INVERSE MODELING AND UNCERTAINTY QUANTIFICATION OF

NONLINEAR FLOW IN POROUS MEDIA MODELS

by

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A Dissertation Presented to the
FACULTY OF THE USC GRADUATE SCHOOL
UNIVERSITY OF SOUTHERN CALIFORNIA
In Partial Fulfillment of the
Requirements for the Degree
DOCTOR OF PHILOSOPHY
(CIVIL ENGINEERING)

May 2014

Dedication

To my family

Acknowledgments

I would like to express my greatest appreciation to everyone who was with me during the entire or part of my journey of Ph.D study.

I would like to thank my advisor, Professor Dongxiao Zhang, for his consistent guidance, support and all the research resources and opportunities he introduced to me, without which this dissertation would never have been accomplished.

I would like to thank the professors on my dissertation committee: Dr. Felipe de Barros, Dr. Roger Ghanem and Dr. Behnam Jafarpour, as well as Dr. Erik Jonhson who served on my qualifying exam committee, for their valuable suggestions and comments.

I would like to extend my sincere thanks to my mentors and collaborators out of USC. They are Dr. Adedayo Oyerinde, Dr. David Stern and Dr. Xiao-hui Wu from ExxonMobil upstream research company, Dr. Guang Lin and Dr. Bin Zheng from Pacific Northwest National Laboratory.

I would like to thank the former and current fellow students and post-doctors in our

and other research groups at USC, Heli Bao, Dr. Haibin Chang, Dr. Parham Ghods, Dr. Ziyi Huang, Dr. Hamid Reza Jahangiri, Woonhoe Kim, Dr. Heng Li, Qinzhuo Liao, Le Lu, Dr. Liangsheng Shi, Charanraj Thimmisetty, Dr. Ramakrishna Tipireddy, Dr. Hamed Haddad Zadegan, Dr. Lingzao Zeng, Ruda Zhang,..., not only for the discussions and shared thoughts that inspired my research, but also for the friendships that made my life through the PhD study so much easier.

Finally, I would like to thank my wife Jie Yang and everyone in my family, for your endless and unconditional love.

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Abstract

When using computer models to predict flow in porous media, it is necessary to set parameter values that correctly characterize the geological properties like permeability and porosity. Besides direct measurements of these geological properties, which may be expensive and difficult, parameter values could be obtained from inverse modeling which calibrates the model to any available observations on flow behaviors such as pressure, saturation and well production rates. A typical inverse problem has non-unique solutions because the information contained in the observations is usually insufficient to identify all uncertain parameters. Finding a single solution to the inverse problem that well matches all observations does not guarantee the correct representation of the real geological system. In order to capture multiple solutions and quantify remaining uncertainty we solve an inverse problem from a probabilistic point of view: seek the posterior distribution of parameters given the observations using Bayes' theorem. In the situation where the model is nonlinear, which is often the case of subsurface flow problems, the posterior distribution cannot be analytically derived. Instead we implement numerical algorithms to find approximate results. The key to running an inversion algorithm is to understand how the

model input (parameters) and model output (simulation results) are related to each other. For complex models where direct derivation is difficult this task can be done by running a large number of trial simulations with different parameter values. These algorithms work well for simple small scale models but are prohibitively expensive to apply to subsurface flow models since each single run may take a long time and we do not have unlimited time and resource to run the trial simulations.

The main contribution of this research is the development and test of two approaches—the "adaptive ANOVA-based probabilistic collocation Kalman filter (PCKF)" and "adaptive sampling via Gaussian process (GP)-based surrogates"—for inverse modeling of nonlinear flow in porous media models. Both approaches fall into the category of probabilistic inversion and have the capability to quantify remaining uncertainty. This study focuses on computational efficiency, which is often the bottleneck of implementing inverse modeling and uncertainty quantification (UQ) algorithms for nonlinear models. The selection of proper inversion approach to be used is problem dependent. The "adaptive ANOVA-based PCKF", is a nonlinear variant of the classic Kalman filter approach, which estimates the first two statistical moments, i.e., mean and covariance, of the posterior distribution. It applies to the problems where the nonlinearity is mild and the posterior distribution is approximately Gaussian. The main idea is to represent and propagate uncertainty with a proper polynomial chaos expansion (PCE) that is adaptively selected for the specific problem. The second method is more general and deals with stronger nonlinearity and non-Gaussian, even multi-modal, posterior distributions. Sampling approaches usually cost even more computational effort comparing with Kalman filter methods. But in our al-

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gorithm, the efficiency is greatly enhanced by the following four features: a GP surrogate for simulation acceleration, an adjustment of the posterior considering surrogate error, an importance sampler using Gaussian mixture proposal distribution, and an adaptive refinement scheme. The developed approaches are demonstrated and tested with different models.

Chapter 1

Introduction

1.1 Subsurface Flow Simulations under Uncertainty

Numerical models are powerful tools to simulate the fluid flow through porous media. It has many research and industrial applications in the areas such as oil and gas recovery, groundwater management, pollutant transport assessment, and geological sequestration of greenhouse gases. After decades of development, the state-of-the-art simulators are now capable of solving coupled partial differential equations governing the complex subsurface multiphase flow system within a practically large spatial and temporal domain. However, despite the advances in numerical approaches and computing capabilities, researchers and engineers still find it challenging to make accurate predictions for real practical problems. One of the biggest difficulties is to assign the correct values to the model parameters when they are subject to uncertainty.

Subsurface flow behaviors depend on the geological properties such as permeability, porosity, fault transmissibility, etc. Thus it is necessary for a modeler to find the parameter values that correctly characterize these properties. But this is not an easy task. The geological properties are location dependent and often reveal a strong heterogeneity. In addition precise and comprehensive measurements are difficult and usually very expensive. These facts prevent modelers from obtaining the complete information of these properties. In addition to the geological properties, uncertain parameters also may arise from our incomplete knowledge about boundary and initial conditions, e.g., the rate of recharge to an aquifer, or the initial position of the oil-water contact in a petroleum reservoir. These uncertain parameters could be a major contributor to the discrepancy between simulation results and reality.

To address this problem one could consider all possible parameter values that are consistent with the available measurement data and other pre-given geological descriptions such as experts' opinion. Mathematically, the model parameters are expressed as random variables (or stochastic processes if the parameters are location/time dependent), which are characterized by the corresponding probability distributions. For models with stochastic parameters, the model output also becomes random. To make reliable prediction one needs to study how the parameter uncertainty propagates through model and affects the simulation results. For example, we may give an estimated error bound for the simulated output. This process is referred to as "(forward) UQ". The studies regarding the stochastic flow in porous media and uncertainty quantification are summarized in the books by Zhang (2001), Rubin (2003), and Dagan and Neuman (2005).

1.2   Uncertainty Reduction by Inverse Modeling

If we hope to reduce the uncertainty and make more accurate predictions, we need to gather more information about the parameters. Besides direct measurements of the input parameters, the field measurement/observation of flow behaviors is another important source of information which helps us improve the estimation of parameters as well as the credibility of predictions about other output variables. The idea is straightforward: only the parameter values from which the simulation results match the observed field data should be trusted and used for prediction. Examples of such field data include the water head observations in a groundwater problem, the concentration measurements in a pollutant transport problem, the bottom-hole pressure and production rates recorded at wells in an oil recovery problem, etc. The work of calibrating model parameters to field data is known as "data assimilation". Since this process infers the input variables (parameters) from the observations on some of the output variables, we also call it "inverse modeling". Previous studies on inverse modeling of flow in porous media problems are seen in the review papers by Yeh (1986) and Oliver and Chen (2011). The calibrated parameters are then used to make predictions to other output variables in a forward modeling procedure. The work flow of forward and inverse modelings is illustrated in Fig. 1.1.

Solving inverse modeling problems is challenging, especially when one has multiple parameters to estimate and multiple field observations to match. Usually, what we have at hand is a simulator that solves the deterministic forward problem. The forward problem is well defined, i.e. for a deterministic input submitted to the simulator we get a unique
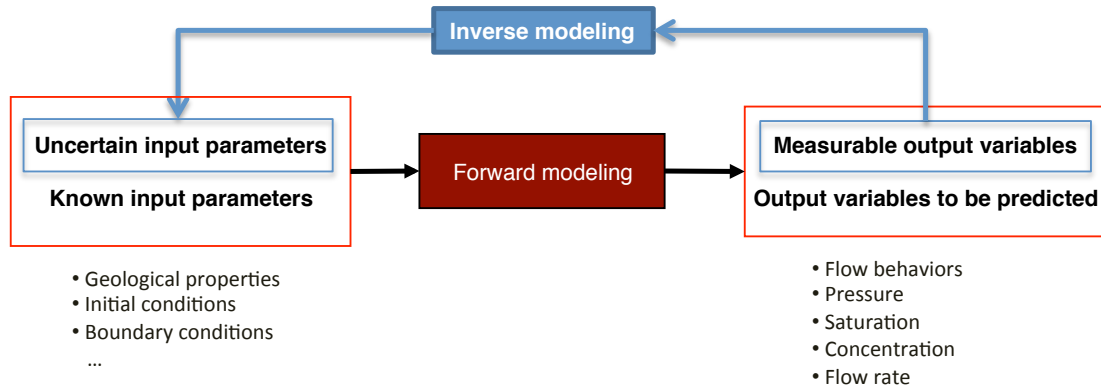
Figure 1.1: Work flow of forward and inverse modelings.

output returned by the simulator. In contrast, the simulator does not generate a model "input" with a given "output". In fact, one should note that an inverse problem is usually ill-posed and has non-unique solutions. This means that for a single deterministic observed value of the output one may find multiple corresponding input values that all give a match to the output value. Essentially, this is because the information contained in the data measurement is insufficient to determine all the uncertain model parameters. Specific reasons causing non-unique solutions include the following ones.

First, in most inverse problems we have less number of independent observations than the independent uncertain parameters. Like solving equations, this implies that we do not have enough constraints to determine all the parameters, and there are different combinations of parameter values that all result in a match to the observations. The second typical reason is the nonlinear input-output relationship. Most subsurface flow models are nonlinear and this may cause non-unique solutions even if the model parameters are constrained by the same number of observations. The third reason is acceptable mismatch.

Besides inaccurate model parameters, there are other causes of the discrepancy between real field measurements and simulation results. For instance, measurement errors associated with observations. In addition, the model used in the simulation could be imperfect and results in a modeling error comparing with the real physical process to be simulated. These errors contribute to the mismatch between the simulation result and the observation made in the real world even if we have accurate parameter values. Considering this fact, one should keep all those parameter points if their corresponding mismatch is within an acceptable error range, rather than requiring a strict zero mismatch.

Approaches solving inverse problems can be roughly divided into two categories: deterministic inversion and probabilistic inversion. In deterministic inversion approaches, we seek a single point in the parameter space that results in the best match to the observed data. This is done by searching for the minimum point of an objective function which quantifies the difference between the simulation results and the observations. The minimization could be implemented by typical numerical optimization algorithms such as gradient-based approaches or genetic algorithms. Once an optimal parameter point is obtained, it is then used for predicting quantities of our interest. For ill-posed inverse problems with non-unique solutions, a regularized term that reflects the modeler's prior preference may be added to the objective function to help identify a single solution.

Non-unique solutions of an inverse problem indicate that the uncertainty associated with model parameters is not eliminated by the observations, but usually only greatly reduced. For example, the variances of uncertain parameters become smaller but not negligible.

In this situation, the single solution provided by the deterministic inversion approach, which omits the remaining uncertainty, does not lead to a reliable prediction of future, because such a solution could deviate from reality even it nicely matches all the field data. Instead, we prefer to keep all possible scenarios in the solution of the inverse problem, which brings the idea of probabilistic inversion approaches. With multiple solutions one can re-assess the remaining uncertainty in the parameters and the simulation results after the data assimilation. In this sense, we also call the probabilistic inverse modeling "inverse uncertainty quantification".

In order to capture multiple solutions and quantify the remaining parameter uncertainty we formulate an inverse modeling problem from a probabilistic point of view, rather than the optimization approaches talked previously. Tarantola (2005) proposed a method of "combination of states of information" to quantify parameter uncertainty. In our study we adopt the more widely used approach of Bayesian inversion. See the book by Kaipio and Somersalo (2006) and the book by Oliver et al. (2008) for reference. In Bayesian probabilistic inversion approaches different solutions are represented by the "posterior probability distribution" of the model parameters given the observations. By the Bayes' theorem the posterior distribution is calculated from the pre-specified prior distribution as well as the likelihood function. While the likelihood function represents the information about model parameters obtained from observations, the prior distribution reflects the information from all other sources, e.g., a physically meaningful range constraining the parameter value, experts' opinions, or direct measurements. Although the posterior distribution provides the complete information of the remaining uncertainty associated

with model parameters, it in general cannot be analytically derived except for a few special cases, e.g., linear models with Gaussian pdfs, or models where the parameters can take only finite number of discrete values. Often we rely on numerical algorithms to find approximate representations of the posterior distributions. In most of the current available numerical algorithms solving inverse modeling problems, the key procedure is to make a large number of trial model simulations with different parameter values, which are used to detect the nonlinear input-output relationship in a model. While these algorithms work well for some other models they cannot be simply applied to subsurface flow models because each single simulation may take a long time and running a large number of simulations is impractical.

1.3   Inversion Approaches: Dealing with Nonlinearity

One special case in which the posterior distribution can be analytically derived is linear models with the prior density of parameters and measurement errors both normally distributed. Under these conditions, the posterior distribution of model parameters is also normal and hence fully characterized by its first two statistical moments, mean and covariance. The classic algorithm to solve such kind of inverse problems is Kalman filter (Kalman, 1960). In addition, the Kalman filter is usually implemented in a recursive manner. Suppose the data (measurements) come available as a time sequence. For each node on this data sequence, we solve an inverse modeling problem. The posterior mean and covariance computed from the previous step serve as the prior for the next step. When-

ever new data are collected, the parameters are updated correspondingly. This process is known as sequential data assimilation.

For nonlinear systems, the posterior distribution generally is non-Gaussian, regardless of whether or not the prior density and observation error are Gaussian. As long as the nonlinearity is not strong, the Kalman filter still yields a good approximate solution of the posterior mean and covariance. The key step in implementing the Kalman filter is to compute the "Kalman gain," which requires knowledge of the covariance of the (prior) joint distribution of model parameters and output variables. While this covariance is easily computed for linear systems, extra computational effort is necessary to estimate it for nonlinear models. Indeed, a forward UQ problem must be solved to study how the parametric uncertainty propagates through the nonlinear system to affect the output quantities. This becomes the main difficulty and computational overhead in extending the Kalman filter to nonlinear models.

A straightforward way to apply Kalman filter to nonlinear models is to implement a first-order linearization to the model around its prior mean. This method is known as "extended Kalman filter (EKF)" (Anderson and Moore, 1979). One of the disadvantages of EKF is its instability when the prior estimation is far away from the true state. Moreover, EKF requires computing the Jacobian matrix, i.e., the partial derivatives of the model outputs with respect to the model parameters. This could be extremely costly for models with a large number of parameters.

The ensemble Kalman filter (EnKF), a relatively new nonlinear variant of the Kalman filter, represents and propagates uncertainty using the Monte Carlo method (Evensen,

1994, 2009). First, a number of realizations (an ensemble) of model parameters are randomly sampled from the prior distribution. Then, for each realization, a simulation is run to predict the corresponding realization of model outputs, and the required covariance is estimated from the joint ensemble. Finally, each realization is updated by the Kalman filter to form a new ensemble that represents the posterior distribution of model parameters. Due to the simplicity in its implementation, EnKF has gained great popularity within the past two decades. Since its invention, EnKF has been applied to many different research fields including the modeling of flow in porous media (Chen and Zhang, 2006; Aanonsen et al., 2009) and has demonstrated great effectiveness. Evensen (2003) has provided a review of the development and applications of EnKF. However, like all Monte Carlo approaches, EnKF's accuracy relies on a sufficiently large ensemble, which causes an enormous computational burden for large-scale computational models.

An alternative to the Monte Carlo method for studying uncertainty propagation is the PCE. In this approach, the random quantities under study are expanded using a polynomial chaos basis, which are the orthogonal polynomials with respect to a set of independent random variable with known distributions (Wiener, 1938; Ghanem and Spanos, 2003; Xiu and Karniadakis, 2003). Once the PCE representation is obtained, the statistical moments of our interest (e.g., mean and covariance of the random quantities) can be easily computed from the coefficients in front of the polynomial chaos basis.

The key–and computationally demanding–step of implementing the PCE approach is solving for the PCE coefficients. Among different methods available to tackle this problem, such as the stochastic Galerkin projection (Ghanem and Spanos, 2003) and regression

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method (Isukapalli et al., 1998), the probabilistic collocation method (PCM) (Tatang et al., 1997) is particularly convenient and effective. PCM constructs the PCE approximation by interpolation, where the interpolation points are called "collocation points." Similar to Monte Carlo, PCM is a non-intrusive approach, which means it treats the model as a black box and requires only repetitive evaluations of the model at the collocation points with a deterministic simulator. To achieve high accuracy in estimating the statistical moments, which by definition are integrals over the random space, the collocation points usually are deployed the same way as the quadrature points used in numerical integration schemes, such as Gauss quadrature points. For high-dimensional PCM, commonly used collocation schemes include sparse grid and Stroud quadrature points (Xiu and Hesthaven, 2005). A discussion regarding the selection of collocation points is given by Eldred and Burkardt (2009). PCM was compared with the Monte Carlo method in previous studies and demonstrated better efficiency in solving forward UQ problems for flow in porous media models (Li and Zhang, 2007, 2009; Li et al., 2009; Lin and Tartakovsky, 2009).

Similar to the EnKF, which combines the Monte Carlo method with the Kalman filter, the so-called "PCKF" or "polynomial chaos-based ensemble Kalman filter", which combines the PCE with the Kalman filter, was developed to solve inverse modeling problems (Saad and Ghanem, 2009; Li and Xiu, 2009; Zeng and Zhang, 2010; Zeng et al., 2011; Li et al., 2011). PCKF resembles EnKF in almost every aspect except that it uses the PCE to represent uncertainty. While an EnKF user must decide on the size of the ensemble before running the algorithm, a PCKF user has to determine in advance the truncation of the PCE, i.e., to select the basis functions to form the PCE approximation. The trade-off is

that keeping more PCE basis functions helps to capture uncertainty more accurately, but it increases the computational cost. An ideal PCE should accurately represent the model uncertainty but keep the number of basis functions as small as possible. Dealing with this issue is particularly vital in solving high-dimensional problems (i.e., stochastic models with a large number of uncertain parameters) because the total number of PCE terms can grow dramatically fast as the dimensionality increases.

