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GAUSSIAN PROCESS REGRESSION AND CONDITIONAL KARHUNEN-LOÈVE EXPANSION FOR FORWARD UNCERTAINTY QUANTIFICATION AND INVERSE MODELING IN THE PRESENCE OF MEASUREMENT NOISE

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We propose a new machine learning framework for uncertainty quantification (UQ) and parameter estimation in partial differential equation (PDE) models using sparse noisy measurements of the parameter field. In our approach, the Gaussian process regression (GPR) is used to estimate the distribution of the unknown parameter κ*, including mean and variance, conditioned on its measurements. Then, the conditional Karhunen-Loève (KL) expansion of* κ *and generalized polynomial chaos (gPC) expansion of the state variable* u *are constructed in terms of the parameter's conditional mean and the eigenfunctions and eigenvalues of the parameter's conditional covariance function. In the forward UQ application, the conditional gPC surrogate is used to estimate the mean and variance of* u*. Our results show that conditioning reduces the* u *variance and that the variance decreases with decreasing measurement noise. In the inverse solution, we use the conditional KL and gPC expansions to find a realization of conditional* κ *distribution that satisfies an appropriate maximum a posteriori minimization problem. We find that the error in the estimated* κ *decreases with the decreasing observation error.*

KEY WORDS: *Guassian process regression, conditional Karhunen-Loève expansion, conditioning on noisy measurements, uncertainty quantification, inverse modeling*

1. INTRODUCTION

Conditional forward uncertainty quantification (UQ) in partial differential equation (PDE) models with sparsely measured parameter fields by means of the conditional Monte Carlo (MC) and moment equation methods dates back to the 1990s (e.g., Neuman, 1993; Tartakovsky and Neuman, 1998). However, MC has a low convergence rate ($1/\sqrt{N_s}$, where N_s is the number of samples) and the moment approach is limited to the small variances (less than 1) of parameter fields. As a result, generalized polynomial chaos (gPC) methods based on the Karhunen-Loève

(KL) representation of the unknown parameter fields have emerged as a method of choice in forward UQ (Xiu and Karniadakis, 2003). However, very limited research exists on conditioning KL-gPC models on the measurements of the parameters and state variables [see Li and Tartakovsky (2020) and references therein]. Furthermore, the existing work on forward UQ with conditional KL-gPC expansions is limited to conditioning on noiseless measurements (Tipireddy et al., 2020). In this work, we propose a method for conditioning KL-gPC expansions on noisy measurements.

Unconditional KL expansions were used in Marzouk et al. (2007) for conditioning a KL-gPC model on state measurements. In Li and Tartakovsky (2020), a conditional KL-gPC model was used for conditioning the estimation of parameters and states on both the parameter and state measurements. The work on conditional KL expansion revealed that conditioning reduces parametric uncertainty and, for the same order of expansions, increases the accuracy of the KL-gPC methods (Tipireddy et al., 2020). In the case of noiseless measurements, the latter is because the conditioning on the parameter measurements reduces the dimensionality of the KL representation of the parameter space and the variance of the parameter space (Li and Tartakovsky, 2020). Both these factors reduce the number of terms in the gPC expansion of the state variable that are required to achieve the desired accuracy.

Here, we extend the work of Tipireddy et al. (2020) for forward UQ and of Li and Tartakovsky (2020) for inverse modeling using KL and gPC expansions conditioned on noiseless measurements for conditioning on noisy measurements. This is important because in most sustainability-related research, the measurements of the parameters of natural systems are prone to measurement errors. We accomplish this by proposing a scheme for conditioning KL expansions on noisy measurements.

2. PROBLEM SETUP

Consider a physical system with the unknown parameter $\kappa(\mathbf{x})$ and described by the PDE,

$$\mathcal{L}(\mathbf{x}, u(\mathbf{x}), \kappa(\mathbf{x})) = 0, \quad \text{for} \quad \mathbf{x} \in D, \tag{1}$$

with known differential operator $\mathcal{L}$ and appropriate boundary conditions $\mathcal{B}(\mathbf{x})_{\partial D} = 0$. In the probabilistic framework, the forward uncertainty propagation in this PDE problem consists of estimating the statistical distribution of $u(\mathbf{x})$ given a prior distribution of $\kappa(\mathbf{x})$, i.e., the distribution of κ given some measurements of κ and/or expert knowledge of the properties of the physical system expressed by $\kappa(\mathbf{x})$. The inverse UQ problem is to estimate the posteriori distribution of κ given its prior distribution and the observations of u. One might be only interested in the most probable realization of the posteriori κ distribution, i.e., the maximum (most probable point) of the posteriori distribution, that can be found as a solution of a deterministic maximum a posteriori (MAP) inverse problem (Li and Tartakovsky, 2020; Tartakovsky et al., 2021). The first step in both forward and inverse problems is the construction of the prior model of $\kappa(\mathbf{x})$. In this work, we assume that the true field κ is a realization of a Gaussian process $\kappa(\mathbf{x}, \omega)$ with a known covariance function (kernel) that is determined from the noisy observations of $\kappa(\mathbf{x})$, $\kappa := \left(\kappa^1, \ldots, \kappa^{N_\kappa}\right)$, located at $\mathbf{x}_\kappa := \left(\mathbf{x}_\kappa^1, \ldots, \mathbf{x}_\kappa^{N_\kappa}\right)$. Furthermore, we consider the diffusion operator $\mathcal{L}(\mathbf{x}, u(\mathbf{x}), \kappa(\mathbf{x})) = \nabla \cdot \exp(\kappa(\mathbf{x}))\nabla u(\mathbf{x})$. In this form, among other problems, Eq. (1) describes steady-state saturated flow in a heterogeneous porous medium, where $\kappa(\mathbf{x})$ is the log conductivity of the said porous medium. We are interested in cases where no measurements of u are available (a forward UQ problem) and where some measurements of u are available (an inverse problem).

The basis of our approach—and its main novelty—is the truncated KL representation of $\kappa(x)$ that is conditioned on the noisy measurements of $\kappa(\mathbf{x})$. The conditional KL expansion is used to obtain the (conditional on κ measurements) gPC approximation of u. In the forward UQ problem, the gPC surrogate is used to compute the mean and variance of u. In the inverse problem, the conditional KL expansion is used to model the unknown parameter field as a realization of the random spatially correlated field with known mean and covariance functions, and a gPC surrogate is used to solve the MAP minimization problem.

3. KARHUNEN-LOEV́E (KL) EXPANSION OF UNCONDITIONAL GAUSSIAN FIELD

A square integrable continuous stochastic process $\kappa(\mathbf{x},\omega)_{\mathbf{x}\in D}$ with the covariance function $C_\kappa(\mathbf{x},\mathbf{y}) := E[\kappa(\mathbf{x},\omega)\kappa(\mathbf{y},\omega)]$, $\mathbf{x},\mathbf{y}\in D$ can be exactly represented by an infinite KL expansion,

$$\kappa(\mathbf{x},\omega) = E[\kappa(\mathbf{x},\omega)] + \sum_{n=1}^{\infty}\sqrt{\lambda_n}\xi_n(\omega)\epsilon_n(\mathbf{x}), \quad \text{in } L^2(\Omega), \tag{2}$$

where $E[\cdot]$ denotes the expectation operator, λ_n are positive eigenvalues, $\epsilon_n(\mathbf{x})$ are mutually orthogonal eigenfunctions such that $\int_D \epsilon_n(\mathbf{x})\epsilon_l(\mathbf{x})d\mathbf{x} = \delta_{n,l}$, and $\delta_{n,l}$ is the Kronecker delta. The eigenfunctions are found as the solution to the Fredholm integral equation of the second kind:

$$\lambda\epsilon(\mathbf{x}) = \int_D C_\kappa(\mathbf{x},\mathbf{y})\epsilon(\mathbf{y})d\mathbf{y}. \tag{3}$$

