} \sigma_{\max}((B^{y})^{T} B^{y})\|\theta\|^{2} + \|z\|^{2})
\[
\leq 2(a_\max^{2} \sigma_{\max}((B^{y})^{T} B^{y}) + 1)\|x\|^{2}.
\]

\[
\square
\]

Theorem 16 Let \( \alpha > 0 \) and \( B^{y} \) injective for all \( y \in U \), then a surrogate of the form (32) satisfies the assumptions of Theorem 12.

Proof Firstly, we show that
\[
\inf_{x \in \mathbb{R}^{n} \times \mathbb{R}^{d}} (x - x^{*})^{T} \nabla_{x} \Psi_{\lambda}(x) > c\|x - x^{*}\|^{2}
\]
is true for a constant \( c > 0 \). To verify this assumption, we first show that \( \Psi_{\lambda} \) is \( c \)-strongly convex. The \( c \)-strong convexity is equivalent to
\[
(x - x^{*})^{T} (\nabla_{x} \Psi_{\lambda}(x) - \nabla_{x} \Psi_{\lambda}(x^{*})) \geq c\|x - x^{*}\|^{2}.
\]

Using the linearity of the surrogate in its parameters, i.e., \( u(\theta, y) := B^{y} \theta \), we obtain
\[
(x - x^{*})^{T} (\nabla_{x} \Psi_{\lambda}(x) - \nabla_{x} \Psi_{\lambda}(x^{*}))
\]
\[
= (\theta - \theta^{*}, z - z^{*})^{T} \mathbb{E}[(2(B^{y})^{T} B^{y} + \lambda(A^{y} B^{y})^{T} (A^{y} B^{y}))(\theta - \theta^{*})
\]
\[
- \lambda(A^{y} B^{y})^{T}(z - z^{*}), (\alpha + \bar{\lambda})(z - z^{*}) - \bar{\lambda}A^{y} B^{y}(\theta - \theta^{*}))]
\]
\[
= 2(\theta - \theta^{*})^{T} \mathbb{E}[(B^{y})^{T} B^{y}](\theta - \theta^{*}) + \bar{\lambda}\|A^{y} B^{y}(\theta - \theta^{*})\|^{2} - (\theta - \theta^{*})^{T} \lambda(A^{y} B^{y})^{T}(z - z^{*})
\]
\[
+ (\alpha + \bar{\lambda})\|z - z^{*}\|^{2} - (z - z^{*})^{T} \lambda A^{y} B^{y}(\theta - \theta^{*})
\]
\[
= 2(\theta - \theta^{*})^{T} \mathbb{E}[(B^{y})^{T} B^{y}](\theta - \theta^{*}) + \alpha\|z - z^{*}\|^{2} + \bar{\lambda}\|(z - z^{*}) - A^{y} B^{y}(\theta - \theta^{*})\|^{2}
\]
\[
\geq 2(\theta - \theta^{*})^{T} \mathbb{E}[(B^{y})^{T} B^{y}](\theta - \theta^{*}) + \alpha\|z - z^{*}\|^{2}
\]
\[
\geq c\|x - x^{*}\|^{2},
\]
where \( c = \min(2\sigma_{\min}(\mathbb{E}[(B^{y})^{T} B^{y}]), \alpha) \). Noting that \( x^{*} \) is a stationary point of \( \Psi_{\lambda}(x) \), we conclude that the assertion is true if \( B^{y} \) is injective for all \( y \in U \).

Secondly, we show that
\[
\mathbb{E}[\|\nabla_{x}(f(x, y) + \lambda_{k} g(x, y))\|^{2}] \leq a_{k} + b_{k}\|x - x^{*}\|^{2}.
\]
For a stationary point $x^*$ of $\Psi_\lambda(x)$ have that

$$0 = \nabla_x (f(x^*, y) + \bar{\lambda} g(x^*, y))$$

and thus

$$\|\nabla_x (f(x, y) + \lambda_k g(x, y))\|^2 = \|\nabla_x (f(x, y) + \lambda_k g(x, y)) - \nabla_x (f(x^*, y) + \bar{\lambda} g(x^*, y))\|^2$$

$$= \|\nabla_x f(x, y) - \nabla_x f(x^*, y) + \lambda_k \nabla_x g(x, y) - \bar{\lambda} \nabla_x g(x^*, y)\|^2$$

$$\leq 2\|\nabla_x (f(x, y) - f(x^*, y))\|^2 + 2\|\lambda_k \nabla_x g(x, y) - \bar{\lambda} \nabla_x g(x^*, y)\|^2.$$ 