A general guideline for choosing the PCE bases for PCKF was lack in previous researches. In this study, we develop a new algorithm (Li et al., 2014) that adaptively selects active PCE basis functions for uncertainty representation in different problems and automatically adjusts the number of basis functions in different Kalman filter loops. We construct the PCE based on adaptive functional analysis of variance (ANOVA) decomposition. Functional ANOVA, also referred to as "high-dimensional model representation" (HDMR), was shown as an effective dimensionality reduction method (Rabitz and Alis, 1999; Li et al., 2001)and was combined with PCE approximation to solve forward UQ problems (Foo and Karniadakis, 2010). Now, we extend this methodology toward solving inverse modeling problems. Because in many physical models the coupling effect of a large number of input parameters on the model output can be reduced to the coupling effect of only a few, functional ANOVA decomposition is able to approximate a high-dimensional function with the summation of a set of low-dimensional functions, known as ANOVA components. For different models, the components of the ANOVA decomposition may be adaptively calculated following some adaptive criterion, which greatly reduces the computational cost and improves efficiency (Ma and Zabaras, 2010; Yang et al., 2012). Once

an ANOVA decomposition is done, the ANOVA components (low-dimensional) can be expanded with PCE, which is much less costly than expanding the original model (high-dimensional).

Although the above mentioned Kalman filter's variants have been shown working well in many studies of nonlinear inverse problems, one should note that all these methods could fail for highly nonlinear models when the assumptions on which Kalman filter is based are severely violated. Kalman filter only uses the first two statistical moments (mean and covariance) to describe the joint distribution of the parameters and model outputs when solving inverse problems. The information contained in higher-order moments is not seen by the algorithm. In an extreme case, it is possible that model input and output are nonlinearly dependent with each other but statistically uncorrelated, i.e., their covariance is zero. In this situation Kalman filter and its variants cannot infer input from the observations of the output. Strong non-linearity also may lead to multimodal posterior distributions in which situation only estimating the first two statistical moments simply does not provide enough insight into the posterior.

To deal with strong nonlinearity and to characterize an arbitrary posterior density, we put down the Kalman filters and go back to solve the Bayesian inverse problem directly. If the posterior density cannot be analytically derived, we could draw a sample of realizations to represent it, which is again the idea of Monte Carlo methods. (Note that in EnKF the purpose of using Monte Carlo method is to estimate the required prior statistical moments and the updated ensemble does not accurately represent the posterior distribution unless the model is indeed linear). Examples of Monte Carlo approaches include the

Particle filter (Gordon et al., 1993), the Markov chain Monte Carlo (MCMC) (Metropolis et al., 1953; Hastings, 1970), etc. Implementing a typical Monte Carlo algorithm requires to randomly sample a set of points in the parameter space according to the prior distribution. For each parameter point the model is evaluated to generate the corresponding output which is then compared with the field data. Only those parameter points that match the field data are kept (following certain rules) to represent the posterior distribution. In many cases, the probability that a randomly selected point hit the target is small. To have enough points representing the posterior distribution one has to sample and evaluate an extremely large number of parameter points. This makes Monte Carlo methods intractable for large scale models which are time consuming to run.

A practical inversion algorithm is expected to keep the computational cost as low as possible. One of the straightforward ideas to lessen the computational cost is to use surrogate models. A surrogate (also called a meta-model, or a reduced order model in different studies) is an approximation of the original true model that can be quickly evaluated. With a surrogate replacing the original model, drawing a large enough sample becomes affordable and hence makes Monte Carlo methods applicable. A good surrogate should be both economical and accurate. Various types of surrogate models have been studied in previous researches to approximate parameter-output relationships for objectives including prediction, optimization, sensitivity analysis, uncertainty analysis and inverse modeling/calibration. Razavi et al. (2012) gave a review of the surrogate models used in the field of water resources research, which are divided into two categories: statistical data-driven models and lower-fidelity physically based surrogates. The construction of the first type of

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surrogate models often requires a number of simulations of the original model at a group of parameter points based on an experimental design scheme, from which a response surface over the entire parameter space is then quickly generated using some technique. In the context of inverse modeling, examples of such techniques include polynomial approximations like the PCE (also known as "stochastic response surface" in some literature) (Balakrishnan et al., 2003), radial basis functions interpolation (Bliznyuk et al., 2008), and the neural network (Zou et al., 2009). Examples of the second category of surrogates include models built on coarser spatial and/or temporal grid size, simplified mathematical equations or physical models.

In previous studies on surrogate-based sampling algorithms for inverse modeling, the original models usually were simply replaced with selected surrogate models under the assumption that the approximation error is negligible. However, surrogate accuracy is indeed a crucial issue. One needs to keep in mind that an inaccurate surrogate in a sampling algorithm causes extra sampling error and results in a biased estimation of the parameters. For example, a parameter point that matches the field data through the original model but not through the inaccurate surrogate may be mistakenly ruled out of the sample. On the other hand, a parameter point out of the true posterior distribution may be sampled if it happens to fit the observations through the inaccurate surrogate.

To reduce such mistakes, we need an error estimation for the surrogate approximation. Note that the approximation error, which is defined as the difference between the output values given by the original model and the surrogate, is deterministic in the sense that repeated computational experiments with the same input parameter point would yield the

same output difference. However, in practice the output value of the original model is not known without running simulations, so the approximation error at each parameter point is generally uncertain and is expressed as a random variable. The accuracy of the surrogate is measured by the spread, e.g., estimated standard deviation, of the approximation error. This quantity indicates how reliable the surrogate is when we use it for inverse modeling. With an error estimation of the surrogate, we can modify sampling algorithms accordingly to avoid the above mentioned mistakes caused by inaccurate surrogate. Specifically, we sample from an adjusted posterior distribution, which incorporate the estimation of approximation error. When the surrogate is accurate, i.e., with a small approximation error, the modified sampling algorithm works almost the same way as sampling via the true model response. However, a large estimated surrogate error would have an effect on the sampling rule. The sampling algorithm should tolerate those parameter points that do not match the observation but lead to a mismatch within a reasonable range considering the estimated approximation error. The reason is that the mismatch could be induced by either an incorrect parameter point or the surrogate error. Before we make any further investigation we should not rashly conclude that the parameter point is wrong and rule it out. Similarly, for those parameter points that do match the observation via the surrogate, the sampling rule should be less assertive to keep them as solutions if the estimated surrogate error is not negligible.

Another prominent byproduct of error estimation is that it provides an indicator of whether a refinement is necessary if a more accurate surrogate is desired. For the majority of nonlinear flow in porous media models, it is extremely difficult to find accurate yet

inexpensive surrogates. However, in the context of inverse modeling, the surrogate does not have to be globally accurate. In fact, we only need the surrogate to be accurate in the regions where the posterior density distributes since most model evaluations are computed here, whereas the accuracy requirement can be relaxed elsewhere. Fortunately, the posterior density in most inverse problems covers only a small portion of the prior distribution, which makes it possible to build such a locally accurate surrogate with affordable computational cost. This motivates us to develop an adaptive re-sampling and surrogate refinement algorithm. We first draw a sample using an initial surrogate which could be associated with some non-negligible error. This initial sample outlines the regions where the solutions could exist. Next we check the estimated surrogate error in these regions and make refinements to locally improve the surrogate accuracy if necessary. Then a new sample is drawn using the improved surrogate. This re-sampling and refinement loops proceed until the surrogate is accurate enough at all the solution regions and the sample points are verified to be reliable solutions via this accurate surrogate.

According to above discussions, we prefer a surrogate model for our algorithm if it has the following two features. 1) At a given parameter point, the surrogate model should provide not only an approximate model output, but also an estimation of the approximation error. 2) The surrogate has the flexibility to be refined adaptively to improve local accuracy in the important regions if necessary. Through adaptive refinement, we are able to achieve a surrogate that is accurate enough for the inverse problem yet costs a minimum computational resource to build. One of such surrogate models that provide these features is GP. The method of approximating a deterministic function with a GP was first

used in geostatistics, known as Kriging interpolation, to estimate the spacial distribution of a geological property. The same idea was later applied to approximation of computer model responses (Sacks et al., 1989; Currin et al., 1991; Kennedy and O'Hagan, 2001). The basic idea of GP-based surrogate, or Kriging, is assuming that the input-output relationship of a model, or a function, resembles a realization of a Gaussian stochastic process that bears some spatial correlation structure. The surrogate is obtained by conditioning this stochastic process to the (original) model output values evaluated at a number of parameter points. The approximate model response and the error estimation of the surrogate are represented by the mean and the variance of the conditional process, respectively. Furthermore, the surrogate model can be adaptively refined by adding more conditioning points to the regions of interest.

Jones et al. (1998) developed an optimization algorithm called "efficient global optimization (EGO)" using Kriging interpolation to approximate the objective function and accelerate the searching process. EGO may be used in the context of inverse modeling in which the objective function to be optimized is defined as the mismatch between surrogate output and the observations. Nevertheless, as we discussed in an earlier paragraph, optimization approaches result in only a single solution, a global minimum, and does not reflect the posterior uncertainty. In addition, we point out that the GP is not a good candidate to approximate the mismatch function in the targeted regions of the posterior distribution because the mismatch would be very close to zero but always positive (hence non-Gaussian).

We adopt the idea of Kriging interpolation in our approach. However, unlike EGO, our

focus is to solve inverse problems rather than a general optimization problem. First, instead of defining and approximating an objective function, we approximate the dependent relation between model parameters and outputs. Secondly, we develop a GP surrogate-based sampling algorithm to sample from the posterior distribution. The objective is to capture multiple solutions of an inverse modeling problem and to quantify the remaining uncertainty.

Besides the estimation of approximation error, several other features of GP/Kriging make it particularly suitable for inverse modeling. 1) The selection of interpolation points (the parameter points where original model is evaluated) is flexible. This allows us to freely and adaptively add more interpolation points wherever we want to refine the surrogate model without abandoning previously evaluated points. Whereas in many other surrogate models (e.g., interpolation on sparse grid) the selection of parameter points for model evaluation must follow a certain scheme (e.g., quadrature schemes). In this case not only local refinement becomes difficult, the total number of model evaluations required by the scheme usually grows dramatically as the dimension of parameter space increases. 2) For model with multiple input parameters, a GP is able to detect the "important" input dimensions among all parameters (sensitivity analysis). This information is crucial since it provides guidance about how to allocate the interpolation points to best capture the dependent relationship between parameters and model output. The sensitivity analysis is embedded in the spatial correlation structure of the GP. The correlation lengths along different dimensions generally is different. In other words, the correlation structure is anisotropic. A strong correlation (long correlation length) along a dimension implies a rel-

atively small and smooth variation and thus a few model evaluation points are sufficient to represent it, whereas a weak correlation (short correlation length) along a dimension means large and frequent variation and so more points are needed. 3) By adjusting the mean and covariance functions of a GP model, we are able to obtain realization functions at different levels of nonlinearity and smoothness, which makes the GP model flexible to mimic model responses with different complexities.

1.4 Objective and Scope

The main contribution of this research is the development and test of two approaches—the "adaptive ANOVA-based PCKF" and "adaptive sampling via GP-based surrogates"—for inverse modeling of nonlinear flow in porous media models. Both approaches fall into the category of probabilistic inversion and have the capability to quantify remaining uncertainty. This study focuses on computational efficiency, which is often the bottleneck of implementing inverse modeling and UQ algorithms for nonlinear models.

The "adaptive ANOVA-based PCKF", is a nonlinear variant of the classic Kalman filter approach. It applies to the problems where the nonlinearity is mild and the posterior distribution is approximately Gaussian. The main idea is to represent and propagate uncertainty with a proper PCE that is adaptively selected for the specific problem.

The second method is more general and deals with stronger nonlinearity and non-Gaussian, even multi-modal, posterior distributions. Four major ingredients of this algorithm are: a GP surrogate for simulation acceleration, an adjustment of the posterior

considering surrogate error, an importance sampler using Gaussian mixture proposal distribution, and an adaptive refinement scheme.

This dissertation is organized as follows. In chapter 2, we formulate the problem of inverse modeling and UQ with Bayes' theorem. The two approaches are presented and discussed in detail in chapters 3 and 4, respectively. Each proposed approach is also illustrated and tested with models relate to different flow in porous media problems. Finally, chapter 5 summarizes the study and outlines the areas for future research work.

Chapter 2

Bayesian Inversion

A subsurface flow system can generally be expressed as

$$\mathbf{d} = g(\mathbf{m}), \tag{2.1}$$

where $\mathbf{m} \in \mathbb{R}^{n_m}$ is a vector that contains all the uncertain input variables/parameters such as those representing the geological properties without a comprehensive and precise measurement. $\mathbf{d}$ is the output vector that contains the simulated output variables which are to be checked against the real field observations. Usually, $g(\cdot)$ is a nonlinear model and time consuming to evaluate. Without knowing the exact values of the parameters, $\mathbf{m}$ is expressed as a random vector characterized by a prior density function that reflects our limited knowledge about the real world system. Inverse modeling is a means to reduce the uncertainty associated with $\mathbf{m}$ by calibrating the simulation results to the observations

$\mathbf{d}^*$. The problem of inverse modeling may be formulated with Bayes' theorem,

$$p(\mathbf{m}|\mathbf{d}^*) = h \cdot p(\mathbf{d}^*|\mathbf{m})p(\mathbf{m}), \qquad (2.2)$$

where $p(\mathbf{m}|\mathbf{d}^*)$, the solution we seek in this inverse problem, is the conditional distribution of $\mathbf{m}$ given the observation $\mathbf{d}^*$, also known as the posterior distribution. According to Bayes' rule (2.2), $p(\mathbf{m}|\mathbf{d}^*)$ is proportional to the product of the prior distribution $p(\mathbf{m})$ and the likelihood function $p(\mathbf{d}^*|\mathbf{m})$, which is defined as the conditional distribution of the observation given a specific parameter value. h is the scaling factor which is constant with respect to $\mathbf{m}$ and makes the integral of the posterior density function equal to 1. While the prior distribution represents our prior knowledge about the model parameters, the likelihood reflects the additional information gained from the observed data. In a Bayesian inversion problem, the prior distribution is given as known, whereas the likelihood function has to be computed based on the relationship between $\mathbf{m}$ and $\mathbf{d}^*$. Consider the following cases.

Case 1: accurate model, accurate observation. If the observation and the model are both free of error, the only possible observation, given the condition that the true model parameter is $\mathbf{m}$, is the simulated output: $\mathbf{d}^* = \mathbf{d} = g(\mathbf{m})$. As a result, the likelihood is expressed with a Dirac-delta function:

$$p(\mathbf{d}^*|\mathbf{m}) = \delta(\mathbf{d}^* - g(\mathbf{m})). \qquad (2.3)$$

Case 2: accurate model, inaccurate observation. In this situation, the observed data

deviate from the model prediction because of an observation error: $\mathbf{d}^* = \mathbf{d} + \mathbf{e}_o = g(\mathbf{m}) + \mathbf{e}_o$. Assuming the observation error follows a probability distribution function $\mathbf{e}_o \sim f_{eo}(\cdot)$, the likelihood is then expressed as

$$p(\mathbf{d}^*|\mathbf{m}) = f_{eo}(\mathbf{d}^* - g(\mathbf{m})). \tag{2.4}$$

Case 3: inaccurate model, accurate observation. Consider the situation when the model does not accurately reflect the dependent relationship between $\mathbf{d}$ and $\mathbf{m}$. For example, we will study in this paper the situation that a surrogate model $\tilde{g}(\cdot)$ is used to replace $g(\cdot)$, and the output of the surrogate may differ from the original accurate model due to an modeling error: $\mathbf{d}^* = \mathbf{d} = g(\mathbf{m}) = \tilde{g}(\mathbf{m}) + \mathbf{e}_g$. When the modeling error follows a distribution function $\mathbf{e}_g \sim f_{eg}(\cdot)$, the likelihood function is expressed as

$$p(\mathbf{d}^*|\mathbf{m}) = f_{eg}(\mathbf{d}^* - \tilde{g}(\mathbf{m})). \tag{2.5}$$

Case 4: inaccurate model, inaccurate observation. In a more general case, the observation and the model could be both subject to errors, so we have $\mathbf{d}^* = g(\mathbf{m}) + \mathbf{e}_o = \tilde{g}(\mathbf{m}) + \mathbf{e}_g + \mathbf{e}_o$. Let $f_e(\cdot)$ denote the pdf of the total error $\mathbf{e} = \mathbf{e}_g + \mathbf{e}_o$, we have the likelihood function in the following form

$$p(\mathbf{d}^*|\mathbf{m}) = f_e(\mathbf{d}^* - \tilde{g}(\mathbf{m})). \tag{2.6}$$

Note that in most situations the original model itself also contains some sources of mod-

eling error (e.g., simplified physics, numerical error, etc.), though here we assume these errors are negligible in comparison with the surrogate error. Otherwise, we need to further modify the likelihood function to reflect these errors.

Although Bayes' rule (Eq.2.2) provides the theoretical foundation for computing the posterior distribution, it usually cannot be analytically and explicitly derived when the model $g(\cdot)$ is nonlinear. In the following chapters, we discuss the numerical approaches, including existing and newly developed ones, that provide approximate solutions to the posterior.

Chapter 3

Nonlinear Kalman Filter Approaches

The Kalman filter is a classic approach solving linear inverse modeling problems. It also has several variants that were successfully applied to nonlinear models. In an effort to improve the efficiency of existing nonlinear Kalman filter methods, we developed a new approach, the adaptive ANOVA-based PCKF (Li et al., 2014). In this chapter we first give a short review of the Kalman filter and its nonlinear extensions, and then present the new approach in detail. Finally, the approach is demonstrated with two different flow in porous media problems.

3.1 Kalman Filter and its Nonlinear Variants

3.1.1 Kalman Filter

Kalman filter is a set of equations which provide the analytic solution of the posterior distribution (Eq. 2.2) when the following conditions are held:

1. Model $g(\cdot)$ is linear. For simplicity we can further assume that $\mathbf{d} = \mathbf{Gm}$, where $\mathbf{G}$ is a matrix. Note that we can always shift the coordinates such that $\mathbf{d} = 0$ when $\mathbf{m} = 0$.