The random variables ξ_n are mutually uncorrelated and have zero mean and unit variance. If $\kappa(\mathbf{x},\omega)$ is a Gaussian process, then ξ_n are i.i.d. standard normal random variables. To use the KL expansion for solving a forward UQ or an inverse problem, Eq. (2) has to be truncated as

$$\kappa_{N_\kappa}(\mathbf{x},\omega) := E[\kappa(\mathbf{x},\omega)] + \sum_{n=1}^{N}\sqrt{\lambda_n}\epsilon_n(\mathbf{x})\xi_n(\omega), \tag{4}$$

where the eigenvalues λ_n are arranged in decreasing order. In the remainder of this paper, we use $\overline{\kappa}(\mathbf{x})$ to denote the expectation $E[\kappa(\mathbf{x},\omega)]$.

4. CONDITIONAL GAUSSIAN FIELD AND ITS KL EXPANSION

We assume that the measurements of κ, $\boldsymbol{\kappa} := \left(\kappa^1,\dots,\kappa^{N_\kappa}\right)$ are available at locations $\mathbf{x}_\kappa := \left(\mathbf{x}_\kappa^1,\dots,\mathbf{x}_\kappa^{N_\kappa}\right)$ with i.i.d. Gaussian noise $\eta^i \sim \mathcal{N}(0,\sigma_\eta^2)$ for $i = 1,\dots,N_\kappa$. The Gaussian process regression (GPR) model (Rasmussen, 2003) defines the covariance function of the conditional field $\kappa^c(\mathbf{x},\omega)$ [i.e., the field $\kappa(\mathbf{x},\omega)$ conditioned on the κ measurements] as

$$C_\kappa^c(\mathbf{x},\mathbf{y}) = C_\kappa(\mathbf{x},\mathbf{y}) - R(\mathbf{x})(\Sigma + \sigma_\eta^2 I_{N_\kappa\times N_\kappa})^{-1}R(\mathbf{y}), \tag{5}$$

while the mean of $\kappa^c(\mathbf{x},\omega)$ follows:

$$\overline{\kappa}^c(\mathbf{x}) = \overline{\kappa}(\mathbf{x}) + R(\mathbf{x})(\Sigma + \sigma_\eta^2 I_{N_\kappa\times N_\kappa})^{-1}K, \tag{6}$$

where $R(\mathbf{s}) = [C_\kappa(\mathbf{s},\mathbf{x}_\kappa^1), C_\kappa(\mathbf{s},\mathbf{x}_\kappa^2),\dots,C_\kappa(\mathbf{s},\mathbf{x}_\kappa^{N_\kappa})]^T$ for any $\mathbf{s}\in D$, Σ is the $N_\kappa\times N_\kappa$ matrix with (i,j)th entry $\Sigma_{i,j} = C_\kappa(\mathbf{x}_\kappa^i,\mathbf{x}_\kappa^j)$, and $K = [\kappa^1 - \overline{\kappa}(\mathbf{x}_\kappa^1), \kappa^2 - \overline{\kappa}(\mathbf{x}_\kappa^2),\dots,\kappa^{N_\kappa} - \overline{\kappa}(\mathbf{x}_\kappa^{N_\kappa})]^T$.

After computing the eigenpairs $\{\lambda_i^c, \epsilon_i^c\}$ of the covariance function C_κ^c, the truncated conditional KL expansion of κ (i.e., the truncated KL expansion of κ^c) takes the form

$$\kappa^c(\mathbf{x},\omega) \sim \overline{\kappa}^c(\mathbf{x}) + \sum_{i=1}^{N} \lambda_i^c \epsilon_i^c(\mathbf{x}) \xi_i(\omega). \tag{7}$$

Below we proof a theorem stating that conditioning of κ on its noisy measurements reduces the variance of κ. Our numerical results in Section 7 show that the reduction of variance in the uncertain parameter field leads to the reduction of uncertainty in the forward UQ problems and improves the accuracy of parameter estimation.

Theorem 1. *If $\kappa(\mathbf{x},\omega)$ is a stationary Gaussian process with the covariance function $C_\kappa(\cdot,\cdot)$, $\boldsymbol{\kappa}$ is the vector of noisy measurements at points $\mathbf{x}_\kappa^i, i = 1,\dots,N_\kappa$ with i.i.d. noise $\sim \mathcal{N}(0,\sigma_\eta^2)$, and N_m grid points fully resolve the correlation function (i.e., the grid size is much smaller than the correlation length), then the ratio q of the total variance of the conditional κ field w.r.t. that of the original field at all grid points satisfies*

$$q \approx 1 - \frac{1}{N_m} \sum_{\mathbf{x}\in D_\mathbf{x}} \sum_{i=1}^{N_k} \frac{(V_i' R(\mathbf{x}))^2}{(\tilde{\lambda}_i + \sigma_\eta^2)\sigma_\kappa^2}, \tag{8}$$

where $\{\tilde{\lambda}_i, V_i\}_{i=1}^{N_\kappa}$ are the eigenpairs of Σ, σ_κ^2 is the variance at each grid point, and $D_\mathbf{x}$ is the set of all grid points.

Proof. From Eq. (5), the conditional variance of κ at each point $\mathbf{x}$ is

$$\sigma_c^2(\mathbf{x}) = C_\kappa(\mathbf{x},\mathbf{x}) - R(\mathbf{x})'(\Sigma + \sigma_\eta^2 I_{N_\kappa\times N_\kappa})^{-1} R(\mathbf{x}). \tag{9}$$

Then, the total conditional variance of κ is

$$\begin{aligned} \mathrm{Var}_\kappa^c := \int_D \sigma_c^2(\mathbf{x}) d\mathbf{x} &\approx \sum_{\mathbf{x}\in D_\mathbf{x}} \Delta\mathbf{x}(C_\kappa(\mathbf{x},\mathbf{x}) - R(\mathbf{x})'(\Sigma + \sigma_\eta^2 I_{N_\kappa\times N_\kappa})^{-1} R(\mathbf{x})), \\ &= \sum_{\mathbf{x}\in D_\mathbf{x}} \Delta\mathbf{x} \left[C_\kappa(\mathbf{x},\mathbf{x}) - \sum_{i=1}^{N_\kappa} \frac{(V_i' R(\mathbf{x}))^2}{\tilde{\lambda}_i + \sigma_\eta^2} \right], \end{aligned} \tag{10}$$

while the total variance of the unconditional κ field has the form

$$\mathrm{Var}_\kappa := \int_D \sigma^2(\mathbf{x}) d\mathbf{x} \approx \sum_{\mathbf{x}\in D_\mathbf{x}} \Delta\mathbf{x}(C_\kappa(\mathbf{x},\mathbf{x})) = \Delta\mathbf{x} N_m \sigma_\kappa^2.$$

Therefore, Eq. (8) is satisfied. □

According to this theorem, q increases as the noise variance σ_η^2 increases and the maximum reduction in the total variance due to conditioning is achieved when $\sigma_\eta^2 = 0$. It is important to note that the conditioning on the noise-free measurements reduces the dimensionality of the unconditional field by the number of its measurements (Li and Tartakovsky, 2020). The same result cannot be proved for conditioning on noisy measurements.

