Optimization-Based Estimation of Random Distributed Parameters in Elliptic Partial Differential Equations
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Abstract—As simulation continues to replace experimentation in the design cycle, the need to quantify uncertainty in model outputs due to uncertainties in the model parameters becomes critical. For distributed parameter models, current approaches assume the mean and variance of parameters are known, then use recently developed efficient numerical methods for approximating stochastic partial differential equations. However, the statistical descriptions of the model parameters are rarely known. A number of recent works have investigated adapting existing variational methods for parameter estimation to account for parametric uncertainty. In this paper, we formulate the parameter identification problem as an infinite dimensional constrained optimization problem for which we establish existence of minimizers and the first order necessary conditions. A spectral approximation of the uncertain observations (via a truncated Karhunen-Loève expansion) allows an approximation of the infinite dimensional problem by a smooth, albeit high dimensional, deterministic optimization problem, the so-called ‘finite noise’ problem, in the space of functions with bounded mixed derivatives. We prove convergence of ‘finite noise’ minimizers to the corresponding infinite dimensional solutions, and devise a gradient based strategy for locating these numerically. Lastly, we illustrate our method with a numerical example.

I. INTRODUCTION

We discuss a variational approach to estimating the parameter $q$ in the elliptic system

$$-\nabla \cdot (q \nabla u) = f \quad \text{on} \quad D \subset \mathbb{R}^d, \quad u = 0 \quad \text{on} \quad \partial D,$$

based on noisy measurements $\hat{u}$ of $u$, when $q$ is modeled as a spatially varying random field. Variational formulations, where the identification problem is posed as a constrained optimization, have been studied extensively for the case when $q$ is deterministic, cf. [1], [2], [3], [4], [5]. The aleatoric uncertainty in these problems arising from imprecise, noisy measurements, variability in operating conditions, or unresolved scales are traditionally modeled as perturbations and addressed by means of regularization techniques. These techniques approximate the original inverse problem by one in which the parameter depends continuously on the data $\hat{u}$, thus ensuring an estimation error commensurate with the noise level. However, when a statistical model for uncertainty in the system is available, it is desirable to incorporate this information more directly into the estimation framework to obtain an approximation not only of $q$ itself but also of its probability distribution.

Bayesian methods provide a sampling-based approach to statistical parameter identification problems with random observations $\hat{u}$. By relating the observation noise in $\hat{u}$ to the uncertainty associated with the estimated parameter via Bayes’ Theorem [6], [7], these methods allow us to sample directly from the joint distribution of $q$ at a given set of spatial points, through repeated evaluation of the deterministic forward model. The computational efficiency of numerical implementations of Bayesian methods, most notably Markov chain Monte Carlo schemes, depends predominantly on the statistical complexity of the input $q$ and the measured output $\hat{u}$, as well as the cost of evaluating the forward model.

There has also been continued interest in adapting variational methods to estimate parameter uncertainty, e.g. [8], [9], [10], [11]. Benefits include a well-established infrastructure of existing theory and algorithms, the possibility of incorporating multiple statistical influences arising from uncertainty in boundary conditions or source terms for instance, and clearly defined convergence criteria. The present work follows this approach. Thus, let $(\Omega, \mathcal{F}, d\omega)$ be a complete probability space and suppose we have a statistical model of the measured data $\hat{u}$ in the form of a random field $\hat{u} = \hat{u}(x, \omega)$ contained in the tensor product $\mathcal{H}(D) := H^1_0(D) \otimes L^2(\Omega)$. A least squares formulation of the parameter identification problem in (1), when $q(x, \omega)$ is a random field, may take the form

$$\min_{(q, \omega) \in \mathcal{H} \times \mathcal{H}_0} J(q, \omega) := \frac{1}{2} \| u - \hat{u} \|^2_{\mathcal{H}_0} + \beta \| q \|^2_{\mathcal{H}_0} \quad \text{s.t.} \quad \omega \in \mathcal{Q}_{ad}, \quad e(q, \omega) = 0,$$

where the regularization term with $\beta > 0$ is added to ensure continuous dependence of the minimizer on the data $\hat{u}$. Here $\mathcal{H}_0 := H(D) \otimes L^2(\Omega)$, where $H(D)$ is any Hilbert space that imbeds continuously in $L^\infty(D)$, which may be taken to be the Sobolev space $H^1(D)$ when $d = 1$ or $H^2(D)$ when $d = 2, 3$ (see [2]). The feasible set $\mathcal{Q}_{ad}$ is given by

$$\mathcal{Q}_{ad} = \{ q \in \mathcal{H}_0 : 0 < q_{\min} \leq q(x, \omega) \text{ a.s. on } D \times \Omega, \quad \| q(\cdot, \omega) \|_H \leq q_{\max} \text{ a.s. on } \Omega \}.$$

while the stochastic equality constraint $e(q, \omega) = 0$ can be written in it’s weak form as

$$\int_{\Omega} \int_D q(x, \omega) \nabla \phi(x, \omega) \cdot \nabla \psi(x, \omega) \, dx \, d\omega = \int_{\Omega} \int_D f(x) \psi(x, \omega) \, d\omega, \quad \forall \psi \in \mathcal{H}_0(D),$$

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where \( u \in \widetilde{H}^1_0(D) \) [12]. We assume for the sake of simplicity that \( f \in L^2(D) \) is deterministic.

This formulation poses a number of theoretical, as well as computational challenges. The lack of smoothness of the random field \( q = q(x, \omega) \) in its stochastic component \( \omega \) limits the regularity of the equality constraint as a function of \( q \), making it difficult to reuse the theory from the deterministic case to establish first order necessary optimality conditions, as will be shown in Section II. The most significant computational hurdle is the need to approximate stochastic integrals required when evaluating the cost functional \( J \) and when imposing with the equality constraint (2). Monte Carlo type schemes are inefficient, especially when compared with Bayesian methods. However, the recent success of stochastic Galerkin methods [12], [13] and stochastic collocation approaches [12], [14] to efficiently estimate the integrals appearing in stochastic (forward) problems has motivated investigations into their potential use for inverse and design problems.