2. Both the prior pdf $p(\mathbf{m})$ and the observation error $\mathbf{e}_o$ follow Gaussian distributions.

In this situation, the posterior distribution $p(\mathbf{m}|\mathbf{d}^*)$ is also Gaussian and its mean $\boldsymbol{\mu}_{\mathbf{m}|\mathbf{d}^*}$ and covariance $\mathbf{C}_{\mathbf{m}|\mathbf{d}^*}$ are given by the following formulas:

$$\boldsymbol{\mu}_{\mathbf{m}|\mathbf{d}^*} = \boldsymbol{\mu}_{\mathbf{m}} + \mathbf{K}(\mathbf{d}^* - \boldsymbol{\mu}_{\mathbf{d}}), \tag{3.1}$$

$$\mathbf{C}_{\mathbf{m}|\mathbf{d}^*} = \mathbf{C}_{\mathbf{mm}} - \mathbf{K}\mathbf{C}_{\mathbf{dm}}, \tag{3.2}$$

where $\boldsymbol{\mu}_{\mathbf{m}}$ and $\mathbf{C}_{\mathbf{mm}}$ are the prior mean and covariance of parameter vector $\mathbf{m}$, respectively. $\boldsymbol{\mu}_{\mathbf{d}}$ is the predicted/prior mean of $\mathbf{d}$. $\mathbf{C}_{\mathbf{dm}}$ is the prior covariance between vectors $\mathbf{d}$ and $\mathbf{m}$. $\mathbf{K}$ is a matrix named Kalman gain:

$$\mathbf{K} = \mathbf{C}_{\mathbf{dm}}(\mathbf{C}_{\mathbf{dd}} + \mathbf{R})^{-1}, \tag{3.3}$$

where $\mathbf{C_{md}} = \mathbf{C_{dm}}^T$, $\mathbf{C_{dd}}$ is the predicted/prior covariance of vector $\mathbf{d}$, and $\mathbf{R}$ is the covariance of the error $\mathbf{e}_o$, which usually is pre-set based on users' knowledge of the error. Implementation of the Kalman filter requires first solving a forward UQ problem, i.e., to estimate the predicted mean $\boldsymbol{\mu_d}$, as well as the covariance matrices $\mathbf{C_{dm}}$ and $\mathbf{C_{dd}}$. They are easily solved for linear models:

$$\boldsymbol{\mu_d} = \mathbf{G}\boldsymbol{\mu_m}, \tag{3.4}$$

$$\mathbf{C_{dm}} = \mathbf{G}\mathbf{C_{mm}}, \tag{3.5}$$

$$\mathbf{C_{dd}} = \mathbf{G}\mathbf{C_{mm}}\mathbf{G}^T. \tag{3.6}$$

Often, the observations of the output variables become available as a sequence: $\mathbf{d} = \left[\mathbf{d}^{(1)T}, \mathbf{d}^{(2)T}, ...\right]^T$, where $\mathbf{d}^{(i)}$ contains the variables on the ith node of the sequence. For instance, the output vector $\mathbf{d}$ may consist of the same quantities (e.g., pressure, flow rate) to be measured at different time points, and each time point makes a node on the data sequence. In this situation, the Kalman filter may be implemented in a recursive manner. For each node $\mathbf{d}^{(i)}$ on the data sequence, we solve an inverse problem with Eqs. (3.1)-(3.6). The resulting posterior then serves as the prior for the next Kalman filter loop when the new data $\mathbf{d}^{(i+1)}$ is available.

3.1.2 Extended Kalman Filter

The Kalman filter can be extended to inverse problems of nonlinear models for which it gives an approximate solution provided that the nonlinearity is not strong, in which case the posterior distribution still is unimodal and well described by its first two statistical moments. However, to propagate uncertainty from $\mathbf{m}$ to $\mathbf{d}$ is not a simple task when a model is nonlinear. One approach is to replace the nonlinear model $g(\cdot)$ with a linear approximation around the mean of $\mathbf{m}$

$$g(\mathbf{m}) \approx \mathbf{G}(\mathbf{m} - \boldsymbol{\mu_m}) + g(\boldsymbol{\mu_m}), \tag{3.7}$$

where $\mathbf{G}$ is the Jacobi matrix

$$\mathbf{G}_{i,j} = \frac{\partial d_i}{\partial m_j}. \tag{3.8}$$

With the linear approximation, the formulas of Kalman filter are applicable and this method is known as EKF. EKF is one of the most straightforward methods to apply Kalman filter to nonlinear inverse problems. But in practice, EKF has some disadvantages. First, the calculation of the Jacobi matrix causes an extra computation burden, especially for high-dimensional problems. Second, EKF may easily diverge if the prior mean is not close to the true parameter point.

3.1.3 Ensemble Kalman Filter

Besides linearization, another commonly used approach to estimate the required statistical moments is the Monte Carlo method, which leads to a variant of the Kalman filter: the EnKF. In EnKF we initially draw a random ensemble of realizations from the prior distribution of the parameters, then propagate the uncertainty by running simulations for each individual realization to generate the corresponding ensemble of output $\mathbf{d}$.

$$\mathbf{d}_i = g(\mathbf{m}_i), \quad i = 1, 2, ..., n_e, \tag{3.9}$$

where n_e is ensemble size (the number of realizations in the ensemble). The required statistical moments are estimated from the ensemble:

$$\hat{\boldsymbol{\mu}}_{\mathbf{d}} = \frac{1}{n_e} \sum_{i=1}^{n_e} \mathbf{d}_i, \tag{3.10}$$

$$\hat{\mathbf{C}}_{\mathbf{dd}} = \frac{1}{n_e - 1} \sum_{i=1}^{n_e} (\mathbf{d}_i - \hat{\boldsymbol{\mu}}_{\mathbf{d}})(\mathbf{d}_i - \hat{\boldsymbol{\mu}}_{\mathbf{d}})^T, \tag{3.11}$$

$$\hat{\mathbf{C}}_{\mathbf{dm}} = \frac{1}{n_e - 1} \sum_{i=1}^{n_e} (\mathbf{d}_i - \hat{\boldsymbol{\mu}}_{\mathbf{d}})(\mathbf{m}_i - \hat{\boldsymbol{\mu}}_{\mathbf{m}})^T. \tag{3.12}$$

Furthermore, instead of updating the first two statistical moments, EnKF updates each realization with the equation of Kalman filter:

$$\mathbf{m}_i^u = \mathbf{m}_i + \mathbf{K}(\mathbf{d}_i^* - g(\mathbf{m}_i)), \quad i = 1, 2, , ..., n_e, \tag{3.13}$$

where the superscript "u" implies "updated." The updated realizations form a new ensemble representing the posterior uncertainty of the parameters and serve as the prior ensemble for the next data assimilation loop.

Remark 3.1. The observation ensemble $\mathbf{d}_i^*$ used in Eq. (3.13) is synthetically generated by perturbing the actually observed value according to $\mathbf{R}$. If a single deterministic observation is used to update all of the realizations, the posterior covariance would be systematically underestimated (Burgers et al., 1998). However, generating perturbed $\mathbf{d}_i^*$ would introduce additional sampling errors. Whitaker and Hamill (2002) have proposed a method termed "ensemble square root filter (EnSRF)," which uses the deterministic observation but yields a consistent estimation of the posterior covariance. It updates the mean and perturbation of m separately. While the mean is updated with the standard Kalman gain (3.3), the perturbation is updated with a modified gain:

$$\tilde{\mathbf{K}} = \mathbf{C_{md}}((\sqrt{\mathbf{C_{dd}} + \mathbf{R}})^{-1})^T (\sqrt{\mathbf{C_{dd}} + \mathbf{R}} + \sqrt{\mathbf{R}})^{-1}. \tag{3.14}$$

EnSRF is adopted in this study.

3.1.4 Probabilistic Collocation Kalman Filter

An intrinsic property of the Monte Carlo method is that its accuracy is guaranteed only when the ensemble size is sufficiently large, which could cause an enormous computational burden for using EnKF when the model $g(\cdot)$ is costly to simulate. An effort to minimize the number of simulations for a given required accuracy has led to the development

of another variant of the Kalman filter: PCKF. PCKF is similar to EnKF in every aspect except that it employs the PCE instead of an ensemble for uncertainty representation and propagation. By PCE, the input and output random vectors $\mathbf{m}$ and $\mathbf{d}$ are expressed as two truncated series:

$$\mathbf{m}(\boldsymbol{\xi}) \approx \sum_{i=0}^{n_\psi} \mathbf{c}_i^{\mathbf{m}} \psi_i(\boldsymbol{\xi}), \tag{3.15}$$

$$\mathbf{d}(\boldsymbol{\xi}) \approx \sum_{i=0}^{n_\psi} \mathbf{c}_i^{\mathbf{d}} \psi_i(\boldsymbol{\xi}), \tag{3.16}$$

where $\boldsymbol{\xi} = \left[\xi_1, \xi_2, ...\xi_{n_\xi}\right]^T$ is a random vector comprising a set of independent random variables with given pdfs, such as normal distribution, uniform distribution, and so on. $\psi_i(\boldsymbol{\xi})$ are the orthogonal polynomial basis with respect to $\boldsymbol{\xi}$: $E\left(\psi_i(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi}))\right) = \delta_{ij}$, where $E(\cdot)$ denotes the expectation operator, δ_{ij} is the Kronecker delta function. The first basis function $\psi_0(\boldsymbol{\xi}) = 1$ represents the mean (deterministic) term, whereas the following terms are the perturbation (random) terms, which have zero means. Vectors $\mathbf{c}_i$ are the deterministic coefficients. In the implementations of PCKF, PCE representation of input parameters (3.15) is set according to the prior distribution of $\mathbf{m}$ (see Section 3.2.3), whereas (3.16) is obtained by solving a forward uncertainty propagation problem (discussed in detail in Sections 3.2.1 and 3.2.2). Note that the numbers of PCE basis functions used in (3.15) and (3.16) are not necessarily the same, but we can always extend (3.15) and (3.16) by adding the missing terms with zero coefficients so that they include the same basis.

With PCE expressions (3.15) and (3.16), the statistical moments needed for implement-

ing the Kalman filter can be easily calculated from the coefficients:

$$\boldsymbol{\mu_{d}} = \sum_{i=0}^{n_{\psi}} \mathbf{c}_i^{\mathbf{d}} E\left(\psi_i(\boldsymbol{\xi})\right) = \mathbf{c}_0^{\mathbf{d}}, \tag{3.17}$$

$$\mathbf{C_{dd}} = E\left((\mathbf{d} - \mu_{\mathbf{d}})(\mathbf{d} - \mu_{\mathbf{d}})^T\right) = E\left((\sum_{i=1}^{n_{\psi}} \mathbf{c}_i^{\mathbf{d}}\psi_i(\xi))(\sum_{j=1}^{n_{\psi}} \mathbf{c}_j^{\mathbf{d}}\psi_j(\xi))^T\right) = \sum_{i=1}^{n_{\psi}} \mathbf{c}_i^{\mathbf{d}}\mathbf{c}_i^{\mathbf{d}T}, \tag{3.18}$$

$$\mathbf{C_{dm}} = E\left((\mathbf{d} - \mu_{\mathbf{d}})(\mathbf{m} - \mu_{\mathbf{m}})^T\right) = E\left((\sum_{i=1}^{n_{\psi}} \mathbf{c}_i^{\mathbf{d}}\psi_i(\xi))(\sum_{j=1}^{n_{\psi}} \mathbf{c}_j^{\mathbf{m}}\psi_j(\xi))^T\right) = \sum_{i=1}^{n_{\psi}} \mathbf{c}_i^{\mathbf{d}}\mathbf{c}_i^{\mathbf{m}T}.$$
$$\tag{3.19}$$

Note that the orthogonal property of $\psi_i(\boldsymbol{\xi})$ is used in Eqs. (3.17)-(3.19).

Similar to EnKF, the majority of the computational cost in PCKF is spent on propagating the uncertainty, i.e., building the PCE representation/calculation of the deterministic coefficients of output vector (3.16) given the PCE representation of the input vector (3.15). The required computational cost for this task depends on the number of PCE basis functions included in (3.16). Usually, this cost is much smaller than running the simulations for all realizations in EnKF if the dimensionality of the problem, i.e., the number of random variables ξ_i, is relatively low. However, PCKF may lose its advantage over EnKF for relatively high-dimensional problems because the number of PCE basis functions grows very fast as the dimensionality increases. For these problems, we need a carefully designed method to select the basis functions that form the PCE approximation (3.16).

3.2 Adaptive ANOVA-based PCKF

A key step in PCKF is to determine the truncation of the PCE for the output vector, i.e., to select the PCE basis to form the approximation. Having more basis functions retained in the truncated PCE gives a better approximation but increases the computational cost. An ideal set of basis for PCE approximation should find a balance between accuracy and computational cost. Nevertheless, there were no clear guidelines for picking the PCE basis functions for PCKF. A common selection is to keep all of the polynomial chaos terms whose degree is smaller than or equal to a certain integer k. This results in a total number of basis functions equal to $(n_\xi! + k)!/(n_\xi!k!)$, where n_ξ is the number of independent random variables ξ_j. In most PCKF applications, setting $k = 2$ was sufficient to yield a good result. However, the total number of basis functions still grows very fast as n_ξ increases, which could make PCKF even more computationally demanding than EnKF for high-dimensional problems. Also, in previous applications of PCKF on sequential data assimilation problems, the PCE basis functions were selected in advance and remained fixed through the entire process.

Demonstrated in this section, we develop an algorithm that improves the efficiency of PCKF by adaptively determining the appropriate PCE truncations for the specific problem under study. For sequential data assimilation problems, the algorithm also adjusts the PCE basis in different loops because the uncertainty changes as more and more information comes in.

We note that most of the terms in the PCE approximation for a high-dimensional func-

tion are those high-dimensional polynomials used to represent the coupling effects of multiple input parameters on the model output. However, in many practical problems, these effects are weak and negligible. This observation leads to the idea of functional ANOVA decomposition. Functional ANOVA is a dimensionality reduction technique widely used in forward UQ problems and can be conveniently combined with PCE approximation. It partitions a high-dimensional random function into a group of lower-dimensional components called "ANOVA components," and the total variance of the random function is distributed among the ANOVA components. With the decomposition, the PCE terms needed for representing this group of low-dimensional random functions are much less than those needed for the original high-dimensional function. In addition, adaptive algorithms have been developed in previous studies (Ma and Zabaras, 2010; Yang et al., 2012) to select active ANOVA components for specific random functions, and this directly leads to an adaptive approach to construct PCE approximation in PCKF.

3.2.1 PCE Approximation based on ANOVA Decomposition

In this subsection, we introduce the functional ANOVA decomposition and explain how to construct the PCE approximation of the output vector d given its ANOVA decomposition. Following the notations defined in Chapter 2, our model can be rewritten as a function with respect to the n_ξ random variables $\mathbf{d} = g(\mathbf{m}(\boldsymbol{\xi})) = f(\boldsymbol{\xi}) = f(\xi_1, ... \xi_{n_\xi})$. Functional ANOVA decomposes this function into a finite group of component functions—each of

which takes a subset of $(\xi_1, ... \xi_{n_\xi})$ as argument:

$$f(\boldsymbol{\xi}) = f_0 + \sum_{1 \leq j_1 \leq n_\xi} f_{j_1}(\xi_{j_1}) + \sum_{1 \leq j_1 < j_2 \leq n_\xi} f_{j_1, j_2}(\xi_{j_1}, \xi_{j_2}) + \cdots + f_{1,2,\cdots,n_\xi}(\xi_1, \xi_2, \cdots, \xi_{n_\xi}), \quad \boldsymbol{\xi} \in \mathbb{R}^{n_\xi},$$

$$(3.20)$$

where the function $f_{j_1, j_2, \cdots, j_v}$ with v argument variables $\xi_{j_1}, \xi_{j_2}, \cdots, \xi_{j_v}$ is called a "vth-order ANOVA component." Each component is computed by integration:

$$f_V(\boldsymbol{\xi}_V) = \int_{\mathbb{R}^{n_\xi - v}} f(\boldsymbol{\xi}) d\mu(\boldsymbol{\xi}_Q) - \sum_{P \subset V} f_P(\boldsymbol{\xi}_P), \tag{3.21}$$

where $V = \{j_1, j_2, \cdots, j_v\}, \boldsymbol{\xi}_V = \{\xi_{j_1}, \xi_{j_2}, \cdots, \xi_{j_v}\}$, P indicates every strict subset of V, and Q is the compliment of V. Note that the computation of f_V requires first computing the lower-order components f_P. So, we first compute the 0th-order component:

$$f_0 = \int_{\mathbb{R}^{N_\xi}} f(\boldsymbol{\xi}) d\pi(\boldsymbol{\xi}). \tag{3.22}$$

Then, the following 1st- and higher-order component functions are computed with (3.21) in a recursive manner.