5. gPC APPROACH FOR THE FORWARD PROBLEM

Given the conditional stochastic representation (7) of the sparsely sampled parameter field κ, the governing equation (1) becomes stochastic with the random state variable $u(\mathbf{x}, \boldsymbol{\xi})$ and can be solved using the gPC Galerkin method or stochastic collocation method. Here, we briefly introduce the gPC collocation method that we later use for constructing the surrogate model of $u(\mathbf{x}, \boldsymbol{\xi})$. The gPC method for Eq. (1) is based on an orthogonal polynomial approximation of $u(\mathbf{x}, \boldsymbol{\xi})$. Let $\mathbf{i} = (i_1, \ldots, i_N) \in (\mathbf{N})_0^n$ be a multi-index with $|\mathbf{i}| = i_1 + \cdots + i_N$ and $P \geq 0$ being an integer. Then, the Pth-degree gPC expansion of function $u(\mathbf{x}, \boldsymbol{\xi})$ is defined as

$$u(\mathbf{x}, \boldsymbol{\xi}) \approx \tilde{u}(\mathbf{x}, \boldsymbol{\xi}) = \sum_{|\mathbf{i}|=0}^{P} c_{\mathbf{i}}(\mathbf{x}) \Phi_{\mathbf{i}}(\boldsymbol{\xi}), \tag{11}$$

where

$$c_{\mathbf{i}}(\mathbf{x}) = \mathbb{E}[\tilde{u}(\mathbf{x}, \boldsymbol{\xi}) \Phi_{\mathbf{i}}(\boldsymbol{\xi})] = \int \tilde{u}(\mathbf{x}, \boldsymbol{\xi}) \Phi_{\mathbf{i}}(\boldsymbol{\xi}) \rho(\boldsymbol{\xi}) d\boldsymbol{\xi}\,,$$

are the coefficients of the expansion, $\Phi_{\mathbf{i}}(\boldsymbol{\xi})$ are the basis functions

$$\Phi_{\mathbf{i}}(\boldsymbol{\xi}) = \phi_{i_1}(\xi_1) \ldots \phi_{i_N}(\xi_N), \quad 0 \leq |\mathbf{i}| \leq P,$$

and $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_N)$ is an N-dimensional random vector with the probability density function $\rho(\boldsymbol{\xi})$. Here, $\phi_j(\xi_k)$ is the jth-degree one-dimensional orthogonal polynomial in the ξ_k direction that satisfies

$$\mathbb{E}[\phi_m(\xi_k)\phi_n(\xi_k)] = \delta_{m,n}, \quad 0 \leq n, m \leq P.$$

For i.i.d. Gaussian random variables $\{\xi_i\}_{i=1}^N$, $\Phi_{\mathbf{i}}(\boldsymbol{\xi})$ are products of Hermite polynomials. The number of $\Phi_{\mathbf{i}}(\boldsymbol{\xi})$ is

$$\begin{pmatrix} N+P \\ P \end{pmatrix},$$

(Xiu, 2009; Xiu and Karniadakis, 2002). The gPC approximation (11) converges to $\tilde{u}(\mathbf{x}, \boldsymbol{\xi})$ in L^2-norm as the degree P increases when $\tilde{u}(\mathbf{x}, \boldsymbol{\xi})$ is square integratable with respect to the probability measure (Xiu, 2007; Xiu and Hesthaven, 2005). The expansion coefficients $c_{\mathbf{i}}(\mathbf{x})$ can be approximated as

$$c_{\mathbf{i}}(\mathbf{x}) \approx \tilde{c}_{\mathbf{i}}(\mathbf{x}) = \sum_{m=1}^{M} \tilde{u}(\mathbf{x}, \boldsymbol{\xi}^{(m)}) \Phi_{\mathbf{i}}(\boldsymbol{\xi}^{(m)}) w^{(m)}, \tag{12}$$

where $\{\boldsymbol{\xi}^{(m)}\}_{m=1}^M$ is a set of quadrature points and $w^{(m)}, m = 1, \ldots, M$ are the corresponding weights in the stochastic collocation method. For each collocation point $\boldsymbol{\xi}^{(i)}$, $u(\mathbf{x}, \boldsymbol{\xi}^{(i)})$ is obtained by solving Eq. (1) with $\tilde{\kappa}(\mathbf{x}, \boldsymbol{\xi})$ replaced by $\tilde{\kappa}(\mathbf{x}, \boldsymbol{\xi}^{(i)})$. Then, the mean and variance of $\tilde{u}(\mathbf{x}, \boldsymbol{\xi})$ can be approximated as

$$\mathbb{E}[\tilde{u}(\mathbf{x}, \boldsymbol{\xi})] \approx \mathbb{E}[\tilde{u}_C(\mathbf{x}, \boldsymbol{\xi})] = \tilde{c}_0(\mathbf{x}), \tag{13}$$

and

$$\mathbb{E}[\tilde{u}(\mathbf{x}, \boldsymbol{\xi}) - E[\tilde{u}(\mathbf{x}, \boldsymbol{\xi})]]^2 \approx \mathbb{E}[\tilde{u}_C(\mathbf{x}, \boldsymbol{\xi}) - E[\tilde{u}_C(\mathbf{x}, \boldsymbol{\xi})]]^2 = \sum_{|\mathbf{i}|=1}^{P} \tilde{c}_{\mathbf{i}}(\mathbf{x})^2. \tag{14}$$

Various quadrature rules can be employed to estimate $c_{\mathbf{i}}$, including tensor product quadrature rules for low-dimensional $\boldsymbol{\xi}$ and sparse grid methods for moderately dimensional $\boldsymbol{\xi}$ (Jakeman and Roberts, 2013; Ma and Zabaras, 2009; Nobile et al., 2008; Xiu and Hesthaven, 2005). The compressive sensing (Hampton and Doostan, 2015; Yan et al., 2012; Yang and Karniadakis, 2013) or the low-rank decomposition methods (Chevreuil et al., 2015; Doostan et al., 2013; Gorodetsky and Jakeman, 2018) are used to further reduce the computational cost to estimate the coefficients $c_{\mathbf{i}}$ whenever the solution has a sparse representation or has a low-rank structure, respectively. We note that given the conditional representation (7) of κ, the gPC expansion (11), gives the approximation of the random state variable u conditioned on the measurements $\boldsymbol{\kappa}$.

6. INVERSE PROBLEM FOR ESTIMATING PARAMETER FIELD

In this section, we use the conditional KL representation $\kappa^c(\mathbf{x},\boldsymbol{\xi})$ of κ and the conditional gPC representation $\tilde{u}(\mathbf{x},\boldsymbol{\xi})$ of u, where $\boldsymbol{\xi}$ is a vector of unknown parameters (as opposed to a vector of random variables in the forward UQ problem), to solve the inverse parameter estimation problem related to the deterministic equation (1) with the unknown parameter field $\kappa(\mathbf{x})$. We assume that in addition to the noisy measurements $\boldsymbol{\kappa}$, we have $\{u^j\}_{j=1}^{N_u}$ noise-free observations of u. Then, the estimation of $\kappa(\mathbf{x})$ reduces to the estimation of the N-dimensional parameter vector $\boldsymbol{\xi}$. The latter can be done by solving the MAP optimization problem (Li and Tartakovsky, 2020),

$$\boldsymbol{\xi}^* = \mathrm{argmin}_{\boldsymbol{\xi}\in\mathbb{R}^N}\mathcal{C}(\boldsymbol{\xi};\mathbf{x}^1,\ldots,\mathbf{x}^{N_u},\boldsymbol{\xi}^o), \tag{15}$$