In forward simulations, collocation methods make use of spectral expansions, such as the Karhunen-Łoève (KL) series, to approximate the known input random field \( q \) by a smooth function of finitely many random variables, a so-called ‘finite noise’ approximation. Standard PDE regularity theory [12] ensures that the corresponding model output \( u \) depends smoothly (even analytically) on these random variables. This facilitates the use of high-dimensional quadrature techniques, based on sparse grid interpolation by high order global polynomials. Inverse problems on the other hand are generally ill-posed and consequently any smoothness of a ‘finite noise’ approximation of the given measured data \( \hat{u} \) does not necessarily carry over to the unknown parameter \( q \). In variational formulations, explicit assumptions should therefore be made on the smoothness of ‘finite noise’ approximations of \( q \) to facilitate efficient implementation, while also accurately estimating problem (P).

We approximate (P) in the space of functions with bounded mixed derivatives. Posing the ‘finite noise’ minimization problem \( (P^n) \) in this space not only guarantees that the equality constraint \( e(q, u) \) is twice Fréchet differentiable in \( q \) (see Section IV), but also allows for the use of numerical discretization schemes based on hierarchical finite elements, approximations known for their effectiveness in mitigating the curse of dimensionality [15]. In [10], Zabaras et al. demonstrate the use of piecewise linear hierarchical finite elements to approximate ‘finite noise’ design parameters in least squares formulations of heat flux control problems subject to system uncertainty with gradient-based methods.

This paper aims to provide a rigorous framework within which to analyze and numerically approximate problems of the form (P) and is structured as follows. In Section II, we establish existence and first order necessary optimality conditions for the infinite dimensional problem (P). Section III, makes use of standard regularization theory to analytically justify the approximation of (P) by the ‘finite noise’ problem \( (P^n) \), while Section IV discusses existence and first order necessary optimality of \( (P^n) \), and outlines a descent method for finding the solution. Finally, a numerical example in Section V illustrates the implementation of the method.

### II. The Infinite Dimensional Problem

In order to accommodate the lack of smoothness of \( q \) as a function of \( \omega \) in our analysis, we impose inequality constraints uniformly in the random space. Any function \( q \) in the feasible set \( Q_{ad} \), satisfies the norm bound \( \|q(\cdot, \omega)\|_H \leq q_{\text{max}} \) uniformly on \( \Omega \), which by the continuous imbedding of \( H(D) \) into \( L^\infty(D) \), implies \( 0 < q_{\text{min}} \leq q(x, \omega) \leq q_{\text{max}} \) for all \((x, \omega) \in D \times \Omega \). This assumption, while ruling out unbounded processes, nevertheless reflects actual physical constraints. The uniform coercivity condition \( 0 < q_{\text{min}} \leq q(x, \omega) \), guarantees that for each \( q \in Q_{ad} \), there exists a unique solution \( u = u(q) \in \widetilde{H}^1_0(D) \) to the weak form (2) of the equality constraint \( e(q, u) = 0 \) [16] satisfying the bound

\[
\|u\|_{\widetilde{H}^1_0}^2 \leq \frac{C_D}{q_{\text{min}}} \|f\|_{L^2}.
\]

Hence all \( q \in Q_{ad} \) and their respective model outputs \( u(q) \) have statistical moments of all orders.

#### A. Existence of Minimizers

An explicit stability estimate of \( u(q) \) in terms of the \( L^p(D \times \Omega) \) norm of \( q \) was given in [12], [16] for \( 2 < p \leq \infty \). These norms, besides lacking a Hilbert space structure, give rise to topologies that are too weak for our purposes. The following lemmas establish the weak compactness of the feasible set, continuity of the solution mapping \( q \mapsto u(q) \) restricted to \( Q_{ad} \), as well as the weak closedness of its graph in the stronger \( \widetilde{H} \) norm and will be used to prove the existence of solutions to (P).

**Lemma II.1** The set \( Q_{ad} \) is closed, convex, and hence weakly compact in \( \widetilde{H} \).

**Proof:** The convexity of \( Q_{ad} \) is easily verified. To show that \( Q_{ad} \) is closed, let \( \{q^n\} \subset Q_{ad} \) and \( q \in \widetilde{H} \) be such that

\[
\|q^n - q\|_{\widetilde{H}}^2 = \int_\Omega \|q^n(\cdot, \omega) - q(\cdot, \omega)\|_H^2 d\omega \to 0 \quad \text{as } n \to \infty
\]

and since convergence in \( L^2(\Omega, d\omega) \) implies pointwise almost sure (a.s.) convergence of a subsequence on \( \Omega \), we have

\[
\|q^{n_k}(\cdot, \omega) - q(\cdot, \omega)\|_H \to 0 \quad \text{a.s. on } \Omega
\]

for some subsequence \( \{q^{n_k}\} \subset Q_{ad} \). Additionally, \( \|q^{n_k}(\cdot, \omega)\|_H \leq q_{\text{max}} \text{ a.s. on } \Omega \) for \( k \in \mathbb{N} \) and therefore \( q \) also satisfies this constraint. Finally, \( H(D) \) imbeds continuously in \( L^\infty(D) \), from which it follows that the subsequence \( \{q^{n_k}\} \) converges to \( q \) pointwise a.s. on \( D \times \Omega \), ensuring that \( q \) also satisfies pointwise constraint \( q(x, \omega) \geq q_{\text{min}} \text{ a.s. on } D \times \Omega \).

**Lemma II.2** The mapping \( u : q \in Q_{ad} \mapsto u(q) \in \widetilde{H}^1_0 \) is continuous.

**Proof:** Suppose \( q^n \to q \) in \( Q_{ad} \). As in the proof of the previous lemma, there exists a subsequence \( q^{n_k} \to q \)
pointwise a.s. on $D \times \Omega$. The upper bound on the function $u$ established in [12, p. 1261] ensures that
\[ \|u(q^n_k)-u(q)\|_{H_0^1} \leq \left( \frac{C_D \|f\|_{L^2}}{d_{\min}^2} \right) \|q^n_k-q\|_{L^\infty(\Omega;L^\infty(D))}, \]
where $C_D$ is the constant appearing in the Poincaré inequality on $D$. Furthermore, since any subsequence of $u(q^n)$ has a subsequence converging to $u(q)$, $u(q^n) \to u(q)$.