For the first summand we have $\nabla_x (f(x, y) - f(x^*, y)) = ((2(B^y)^\top B^y)(\theta - \theta^*), \alpha(z - z^*))$ and thus

$$\mathbb{E}[\|\nabla_x (f(x, y) - f(x^*, y))\|^2] \leq \bar{c}^2\|x - x^*\|^2,$$

with $\bar{c} = 2\mathbb{E}[\sigma_{\text{max}}((B^y)^\top B^y)] + \alpha$. Moreover, for the second summand we have

$$\nabla_x (\lambda_k g(x, y) - \bar{\lambda} g(x^*, y)) = (2(A^y B^y)\top (A^y B^y)(\lambda_k \theta - \bar{\lambda} \theta^*)$$

$$-(\lambda_k z - \bar{\lambda} z^*), 2((\lambda_k z - \bar{\lambda} z^*) - A^y B^y(\lambda_k \theta - \bar{\lambda} \theta^*))$$

$$= \nabla_x g(\lambda_k x - \bar{\lambda} x^*, y).$$

We can use this together with Lemma 14 and Lemma 15 to obtain

$$\mathbb{E}[\|\nabla_x g(\lambda_k x - \bar{\lambda} x^*, y)\|^2]$$

$$\leq \mathbb{E}[4(a_{\text{max}}^2 \sigma_{\text{max}}(B^y(B^y)^\top) + 1)g(\lambda_k x - \bar{\lambda} x^*, y)]$$

$$\leq \mathbb{E}[4(a_{\text{max}}^2 \sigma_{\text{max}}(B^y(B^y)^\top) + 1)2(a_{\text{max}}^2 \sigma_{\text{max}}((B^y)^\top B^y) + 1)\|\lambda_k x - \bar{\lambda} x^*\|^2]$$

$$= 8(a_{\text{max}}^4 \mathbb{E}[\sigma_{\text{max}}((B^y)^\top B^y)\sigma_{\text{max}}(B^y(B^y)^\top)] + 1$$

$$+ a_{\text{max}}^2 (\mathbb{E}[\sigma_{\text{max}}((B^y)^\top B^y)] + \sigma_{\text{max}}(B^y(B^y)^\top))\|\lambda_k x - \bar{\lambda} x^*\|^2$$

$$\leq 8(a_{\text{max}}^4 \mathbb{E}[\sigma_{\text{max}}((B^y)^\top B^y)\sigma_{\text{max}}(B^y(B^y)^\top)] + 1$$

$$+ a_{\text{max}}^2 (\mathbb{E}[\sigma_{\text{max}}((B^y)^\top B^y)] + \sigma_{\text{max}}(B^y(B^y)^\top)))$$

$$\times 2(\lambda_k^2\|x - x^*\|^2 + (\lambda_k - \bar{\lambda})^2\|x^*\|^2).$$

We conclude that

$$\mathbb{E}[\|\nabla_x (f(x, y) + \lambda_k g(x, y))\|^2] \leq a_k + b_k\|x - x^*\|^2$$

holds for $a_0 \geq a_k = 2C_{ab}2(\lambda_k - \bar{\lambda})^2\|x^*\|$ and $b_k = 2\bar{c}^2 + 2C_{ab}2\lambda_k^2$, where $C_{ab} = 8(a_{\text{max}}^4 \mathbb{E}[\sigma_{\text{max}}((B^y)^\top B^y)\sigma_{\text{max}}(B^y(B^y)^\top)] + 1 + a_{\text{max}}^2 (\mathbb{E}[\sigma_{\text{max}}((B^y)^\top B^y)] + \sigma_{\text{max}}(B^y(B^y)^\top))).$

Thirdly, we show that

$$\inf_{x \in M} \mathbb{E}[(\lambda_k - \bar{\lambda})\nabla_x g(x, y)]^2 \leq \kappa_1 |\lambda_k - \bar{\lambda}|^2,$$

for some $\kappa_1 > 0$. 

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We observe that
\[
\|E[(\lambda_k - \bar{\lambda})\nabla_x g(x, y)]\|^2 \leq |\lambda_k - \bar{\lambda}|^2 \|E[\nabla_x g(x, y)]\|^2
\]
\[
\leq |\lambda_k - \bar{\lambda}|^2 E[\|\nabla_x g(x, y)\|^2]
\]
\[
\leq |\lambda_k - \bar{\lambda}|^2 E[4(a_{\text{max}}\sigma_{\text{max}}(B^y(B^y)^\top) + 1)g(x, y)]
\]
\[
\leq |\lambda_k - \bar{\lambda}|^2 E[4(a_{\text{max}}\sigma_{\text{max}}(B^y(B^y)^\top) + 1)
\times 2(a_{\text{max}}\sigma_{\text{max}}((B^y)^\top B^y) + 1)||x||^2].
\]

This inequality then clearly holds for the infimum over the compact set $M$, so we have shown the assertion for $\kappa_1 = E[4(a_{\text{max}}\sigma_{\text{max}}(B^y(B^y)^\top) + 1) 2(a_{\text{max}}\sigma_{\text{max}}((B^y)^\top B^y) + 1)||x||^2]$. 