Different choices of integration measure $d\pi(\boldsymbol{\xi})$ result in different ANOVA decompositions. If $d\pi(\boldsymbol{\xi})$ is chosen to be the same as the probability measure of $\boldsymbol{\xi}$, we have the following property:

$$\sigma^2(f) = \sum_{1 \leq j_1 \leq n_\xi} \sigma^2(f_{j_1}) + \sum_{1 \leq j_1 < j_2 \leq n_\xi} \sigma^2(f_{j_1, j_2}) + \cdots + \sigma^2(f_{1,2,\cdots,n_\xi}), \tag{3.23}$$

which means the total variance of f is exactly equal to the sum of the variances of all

the ANOVA components. However, in practice, the integration with respect to the probability measure generally is difficult to compute. Instead, the Dirac measure is used as a convenient alternative: $d\pi(\boldsymbol{\xi}) = \delta(\boldsymbol{\xi} - \boldsymbol{\theta})d\boldsymbol{\xi}$, where $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_{n_\xi}) \in \mathbb{R}$ is a constant point, usually chosen to be the mean of $\boldsymbol{\xi}$, and called the "anchor point." The corresponding ANOVA decomposition is termed "anchored-ANOVA." In anchored-ANOVA, (3.21) becomes:

$$f_V(\boldsymbol{\xi}_V) = f(\boldsymbol{\xi}_V, \boldsymbol{\theta}_Q) - \sum_{P \subset V} f_P(\boldsymbol{\xi}_P). \tag{3.24}$$

The computation of an anchored-ANOVA component requires only evaluating the model at corresponding points. For example, the first few components of anchored-ANOVA decomposition are listed as follows:

$$f_0 = f(\boldsymbol{\theta}), \tag{3.25}$$

$$f_1(\xi_1) = f(\xi_1, \theta_2, ..., \theta_{n_\xi}) - f_0, \tag{3.26}$$

$$f_2(\xi_2) = f(\theta_1, \xi_2, \theta_3, ..., \theta_{n_\xi}) - f_0, \tag{3.27}$$

$$f_{1,2}(\xi_1, \xi_2) = f(\xi_1, \xi_2, \theta_3, ..., \theta_{n_\xi}) - f_1(\xi_1) - f_2(\xi_2) - f_0. \tag{3.28}$$

In many practical problems, the variance of the function f distributes mainly on low-order ANOVA components. In other words, the coupling effect between multiple dimensions usually is small and negligible. This allows us to truncate the high-order ANOVA components in (3.20) and obtain an approximation of the original high-dimensional func-

tion f with its low-dimensional components:

$$f(\boldsymbol{\xi}) \approx \sum_{i=1}^{n_A} f_{V_i}(\boldsymbol{\xi}_{V_i}). \tag{3.29}$$

With the truncated ANOVA decomposition (3.29), we construct the PCE for the random function by expanding each component into PCE. For a component function $f_V(\boldsymbol{\xi}_V)$, we form its polynomial chaos basis from the tensor product of the one-dimensional basis:

$$f_{j_1,j_2,\ldots,j_v}(\xi_{j_1},\cdots,\xi_{j_v}) \approx \sum_{i_1=0}^{k}\cdots\sum_{i_v=0}^{k} c_{i_1\ldots i_v}\phi_{i_1}(\xi_{j_1})\ldots\phi_{i_v}(\xi_{j_v}), \tag{3.30}$$

where $\phi_i(\xi_j)$ is the ith-degree one-dimensional polynomial chaos with respect to the random variable ξ_j, while $c_{i_1\cdots i_t}$ are the deterministic coefficients. For example, the first three one-dimensional polynomial chaos basis functions (including the deterministic one) for standard normal random variable are: $\phi_0(\xi) = 1$, $\phi_1(\xi) = \xi$, and $\phi_2(\xi) = (\xi^2 - 1)/\sqrt{2}$ (known as Hermite polynomials). The 1st-order ANOVA component f_1 with respect to a single standard normal random variable is expanded as follows:

$$f_1(\xi_1) \approx \sum_{i_1=0}^{2} c_{i_1}\phi_{i_1}(\xi_1) = c_0 + c_1\xi_1 + c_2(\xi_1^2 - 1)\Big/\sqrt{2}, \tag{3.31}$$

and the 2nd-order ANOVA component $f_{1,2}$ with respect to two standard normal random

variables is expanded as follows:

$$
\begin{aligned}
f_{1,2}(\xi_1, \xi_2) &\approx \sum_{i_1=0}^{2} \sum_{i_2=0}^{2} c_{i_1 i_2} \phi_{i_1}(\xi_1) \phi_{i_2}(\xi_2) \\
&= c_{00} + c_{01}\xi_2 + c_{02}(\xi_2^2 - 1)/\sqrt{2} \\
&\quad + c_{10}\xi_1 + c_{11}\xi_1\xi_2 + c_{12}\xi_1(\xi_2^2 - 1)/\sqrt{2} \\
&\quad + c_{20}(\xi_1^2 - 1)/\sqrt{2} + c_{21}\xi_2(\xi_1^2 - 1)/\sqrt{2} + c_{22}(\xi_1^2 - 1)(\xi_2^2 - 1)/2.
\end{aligned}
\tag{3.32}
$$

To determine the PCE coefficients, we use PCM (Tatang et al., 1997). In PCM, we evaluate the component $f_{j_1, j_2, \cdots, j_v}(\xi_{j_1}, \xi_{j_2}, \cdots, \xi_{j_v})$ following the anchored-ANOVA procedures at a set of collocation points. The number of collocation points is chosen to be the same as the number of polynomial basis functions. By requiring the PCE approximation to be equal to the true function at these points (i.e., interpolation), one solves for the coefficients. PCM is a non-intrusive approach where we may treat the function f as a black box. The accuracy of PCM depends on the positions of collocation points. Commonly, the collocation points are positioned at the quadrature points (e.g., Gauss points), resulting in accurate computations of the statistical moments of $f(\boldsymbol{\xi})$. Specifically, for a one-dimensional PCE with the highest polynomial degree of k, the collocation points/Gauss quadrature points are the roots of the $(k+1)$st polynomial chaos. For a multidimensional PCE, the collocation points are formed from the tensor product of the one-dimensional collocation points. For instance, the PCE representation of a two-dimensional component, such as (3.32), may be built by interpolation on a 3 by 3 tensor product of one-dimensional Gaussian quadrature points. After expanding each ANOVA component with PCE, we sum up all of the PCE terms to form the final PCE approximation for the original function (3.16).

With the PCE representation of an ANOVA component f_V, we can easily calculate its variance $\sigma^2(f_V)$ from the PCE coefficients. Note that the PCE representation for an ANOVA component built with PCM may include the PCE terms that, in fact, belong to lower-order ANOVA components. For example, take representation (3.32): c_{00} belongs to the 0th-order component f_0 , and $c_{10}\xi_1$ belongs to the 1st-order component f_1. These terms are not necessarily zero. When the same PCE basis function appears in the PCE representations of different ANOVA components, the resulting variances of different components are not additive, e.g., $\sigma^2(f_1 + f_{1,2}) \neq \sigma^2(f_1) + \sigma^2(f_{1,2})$ when $c_1\xi_1$ in (3.31) and $c_{10}\xi_1$ in (3.32) are both non-zero. This is because the Dirac measure is used in anchored-ANOVA. To regain the additive property, we may rearrange and lump the PCE terms according to their arguments. For example, we amend the PCE representation (3.32) for $f_{1,2}$ by removing the term $c_{10}\xi_1$ and adding it to the PCE representation for f_1 (3.31). Other terms in (3.32), such as c_{00}, $c_{01}\xi_2$, $c_{02}(\xi_2^2 - 1)/\sqrt{2}$ and $c_{20}(\xi_1^2 - 1)/\sqrt{2}$, should be moved similarly.

The approach of forming collocation points and polynomial chaos basis using tensor product would suffer the so-called "curse of dimensionality" for high-dimensional functions because the tensor product yields a huge number of points and basis functions. Still, it works well in our algorithm if we have most high-order ANOVA components truncated and mainly compute the low-dimensional components. This truncation may be obtained for a specific function f based on some adaptive criterion, which will be discussed in detail in Section 3.2.2.

3.2.2 Adaptive Selection of ANOVA Components

As mentioned in Section 3.2.1, when computing the ANOVA decomposition for a specific function, we can use some criteria to decide which ANOVA components are computed and which are truncated. This leads to the adaptive ANOVA decomposition.

Remark 3.2. In our context, "computing an ANOVA component" does not imply evaluating the component at every possible point with Eq. (3.24), but to give the PCE approximation (3.30) and estimate the statistical moments from the PCE coefficients.

The idea of the adaptive ANOVA is to identify the important dimensions, called "active dimensions," and only compute the high-order components on these dimensions. In the first step of this process, we choose the 1st-order active dimensions $i \in A_1$ and compute their corresponding 1st-order ANOVA components:

$$f(\boldsymbol{\xi}) = f_0 + \sum_{i \in A_1} f_i(\xi_i). \tag{3.33}$$

Note that this step is much easier than computing 2nd- and higher-order ANOVA components because the number of PCE basis functions, as well as the number of required model evaluations in this step, grows only linearly with the number of dimensions included in A_1. Usually, if we do not have any prior information to determine which dimensions can be safely neglected, we could afford to keep all dimensions 1st-order active. Next, we select the 2nd-order active dimensions by examining the statistical moments of the 1st-order ANOVA components. For example, we may check how the total variance of (3.33) is distributed to each individual dimension $\sigma^2(f) = \sum_{i \in A_1} \sigma^2(f_i)$. The dimensions with large

portions of variance are identified as important and chosen to be 2nd-order active. For each pair of the 1st-order active dimensions (i,j) $i,j \in A_2$ we compute the corresponding 2nd-order ANOVA component $f_{i,j}(\xi_i, \xi_j)$. Similarly, we can adaptively select the 3rd- and higher-order active dimensions by examining the statistical moments of lower-order ANOVA components. However, when using ANOVA-based PCKF, our numerical results suggest computing the ANOVA components no further than the 2nd-order. This is not simply because the computation of 3rd- and higher-order components is much more expensive. More importantly, the Kalman filter and its variants assume that the nonlinearity of the studied model is mild. Thus, using only the first two statistical moments is sufficient to infer the input from the observations of the output. For these models, 2nd-order ANOVA usually is capable of providing a good approximation. For those models where nonlinearity is strong–such that keeping higher-order ANOVA components is necessary– other inversion approaches, rather than Kalman filters, should be considered. This study focuses on the adaptive criteria for choosing the 2nd-order active dimensions. Three different criteria are discussed here and will be tested in Section 3.3 with illustrative examples.

Remark 3.3. In the following discussions on adaptive criteria, we consider the situation when there is only one observable output variable. For the general case when the model has multiple observable output variables, we apply the adaptive criteria to the ANOVA decomposition for each individual output variable. Because different output variables may be sensitive to different input dimensions, the selected ANOVA components and resulting PCE basis functions for different output variables generally are not the same. Finally, the entire output vector is represented with the union of all selected basis functions.

Criterion 1

Yang et al. (2012) showed an adaptive criterion that assesses the "importance" of each dimension based on the variances of the 1st-order ANOVA components $\sigma^2(f_i)$. This requires sorting the dimensions according to $\sigma^2(f_i)$ in descending order and keeping the first N_2 in the set of 2nd-order active dimensions A_2 such that:

$$\sum_{j=1}^{n_2} \sigma^2(f_j) \geq (1 - \epsilon) \sum_{i \in A_1} \sigma^2(f_i), \tag{3.34}$$

where ϵ is a proportional constant between 0 and 1. Smaller ϵ retains more dimensions in A_2. Then, we compute the 2nd-order ANOVA components for each pair (i, j) $i, j \in A_2$.

This criterion determines the relative importance between different dimensions, but it does not compare the relative importance between 1st- and 2nd-order ANOVA components. For example, consider two functions $f^{(1)}$ and $f^{(2)}$, which have approximately the same 1st-order ANOVA components. Their difference is that the variance distributed on the 2nd-order ANOVA components of $f^{(1)}$ is comparable with its 1st-order components, whereas the 2nd-order components of $f^{(2)}$ are negligible. Ideally, an adaptive criterion should compute more 2nd-order ANOVA components for $f^{(1)}$ than for $f^{(2)}$. However, Criterion 1 cannot distinguish these two different situations because it does not check the variances of the 2nd-order ANOVA components. To solve this issue, we propose a more sophisticated adaptive criterion.

Criterion 2

We propose a new adaptive criterion that compares the relative importance not only between different dimensions but also between the 1st- and 2nd-order ANOVA components. This criterion is based on the estimation of the variance distributed on the 2nd-order components that are excluded from the ANOVA decomposition. To obtain this estimation we build a regression model that can be used to approximately predict $\sigma^2(f_{i,j})$ for a dimension pair (i, j) before actually computing $f_{i,j}$. Specifically, we assume that $\sigma^2(f_{i,j})$ is related to the variances of 1st-order components $\sigma^2(f_i)$ and $\sigma^2(f_j)$ through the following equation

$$\sigma^2(f_{i,j}) = \beta \sigma^2(f_i) \sigma^2(f_j) + e_{i,j}, \tag{3.35}$$

where β is a ratio coefficient and $e_{i,j}$ is an error term. Eq. (3.35) is based on two simple assumptions which are valid for many models: (i) a dimension pair (i, j) is likely to have larger coupling effect (measured by $\sigma^2(f_{i,j})$) comparing with other pairs if dimensions i and j both have relatively large individual effect (measured by $\sigma^2(f_i)$ and $\sigma^2(f_j)$); (ii) If both dimensions i and j have relatively small individual effect, the corresponding dimension pair (i, j) is likely to have relatively small coupling effect. Based on the second assumption, we prefer Eq. (3.35) to an additive model such as

$$\sigma^2(f_{i,j}) = \beta[\sigma^2(f_i) + \sigma^2(f_j)] + e_{i,j}, \tag{3.36}$$

or a regression model that includes a constant term:

$$\sigma^2(f_{i,j}) = \beta_0 + \beta_1 \sigma^2(f_i)\sigma^2(f_j) + e_{i,j}. \tag{3.37}$$

We point out that the regression model (3.35) is a simplified relation that is intended to capture only the big trend and may not accurately fit every dimension pair. Indeed it is impossible to have a general equation that accurately predicts the value of $\sigma^2(f_{i,j})$ for every function f from only the statistical moments of the 1st-order ANOVA components. If more properties of the function f are known in a specific problem, we may replace (3.35) with a better model.

With Eq. (3.35) we develop the new adaptive criterion as follows. After computing all 1st-order active ANOVA components, we sort all of the dimension pairs (i,j) $i,j \in A_1$ into a list according to $\sigma^2(f_i)\sigma^2(f_j)$ in descending order. We then compute the 2nd-order ANOVA components, starting with the important pairs, which are the leading pairs in this list. After computing each 2nd-order component, we give an assessment of the error in calculating the total variance of f , induced by leaving the rest of the pairs out of the ANOVA decomposition:

$$Err^{(D)}_{\sigma^2_f} = \sum_{(i,j)\notin D} \sigma^2(f_{i,j}) \approx \beta \sum_{(i,j)\notin D} \sigma^2(f_i)\sigma^2(f_j), \tag{3.38}$$

where D is the set of all pairs whose 2nd-order ANOVA components have been computed,

and β is computed from

$$\beta = \frac{\sum\limits_{(i,j)\in D} \sigma^2(f_{i,j})}{\sum\limits_{(i,j)\in D} \sigma^2(f_i)\sigma^2(f_j)}. \tag{3.39}$$

This error estimation is based on assumption (3.35), and the ratio coefficient β is estimated from the previously computed pairs. As D expands and more 2nd-order ANOVA components are computed, this error diminishes. Computing stops once this error is small enough when compared to the total variance of all the 1st- and 2nd-order ANOVA components that have been computed:

$$Err_{\sigma_f^2}^{(D)} < \epsilon \left(\sum_{i\in A_1} \sigma^2(f_i) + \sum_{(i,j)\in D} \sigma^2(f_{i,j}) \right). \tag{3.40}$$

This new criterion is able to examine the overall relative importance of the 2nd-order ANOVA components compared with the 1st-order ones (represented by β), and hence decides to keep more or less 2nd-order components in the decomposition. For example, reconsider the two functions $f^{(1)}$ and $f^{(2)}$ described in the discussion of Criterion 1. In that situation, the stop criterion (3.40) is reached much earlier for $f^{(2)}$ than for $f^{(1)}$ because a much smaller ratio coefficient β would be detected for model $f^{(2)}$.

Criterion 3

We point out that Criteria 1 and 2 are designed for forward modeling problems, i.e., to quantify the uncertainty of model output. However, these criteria do not give a consideration to the error associated with the observation $e_o = d^* - d$, which is important in inverse

modeling problems. In most inverse modeling problems, the observations of output variables are not treated as hard data (i.e., the data must be exactly matched by the simulation results) but soft (i.e., mismatches within certain ranges are allowed). This is because the discrepancy between observations and simulation results may be due to a reason other than inaccurate input parameters, such as a modeling or measurement error. In the context of Kalman filter, we focus on quantifying the variance of $d^* = d + e_o$: $\sigma^2_{d^*} = \sigma^2 + R$, where R is the variance of error e_o. Accordingly, we modify criterion (3.40) to a new version:

$$Err^{(D)}_{\sigma^2_f} < \epsilon \left(\sum_{i \in A_1} \sigma^2(f_i) + \sum_{(i,j) \in D} \sigma^2(f_{i,j}) + R \right).$$ (3.41)

Note that larger R makes the stop criterion (3.41) easier to achieve and thus requires a smaller number of 2nd-order ANOVA components to be calculated. Intuitively, this implies that the criterion considers the quality of the observation when running PCKF. A large error variance R indicates the observed data provide little information for inferring the input parameters. Accordingly, we do not need to spend much computational effort on assimilating these data.

3.2.3 Additional Discussions on Implementation

In this section, we discuss the pre- and post-procedures in the implementation of the adaptive ANOVA-based PCKF before summarizing this algorithm in Section 3.2.4.

Representation of Prior Parametric Uncertainty

The first step in PCKF is to provide a PCE representation of the input parameter vector $\mathbf{m}$ that is consistent with its prior statistical moments. In our algorithm, we use principal component analysis (PCA), also known as Karhunen-Loève expansion (KLE). A random parameter vector $\mathbf{m}$ with prior mean $\boldsymbol{\mu_m}$ and covariance matrix $\mathbf{C_{mm}}$ can be expressed in the following form:

$$\mathbf{m} = \boldsymbol{\mu_m} + \sum_{i=1}^{n_P} \sqrt{\lambda_i} \mathbf{m}_i \xi_i, \tag{3.42}$$

in which λ_i and $\mathbf{m}_i$ are the ith eigenvalue and eigenvector of $\mathbf{C_{mm}}$, respectively. ξ_i are a set of uncorrelated random variables with zero mean and unit variance. Eq. (3.42) is equivalent to the PCE form

$$\mathbf{m}(\boldsymbol{\xi}) = \mathbf{c}_0 + \sum_{i=1}^{n_P} \mathbf{c}_i \psi_i(\boldsymbol{\xi}) \tag{3.43}$$

, where $\mathbf{c}_0 = \boldsymbol{\mu_m}$, $\mathbf{c}_i = \sqrt{\lambda_i} \mathbf{m}_i$, $\psi_i(\boldsymbol{\xi}) = \xi_i$, $i = 1, ..., n_P$.

PCA not only decouples the correlation–represents correlated parameters with uncorrelated random variables–but also redistributes the variability of all input parameters mainly to the first few dimensions (i.e., the dimensions with largest eigenvalues). By truncating the dimensions with negligible eigenvalues, we may reduce the dimensionality of the problem to a number less than the parameters.

Remark 3.4. Generally, the pdf of ξ_i depends on the distribution of $\mathbf{m}$ and can be estimated numerically. In our algorithm, we simply set ξ_i to be independent standard normal. It is a reasonable approximation as, in a PCKF problem, the prior distribution should be approximately normal. Also, the first two statistical moments of $\mathbf{m}$, which are all of the

information considered by Kalman filter, still are accurately represented.

Remark 3.5. A special case arises when input parameters are uncorrelated. In such a situation, the PCA does not help to reduce the dimensionality. In fact, PCA (3.42) is equivalent to representing each individual parameter with a random variable.