**Lemma II.3** The graph \( \{ (q, u) \in \widetilde{H} \times \widetilde{H}_0^1 : q \in Q_{ad}, u = u(q) \} \) of $u$ is weakly closed.

**Proof:** Due to space limitations, a detailed proof is omitted. However, the proof is based on showing that a weakly convergent sequence $(q^n, u(q^n)) \to (q, u)$ has $q \in Q_{ad}$ by Lemma II.1 and satisfies $e(q,u) = 0$. The latter condition uses the fact that $e(q^n, u(q^n)) = 0$ along with the Cauchy-Schwarz inequality, the Dominated Convergence Theorem, and the fact that $(\cdot \cdot \cdot, \cdot \cdot \cdot) = (\cdot \cdot \cdot, \cdot \cdot \cdot)$. Dividing (5) by $\alpha_0$ and letting $\alpha_0 = \alpha_0$.

Finally, it follows from Lemma II.3 that $u^* = u^*(q^*)$, hence $u^*$ satisfies the inequality constraint $e(q^*, u^*) = 0$.

**B. A Saddle Point Condition**

Although solutions to (P) exist, the inherent lack of smoothness of $q$ in the stochastic variable $\omega$ complicates the establishment of traditional necessary optimality conditions. A short calculation reveals that the equality constraint $e(q,u)$ is not Fréchet differentiable, as a function of $q$ in $\widetilde{H}$. Additionally, the set of constraints has an empty interior in the $\widetilde{H}$-norm. Instead, we follow [18] in deriving a saddle point condition for the optimizer $(q^*, u^*)$ of (P) with the help of a Hahn-Banach separation argument.

Let \( \langle \cdot, \cdot \rangle \) denote the $L^2(D \times \Omega)$ inner product. For any triple $(q,u,\lambda) \in \widetilde{H} \times \widetilde{H}_0^1 \times \widetilde{H}_0^1$, we define the Lagrangian functional
\[ L(q,u,\lambda) = L(q,u) + \langle e(q,u), \lambda \rangle_{\widetilde{H}^{-1} \times \widetilde{H}_0^1} \]
\[ = \frac{1}{2} \|u-\tilde{u}\|^2_{H_0^1} + \frac{\beta}{2} \|q\|^2_{H} + \langle q \nabla u, \nabla \lambda \rangle - \langle f, \lambda \rangle. \]

The main theorem of this subsection is the following [19]

**Theorem II.5 (Saddle Point Condition)** Let $(q^*, u^*) \in Q_{ad} \times \widetilde{H}_0^1$ solve problem (P). Then there exists a Lagrange multiplier $\lambda^* \in \widetilde{H}_0^1$ so that the saddle point condition
\[ L(q^*, u^*, \lambda) \leq L(q^*, u^*, \lambda^*) \leq L(q,u,\lambda^*) \]
holds for all $(q,u,\lambda) \in Q_{ad} \times \widetilde{H}_0^1 \times \widetilde{H}_0^1$.

**Proof:** Note that the second inequality simply reflects the optimality of $(q^*, u^*)$. To obtain the first inequality, we rely on a Hahn-Banach separation argument. Let
\[ S = \{ (J(q,u) - J(q^*, u^*) + s, e(q,u)) \in \mathbb{R} \times \widetilde{H}_0^1 : (q,u) \in Q_{ad} \times \widetilde{H}_0^1, s \geq 0 \} \]
and
\[ T = \{ (-t, 0) \in \mathbb{R} \times \widetilde{H}_0^1 : t > 0 \}. \]

The Hahn-Banach Theorem (justified by Lemmas II.6–II.8) gives rise to a separating hyperplane, i.e. a pair $(\alpha_0, \lambda_0) \neq (0, 0)$ in $\mathbb{R} \times \widetilde{H}_0^1$, such that
\[ \alpha_0(J(q,u) - J(q^*, u^*) + s) + \langle e(q,u), \lambda_0 \rangle_{\widetilde{H}^{-1} \times \widetilde{H}_0^1} \geq -t \alpha_0 \]
for all $t > 0, s \geq 0$, and $(q,u) \in Q_{ad} \times \widetilde{H}_0^1$. Letting $s = t = 1$ and $(q,u) = (q^*, u^*)$ readily yields $\alpha_0 \geq 0$. In fact $\alpha_0 > 0$. Suppose to the contrary that $\alpha_0 = 0$. Then by (5)
\[ \langle e(q,u), \lambda_0 \rangle_{\widetilde{H}^{-1} \times \widetilde{H}_0^1} = \langle q \nabla u, \nabla \lambda_0 \rangle - \langle f, \lambda_0 \rangle \geq 0 \]
for all $(q,u) \in Q_{ad} \times \widetilde{H}_0^1$. In particular, for $q = q^*$ and $u \in \widetilde{H}_0^1$ satisfying $\langle q^* \nabla u, \nabla \phi \rangle - \langle f - \lambda_0, \phi \rangle = 0$ for all $\phi \in \widetilde{H}_0^1$, we have
\[ \langle q^* \nabla u, \nabla \lambda_0 \rangle - \langle f, \lambda_0 \rangle = -\langle \lambda_0, \lambda_0 \rangle \geq 0, \]
which implies that $\lambda_0 = 0$. This contradicts the fact that $(\alpha_0, \lambda_0) \neq (0, 0)$. Dividing (5) by $\alpha_0$ and letting $\lambda^* = \lambda_0/\alpha_0$.
yields \( J(q^*, u^*) \leq J(q, u) + \langle e(q, u), \lambda^* \rangle_{\bar{H}_1^{-1}, \bar{H}_0^{-1}} \) \( \forall (q, u) \in Q_{ad} \times \bar{H}_0^{-1} \) and hence
\[
L(q^*, u^*, \mu) = J(q^*, u^*) + \langle e(q^*, u^*), \mu \rangle_{\bar{H}_1^{-1}, \bar{H}_0^{-1}} \\
\leq J(q, u) + \langle e(q, u), \lambda^* \rangle_{\bar{H}_1^{-1}, \bar{H}_0^{-1}} = L(q, u, \lambda^*)
\]
for all \( (q, u, \mu) \in Q_{ad} \times \bar{H}_0^{-1} \times \bar{H}_0^{-1} \).