6. Numerical Experiments

The model problem in our numerical experiments is the Poisson equation, (1) (2), on the unit square $D = (0, 1)^2$. We use piecewise-linear finite elements on a uniform triangular mesh with meshwidth $h = 1/8$. The random input field is modelled as
\[
a^y(x) = a_0(x) + \sum_{j=1}^s y_j \frac{1}{(\pi^2(k_j^2 + \ell_j^2) + \tau^2)\vartheta} \sin(\pi x_k k_j) \sin(\pi x_\ell \ell_j),
\]
where $a_0(x) = 0.00001 + \|\sum_{j=1}^s \frac{1}{(\pi^2(k_j^2 + \ell_j^2) + \tau^2)\vartheta} \sin(\pi x_k k_j) \sin(\pi x_\ell \ell_j)\|_{L^\infty(D)}$, $s = 4$, $\vartheta = 0.25$, $\tau = 3$, $(k_j, \ell_j) j \in \{1, \ldots, s\}^2$ and $y_j \sim \mathcal{U}([-1, 1])$ i.i.d. for all $j = 1, \ldots, s$. The variance of the resulting PDE solution $u^y$, with right-hand side $z(x) = x_2^2 - x_1^2$, is illustrated in Figure 1 and Figure 2. The mean and standard deviation is estimated using $10^5$ Monte Carlo samples.

In the following numerical experiments we solve the (pERM) problem
\[
\min_{(z, \theta)} \frac{1}{N} \sum_{i=1}^N \|u(\theta, y) - u_0\|^2 + \frac{\alpha}{2} \|z\|^2 + \lambda_k \frac{1}{N} \sum_{i=1}^N \|A^y u(\theta, y) - z\|^2.
\]
where $\alpha = 0.5$ and the target state $u_0$ is given as $u_0 = \Delta^{-1}100(x_2^2 - x_1^2)$. We solve the optimization problem using the ADAM algorithm as implemented in \texttt{tensorflow} and the \texttt{scipy} implementation of the L-BFGS method. The initial guess for the optimization routines is $(z_0, \theta_0)$ with $z_0 = (0, \ldots, 0) \in \mathbb{R}^n$ and $\theta_0 = (1, \ldots, 1) \in \mathbb{R}^d$. In our experiments we compared to two different surrogate models: the orthogonal Legendre polynomials, which are linear in the parameters $\theta$ and a neural network, which is nonlinear in the parameters $\theta$.

Recall the polynomial expansion from (24): $u(\theta, y) = \sum_{\nu \in \mathbb{N}_0} \theta_\nu P_\nu(y)$ of degree $\ell = 1, 2, 3$, with $P_\nu = \prod_{k=1}^s P_{k_\nu}(y_k)$ and $P_{k_\nu}$ is the k-th order Legendre polynomial. The number of parameters $\theta$ increases rapidly as the order of the polynomials increases. In fact, $\theta \in \mathbb{R}^{n_{\text{FEM}} \times n_{\text{Pol}}}$, where $n_{\text{FEM}}$ denotes the number of degrees of freedoms of the finite element.
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method and $n_{\text{Pol}}$ denotes the number of polynomials given by $n_{\text{Pol}} = \frac{(\ell+s)!}{\ell!s!}$, i.e., $n_{\text{Pol}} = 15$ if $\ell = 2$ and $n_{\text{Pol}} = 35$ if $\ell = 3$ for $s = 4$. Consequently, the Legendre polynomial expansions have 245, 735, and 1715 parameters to be determined during the optimization.

A nonlinear surrogate we are testing is a neural network, as defined in (25) of size $[4, 9, 9, 49]$, i.e., with a total number of 715 parameters. The activation function we are using is the sigmoid function $\sigma(x) := \frac{1}{1 + \exp(-x)}$.

In our first experiment, we verify Lemma 10. To this end, we set $\lambda_k = 1$ for all $k$ and solve the (pERM) problem multiple times for increasing sample size $N = 2^\ell$, with $\ell = 1, \ldots, 13$. In this experiment the surrogate is a Legendre polynomial expansion of degree 2. The reference solution $(z_{\text{ref}}, \theta_{\text{ref}})$ is computed by using $N_{\text{ref}} = 2^{14}$ Monte Carlo samples. The observed rate in Figure 3 aligns nicely with the predicted rate in Lemma 10.