Update Scheme of PCKF

After obtaining the PCE representation of the output vector and computing the needed statistical moments from the PCE coefficients, we update the PCE representation of the parameter vector $\mathbf{m}$ given the observation using the Kalman filter. In this paper, we use an updated scheme of EnSRF, which does not require an artificially perturbed observation. The mean is updated with Kalman gain:

$$\mathbf{c}_0^{\mathbf{m}u} = \mathbf{c}_0^{\mathbf{m}} + \mathbf{K}(\mathbf{d}^* - \mathbf{c}_0^{\mathbf{d}}). \tag{3.44}$$

The perturbation (all PCE terms except the first) is updated with the modified gain defined in (3.14), which yields a consistent estimation of the posterior covariance:

$$\sum_{j=1}^{n_\psi} \mathbf{c}_j^{\mathbf{m}u} \psi_j = \sum_{j=1}^{n_\psi} \mathbf{c}_j^{\mathbf{m}} \psi_j + \tilde{\mathbf{K}} \left(\sum_{j=1}^{n_\psi} \mathbf{c}_j^{\mathbf{d}^*} \psi_j - \sum_{j=1}^{n_\psi} \mathbf{c}_j^{\mathbf{d}} \psi_j \right). \tag{3.45}$$

Note that when using the EnSRF, all of the random terms of the observation are zero ($\mathbf{c}_j^{\mathbf{d}^*} = 0$, $j = 1, ..., n_\psi$) because perturbation is not needed. By multiplying Eq. (3.45) with each basis function and taking the expectation, we have the update equations for the coefficients

other than the mean (first) term:

$$\mathbf{c}_j^{\mathbf{m}u} = \mathbf{c}_j^{\mathbf{m}} - \tilde{\mathbf{K}}\mathbf{c}_j^{\mathbf{d}}, \quad j = 1, ..., n_\psi. \tag{3.46}$$

In our algorithm, we update the PCE of parameters by directly updating its coefficients, which follows (Saad and Ghanem, 2009; Zeng and Zhang, 2010). Another method is seen in (Li and Xiu, 2009), where the PCE approximation is used as a surrogate to generate a large ensemble of realizations and the posterior PCE is obtained from the updated ensemble.

The posterior mean and covariance of the parameters can be calculated from the updated PCE representation:

$$\mu_{\mathbf{m}|\mathbf{d}^*} = \mathbf{c}_0^{\mathbf{m}u}, \tag{3.47}$$

$$\mathbf{C}_{\mathbf{mm}|\mathbf{d}^*} = \sum_{j=1}^{n_\psi} (\mathbf{c}_j^{\mathbf{m}u})(\mathbf{c}_j^{\mathbf{m}u})^T. \tag{3.48}$$

3.2.4 Summary of Adaptive ANOVA-based PCKF Algorithm

The algorithm of adaptive ANOVA-based PCKF is summarized herein. The following procedures consist of a complete data assimilation loop:

1. Represent the parameter vector m with PCE (3.15) according to the prior statistical moments. For a correlated input parameter, PCA (3.42) may be used to reduce the input dimensionality.

2. Compute the PCE representation (3.16) for the output variables d with adaptive ANOVA. This includes:

   (a) Compute the 0th-order ANOVA components by evaluating the model output at the anchored point (3.25).

   (b) Compute the PCE approximations for the 1st-order ANOVA component with respect to each input dimension using the PCM method.

   (c) Select the dimension pairs with an adaptive criterion and compute the corresponding 2nd-order ANOVA components using the PCM method.

   (d) Rearrange all PCE terms to form the final PCE representation (3.16).

3. Estimate the required statistical moments–(3.17), (3.18), and (3.19)–for computing the Kalman gain (3.3) and the modified gain (3.14).

4. Update the PCE representation of m using EnSRF. Mean (i.e., the first PCE term) is updated with standard Kalman gain (3.44). The perturbation (i.e., all PCE terms except the first) is updated with the modified gain (3.46).

5. Compute the posterior mean and covariance of $\mathbf{m}$ from the updated PCE (3.47) and (3.47).

3.3 Illustrative Examples

3.3.1 Problem 1: Saturated Water Flow in a Heterogeneous Aquifer

In the first example, we consider one of the most basic models for flow in porous media: 1-dimensional steady groundwater flow in a saturated but heterogeneous aquifer, which is described by the following differential equation

$$
\begin{cases}
\dfrac{d}{dx}\left[\exp\left(Y(x,\boldsymbol{\xi})\right)\dfrac{d}{dx}h(x,\boldsymbol{\xi})\right] = 0, \quad 0 \leq x \leq 1 \\[2mm]
h(0) = 0, \quad h(1) = 1
\end{cases}
\tag{3.49}
$$

The input parameter of this model is log conductivity $Y(x,\boldsymbol{\xi})$, and the output is the hydraulic head $h(x,\boldsymbol{\xi})$. Both input and output are functions with respect to location coordinate x. We assume that $Y(x,\boldsymbol{\xi})$ is subject to a prior uncertainty and is expressed by a random function with stationary normal distribution. The prior mean and covariance of $Y(x,\boldsymbol{\xi})$ is $E(Y(x)) = 0$ and $C(Y(x_1), Y(x_2)) = \sigma_Y^2 \exp\left[25(x_1 - x_2)^2\right]$, respectively. σ_Y^2 is the prior variance of Y. A realization of $Y(x,\boldsymbol{\xi})$ is sampled from the prior distribution and serves as the reference parameter value. The reference output is solved from the differential equation with the reference parameter. Observations of the output are made on the reference output at 10 locations ($x_1 = 0.05, x_2 = 0.15, ..., x_10 = 0.95$) with the observation errors assumed to be independent normal random variables $N(0, R)$. The objective is to estimate model parameter $Y(x,\boldsymbol{\xi})$ from the observed data. The data sequence $h_i = h(x_i)$ is assimilated with 10 Kalman filter loops recursively. We have tested our adaptive algorithm in three case studies with different prior variances and observation errors (Table 3.1).

Table 3.1: List of case studies of Problem 1 with different prior variances and observation errors.

	σ_Y^2	R
Case 1	2	0.02^2
Case 2	0.5	0.02^2
Case 3	2	0.2^2

Demonstration of Adaptive ANOVA-based PCKF

We first demonstrate the adaptive ANOVA-based PCKF algorithm using the initial case study. The PCE representation for parameter $Y(x)$ is initialized using PCA with 10 random variables, which makes this a 10-dimensional inverse problem. The model output $h(x)$ is approximated using functional ANOVA decomposition. In Fig. 3.1, we plot the variances of the 10 1st-order ANOVA components of $h|_{x=0.05}$. It is apparent that some dimensions have larger contributions to the total output variance (the 3rd, 4th, and 5th dimensions), whereas other dimensions do not affect the output very much (the 8th, 9th, and 10th dimensions). In each Kalman filter loop, the ANOVA components are selected according to the adaptive criteria described in Section 3.2.2 ($\epsilon = 0.05$), and each ANOVA component is expanded into PCE (Eq. 3.30) using the tensor product of the first three one-dimensional Hermite polynomial basis functions.

Fig. 3.2 shows the number of total PCE basis functions, which is the same as the number of required model simulations kept in different data assimilation loops. We can see that all three criteria are capable of adaptively adjusting the PCE basis in different loops. Overall, we recognize a decreasing trend in the number of PCE basis functions as the data assimila-
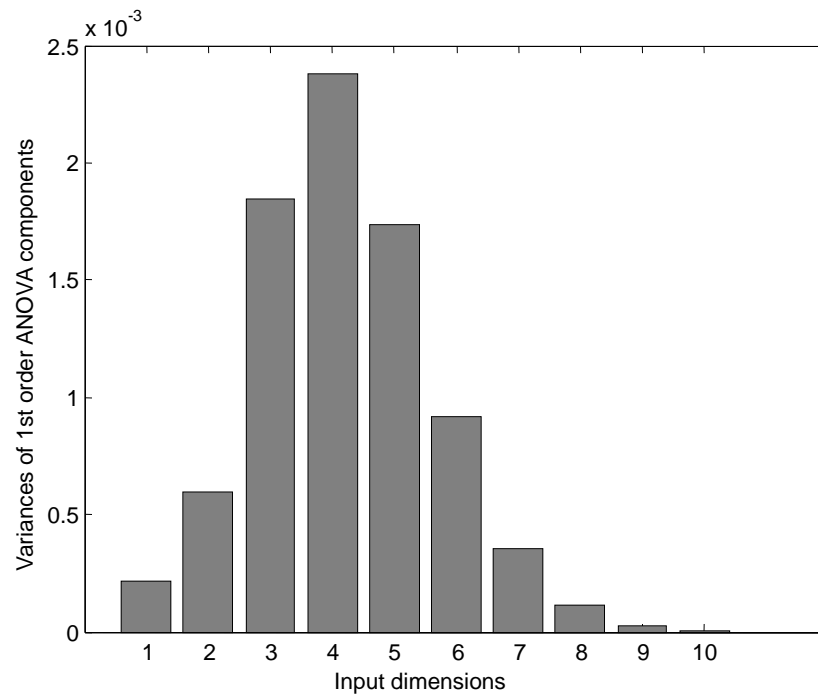
Figure 3.1: First order ANOVA components' variances of model output in Problem 1 $(h|_{x=0.05})$.

tion process goes loop by loop, which means that a smaller number of PCE basis functions are sufficient to represent the remaining uncertainty.
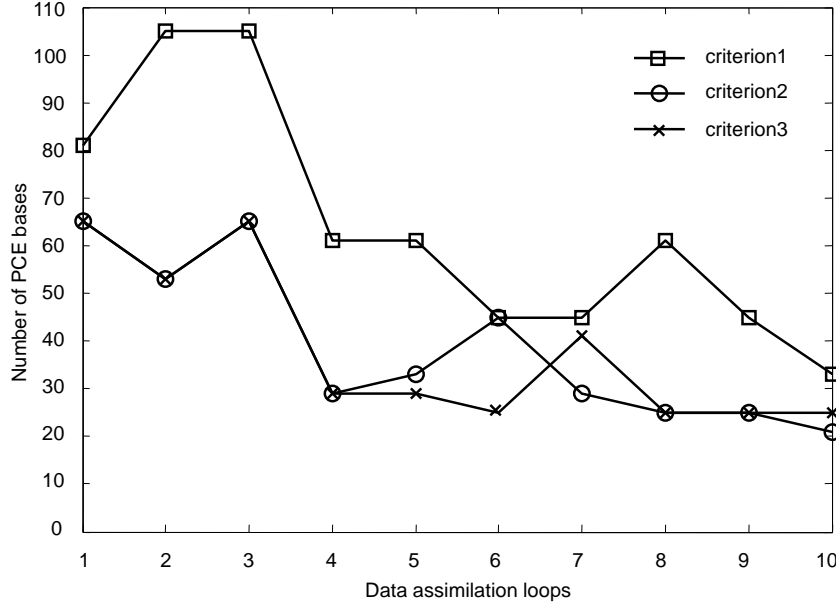
Figure 3.2: Adaptive selection of PCE bases using three criteria for case 1, Problem 1 ($\epsilon = 0.05$).

In each loop, we calculate the means and standard deviations of the model output $h(x, \boldsymbol{\xi})$ and input $Y(x, \boldsymbol{\xi})$ from their PCEs and plot them in Figs. 3.3 and 3.4, respectively. Initially, the mean of $Y(x, \boldsymbol{\xi})$ is zero with standard deviation equal to $\sqrt{2}$ throughout the domain, which is consistent with our assumption of the prior distribution. Also, we see significant uncertainty associated with the initial prediction of the model output $h(x, \boldsymbol{\xi})$– except for the left and right ends $x = 0$ and $x = 1$, where they are constrained by the boundary conditions. As observations are assimilated, we see a trend of uncertainty re-

duction in the estimation of both parameter $Y(x, \boldsymbol{\xi})$ and output $h(x, \boldsymbol{\xi})$. For the latter, where direct observations are made, our estimation converges to the reference case. For the parameter, we obtain a much more accurate posterior estimation with reduced uncertainty compared to the prior one. However, a non-negligible uncertainty still exists, even after 10 data assimilation loops. This shows the ill-posedness of this inverse problem and implies that the reference parameter cannot be exactly identified by observing $h(x, \boldsymbol{\xi})$ at the 10 locations.

Figure 3.3: Uncertainty quantification of model output $h(x)$ and calibration to observations, Adaptive PCKF, criterion 3.

Figure 3.4: Uncertainty quantification of model parameter $Y(x)$, Adaptive PCKF, criterion3.
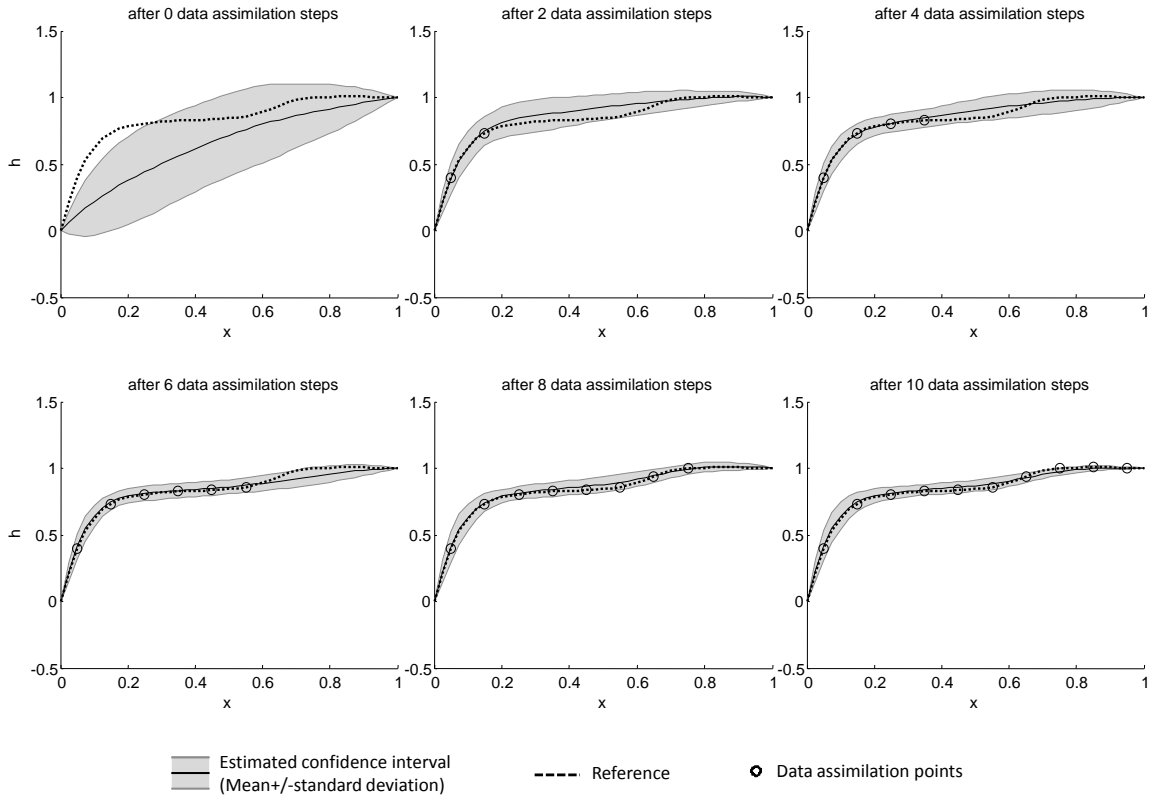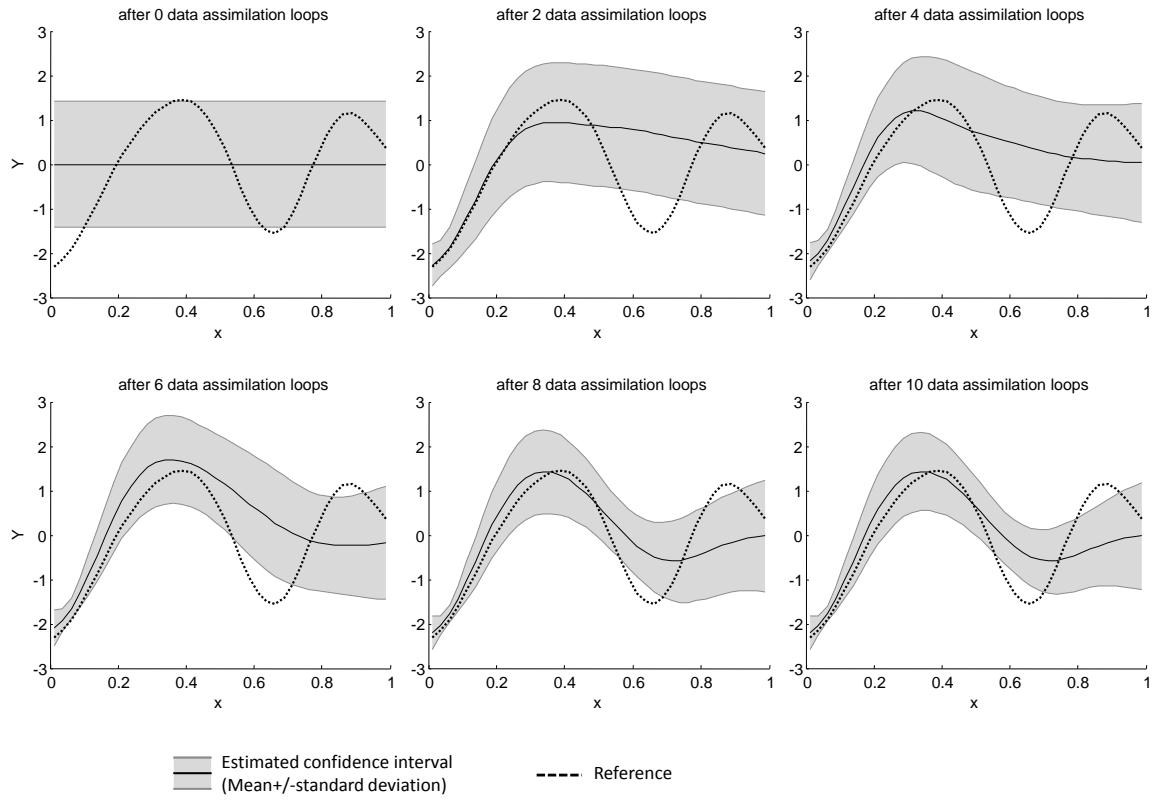
Efficiency Comparison with EnKF and Non-adaptive PCKF

To check the efficiency of our algorithm, we solve the same inverse modeling problem using EnKF methods with different ensemble sizes. Furthermore, we conduct two more non-adaptive PCKF algorithms. All 10 dimensions are expanded to only the 1st-order ANOVA in the first non-adaptive algorithm and to the full 2nd-order ANOVA in the second. The estimated posterior means and standard deviations of $Y(x, \boldsymbol{\xi})$ by different methods are compared in Fig. 3.5. The result given by EnKF with a large number of realizations (10000) is set as the benchmark. From the comparison, we see that the result given by PCKF based on 2nd-order ANOVA is able to aptly capture the posterior uncertainty and is very close to the benchmark, whereas the 1st-order ANOVA-based PCKF gives a result that apparently differs from the benchmark, as well as the reference. The adaptive ANOVA-based PCKFs offer results that also are very close to the benchmark but require much less computational cost compared with the 2nd-order ANOVA-based PCKF. Moreover, the results from the adaptive ANOVA-based PCKFs are more reliable than the EnKFs with similar computational costs. To accurately check the performances of different methods, we compute a single index that simultaneously measures the accuracies of both estimated mean $\mu_Y(x)$ and variance $\sigma_Y^2(x)$ of the model parameter:

$$H^2(\mu_Y(x), \sigma_Y^2(x)) = 1 - \sqrt{\frac{2\sigma_Y(x)\sigma_{Yb}(x)}{\sigma_Y^2(x) + \sigma_{Yb}^2(x)}} \exp\left[-\frac{1}{4}\frac{(\mu_Y(x) - \mu_{Yb}(x))^2}{\sigma_Y^2(x) + \sigma_{Yb}^2(x)}\right], \qquad (3.50)$$

where mean $\mu_{Yb}(x)$ and variance $\sigma_{Yb}(x)$ are the benchmark. Eq. (3.50) is close to 1 if the estimation and benchmark have little overlap and equals 0 if the estimation is identical to

the benchmark. Index H^2 also is known as the squared Hellinger distance between two normal distributions. We plot H^2 (averaged in $x \in [0, 1]$) of the estimated posterior means and variances given by different methods, including adaptive and non-adaptive PCKFs and EnKFs with different ensemble sizes, against their computational cost on a log-log plot (Fig. 3.6). From the plot, we recognize the convergence of EnKF toward the benchmark as the ensemble size increases. Because the result of EnKF depends on the sampling of initial realizations and has some randomness, we run EnKF 10 times for every tested ensemble size with different initial realizations and plot the maximum, average, and minimum H^2 of the 10 experiments. For this specific problem, the 2nd-order ANOVA-based PCKF is more accurate than the EnKF with similar computational cost, while the 1st-order ANOVA-based PCKF is worse than most of the EnKF experiments. The adaptive ANOVA-based PCKFs are more efficient than the non-adaptive PCKFs because they achieved relatively high accuracy with relatively small computational cost. Also, the adaptive PCKFs outperform the EnKFs with similar computational cost.