where

$$\mathcal{C}(\boldsymbol{\xi};\mathbf{x}^1,\ldots,\mathbf{x}^{N_u},\boldsymbol{\xi}^o) := \sum_{j=1}^{N_u}|u^j - \tilde{u}_C(\mathbf{x}^j,\boldsymbol{\xi})|^2 + \lambda\|\boldsymbol{\xi}-\boldsymbol{\xi}^o\|^2, \tag{16}$$

is the cost function. The $\lambda\|\boldsymbol{\xi}-\boldsymbol{\xi}^o\|^2$ term is added to regularize the solution of the optimization problem, where $\boldsymbol{\xi}^o := (\xi_1^o,\ldots,\xi_N) \in \mathbb{R}^N$ and λ are the regularization parameters. We use the trust region method (Shultz et al., 1985) and its implementation in the Matlab software MATLAB (2018) to solve the optimization problem (15) and (16). We set the regularization parameters to $\boldsymbol{\xi}^o = 0$ and λ in the range of 0.0001^2–0.0003^2. In this work, we choose the value of λ to minimize the error with respect to a known reference solution. When a reference solution is not known, λ can be chosen using a cross-validation method. Most of the deterministic optimization methods, including the trust region method, require derivatives of the cost function $\mathcal{C}$ with respect to the optimization parameters. With the gPC surrogate $\tilde{u}_C(\mathbf{x},\boldsymbol{\xi})$, the gradient of $\mathcal{C}$ can be easily evaluated as

$$\frac{\partial}{\partial\xi_i}\mathcal{C}(\boldsymbol{\xi};\mathbf{x}^1,\ldots,\mathbf{x}^{N_u},\boldsymbol{\xi}^o) = \sum_{j=1}^{N_u}2(u^j - \tilde{u}_C(\mathbf{x}^j,\boldsymbol{\xi}))\frac{\partial}{\partial\xi_i}\tilde{u}_C(\mathbf{x}^j,\boldsymbol{\xi}) + 2\lambda(\xi_i - \xi_i^o), \tag{17}$$

where

$$\begin{aligned}\frac{\partial}{\partial\xi_i}\tilde{u}_C(\mathbf{x},\boldsymbol{\xi}) &= \sum_{|\mathbf{j}|=0}^{P}\tilde{c}_{\mathbf{j}}(\mathbf{x})\frac{\partial}{\partial\xi_i}\Phi_{\boldsymbol{j}}(\boldsymbol{\xi})\\ &= \sum_{|\mathbf{j}|=0}^{P}\tilde{c}_{\mathbf{j}}(\mathbf{x})\frac{\partial}{\partial\xi_i}\phi_{j_i}(\xi_i)\prod_{s=1}^{i-1}\phi_{j_s}(\xi_s)\prod_{t=i+1}^{N}\phi_{j_t}(\xi_t).\end{aligned} \tag{18}$$

We note that the uncertainty in the solution in the estimated κ can be quantified by computing the posterior distribution of $\boldsymbol{\xi}$ [and, therefore $\kappa^c(\mathbf{x}, \boldsymbol{\xi})$] using the Bayes rule and the Markov chain Monte Carlo method, as described in Li and Tartakovsky (2020) for noise-free κ measurements.

7. NUMERICAL EXAMPLES

To illustrate the proposed method, we consider the diffusion equation with a partially known (i.e., sparsely sampled) parameter field $\kappa(\mathbf{x})$,

$$\nabla \cdot (e^{\kappa(\mathbf{x})} \nabla u(\mathbf{x})) = 0, \tag{19}$$

subject to the appropriate deterministic boundary conditions. Among various physical problems, this equation describes heat transport in solid bodies and flow in porous media with heterogeneous log conductivity κ. In the case of flow in geological porous media, many studies have shown that the statistical properties of $\kappa(\mathbf{x})$ can be well described by a Gaussian model learned from available observations (Boschan and Nœtinger, 2012; Tartakovsky et al., 2003). In the remainder of this section, we consider one- and two-dimensional forms of Eq. (19), and we assume that the prior Gaussian model of κ is available. In the forward UQ problem, we assume that some noisy measurements of κ are available and we compute the conditional mean and variance of $u(\mathbf{x})$. In the inverse problem, we use noisy measurements of k and noise-free measurements of u to estimate $\kappa(\mathbf{x})$.

7.1 One-Dimensional Diffusion Equation with Unknown Diffusion Coefficient

Here, we consider the one-dimensional steady-state diffusion equation

$$\begin{gathered} \frac{\partial}{\partial x}\left[e^{\kappa(x)} \frac{\partial u(x)}{\partial x}\right] = 0, \quad x \in (0,1), \\ u(0) = u_l, \quad u(1) = u_r, \end{gathered} \tag{20}$$

where $u_l = 0$ and $u_r = 2$. The sparsely measured $\kappa(x)$ is treated as random variable $\kappa(x, \boldsymbol{\xi})$ with the known mean $\overline{\kappa} = 1.4979$ and covariance function

$$C(x_1, x_2) = \sigma_\kappa^2 e^{-|x_1 - x_2|^2/\eta^2}, \quad x_1, x_2 \in [0,1], \tag{21}$$

with the correlation length $\eta = 0.5$ and standard deviation $\sigma_\kappa = 0.4724$. Our objective is to estimate the mean and variance of u conditioned on noisy measurements of κ. In this case, the $N = 7$-term KL expansion retains more than 99.99% of the total variance. The reference parameter field $\kappa(x)$ is obtained as a realization of $\kappa(x, \boldsymbol{\xi})$. We assume that three equidistant observations of κ are available with values drawn from the reference κ field. To study the effect of the measurement noise, in Case 1 we add random noise to the reference κ field values with the standard deviation $\sigma_\eta = 0.5$, in Case 2 we add noise with $\sigma_\eta = 0.1$, and in Case 3 we add the noise with $\sigma_\eta = 0.01$. The reference field κ, its noisy measurements, the conditional mean of the κ field, and the 97.5% confidence interval are shown in Fig. 1 for the three noise levels. It can be seen that the uncertainty (i.e., the conditional variance of κ) decreases as the variance of the noise decreases. The percentage of the total variance w.r.t. the variance of the unconditional κ is presented in Table 1.