\textbf{Lemma II.6} The sets \( S \) and \( T \) are convex.

\textbf{Lemma II.7} The sets \( S \) and \( T \) are disjoint.

\textbf{Proof:} This follows directly from the fact that \( J(q, u) \geq J(q^*, u^*) \) for all points \( (q, u) \) in \( Q_{ad} \times \bar{H}_0^{-1} \).

\textbf{Lemma II.8} The set \( S \) has a non-empty interior.

In the following section, we will show that if the observed data \( \hat{u} \) is expressed as a Karhunen-Loève series \([20],[21]\), we may approximate problem \((P)^n\) by a ‘finite noise’ optimization problem \((P^n)\), where \( q \) is a smooth, albeit high-dimensional, function of \( x \) and intermediary random variables \( \{Y_i\}_{i=1}^n \). The convergence framework not only informs the choice of numerical discretization, but also suggests the use of a dimension-adaptive scheme to exploit the progressive ‘smoothing’ of the problem.

\section{Approximation by the Finite Noise Problem}

According to [20], the random field \( \hat{u} \) may be written as the Karhunen-Loève (KL) series
\[
\hat{u}(x, \omega) = u_0(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} \phi_n(x) Y_n(\omega),
\]
where \( \{Y_n\}_{n=1}^{\infty} \) is an uncorrelated orthonormal sequence of random variables with zero mean and unit variance and \( (\lambda_n, \phi_n) \) is the eigenpair sequence of \( \hat{u} \)’s compact covariance operator \( C : H^2_0(D) \rightarrow H^2_0(D) \) \([21]\). Moreover, the truncated series
\[
\hat{u}^n(x, \omega) = u_0(x) + \sum_{i=1}^{n} \sqrt{\lambda_i} \phi_i(x) Y_i(\omega)
\]
converges to \( \hat{u} \) in \( \bar{H}_1^{-1} \), i.e. \( \|\hat{u} - \hat{u}^n\|_{\bar{H}_1^{-1}} \rightarrow 0 \) as \( n \rightarrow \infty \).

Assume w.l.o.g. that \( \{Y_n\}_{n=1}^{\infty} \) forms a complete orthonormal basis for \( L^2(\Omega) \), the set of functions in \( L^2(\Omega) \) with zero mean. If this is not the case, we can restrict ourselves to \( L^2(\Omega) \cap \text{span} \{Y_i\} \). The following additional assumption relates to the form of the random vector.

\textbf{Assumption III.1} Assume the random variables \( \{Y_n\} \) are bounded uniformly in \( n \), i.e. for some \( y_{\min}, y_{\max} \in \mathbb{R} \),
\[
y_{\min} \leq Y_n(\omega) \leq y_{\max} \quad \text{a.s. on} \ \Omega \quad \text{for all} \ n \in \mathbb{N}.
\]

Furthermore, assume that for any \( n \) the probability measure of the random vector \( Y = (Y_1, ..., Y_n) \) is absolutely continuous with respect to the Lebesgue measure and hence \( Y \) has joint density \( \rho_n : \Gamma^n \rightarrow [0, \infty) \), where the hypercube \( \Gamma^n = \prod_{i=1}^{n} \Gamma_i \subset [y_{\min}, y_{\max}]^n \) denotes the range of \( Y \).

Since \( \hat{u}^n \) depends on \( \omega \) only through the intermediary variables \( \{Y_i\}_{i=1}^n \), it seems reasonable to also estimate the unknown parameter \( q^n \) as a function of these, i.e. \( q^n(x, \omega) = q^n(x, Y_1(\omega), ..., Y_n(\omega)) \in \bar{H}(\Gamma^n) := H(D) \otimes L^2(\Gamma^n) \).

The corresponding model output \( u^n = u(q^n) \), depending continuously on the parameter \( q^n \), would then also be a function of \( Y = (Y_1, ..., Y_n) \), according to the Doob-Dynkin lemma. The ‘finite noise’ equality constraint \( e_n(q^n, u^n) = 0 \) now takes the form of the parameterized partial differential equation \([16]\)
\[
-\nabla \cdot \left( q^n(x, y) \nabla u^n(x, y) \right) - f(x) = 0 \quad \text{a.s. on} \ \Omega \times \Gamma^n
\]
\[
u^n(x, y) = 0 \quad \text{a.s. on} \ \partial\Omega \times \Gamma^n.
\]

This leaves us free to specify the regularity of \( q^n \) as a function of the vector \( y = (y_1, ..., y_n) \in \Gamma^n \subset \mathbb{R}^n \). At the very least, \( q^n \) should be square integrable in \( y \). Moreover, seeing that \( \{Y_n\}_{n=1}^{\infty} \) forms a basis for \( L^2(\Omega) \), the minimizer \( q^* \) of the original infinite dimensional problem \((P)\) takes the form
\[
q^*(x, \omega) = q_n^*(x) + \sum_{n=1}^{\infty} q_n(x) Y_n(\omega),
\]
which is linear in each of the random variables \( Y_n \). Any minimizer \( q_n^* \) of \((P^n)\) that approximates \( q^* \) (even in the weak sense) is therefore expected to depend relatively smoothly on \( y \) when \( n \) is large. At low orders of approximation, on the other hand, the parameter \( q \) that gives rise to the model output \( u(q) \) most closely resembling the partial data \( \hat{u} \) may not exhibit the same degree of smoothness in the variable \( y = (y_1, ..., y_n) \). Since the accuracy in approximation of functions in high dimensions benefits greatly from a high degree of smoothness \([22]\), this suggests the use of a dimension adaptive strategy in which the smoothness requirement of the parameter is gradually strengthened as the stochastic dimension \( n \) increases.