Remark 3.6. When comparing the performances of the different methods, particular attention should be noted in the differences between the following three:

(a)   The reference parameter.

(b)   The posterior distribution of the parameter given by Bayesian theorem.

(c)   The estimation of the parameter given by Kalman filter.

Point (b) is the solution we seek in an inverse problem. It contains all of the possible realizations, including the reference (a), that are consistent with the model and available observations. We cannot identify the reference (a) unless more information is given. Point

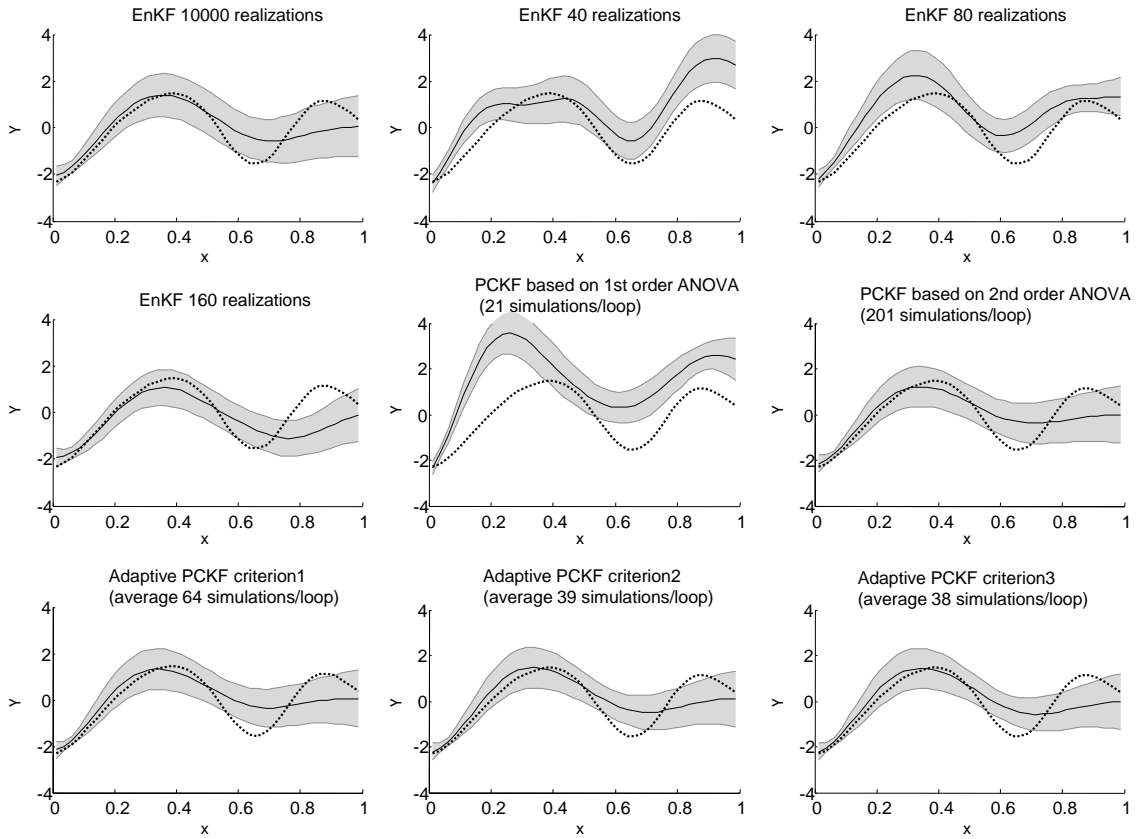**Figure 3.5:** Comparison of the parameter estimations given by EnKFs, non-adaptive PCKFs and Adaptive PCKFs (Problem 1).
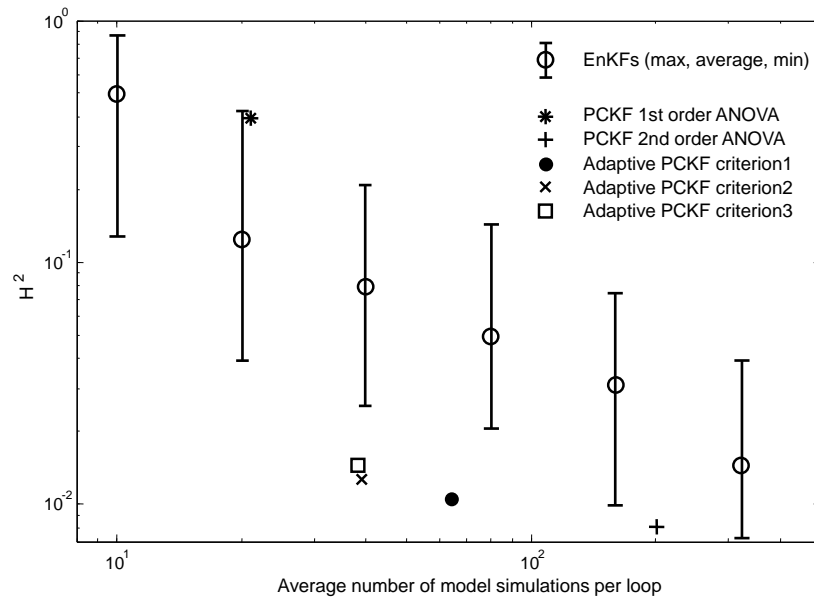
Figure 3.6: Efficiency comparison between EnKFs, non-adaptive PCKFs and Adaptive PCKFs using H^2 index (Case 1, Problem 1).

(c) is an approximation to (b) that may be obtained with less computational cost (e.g., compared with MCMC). The difference between (b) and (c) results from applying the Kalman filter to a nonlinear model, and this error cannot be eliminated by enlarging either the ensemble size in EnKF or the PCE terms in PCKF. Hence, rather than (a) or (b), we choose the EnKF with large ensemble size as the benchmark.

Comparison Between Adaptive Criteria

To further study and compare the different adaptive criteria, we test our algorithm on Case 2 and Case 3. In Case 2, we set a smaller prior parameter variance. Because the parameter varies in a smaller range, this makes input–output relation less nonlinear and results in smaller 2nd-order ANOVA components. This case is designed to study how the adaptive criteria respond to the change in the problem's non-linearity. In Case 3, we assume the observations are less accurate by setting larger observation errors. The purpose is to check how the adaptive criteria react to the change in observation quality. Table 3.2 shows the average number of PCE basis functions selected in the 10 loops by the three different criteria. From Table 3.2, we see that Criterion 3 responds to the changes in Cases 2 and 3 by retaining a smaller number of PCE basis functions compared with Case 1, which implies that fewer 2nd-order components are computed in the ANOVA decomposition. Criterion 2 reduces the number of PCE basis functions for only Case 2 but is not sensitive to the change in Case 3. Criterion 1 retains almost the same number of PCE basis functions in all three cases. This result is consistent with our expectations. Criterion 1 selects 2nd-order ANOVA components by distinguishing the important dimensions among all dimensions

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using 1st-order ANOVA, but it considers neither the nonlinearity of the problem nor the quality of the observations. Criterion 2, which is an improvement upon Criterion 1, examines model nonlinearity. Finally, Criterion 3 improves Criterion 2 by considering the quality of the observations.

To check the accuracies of the adaptive ANOVA-based PCKF using different criteria, we once again solve the last two cases by different KF approaches and plot the index H^2 of their results against the corresponding computational cost for Case 2 and Case 3 (Fig. 3.7 and Fig. 3.8, respectively). Apparently, the accuracies of the three adaptive ANOVA-based PCKF methods are at almost the same level. Considering the computational cost, we conclude that adaptive Criterion 3 offers the most effective selection of the PCE basis. In fact, in the comparison with EnKFs, the 1st-order ANOVA-based PCKF performs much better for Cases 2 and 3 than for Case 1. This also shows that a large number of 2nd-order components are not necessary for the last two cases, and the response of reducing PCE basis functions automatically made by Criterion 3 (also by Criterion 2 in Case 2) is appropriate.

Table 3.2: Number of PCE basis functions selected by three criteria (average number of 10 data assimilation loops).

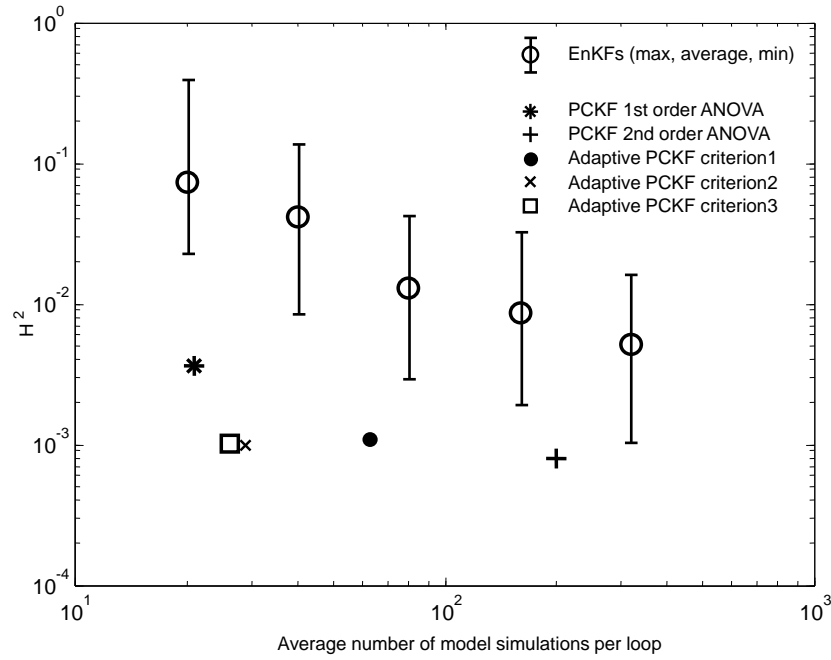|	Criterion 1	Criterion 2	Criterion 3
Case 1	64	39	38
Case 2	63	27	26
Case 3	69	38	26

Figure 3.7: Efficiency comparison between EnKFs, non-adaptive PCKFs and Adaptive PCKFs using H^2 index (Case 2, Problem 1).
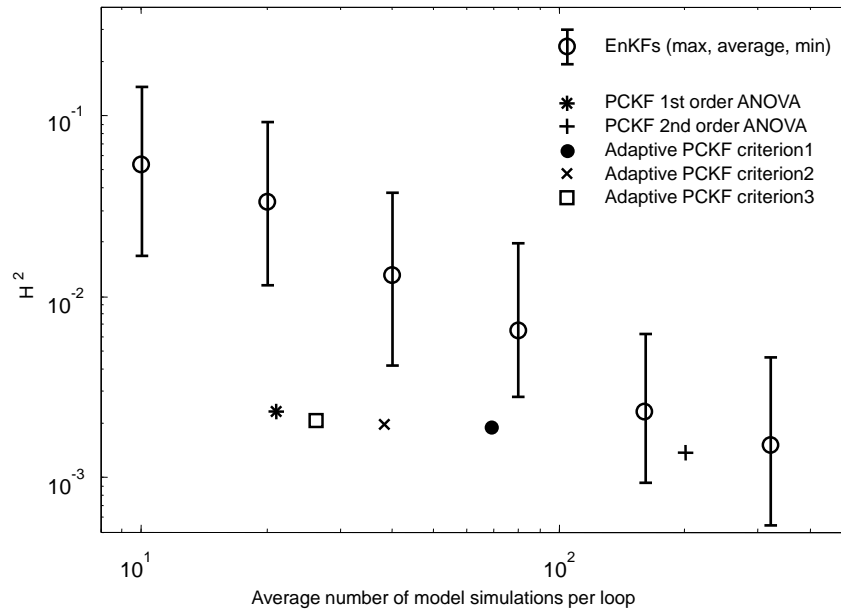
Figure 3.8: Efficiency comparison between EnKFs, non-adaptive PCKFs and Adaptive PCKFs using H^2 index (Case 3, Problem 1).

3.3.2 Problem 2: Waterflooding of a Petroleum Reservoir

To further test and demonstrate the adaptive ANOVA-based PCKF, we apply it to a history matching problem, which is commonly practiced in reservoir engineering. We calibrate a petroleum reservoir model to the recorded well production data. Consider a synthetic, two-dimensional, square-shaped reservoir bounded by no-flow boundaries (Fig. 3.9a). The 1200-ft by 1200-ft domain is partitioned into 40 by 40 grid blocks, and the thickness of every grid block is 30 ft. We simulate the physical process of two-phase flow (oil and water) in the reservoir. Initially, the reservoir is saturated with 75% oil and 25% water (porosity is 0.2). Four wells, two producers, and two water injectors are located at the four corners. The oil is recovered from the reservoir using the waterflooding method: two injectors are used to push oil toward the producers by injecting water, both at the constant rate of 300 stock tank barrels (STB) per day and the two production wells both produce fluids while maintaining a constant bottom hole pressure (BHP) of 3000 psi. This production process is simulated with the reservoir simulator ECLIPSE. In this process, the permeability $k(x, y)$ of the reservoir medium has significant influence on the fluid flow and determines how much of the total oil stored in the reservoir may be recovered. However, due to the heterogeneity of the permeability distribution and difficulty of precise measurement, we usually do not have complete and accurate knowledge of $k(x, y)$. In this example, $k(x, y)$ is assumed to be subject to a prior uncertainty. $Y = \log(k)$ is a stationary Gaussian random function, and its prior mean and covariance are:

$$E(Y(x, y)) = \mu_Y, \tag{3.51}$$

$$\text{Cov}\left(Y\left(x_1, y_1\right), Y\left(x_2, y_2\right)\right) = \sigma_Y^2 \exp\left[-\left(\frac{x_1 - x_2}{\eta_x}\right)^2 - \left(\frac{y_1 - y_2}{\eta_y}\right)^2\right], \qquad (3.52)$$

where the mean of log permeability is $\mu_Y = 2$ (this mean is calculated when permeability is measured in the unit of millidarcy); variance $\sigma_Y^2 = 1$; and the correlation factors in x and y directions, η_x and η_y, are both 400 ft. A realization of Y is sampled from the prior distribution and is assumed to be the true permeability field (Fig. 3.9b). Given the permeability field, we can predict the water saturation in different stages during the waterflooding process (Figs. 3.9c and 3.9d).

In this inverse problem, our objective is to estimate Y from the recorded production data in different stages (also known as the production history). The available data include the bottom hole pressure (BHP) recorded at the two injection wells, as well as the water production rate (WPR) and the oil production rate (OPR) at the two production wells. The data are generated from the true permeability field and are collected every 40 days at a total of 15 time steps. The data observed at different time steps are assimilated sequentially in Kalman filter loops. The errors associated with observations are assumed to be independent normal with zero means and standard deviations being equal to 5% of the observed values.