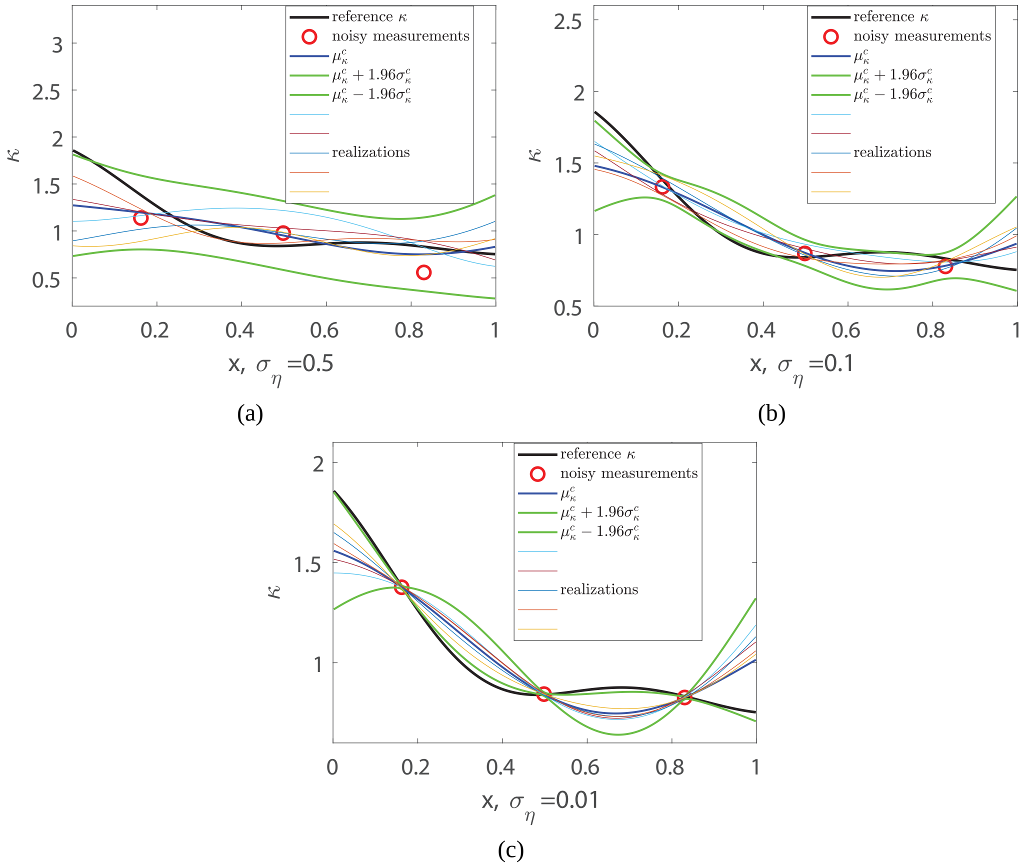


FIG. 1: Noisy measurements κ (open circles), conditional mean μ_κ^c (denoted by blue line), $\mu_\kappa^c \pm 1.96\sigma_\kappa^c$ (green lines), and several realizations of the conditional $\kappa^c(x, \xi)$ for the noise variance (a) $\sigma_\eta = 0.5$, (b) $\sigma_\eta = 0.1$, and (c) $\sigma_\eta = 0.01$. Black line denotes the reference κ field.

TABLE 1: Percentage of the total variance of the one-dimensional conditional κ w.r.t. that of the one-dimensional unconditional κ field

—	**Unconditional**	$\boldsymbol{\sigma_\eta = 0.5}$	$\boldsymbol{\sigma_\eta = 0.1}$	$\boldsymbol{\sigma_\eta = 0.01}$
total variance w.r.t. unconditional field	100%	18.82%	2.54%	1.55%

7.1.1 One-Dimensional Forward UQ Problem

We employ the stochastic collocation method with the level 7 and seven-dimensional sparse grids (Xiu and Hesthaven, 2005) to construct the order 4 gPC surrogate of u that we use to estimate its mean and variance. The reference $u(x)$, the mean field $\overline{u}(x)$, and $\overline{u}(x) \pm \sigma_u$ are presented in Fig. 2 for Cases 1–3. The reference $u(x)$ field is obtained by numerically solving the deterministic governing equation with $\kappa(x)$ given by the reference field on a mesh with 257 nodes using the finite element method.

Figure 3 displays the variances of κ and u conditioned on the noisy measurements of κ for the three different noise levels. For comparison, we also show the unconditional variances of κ

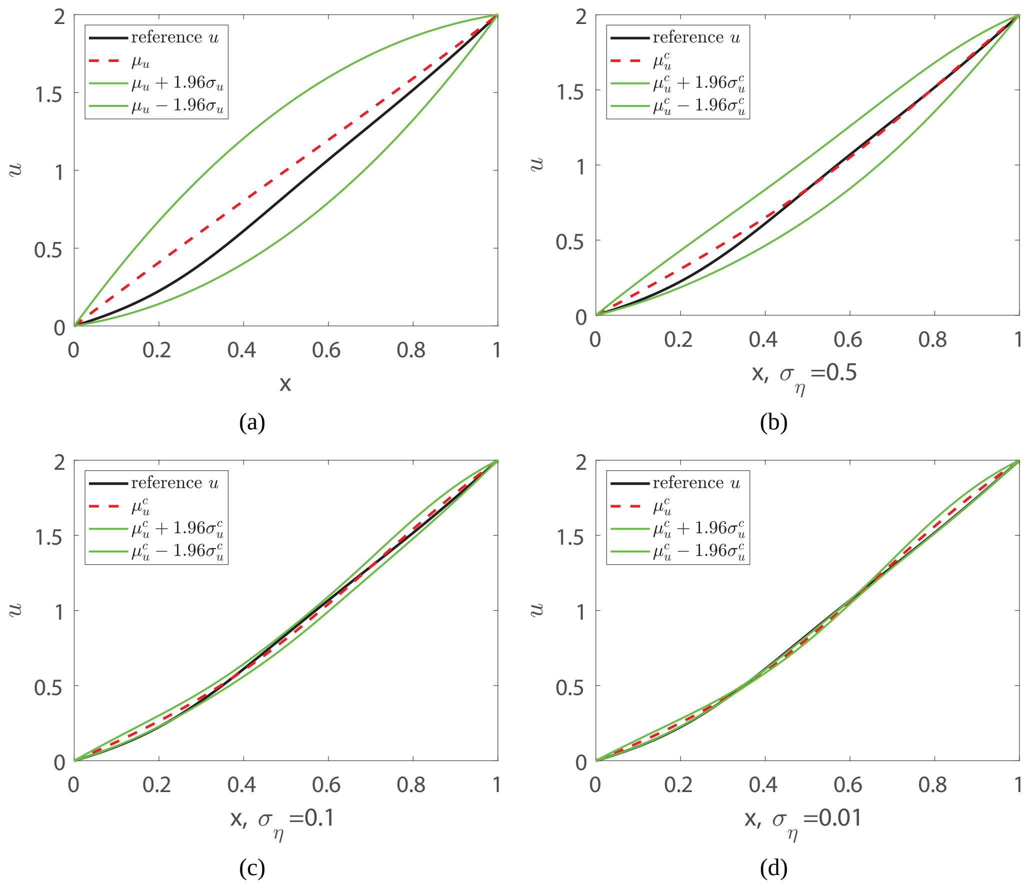


FIG. 2: (a) Unconditional mean and standard deviation of u. (b)–(d) Mean and standard deviation of u conditioned on the noisy measurements of κ with the measurement noise standard deviations $\sigma_\eta = 0.5$, 0.1, and 0.01, respectively. All plots also show the reference u field.

and u. For the largest considered measurement noise, the variance of κ is reduced by more than 66% and the variance of u is reduced by more than 75% compared to the unconditional case. The reduction in the variances of κ and u increases as the measurement noise decreases.

7.1.2 One-Dimensional Inverse Problem

Here, we use the KL expansion of κ and gPC surrogate of u conditioned on noisy measurements to estimate a realization of the κ that solves the inverse problem (15). We assume that the observations of u are noise-free, and we draw eight u measurements from the reference u field, which is generated as described in Section 7.1. For a given number of measurements, the solutions of the inverse problems depend on the measurement locations (Li and Tartakovsky, 2020). Here, we assume that all local maxima of the u variance curve are sampled with the rest of the measurements uniformly spread through the domain. The resulting measurement locations are shown in Fig. 4 for the three considered levels of the κ measurement noise.