For the sake of our analysis, we seek ‘finite noise’ minimizers \( q_n^* \) in the space \( \tilde{H}_0^{-1}(\Omega) := H(D) \otimes \tilde{H}_0^{-1}(\Gamma^n) \), where \( \tilde{H}_0^{-1}(\Gamma^n) \) is the space of functions with bounded mixed derivatives, \( s \geq 1 \) \([15]\). For any function \( v \in \tilde{H}_0^{-1}(\Omega) \subset L^2(D \times \Gamma^n) \), the norm
\[
\|v\|_{\tilde{H}_0^{-1}(\Omega)}^2 = \sum_{|\alpha| \leq s} \sum_{|\nu| \leq \nu_d} \int_D \int_{\Gamma^n} |D^\nu \partial^\alpha v(x, y)|^2 \rho_n(y) dy dx
\]
(7)
is finite, where \( y = (y_1, ..., y_n) \in \mathbb{R}^n \) and \( \alpha = (\alpha_1, ..., \alpha_d) \in \mathbb{N}^d \) are multi-indices, with \( |\alpha| = \max|\alpha_1|, ..., |\alpha_n| \), \( |\nu| = \alpha_1 + ... + \alpha_n \) and \( \nu_d = 1 \) when \( d = 1 \) or \( \nu_d = 2 \) when \( d = 2 \). 3, 2

We can now proceed to formulate a ‘finite noise’ least squares parameter estimation problem for the perturbed, finite noise data \( \hat{u}^n \):
\[
\min_{(q, u) \in \tilde{H}_0^{-1}(\Omega) \times \bar{H}_1^{-1}} J(q, u) := \frac{1}{2} \|u - \hat{u}^n\|_{\bar{H}_1^{-1}}^2 + \frac{\beta_n}{2} \|q\|_{\tilde{H}_0^{-1}(\Gamma^n)}^2
\]
s.t. \( q \in Q_{ad}^{n}, e_n(q, u) = 0 \) \( (P^n) \)
where
\[ Q_{ad}^n := \{ q \in \tilde{H}^n : 0 < q_{\min} - \frac{1}{k_n} \leq q(x, y) \} \]
as on \( D \times \Gamma^n, \| q(\cdot, y) \|_H \leq q_{\max} + \frac{1}{k_n} \) a.s. on \( \Gamma^n \}
and \( k_n \to \infty \) is a monotone increasing approximation parameter to be specified later.

We will justify the use of this approximation scheme by demonstrating that as \( n \to \infty \) and \( \beta_n \to 0 \), the sequence of minimizers \( \tilde{q}_n^* \) of problem \( (P^n) \) has a weakly convergent subsequence and that the limits of all convergent subsequences minimize the infinite dimensional problem (P).

Tikhonov regularization theory for non-linear least squares problems [23] provides the theoretical framework underlying the arguments in this section. In order to mediate between the minimizer \( q_n^* \) of the finite noise problem \( (P^n) \), formulated in the \( H_{mix}^s \) norm, and that of the infinite dimensional problem, whose minimizer \( q^* \) is measured in the \( H \) norm, we make use of the projection of \( q^* \) on the first \( n \) basis vectors:

\[ P^n q^* = q_0(x) + \sum_{i=1}^{n} q_i(x) Y_i(\omega). \]

Evidently, \( P^n q^* \to q^* \) as \( n \to \infty \) in \( \tilde{H} \). Moreover, seeing that \( P^n q^* \) is linear in \( y \), it’s norm in \( H_{mix}^s \) can be bounded in terms of its norm in \( H \) as stated in the following

**Lemma III.2** \( \| P^n q^* \|_{\tilde{H}_{mix}^s} \leq \sqrt{2} \| P^n q^* \|_{\tilde{H}}. \)

The next lemma addresses the feasibility of \( P^n q^* \). Although \( P^n q^* \) does not necessarily lie in the feasible region \( Q_{ad} \), the set on which it \( P^n q^* \notin Q_{ad} \) can be made arbitrarily small as \( n \to \infty \). Let \( A_n \) be the event that \( P^n q^* \) lies inside the approximate feasible region \( Q_{ad} \), i.e.

\[ A_n := \{ \omega \in \Omega : 0 < q_{\min} + \frac{1}{k_n} \leq P^n q^*(x, y) \text{ a.s. on } D \} \]

\[ \| P^n q^*(\cdot, y) \|_H \leq q_{\max} + \frac{1}{k_n} \}. \]

Then we have

**Lemma III.3** There is a monotonically increasing sequence \( k_n \to \infty \) so that \( P(\Omega \setminus A_n) \leq \frac{1}{k_n} \) for all \( n \in \mathbb{N} \).

In order to ensure strict adherence to the inequality constraints of \( (P^n) \) for every \( n \), we modify \( P^n q^*(\cdot, y) \) on \( \Omega \setminus A_n \).

**Definition III.4** For all \( n \in \mathbb{N} \), let \( \tilde{q}_n^* \in \tilde{H}_{mix}^s \subset \tilde{H} \) be defined as follows:

\[ \tilde{q}_n^* := \begin{cases} P^n q^*, & \omega \in A_n \\ q_n^*, & \omega \notin A_n \end{cases} \] \( (8) \)

Evidently \( \tilde{q}_n^* \in Q_{ad} \cap \tilde{H}_{mix}^s \) and in light of Lemma III.3, it is reasonable to expect \( \tilde{q}_n^* \approx P^n q^* \) for large \( n \), except on sets of negligible measure. Indeed

**Lemma III.5** \( \tilde{q}_n^* \to q^* \) in \( \tilde{H} \) as \( n \to \infty \).

---

**Proof:**

\[ \| \tilde{q}_n^* - q^* \|_{\tilde{H}} = \int_{A_n} \| P^n q^*(\cdot, \omega) - q^*(\cdot, \omega) \|_{H}^2 d\omega \]

\[ + \int_{\Omega \setminus A_n} \| q_n^*(\cdot, \omega) - q^*(\cdot, \omega) \|_{H}^2 d\omega \leq \| P^n q^* - q^* \|_{H}^2 \]

\[ + \mathbb{P}(\Omega \setminus A_n) \sup_{\omega \in \Omega} \| q_n^*(\cdot, \omega) - q^*(\cdot, \omega) \|_{H}^2 \leq \| P^n q^* - q^* \|_{H}^2 + \frac{1}{k_n} 4(q_{\max} + \frac{1}{k_1})^2 \to 0. \]

We are now in a position to prove the main theorem of this section. For its proof we will make use of the fact that, due to the lower semicontinuity of norms

\[ x_n \to x, \quad \limsup_{n \to \infty} \| x_n \| \leq \| x \| \Rightarrow x_n \to x \quad (9) \]

for any sequence \( x_n \) in a Hilbert space.