We solve this problem with adaptive ANOVA-based PCKF using Criterion 3. The PCE representation for parameter Y is initialized using PCA with 20 random variables, which results in a 20-dimensional inverse problem. Fig. 3.10 and Fig. 3.11 show the simulation results with error bars of the well production history before and after data assimilations, respectively. We observe that, due to the uncertain parameters, the simulation results in
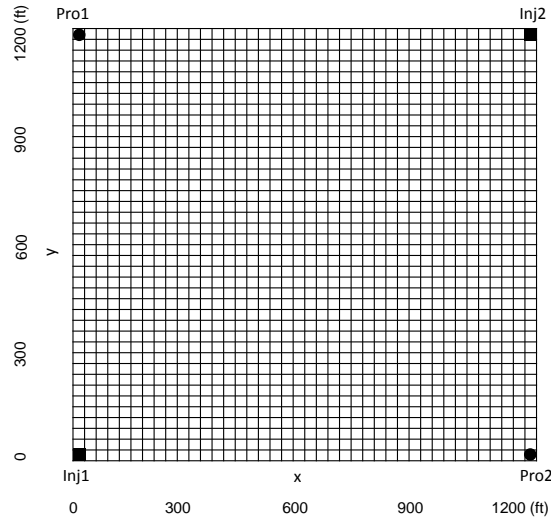
(a) A synthetic 2-d reservoir model.
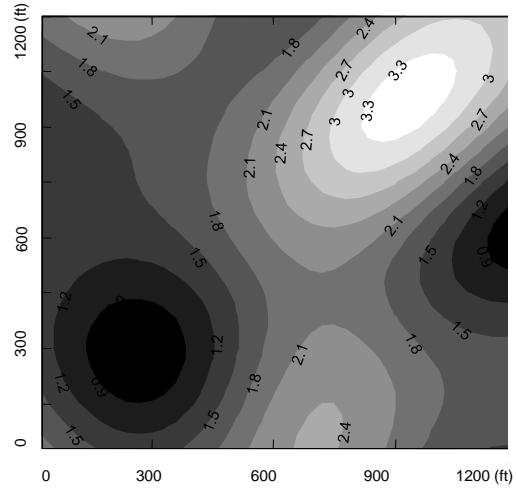
(b) True log permeability field.
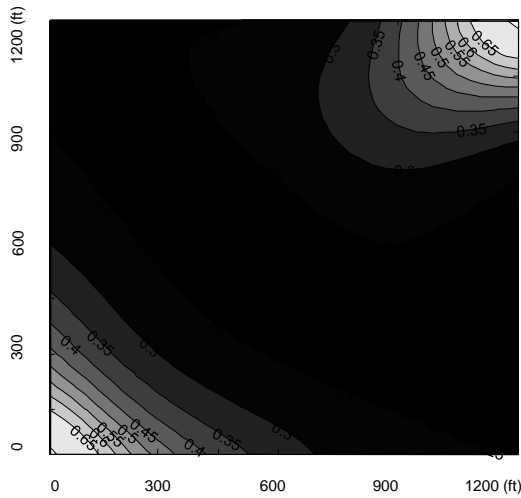
(c) Water saturation at t=180 d.
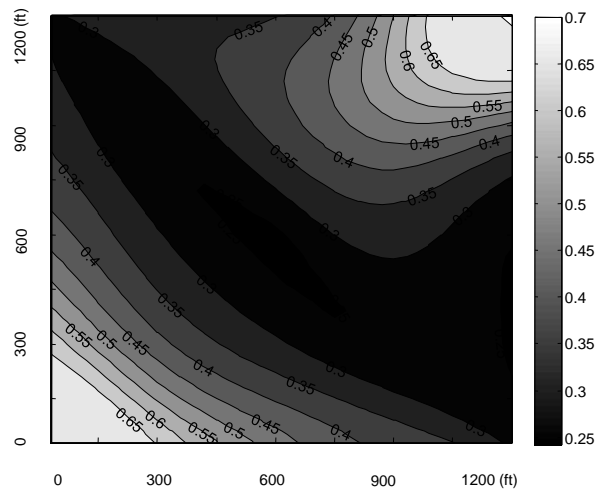
(d) Water saturation at t=500 d.

Figure 3.9: Oil recovery from a reservoir by waterflooding.

Fig. 3.10 do not match the observed production history and are subject to significant uncertainties. After assimilating all of the observations, we note the simulations match the production history well and the uncertainties are greatly reduced (Fig. 3.11). The estimated mean and posterior standard deviation of the log permeability field $Y(x, y)$ by the adaptive ANOVA-based PCKF is plotted in Fig. 3.12. Compared with Fig. 3.9b, we see that the estimated mean is not identical to the true permeability but captures the big trend, i.e., high permeability in the upper right area and low permeability in the lower left area. From Fig. 3.12b, it is apparent that the parametric uncertainty is reduced mainly in the regions near the wells, especially the production wells (note that the prior standard deviation is uniformly equal to 1). In the regions far away from the wells, the uncertainty is less reduced, indicating the production data are less sensitive to the permeability at those locations. To accurately estimate the permeability of the entire domain, other measurements would be necessary.

In Fig. 3.13, we plot the number of adaptively selected PCE basis functions in different data assimilation loops. The most visible trend in this plot is that the adaptive criterion increased the number of PCE basis functions from Day 180 until around Day 380. In fact, this is the early period when the production wells started producing water, known as "break- through." During breakthrough, there are some radical changes in the production history, such as a sudden increase in WPR and a decrease in OPR. Having more PCE terms helps to accurately capture the model response during this period.

Finally, we compare the efficiency of the adaptive ANOVA-based PCKF with non-adaptive PCKFs and EnKFs. Again, we use the EnKF with large ensemble size (2000) as
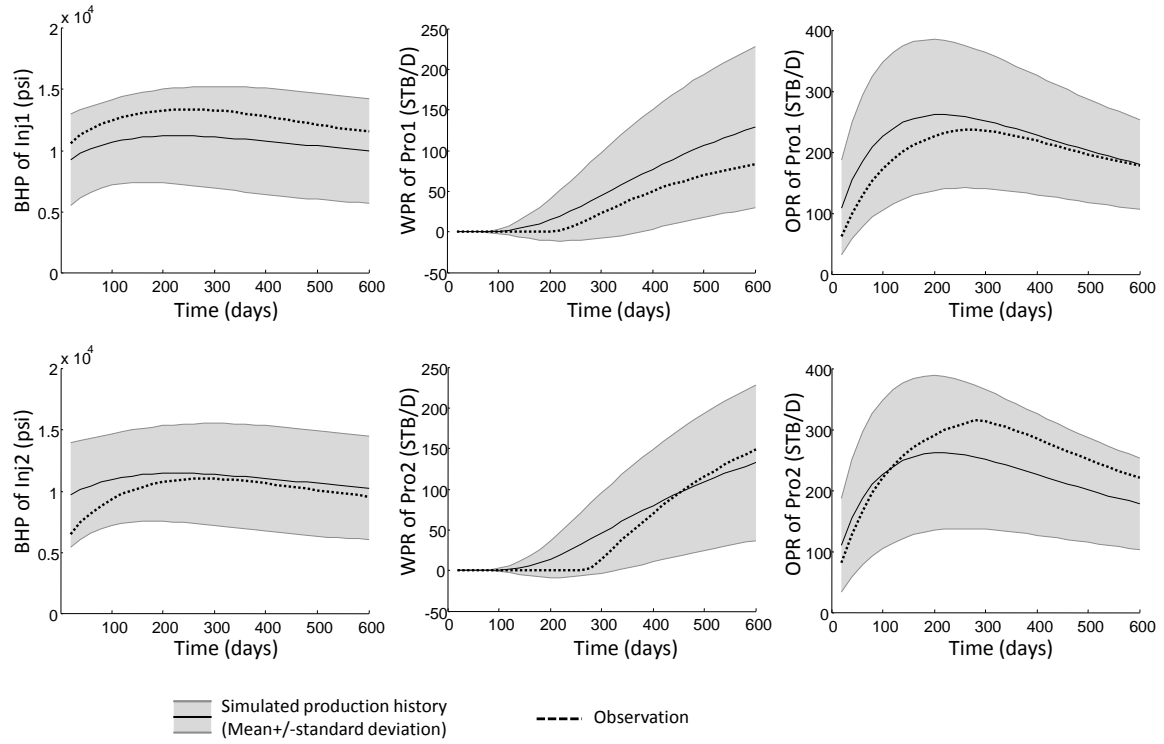
Figure 3.10: Simulated production history with uncertainty quantification, before model calibration (Problem 2).
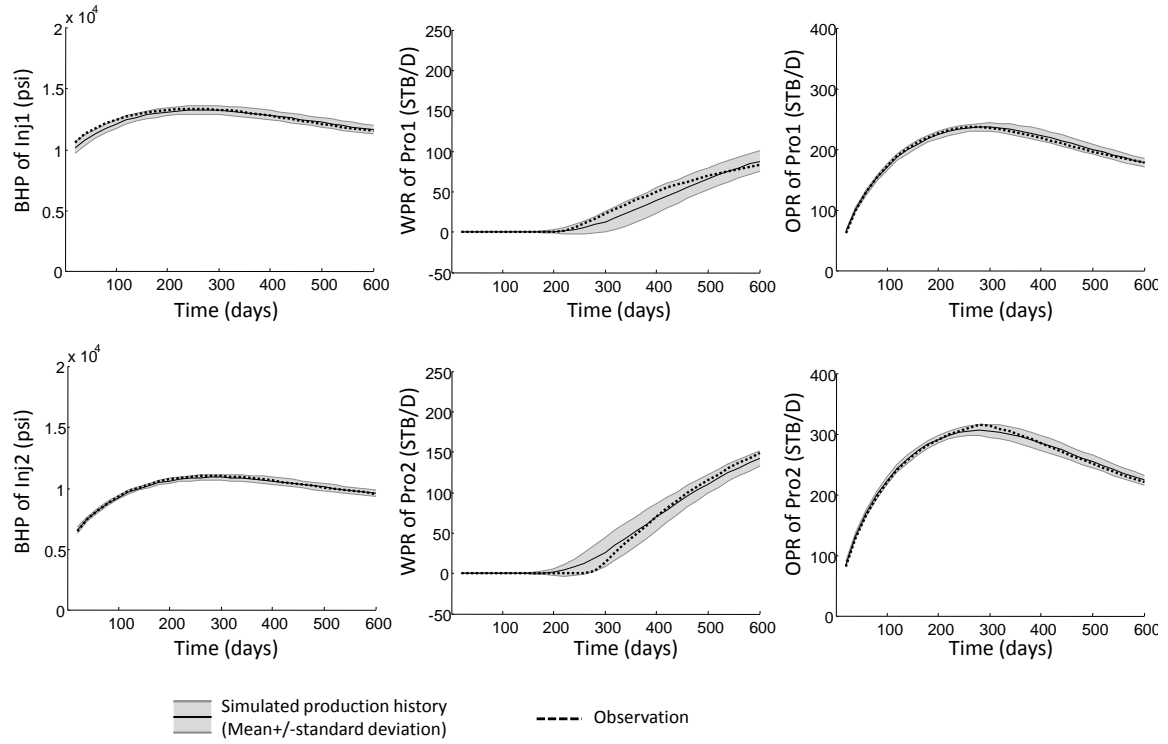
Figure 3.11: Simulated production history with uncertainty quantification, after model calibration (Problem 2).

(a) Mean of log permeability.

(b) Standard deviation of log permeability.
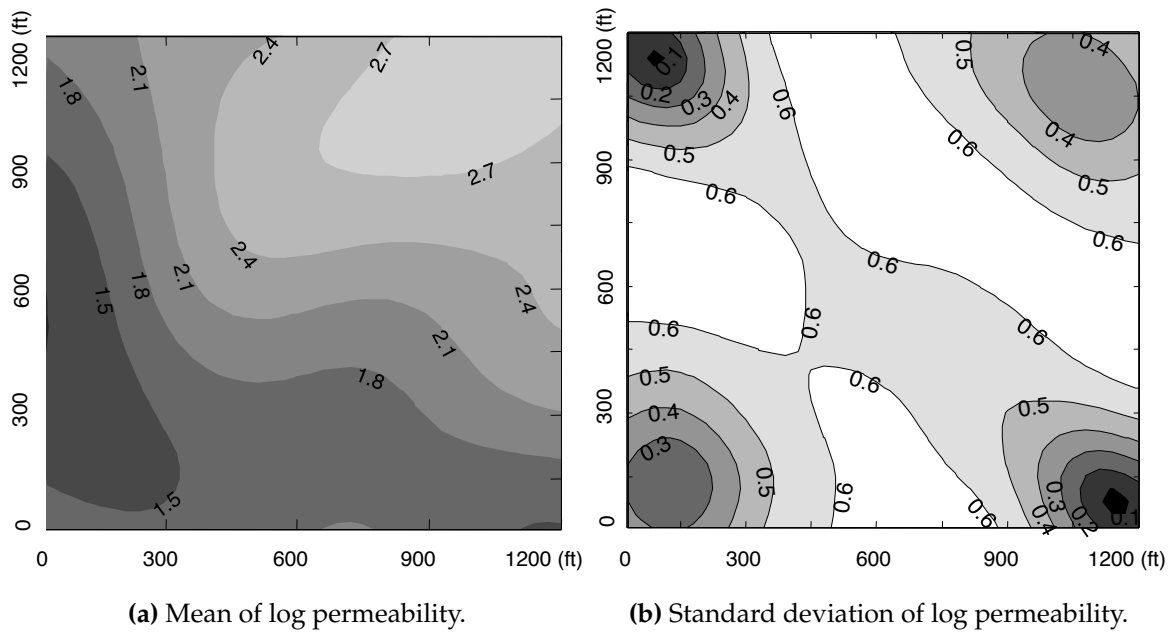
Figure 3.12: Estimated mean and standard deviation of log permeability by adaptive ANOVA-based PCKF (Problem 2).
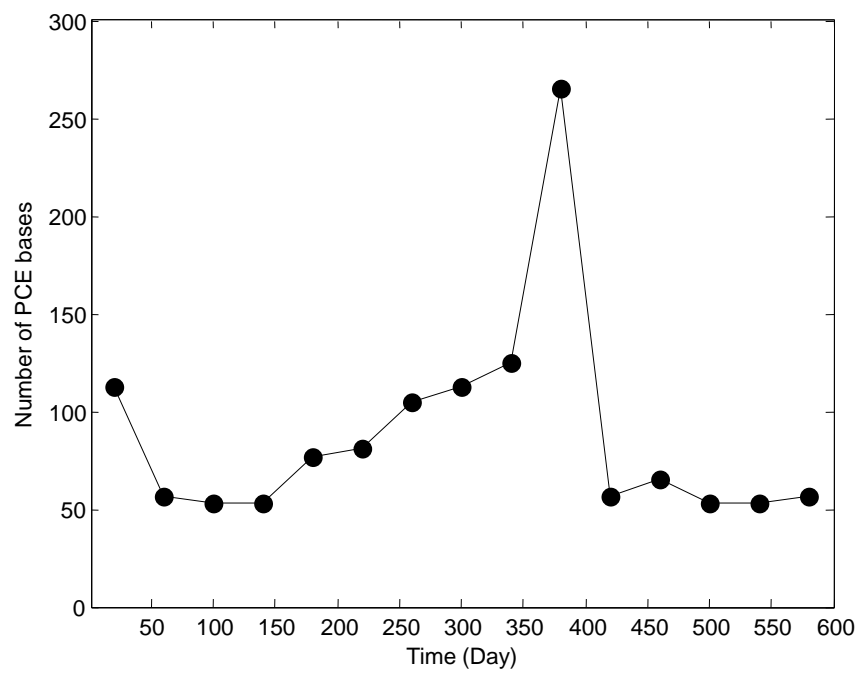
Figure 3.13: Number of PCE bases adaptively selected by criterion 3 (problem 2).

the benchmark and calculate the H^2 indexes of the results given by different approaches to measure their accuracy. Fig. 3.14 depicts the "accuracy versus computational cost" chart. Notably, the non-adaptive PCKFs are almost at the same accuracy levels with the EnKFs with comparable computational cost, but the adaptive ANOVA-based PCKF is able to achieve higher accuracy with relatively low cost, making it the most efficient option among all of the methods tested.
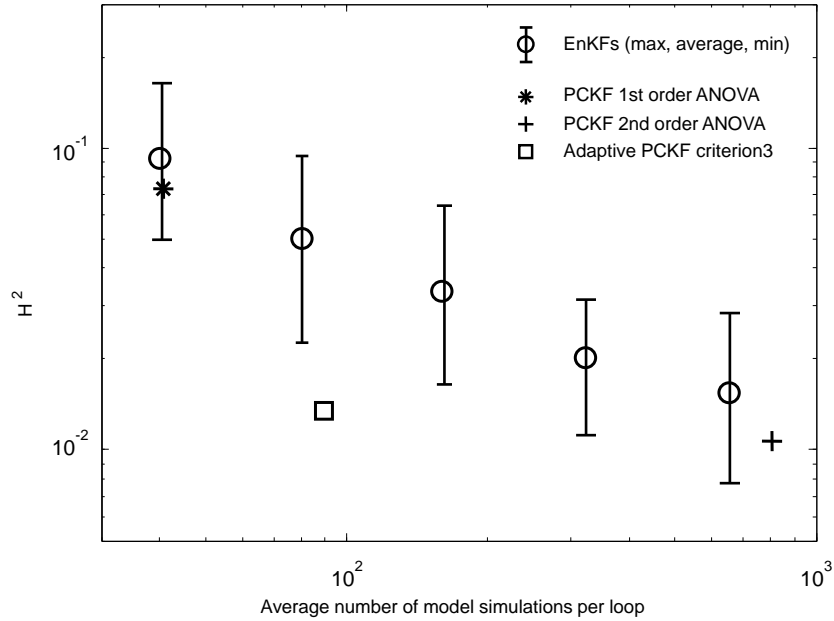
Figure 3.14: Efficiency comparison between EnKFs, non-adaptive PCKFs and Adaptive PCKFs using H^2 index (problem 2).

3.4 Discussions

In this chapter, we develop an adaptive ANOVA-based PCKF algorithm to solve nonlinear inverse modeling problems. Our research contributes to previous studies from the following aspects, and these improvements make the adaptive ANOVA-based PCKF a more flexible and efficient tool for inverse modeling problems when compared with classic PCKF.

(a) Our algorithm adaptively selects the PCE basis functions to represent uncertainties for different models and in different Kalman filter loops of sequential data assimilation problems, while, in classic PCKF methods, the PCE basis are pre-set by users and remain fixed in all loops.

(b) We extend the adaptive functional ANOVA algorithm, which mainly is used in solving forward uncertainty propagation problems, to solving inverse modeling problems.

(c) We propose two new criteria (Criteria 2 and 3 in Section 3.2.2) for adaptive functional ANOVA decomposition, which are more efficient and especially suited for using PCKF. Criterion 2 is not only able to detect the important input dimen- sions among all of them, but it also compares the relative importance between the low- and high-order components. Criterion 3 is a modified version of Criterion 2. It accounts for the quality of the observations and is more effective for inverse modeling problems.

We have tested the developed method by solving the inverse problems for two flow in porous media models. The new method has been demonstrated to be more efficient and

reliable in comparison with non-adaptive PCKF and EnKF approaches.

Finally, there are two other points worth noting: 1) The major computational burden in the new approach still is the model evaluations at collocation points. The extra computational cost caused by manipulating the PCE terms and judging the adaptive criteria does not make a difference in the efficiency competition between the new and old Kalman filter methods. 2) Even with adaptive basis selection, the PCKF approach is not supposed to replace the EnKF for extremely high-dimensional problems, e.g., when the dimension is a few hundred or higher. For these problems, the computational cost of the PCKF based only on 1st-order ANOVA decomposition still may be comparable to or exceed that required by EnKF.

Chapter 4

Adaptive Sampling via GP-based Surrogates

In this chapter we study a more general inversion approach. In order to deal with nonlinear models and non-Gaussian distributions, we abandon the assumptions of Kalman filter and directly sample from the posterior distribution defined by Bayes' theorem. Sampling methods rely on a large number of model evaluations with different parameter points, which is computationally costly and impractical for most inverse modeling problems. To alleviate the computation burden we study the use of a GP-based surrogate to facilitate the sampling process. Like any other surrogate models, the GP-based surrogate is an approximation of the original model that can be evaluated with much less computation effort. In addition, the GP-based surrogate gives an estimation of approximation error. This error estimation is considered in the sampling algorithm to yield a more reliable estimation of

posterior distribution of model parameters. Furthermore this estimation indicates where to do local refinements if a more accurate surrogate is desired. We present a novel inversion algorithm that consists of a series of adaptive sampling and surrogate refinement loops, which captures the posterior accurately while keeping the computational cost as low as possible. To further improve the sampling efficiency and better reproduce non-Gaussian, especially multi-modal posteriors, we propose an importance sampler using Gaussian mixture proposal distributions.