Next, we verify Lemma 9. We fix the sample size $N = 100$ and solve the (pERM) problem for increasing penalty parameter $\lambda_k$. The surrogate in this experiment is again the Legendre polynomial expansion of degree 2. In Figure 4 we observe the rate predicted by Lemma 9. Here the reference solution is computed for $\lambda_k \approx 1.7 \cdot 10^6$. For numerical stability we regularize the problem in this experiment by adding the term $10^{-5}\|\theta\|^2$ to the objective function of the (pERM) problem.

As predicted by the theory, we also observe this rate in the following experiment, where we use the ADAM algorithm as implemented in tensorflow and increase $\lambda_k$ linearly in each iteration $k$ of the ADAM algorithm. The reference solution $(z_{\text{ref}}, u_{\text{ref}})$ of the (cRM) problem is computed using the L-BFGS as implemented in scipy. We perform this experiment for the NN and the Legendre polynomial expansions of order 1, 2 and 3. For each of the surrogates considered, we observe the expected rate of the error in the control, see
Figure 3: Convergence for increasing sample size. Squared error of the optimal controls $\| z - z_{\text{ref}} \|^2$ and squared error of the optimal surrogate parameters $\| \theta - \theta_{\text{ref}} \|^2$.

Figure 4: Convergence for increasing penalty parameter $\lambda_k$. Squared error of the optimal controls $\| z - z_{\text{ref}} \|^2$ and squared error of the optimal surrogate parameters $\| \theta - \theta_{\text{ref}} \|^2$.

Figure 5: Mean squared error of control computed with surrogate and L-BFGS reference solution of the control $\| z - z_{\text{ref}} \|^2$

Figure 6: Mean squared error of surrogate and L-BFGS reference solution of the state $\mathbb{E}[\| u^y_{\theta} - u^y_{\text{ref}} \|^2]$
Figure 5. Clearly, this error is bounded from below by the approximation properties of the surrogates. In Figure 6 we observe the predicted rate only for the largest surrogate, the Legendre polynomial approximation of order 3.

In the same experiment we plot the model error and the difference of the surrogates to the target state \( u_0 \). We observe that the model error is smaller for surrogates with better approximation properties.

Moreover, due to the nonlinearity introduced by the activation function of the NN, our convergence theory does not apply to the problem with the NN surrogate. However, the numerical experiments are demonstrating that the NN can outperform the Legendre polynomials with a comparable number of optimization parameters.

![Graph showing mean squared residual](image)

Figure 7: Mean squared residual

\[ \mathbb{E}[\|A_y u_y - z\|^2] \]

![Graph showing mean squared error](image)

Figure 8: Mean squared error \( \mathbb{E}[\|u_y - u_0\|^2] \) of the surrogate \( u_y \) and the target state \( u_0 \)

Finally, we verify that the ADAM algorithm with adaptive choice of the penalty parameter converges to the solution of the (pERM) problem with large reference value \( \bar{\lambda} \), see Theorem 12. We compute the reference solution \((z_{\text{ref}}, u_{y_{\text{ref}}})\) with \( \bar{\lambda} = 100 \) using the L-BFGS algorithm and plot the error of the ADAM algorithm with adaptive choice of the penalty parameter \( \lambda_k \) against the iterations \( k \) of the ADAM algorithm. We observe convergence for both, the control and the state. The surrogate in this experiment is a Legendre polynomial expansion of degree 2.

7. Conclusions

We proposed a flexible framework for the incorporation of machine learning approximations for optimization under uncertainty. The surrogate is trained only for the optimal control, i.e., no expensive offline training is needed. Further, the one-shot approach allows to consider much smaller surrogates, as the complexity of the underlying approximation problem is significantly reduced by the suggested approach. The numerical experiments show promising results and application to more complex optimization problems under uncertainty will be subject to future work.
We analyzed the stochastic gradient method for the optimization of the one-shot system. In more complex situations, gradients might not be available due to the use of black-box solvers or computational limits. We will explore the generalization of our work to derivative-free optimization techniques, in particular to Kalman based methods, in order to ensure applicability also in this setting.

The penalty approach, which can be motivated by the Bayesian ansatz (cp. Guth et al., 2020), provides an algorithmic framework ensuring the feasibility of the control w.r. to the forward model. The Bayesian viewpoint will guide further work to adaptively learn the penalty function and incorporate model error.

Acknowledgments

PG is grateful to the DFG RTG1953 “Statistical Modeling of Complex Systems and Processes” for funding of this research. The authors acknowledge support by the state of Baden-Württemberg through bwHPC.

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