**Theorem III.6** (van Wyk [19]) Let \( \| \tilde{u} - \tilde{u}^n \|_{H_{mix}^s} \to 0 \) and \( \beta_n \to 0 \) as \( n \to \infty \). Then the sequence of minimizers \( q_n^* \) of \( (P^n) \) has a subsequence converging weakly to a minimizer of infinite dimensional problem \( (P) \) and the limit of every weakly convergent subsequence is a minimizer of \( (P) \). The corresponding model outputs converge strongly to the infinite dimensional minimizer’s model output.

**Proof:** Since \( q_n^* \) is optimal for \( (P^n) \), we have

\[ \| u(q_n^* - \tilde{u}^n \|_{H_{mix}^s} + \beta_n \| q_n^* \|_{H_{mix}^s} \]

\[ \leq \| u(q_n^* - \tilde{u}^n \|_{H_{mix}^s} + \beta_n \| q_n^* \|_{H_{mix}^s}. \] \( (10) \)

Moreover, by definition \( \tilde{q}_n^*(\cdot, Y(\omega)) = q_n^*(\cdot, Y(\omega)) \) for all \( Y \in Y(\Omega \setminus A_n) \) and hence

\[ \| q_n^* \|_{H_{mix}^s}^2 \leq \| q_n^* \|_{H_{mix}^s}^2 \]

\[ = \sum_{|y|_{\infty} \leq 1} \sum_{|z|_{\infty} \leq 1} \left( \int_{Y(\Omega \setminus A_n)} \int_D D_y^2 D_z^2 P^n q^* y^2 \rho_n(y) dxdy \right) \]

\[ \leq \sum_{|y|_{\infty} \leq 1} \sum_{|z|_{\infty} \leq 1} \left( \int_{Y(\Omega \setminus A_n)} \int_D D_y^2 D_z^2 P^n q^* y^2 \rho_n(y) dxdy \right) \]

\[ \leq \| P^n q^* \|_{H_{mix}^s}^2 \leq 2 \| P^n q^* \|_{H}^2 \]

from which it follows that

\[ \| u(q_n^* - \tilde{u}^n \|_{H_{mix}^s} \]

\[ \leq \| u(q_n^* - \tilde{u}^n \|_{H_{mix}^s} + \beta_n \| q_n^* \|_{H_{mix}^s} - \beta_n \| q_n^* \|_{H_{mix}^s} \]

By Lemmas III.5 and II.2

\[ \limsup_{n \to \infty} \| u(q_n^* - \tilde{u}^n \|_{H_{mix}^s} \]

\[ \leq \lim_{n \to \infty} \| u(q_n^* - \tilde{u}^n \|_{H_{mix}^s} + \beta_n \| P^n q^* \|_{H}^2 \]

\[ = \| u(q^*) - \tilde{u}^n \|_{H_{mix}^s}. \]
which, together with the Banach Alaoglu Theorem, guarantees the existence of a subsequence \( u^q_{n_j} \) converging weakly to some \( u_0 \in \overline{H}_0^1 \). Since feasible sets \( Q_{ad}^{n} \) form a nested sequence, all functions \( u^q_{n_j} \in Q_{ad}^{n} \subset Q_{ad}^{n_1} \), which is weakly compact (Lemma II.1). The sequence \( u^q_{n_j} \) therefore has a subsequence, \( u^q_{n_j} \rightarrow q_0 \in Q_{ad}^{1} \) in \( H \). Additionally, since \( Q_{ad}^{n} \) is nested and the graph of u is weakly closed (Lemma II.3) we have \( q_0 \in \bigcap_{n=1}^{\infty} Q_{ad}^{n} = Q_{ad} \) and \( u_0 = u(q_0) \). Therefore

\[
\left\| u(q_0) - \tilde{u} \right\|_{\overline{H}_0^1}^2 = \lim_{j \to \infty} \left( u(q^q_{n_j}) - \tilde{u} \right) = \lim_{j \to \infty} \left( u(q^q_{n_j}) - u(q_0) - \tilde{u} \right)
\]

\[
\left\| u(q^q_{n_j}) - u(q_0) - \tilde{u} \right\|_{\overline{H}_0^1}
\]

(11)

\[
\leq \limsup_{j \to \infty} \left( u(q^q_{n_j}) - u(q_0) - \tilde{u} \right) - \tilde{u} \|
\]

(12)

\[
\leq \left( u(q^q_{n_j}) - \tilde{u} \right) - \tilde{u} \|
\]

which means \( \left\| u(q_0) - \tilde{u} \right\|_{\overline{H}_0^1} \leq \left\| u(q^q_{n_j}) - \tilde{u} \right\|_{\overline{H}_0^1} \) and hence \( q_0 \in Q_{ad} \) is a minimizer for (P). Inequalities (11) and (12) further imply

\[
\lim_{j \to \infty} \left( u(q^q_{n_j}) - \tilde{u} \right) = \left( u(q_0) - \tilde{u} \right)
\]

which, together with the weak convergence \( u(q^q_{n_j}) - \tilde{u} \rightarrow u(q_0) - \tilde{u} \), implies \( u(q^q_{n_j}) - \tilde{u} \rightarrow u(q_0) - \tilde{u} \) due to (9). In addition the fact that \( \tilde{u} \rightarrow \tilde{u} \) implies that \( u(q^q_{n_j}) \rightarrow u(q_0) \). Finally, this argument holds for any convergent subsequence of \( \{q_{n_j}^q\} \) and hence the theorem is proved.