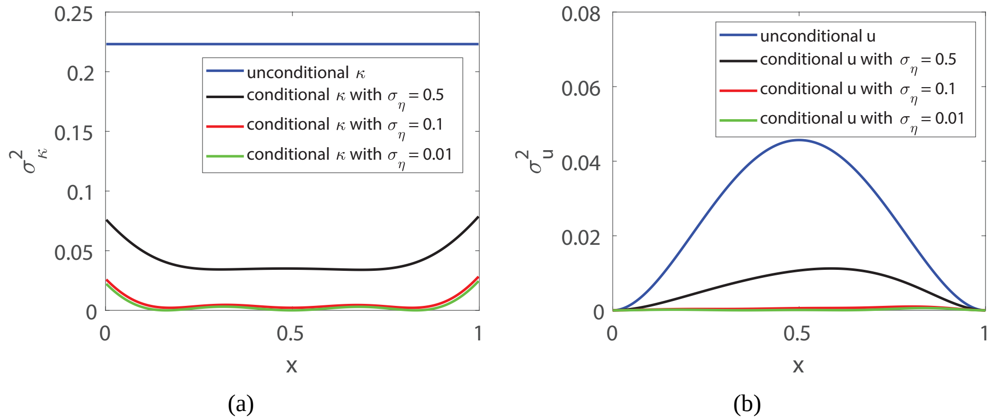


FIG. 3: (a) Unconditional and conditional variances of κ and (b) unconditional and conditional variances of u as functions of x. The conditional variances are given for the κ measurement noise with the standard deviations $\sigma_\eta = 0.5$, 0.1, and 0.01.

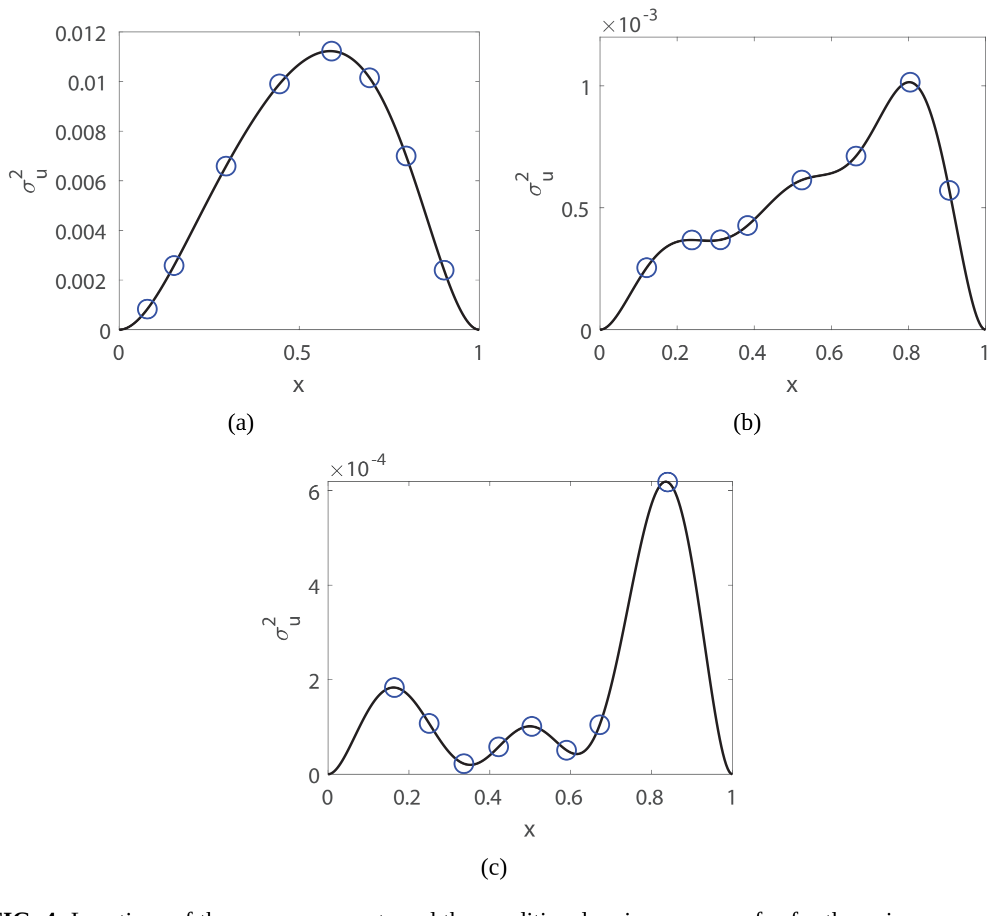


FIG. 4: Locations of the u measurements and the conditional variance curve of u for the noisy measurements of κ with the measurement noise standard deviation (a) $\sigma_\eta = 0.5$, (b) $\sigma_\eta = 0.1$, and (c) $\sigma_\eta = 0.01$

The optimization problem is solved using the Matlab optimization toolbox with the "fminunc/gradients" option. The relative errors in the estimated κ for the three levels of the κ measurement noise are displayed in Fig. 5 as functions of x. The maximum relative errors are approximately 13% for the measurement noise with $\sigma_\eta = 0.5$, 2.3% for $\sigma_\eta = 0.1$, and less than 0.3% for $\sigma_\eta = 0.01$.

7.2 Two-Dimensional Diffusion Equation with Unknown Diffusion Coefficient

In this section, we consider the two-dimensional diffusion equation with the partially observed coefficient $\kappa(x)$,

$$\nabla \cdot (e^{\kappa(\mathbf{x})} \nabla u(\mathbf{x})) = 0, \qquad \mathbf{x} = (x_1, x_2) \in D, \tag{22}$$

subject to the boundary conditions

$$u(0, x_2) = 2, \quad u(2, x_2) = 0, \quad -\mathbf{n} \cdot (e^{\kappa(\mathbf{x})} \nabla u)|_{(x_1,0)} = \mathbf{n} \cdot (e^{\kappa(\mathbf{x})} \nabla u)|_{(x_1,1)} = 0, \tag{23}$$

where $D = [0, 240] \times [0, 60]$ and $\mathbf{n} = (0, 1)$.

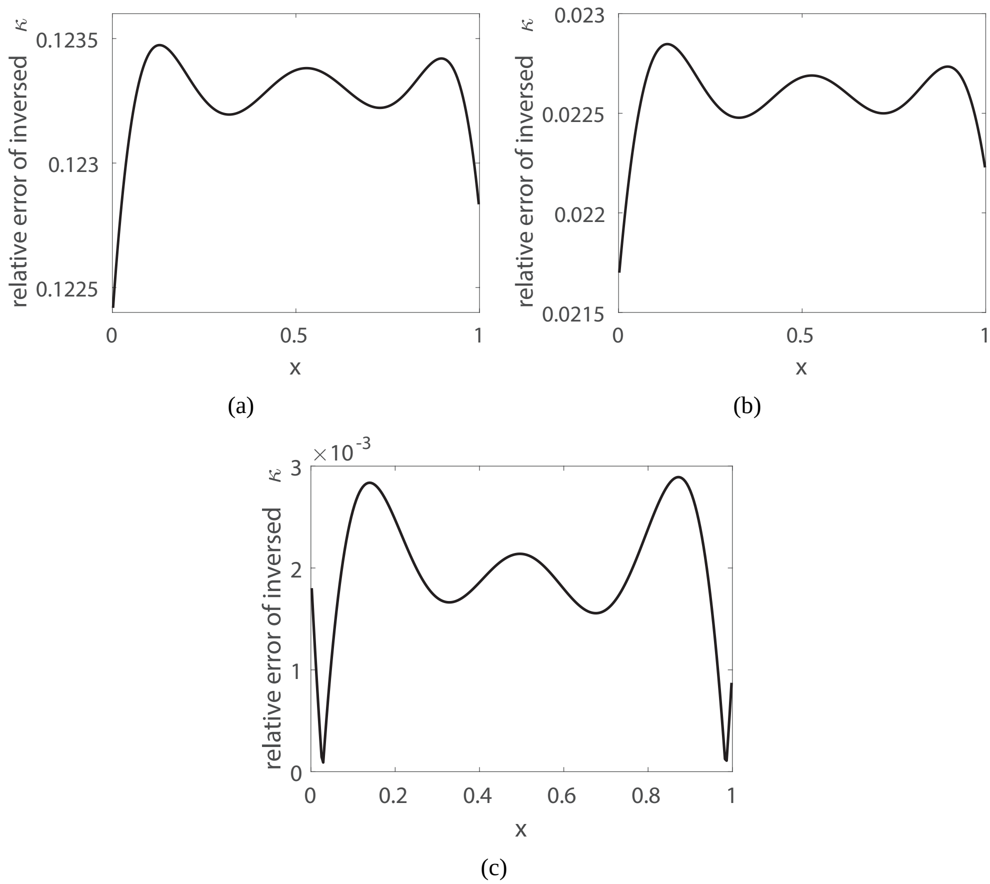


FIG. 5: Relative error of the estimated κ versus x for the standard deviation of the κ measurement noise: (a) $\sigma_\eta = 0.5$, (b) $\sigma_\eta = 0.1$, and (c) $\sigma_\eta = 0.01$

We assume that the sparsely sampled reference field $\kappa(\mathbf{x})$ is a realization of the Gaussian field with mean $\mu_\kappa = 0.8349$, standard deviation $\sigma_\kappa = 0.7262$, and the covariance function

$$C((x_1, x_2), (y_1, y_2)) = \sigma_\kappa^2 e^{-|x_1-y_1|^2/\eta_1^2 - |x_2-y_2|^2/\eta_2^2}, \tag{24}$$

where $\eta_1 = 120$ and $\eta_2 = 100$.

We approximate this Gaussian field with the $N = 7$-term truncated KL expansion,

$$\kappa(\mathbf{x}, \boldsymbol{\xi}) = \mu_\kappa + \sigma_\kappa \sum_{i=1}^{N} \sqrt{\lambda_i} \epsilon_i(\mathbf{x}) \xi_i, \tag{25}$$

which retains 99.67% of the total variance of the infinite-dimensional KL expansion. As in the one-dimensional example, we consider conditioning on κ measurements with three levels of measurement noise characterized by standard deviations $\sigma_\eta = 0.5$ (Case 1), $\sigma_\eta = 0.1$ (Case 2), and $\sigma_\eta = 0.01$ (Case 3). Four equidistant measurements of κ are drawn from the reference κ field, which is generated as a realization of the Gaussian field (24). Then, the i.i.d. Gaussian noise is added to simulate noisy measurements. Fig. 6(a) shows the reference κ field and the locations of the measurements. We present the variance of the conditional κ field for each noise

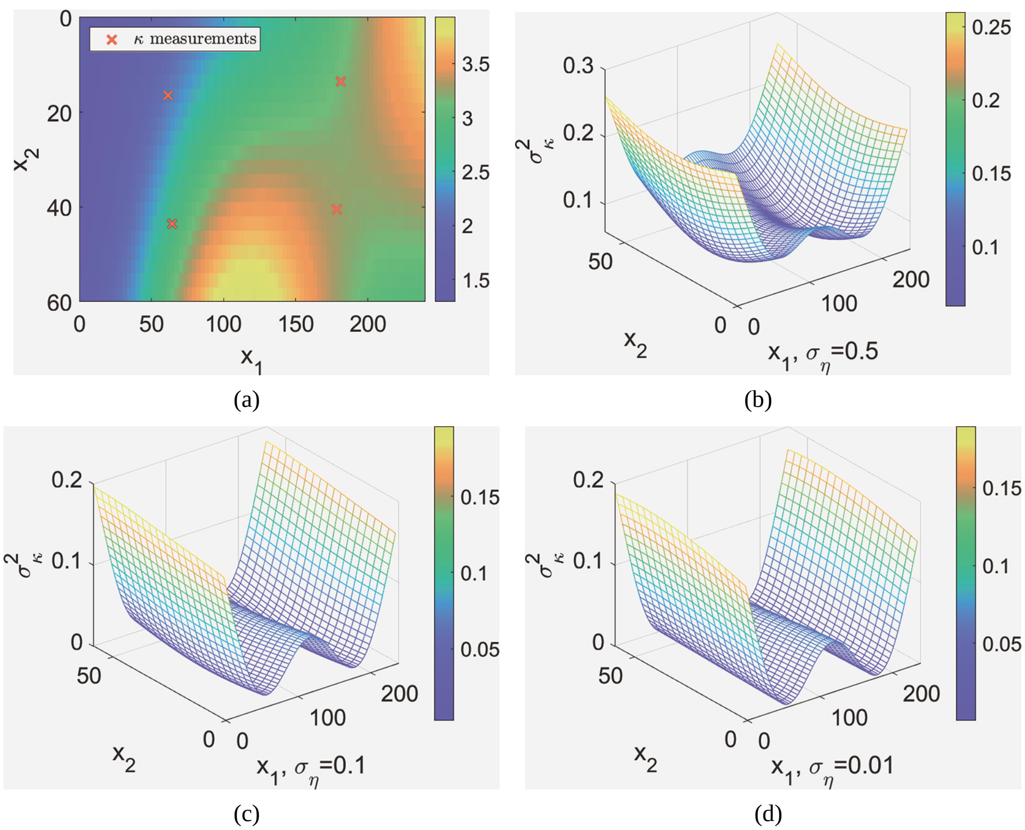


FIG. 6: (a) Two-dimensional reference κ field and measurement locations. (b)–(d) Variance of κ conditioned on noisy measurements with the noise standard deviations $\sigma_\eta = 0.5$, 0.1, and 0.01, respectively.

level in Figs. 6(b)–6(d). The percentage of the total conditional variance of κ w.r.t. the variance of unconditional κ is presented in Table 2. As in the one-dimensional case, conditioning reduces the variance of κ, with the variance reduction increasing with the decreasing noise level. The gPC collocation method with level 7 sparse grids is used to build the surrogate model of u for each level of κ measurement noise. To solve the equation for u for each collocation point, we use the finite volume method with 1600 elements.

7.2.1 Two-Dimensional Forward UQ Problem

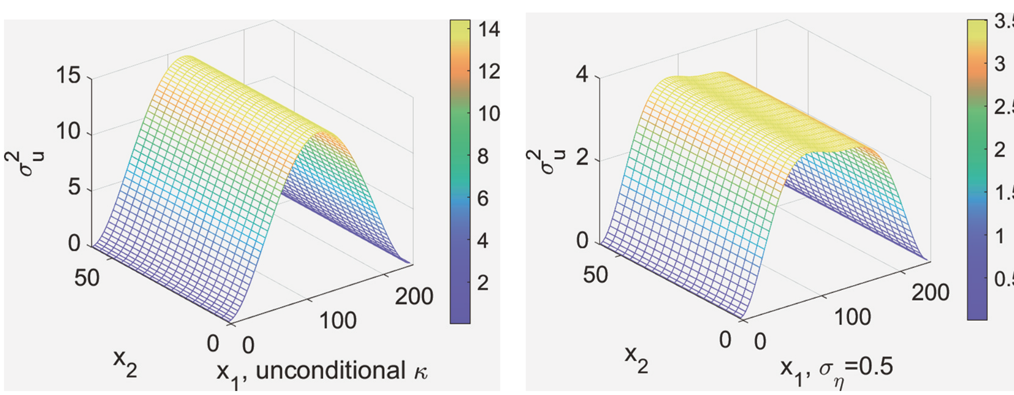
Here, we use the gPC surrogate to estimate the mean and variance of u conditioned on the noisy measurements of κ. The conditional variance of u as a function of the x_1 and x_2 coordinates is shown in Figs. 7(b)–7(d) for the three noise levels. For comparison, Fig. 7(a) depicts the unconditional variance of u. As in the one-dimensional problem, conditioning on the noisy κ measurements reduces the u variance and the reduction in variance increases with decreasing noise level.