IV. THE FINITE NOISE PROBLEM

The immediate benefit of using \( \overline{H}_{mix}^s \) as an approximate search space is that it imbeds continuously in \( L^\infty(D \times \Gamma) \), regardless of the size of the stochastic dimension \( n \). By virtue of the tensor product structure of \( \overline{H}_{mix}^s(\Gamma^n) \) we may consider Sobolev regularity component-wise, which, in conjunction with the compact imbedding of \( H^1(\Gamma) \) in \( L^\infty(\Gamma) \), gives rise to this property summarized in the following lemma.

Lemma IV.1 The space \( \overline{H}_{mix}^s \) imbeds continuously in \( L^\infty(\Gamma^n) \) for all \( n \in \mathbb{N} \).

A. Differentiability and Existence of Lagrange Multipliers

Consider again the right hand side \( e_n(\cdot, \cdot) : \overline{H}_{mix}^s \times \overline{H} \rightarrow \overline{H}^{-1} \) of the equality constraint, given in variational form, i.e. for all \( \phi \in \overline{H}_{mix}^s \)

\[
\langle e_n(q, u), \phi \rangle_{\overline{H}_0^1} :=
\]

\[
\int_D \int_{\Gamma^n} q(x, y) \nabla u(x, y) \cdot \phi(x, y) \rho_n(y) dy \ dx
\]

\[
- \int_D \int_{\Gamma^n} f(x, y) \phi(x, y) \rho_n(y) dy \ dx.
\]

Since \( e(q, u) \) is affine linear in both arguments, it’s Fréchet differentiability with respect to either \( q \) or \( u \) follows directly from its boundedness in these variables. Continuity in \( u \) is straightforward. For \( u, \tilde{u} \in \overline{H}_0^1 \),

\[
\langle e(q, u - \tilde{u}), \phi \rangle_{\overline{H}_0^1} = \int_D \int_{\Gamma^n} q \nabla(u - \tilde{u}) \cdot \nabla \phi \rho_n dy \ dx
\]

\[
\leq \|q\|_\infty \|u - \tilde{u}\|_{\overline{H}_0^1} \|\phi\|_{\overline{H}_0^1} \forall \phi \in \overline{H}_0^1
\]

and hence \( \|e(q, u - \tilde{u})\|_{\overline{H}^{-1}_0} \leq \|q\|_\infty \|u - \tilde{u}\|_{\overline{H}_0^1} \). In order to establish the continuity of \( e(q, u) \) with respect to \( q \in \overline{H}_{mix}^s \), we make use of the imbedding from Lemma IV.1. Let \( \tilde{q}, q \in \overline{H}_{mix}^s \) and \( \phi \in \overline{H}_0^1 \) be an arbitrary test function. Then

\[
\langle e(q - \tilde{q}), \phi \rangle_{\overline{H}_0^1} \leq C_n \|q - \tilde{q}\|_{\overline{H}_{mix}^s} \|\phi\|_{\overline{H}_0^1},
\]

from which it readily follows that \( \|e(q - \tilde{q}, u)\|_{\overline{H}_0^1} \leq C_n \|u\|_{\overline{H}_0^1} \|\phi\|_{\overline{H}_0^1} \) and therefore \( e_n \) is continuously Fréchet differentiable.

A simple calculation then reveals that the first derivative of \( e_n \) in the direction \( (h, v) \in \overline{H}_{mix}^s \times \overline{H}_0^1 \) is given by:

\[
e'(q, u)(h, v) = e_q(q, u) h + e_u(q, u) v
\]

where

\[
\langle e_q(q, u), h \rangle_{\overline{H}_0^1, \overline{H}_0^1} = \int_D \int_{\Gamma^n} h \nabla u \cdot \nabla \phi_n dy \ dx
\]

\[
\langle e_u(q, u), v \rangle_{\overline{H}_0^1, \overline{H}_0^1} = \int_D \int_{\Gamma^n} q \nabla v \cdot \nabla \phi_n dy \ dx
\]

for all \( \phi \in \overline{H}_0^1 \). We can now derive more traditional first order necessary optimality conditions [19]

Theorem IV.2 (Existence of Lagrange Multipliers) Let \( (q^*, u^*) \) be a minimizer for problem (P). Then there exists a unique Lagrange multiplier \( \lambda^* \in \overline{H}_0^1 \) for which the Lagrangian functional

\[
L(q, u; \lambda) = J(q, u) + \langle \lambda, e_n(q, u) \rangle_{\overline{H}_0^1}
\]

satisfies

\[
L'(q^*, u^*; \lambda^*)(h, v) \geq 0 \text{ for all } (h, v) \in C(q^*) \times \overline{H}_0^1
\]

where

\[
C(q^*) = \{l(c - q^*) : c \in Q_{ad}, l \geq 0\}
\]

Particularly, the adjoint equation and complementary condition hold

\[
e_n(q^*, \lambda^*) = -\langle u^* - \tilde{u}^*, \gamma \rangle_{\overline{H}_0^1}
\]

\[
\beta(q^*, q - q^*)_{\overline{H}_{mix}^s} - \langle \nabla \lambda^*, (q - q^*) \nabla u^* \rangle_{L^2(D \times \Gamma)} \geq 0
\]

for all \( q \in Q_{ad} \).
B. A Simple Descent Algorithm

In this section we outline a simple gradient descent algorithm. Consider again our problem \((P^n)\). We rewrite it in simpler notation.

\[
\min_{q \in Q_{ad} \cap \mathcal{H}^s_{mix}} J(q, u(q)) = \frac{1}{2\varepsilon} \|u(q) - \hat{u}\|_{\mathcal{H}^0}^2 + \frac{\beta}{2} \|q\|_{\mathcal{H}^s_{mix}}^2
\]

\[\text{s.t.} \ e(q, u(q)) = 0 \in \mathcal{H}^{-1}, \ (15)\]

where \(e : \mathcal{H}^s_{mix} \times \mathcal{H}^0 \rightarrow \mathcal{H}^{-1}\) is a bounded bilinear form, \(J(q, u(q)) : \mathcal{H}^s_{mix} \times \mathcal{H}^0 \rightarrow \mathbb{R}\). Evidently

\[
J'(q, u(q))h = J_u(q, u(q))u'(q)h + J_q(q, u(q))h = (u(q) - \hat{u}, u'(q)h)_{\mathcal{H}^0} + (q, h)_{\mathcal{H}^s_{mix}}
\]