7.2.2 Two-Dimensional Inverse Problem

As in the one-dimensional case, we assume that the observations of u are noise-free and are drawn from the reference u field that is found by solving the governing equation with the κ field given by the reference κ field. We use ten observations of u. The relative errors in κ estimated from the κ measurements with the three noise levels (and u noiseless measurements) are given in Fig. 8. The relative errors decrease with the noise level, with the maximum relative error of 15% for $\sigma_\eta = 0.5$, 1.6% for $\sigma_\eta = 0.1$, and 1.3% for $\sigma_\eta = 0.01$).

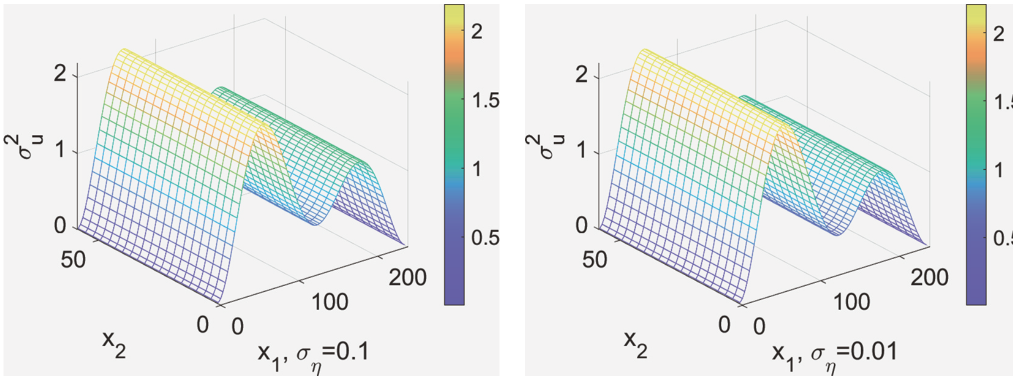
TABLE 2: Percentage of the total variance of the conditional two-dimensional κ w.r.t. that of the unconditional two-dimensional κ field

—	**Unconditional**	$\boldsymbol{\sigma_\eta = 0.5}$	$\boldsymbol{\sigma_\eta = 0.1}$	$\boldsymbol{\sigma_\eta = 0.01}$
total variance w.r.t. unconditional field	100%	22.13%	9.8%	8.76%



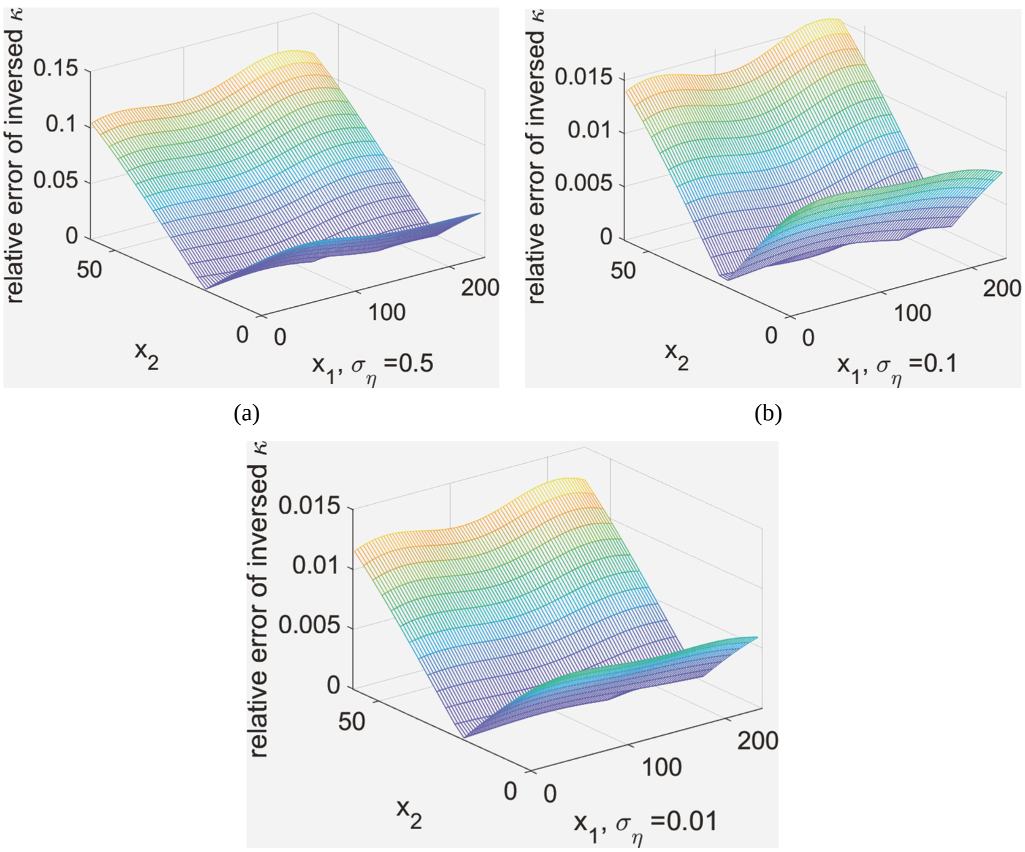
(a) (b)

FIG. 7.



(c) (d)

FIG. 7: (a) Unconditional variance of u as a function of the x_1 and x_2 coordinates. (b)–(d) Variance of u conditioned on κ measurements with the noise levels $\sigma_\eta = 0.5$, 0.1, and $\sigma_\eta = 0.01$, respectively.



(a) (b) (c)

FIG. 8: Relative error of estimated κ field obtained with noiseless u measurements and noisy κ measurements with the measurement noise standard deviations (a) $\sigma_\eta = 0.5$, (b) $\sigma_\eta = 0.1$, and (c) $\sigma_\eta = 0.01$

8. CONCLUSION

We proposed a new form of KL and gPC expansions conditioned on noisy measurements. We use these expansions for forward UQ and inverse problems in PDE models with unknown sparsely sampled parameter fields. In the proposed approach, GPR is used to estimate the distribution of the unknown parameter conditioned on its noisy measurements. Then, the corresponding KL and gPC expansions are constructed in terms of the eigenfunctions and eigenvalues of the conditional covariance function of the parameter obtained from the GPR model. In the forward UQ application, the conditional gPC surrogate was used to estimate the mean and variance of the state variable conditioned on the noisy measurements of the parameter. We found that conditioning reduces the state variable variance, with the variance decreasing as the measurement noise decreases. In the inverse solution, we formulated a MAP minimization problem and used the conditional KL and gPC expansions to find a realization of the conditional parameter field that satisfies the minimization problem. We found that errors in the estimated parameter field with respect to the reference parameter field decrease with the decreasing measurement errors.

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