\[
e' = u'(q)^* J_u(q, u(q))h + J_q(q, u(q))h
\]

and

\[
e(q, u(q)) = 0 \in \mathcal{H}^{-1}
\]

leads to

\[
e_q(q, u(q))h + e_u(q, u(q))u'(q)h = 0 \text{ in } \mathcal{H}^{-1}
\]

for all \(h \in \mathcal{H}^s_{mix}\) and

\[
e'(q)^* J_u(q, u(q)) = -e_q(q, u(q))^{*} e_u(q, u(q))^{*} J_u(q, u(q))
\]

in \(\mathcal{L}(\mathcal{H}^{-1}, \mathcal{H}^s_{mix})\). Equivalently, \(u'(q)^* J_u(q, u(q)) = e_q(q, u(q))^{*} e_u(q, u(q))^{*} p\), where \(p \in (\mathcal{H}^{-1})^{*} = \mathcal{H}^0\) solves

\[
e_u(q, u(q))^{*} p = -J_u(q, u(q)).
\]

Since \(e_u(q, u) : \mathcal{H}^0 \rightarrow \mathcal{H}^{-1} : v \mapsto \langle q\nabla v, \nabla v \rangle\), we can rewrite this adjoint equation as

\[
\langle q\nabla p, \nabla \cdot \rangle = -\langle \nabla u - \nabla \hat{u}, \nabla \cdot \rangle.
\]

Here \(e_q(q, u) : \mathcal{H} \rightarrow \mathcal{H}^{-1} : h \mapsto \langle h\nabla u, \nabla \cdot \rangle\) and \(e_u(q, u) : \mathcal{H}^0 \rightarrow \mathcal{H}^{-1} : v \mapsto \langle q\nabla v, \nabla v \rangle\). Therefore \(e_q(q, u)^{*} : \mathcal{H}^0 \rightarrow \mathcal{H}^s_{mix}\) maps \(p \mapsto \langle \nabla p, \nabla u \rangle\).

\[
J'(q, u(q))h = (h \nabla p, \nabla u)_{L^2} + (q, h)_{\mathcal{H}^s_{mix}}.
\]

It is also evident that the constraint set \(Q_{ad} \cap \mathcal{H}^s_{mix}\) is closed and convex in \(\mathcal{H}^s_{mix}\). We can therefore make use of Algorithms such as the projected Armijo rule [24] to find the optimal \(q\). This method has linear convergence. Moreover, the calculation of the cost functional requires one forward solve = \(N_{colocation}\) deterministic solves, which can be done in parallel however. The computation of the gradient also requires an adjoint solve (one for each stochastic collocation point).

V. NUMERICAL EXAMPLE

To test this formulation on a stochastic parameter estimation problem, we generated model data \(\hat{u}\) using a known stochastic conductivity \(q(x, \omega)\) and source term \(f\) given by

\[
q(x, \omega) = 3 + x^2 + Y_1(\omega) \sin(\pi x) + Y_2(\omega) \sin(2\pi x),
\]

\[
f(x) = -6 + 18x - 8x^2 + 12x^3,
\]

where \((Y_1, Y_2) \sim \text{uniform}(0, 1)^2\). The model data \(\hat{u}\) was computed from the data generated by \(q\) and \(f\) and expanded in the same random basis \((Y_1, Y_2)\). We then implemented an augmented Lagrangian algorithm to identify \(q\). From an initial guess of \(q^0(x, Y_1, Y_2) = 3\), the algorithm converges, albeit slowly, to the correct function. We used 16 quadratic finite elements for the deterministic portion of \(q\) (33 degrees of freedom) and a 3rd level interpolation in stochastic space, yielding 29 sparse grid points. We therefore had to estimate the coefficients of a 957 dimensional vector. In Fig. 1, we compare the values of \(\{q^*(\cdot, Y_1, Y_2)\}_{i=1}^{29}\) and the estimated values of \(\{q^*(\cdot, Y_1, Y_2)\}_{i=1}^{29}\) at all 29 stochastic collocation points. As we can see, there is very good agreement between the interpolated values of the parameter and the estimated parameter. The largest discrepancy occurs near \(x = 0\) where the slope of deterministic solutions are near zero and hinder the identifiability of the parameter.

Access to the ‘finite noise’ stochastic representation of \(q\) allows one to address fundamental questions through integration over the stochastic variables. Using this example, and the moment formulas

\[
q_0 = E[q] \quad \text{and} \quad \mu_k = E[(q - q_0)^k].
\]

we compute the first 9 central moments of the stochastic variable \(q^*\) and compare them with the exact moments in Fig. 2. There is very good agreement between the moments of the true and estimated parameters. For instance, we see that the standard deviation \(\mu_2\) changes significantly across the spatial domain \([0, 1]\) and that aside from the first moment, odd moments are computed to be relatively insignificant.

VI. CONCLUSIONS AND FUTURE WORKS

A. Conclusions

Estimation of random distributed parameters is a natural complement to stochastic simulations and uncertainty quantification. We have developed a mathematical framework for posing the parameter estimation problem where we attempt to approximate the entire random field across the distributed parameter. While other formulations, such as attempting to identify moments, are possible, the present formulation allows one to both answer interesting probabilistic questions...
by computing integrals in the probability space and to have access to a spectral expansion of parameters that are suitable for applying modern stochastic partial differential equation approximation methods. We pose the random parameter estimation problem as an optimization problem using the ‘finite noise’ assumption. We justify the finite noise approximation and the least-squares optimization framework when the covariance function is smooth enough. A differentiating feature of this work is the setup of the problem in $H_{mix}^s$, the space of bounded mixed derivatives. This space is used in the analysis of hierarchical collocation rules used in sparse grid methods. Thus, it is a natural space for approximation of the first-order necessary conditions as well as for implementing regularization.

B. Future Works

In future work, we plan to address more efficient optimization algorithms such as simultaneously solving the state, adjoint and gradient equations using sparse grid collocation. In addition, we will investigate other strategies for post-processing the distributed ‘finite noise’ parametric variables such as computing the likelihood the parameter lies between given ranges.

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