The structure of this chapter is as follows: first, we briefly discuss the sampling techniques that are used in inverse modeling; we then review some necessary background knowledge about GP-based surrogates before presenting the main algorithm, which will be demonstrated with three examples; finally, we summarize the chapter with conclusions and further discussions.

4.1 Sampling Methods

4.1.1 Markov Chain Monte Carlo

MCMC is able to sample from a posterior density of any form and in high dimensionality. It forms a Markov chain which evolves in the parameter space under some rules. Those rules make the chain equivalent to a sample from the objective density function. The classic MCMC algorithm with Metropolis-Hastings sampling rule was developed by Metropolis et al. (1953). A brief summary of the Metropolis-Hastings algorithm is described here.

To sample from the posterior $p(\mathbf{m}|\mathbf{d}^*)$, we start with an randomly selected initial point $\mathbf{m}^{(0)}$ and then build a Markov chain step by step. In the $(j+1)$st step, a new point is selected with the following rule:

1. A candidate point $\mathbf{m}_q$ is generated from a proposal distribution $q(\cdot)$ which is easy to sample from but may differ from our objective density $p(\mathbf{m}|\mathbf{d}^*)$. $q(\cdot)$ could depend on the point at previous step: $q(\cdot|\mathbf{m}^{(j)})$.

2. The candidate point $\mathbf{m}_q$ is accepted to be the $(j+1)$st point on the chain with probability γ, which depends on $\mathbf{m}^{(j)}$ and $\mathbf{m}_q$ through the following equation:

$$\gamma = \min\left(1, \frac{p(\mathbf{m}_q|\mathbf{d}^*)q(\mathbf{m}^{(j)}|\mathbf{m}_q)}{p(\mathbf{m}^{(j)}|\mathbf{d}^*)q(\mathbf{m}_q|\mathbf{m}^{(j)})}\right). \tag{4.1}$$

If $\mathbf{m}_q$ is rejected, the Markov chain stays at the previous point, $\mathbf{m}^{(j+1)} = \mathbf{m}^{(j)}$.

The second step reshapes the sample from the proposal distribution q to the objective distribution. Note that: 1) for each proposed candidate point $\mathbf{m}_q$, one needs to call the simulator once to evaluate the model and compute the acceptance probability. This makes MCMC a computationally expensive method; 2) the computation of γ does not require to know h, the normalizing constant in the Bayesian theorem since it cancels in the ratio expression.

4.1.2 Importance Sampling

Similar to MCMC, importance sampling draws a sample from an arbitrary pdf in two steps: proposal and correction. In the first step, a sample of points $\{\mathbf{m}_q^{(1)}, \mathbf{m}_q^{(2)}, ..., \mathbf{m}_q^{(n_S)}\}$ is generated from a proposal distribution $q(\mathbf{m})$, which may be different from the targeted distribution but takes some simple form that is easy to sample from. In the second step, we make this proposed sample reflect the distribution of $p(\mathbf{m}|\mathbf{d}^*)$ by assigning each sample point a weight

$$w_j = \frac{p(\mathbf{m}_q^{(j)}|\mathbf{d}^*)}{q(\mathbf{m}_q^{(j)})}, \quad j = 1, 2, ..., n_S, \tag{4.2}$$

The weight factors w_j are then normalized such that their summation equals 1. Because of this normalization, the normalizing constant h in the expression of posterior distribution again does not have to be explicitly calculated. The calculation of the weights requires model evaluations at each proposed points, which again makes the algorithm computational demanding. However, one advantage of importance sampling over MCMC is that the model evaluations at different points may be run in parallel.

If a equal-weight sample is desired, we can draw a new sample among the points of $\{\mathbf{m}_q^{(1)}, \mathbf{m}_q^{(2)}, ..., \mathbf{m}_q^{(n_S)}\}$ with probability of picking the point $\mathbf{m}_q^{(j)}$ being w_j. In our algorithm, we use the method of systematic re-sampling (Arulampalam et al., 2002): generate n_S i.i.d. random numbers u_j from the uniform distribution $U(0, 1)$, and let $\mathbf{m}^{(j)} = \mathbf{m}_q^{(r)}$, such that $\sum_{l=1}^{r} w_l \geq u_j$ and $\sum_{l=1}^{r-1} w_l < u_j$. Finally, $\{\mathbf{m}^{(1)}, \mathbf{m}^{(2)}, ..., \mathbf{m}^{(n_S)}\}$ form an equal-weight sample representing the objective posterior distribution.

Importance sampling also may be used for sequential data assimilation problems, which

leads to the algorithm of sequential importance sampling, also known as particle filter (Gordon et al., 1993). In particle filter, the weight associated with each point is updated whenever new data become available so that the new information is assimilated.

4.1.3 Simulated Annealing

In most inverse modeling problems, the regions in the parameter space with non-negligible posterior distribution only covers a tiny portion of that of the prior, which results in spiky and rugged posterior pdf. As a result, in a MCMC implementation, most of the proposed points do not hit the posterior and hence are rejected, whereas in importance sampling, most of the proposed points would end up with nearly-zero weights. For such problems, an extremely long chain or an extremely large sample size is necessary to achieve a reliable representation of the posterior distribution. To alleviate the difficulty, one may sample from a pdf that is modified from the original posterior distribution

$$p_\tau(\mathbf{m}|\mathbf{d}^*) = h \cdot \exp\left[\frac{\ln p(\mathbf{m}|\mathbf{d}^*)}{\tau}\right], \tag{4.3}$$

where $\tau \geq 1$ is a parameter called temperature. When $\tau = 1$, the modified pdf (4.3) is equivalent to the original posterior pdf. When a larger temperature is used, the pdf (4.3) becomes a flattened version of the original posterior and hence easier to sample from. See Fig. 4.1 for an example. In practice, one can start with a high temperature, which is then gradually decreased to approach the real posterior.
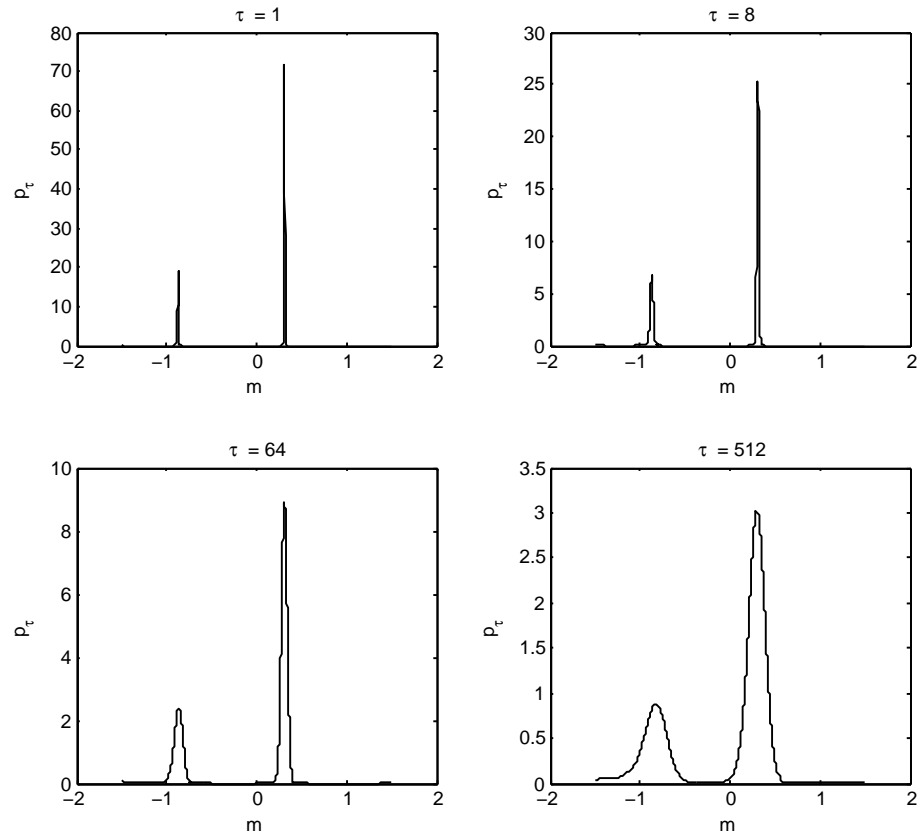
Figure 4.1: An example of a pdf at different temperatures.

4.2 Gaussian Process-based Surrogates

4.2.1 Basic Idea

In this section, we give a review of Gaussian process-based surrogates and demonstrate how they can be used to facilitate the Bayesian inversion. For simplicity, we first consider models with only one output variable, and then extend the methodology to general models with multidimensional output.

The methods of using Gaussian processes to approximate deterministic computer model outputs were previously developed in different studies (Sacks et al., 1989; Currin et al., 1991; Kennedy and O'Hagan, 2001). Though formulated by different researchers and from different perspectives, these methods share the same fundamental philosophy. Essentially, the true model response $g(\mathbf{m})$ is assumed to be a realization of a stochastic process $G(\mathbf{m})$. For mathematical convenience, this stochastic process is often chosen to be a Gaussian/normal process:

$$G(\mathbf{m}) \sim N\left(\mu(\cdot), C\left(\cdot, \cdot\right)\right), \tag{4.4}$$

which is characterized by its mean function $\mu(\cdot)$ and covariance function $C\left(\cdot, \cdot\right)$ (see next subsection for detailed discussion about the covariance function). Eq. (4.4) means that the model response at n different parameter points $\{\mathbf{m}^{(1)}, \mathbf{m}^{(2)}, ..., \mathbf{m}^{(n)}\}$ follow a multivariate Gaussian distribution $N(\boldsymbol{\mu}, \mathbf{C})$, where the mean vector and covariance matrix are $\boldsymbol{\mu}_i = \mu(\mathbf{m}^{(i)})$, $\mathbf{C}_{ij} = C(\mathbf{m}^{(i)}, \mathbf{m}^{(j)})$, $i, j = 1, ...n$. Specifically, at any parameter point $\mathbf{m}$, the model response is expressed as a Gaussian random variable.

The uncertainty associated with the model output is caused by the fact that we are not able to actually evaluate the original model at that parameter point due to the computational cost, but can only give an approximate estimation. To reduce this uncertainty, we may condition this process (Eq.4.4) to model evaluations at n_B parameter points, which we call the base points: $B = \{\mathbf{m}_B^{(1)}, \mathbf{m}_B^{(2)}, ..., \mathbf{m}_B^{(n_B)}\}$. The conditional process, $G_{|B}(\mathbf{m})$, is still a a Gaussian process, and its mean and variance at a parameter point $\mathbf{m}$ are given by

$$\mu_{|B}(\mathbf{m}) = \mu(\mathbf{m}) + C_{\mathbf{m}B}C_{BB}^{-1}\left(g(B) - \mu(B)\right), \tag{4.5}$$

and

$$\sigma_{|B}^2(\mathbf{m}) = C(\mathbf{m}, \mathbf{m}) - C_{\mathbf{m}B}C_{BB}^{-1}C_{B\mathbf{m}}, \tag{4.6}$$

respectively. $\mu(\cdot)$ and $C(\cdot, \cdot)$ are the mean and covariance functions defined in the unconditional process (4.4). $C_{\mathbf{m}B}$ is a 1 by n_B vector where the ith element is $C(\mathbf{m}, \mathbf{m}_B^{(i)})$. C_{BB} is a n_B by n_B matrix where the element on the ith row and the jth column is $C(\mathbf{m}_B^{(i)}, \mathbf{m}_B^{(j)})$. $g(B)$ and $\mu(B)$ are both n_B by 1 vectors. While the former contains the evaluated model output at the n_B base points, the latter includes the unconditional mean defined on the same points. Note that the conditioned variance (Eq.4.6) at the base points becomes zero, which shows our knowledge of the exact model output at these points. Moreover, the uncertainty at any other point $\mathbf{m}$ is also reduced because of the information gained through the correlations between $\mathbf{m}$ and the base points.

The conditional distribution provides a surrogate to the original model: $g(\mathbf{m}) = \tilde{g}(\mathbf{m}) + e_g$, where $\tilde{g}(\mathbf{m}) = \mu_{|B}(\mathbf{m})$ can be used as an approximation of the true model response,

and e_g is the estimated surrogate error which follows the normal distribution $N\left(0, \sigma_{|B}^2\right)$. The likelihood function may be derived from this surrogate. Consider an example of case 4 discussed in Chapter 2. Suppose the observation of the model output has an error of $e_o \sim N(0, \sigma_o^2)$ independent of the surrogate error, then the total error, $e = e_g + e_o$, is also a Gaussian random variable with the distribution of $N(0, \sigma_{|B}^2 + \sigma_o^2)$. The likelihood function takes the form of $f_e(\mathbf{d}^* - \tilde{g}(\mathbf{m}))$, where $f_e(\cdot)$ is the pdf of e.

To illustrate the GP surrogate-based Bayesian inversion, we consider a simple nonlinear model with only one input parameter and one output variable: $d = g(m)$. The model parameter is subject to a prior uncertainty: $m \sim N(0, 0.5^2)$. To estimate the parameter, an observation of the model output is made: $d^* = 1.1$, which is also associated with an observation error: $e_o \sim N(0, 0.02^2)$. When the model is expensive to evaluate, we cannot afford to compute the exact model response at every points, but we assume it resembles a realization of a Gaussian process described by Eq.(4.4) with a constant mean $\mu(m) = 1.5$ for any m and a covariance function $C(m^{(1)}, m^{(2)}) = 4 \exp\left(-0.75(m^{(1)} - m^{(2)})^2\right)$. Note that according to this assumption, the model output at any parameter point m is a Gaussian random variable with standard deviation of 2. To reduce this uncertainty, we evaluate the model $d = g(m)$ at three base points $B = \{m_B^{(1)} = -\sqrt{3}/2, m_B^{(2)} = 0, m_B^{(3)} = \sqrt{3}/2\}$, and condition the Gaussian process to these base points. This conditional process as a surrogate to the original model is plotted in Fig. 4.2. We see that the conditional mean approximates the true model response, whereas the conditional standard deviation shows the estimated approximation error. The surrogate is accurate at the points where original model is evaluated while some surrogate uncertainty remains at other parameter points.

Nonetheless, the overall uncertainty is greatly reduced after the conditioning. We also plot in Fig.4.2 two posterior distributions of m, one derived from the GP-based surrogate and the other from the true model response. The latter one is the true solution of this Bayesian inverse problem, however, it requires the evaluation of model $g(m)$ at a large number of parameter points. Two spikes are seen in this distribution, showing two distinct parameter values that may result in the observed output value. Also, the right spike is taller than the left one, which is because the prior distribution puts more weight on the right solution. The posterior pdf derived from the surrogate also accurately captures the left solution. But the exact location of the right solution is not identified because the surrogate is subject to a relatively large error in that region. Instead, we observe that the posterior pdf outlines a larger region where the right solution might exist. This observation motivates us to add one refinement base point ($m = 0.4$) in that region to improve the local accuracy. The refined surrogate and the corresponding posterior distribution are shown in Fig. 4.3. With one more refinement point (and a total of four base points and four model evaluations), the GP-based surrogate is accurate enough around both solutions, and the resulting posterior pdf is in a good agreement with the one obtained from the true model response. Finally, Fig. 4.4 demonstrates the posterior computed from the surrogate without considering the surrogate error. Assuming the surrogate is accurate enough, we simply substitute the original model $g(\cdot)$ with the mean response of the GP $\tilde{g}(\cdot)$ when calculating the likelihood (2.4). However, we see that the estimated right spike is biased due to the inaccurate approximation of the surrogate, and the true solution is mistakenly excluded from the posterior. The posterior estimation of the right solution is precise (small reported uncertainty) but wrong. Moreover, without an estimation of the surrogate, we have no clue of whether refinement

points are needed.

Figure 4.2: Comparison between the true and GP-based surrogate model responses, and their corresponding posterior distributions of the model parameter given an observation of the model output. The surrogate and its error estimation are represented by a Gaussian process conditioned to model evaluations at three base points.

Figure 4.3: Comparison between the true and GP-based surrogate model responses, and their corresponding posterior distributions of the model parameter given an observation of the model output. The surrogate and its error estimation are represented by a Gaussian process conditioned to the model evaluations at three initial base points and one refinement point.
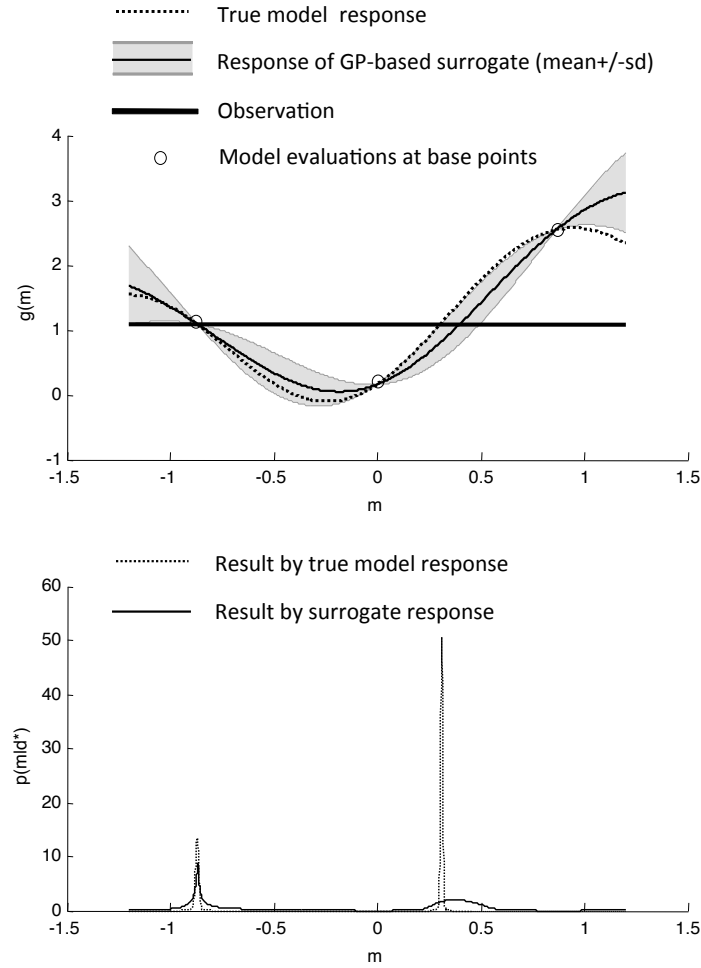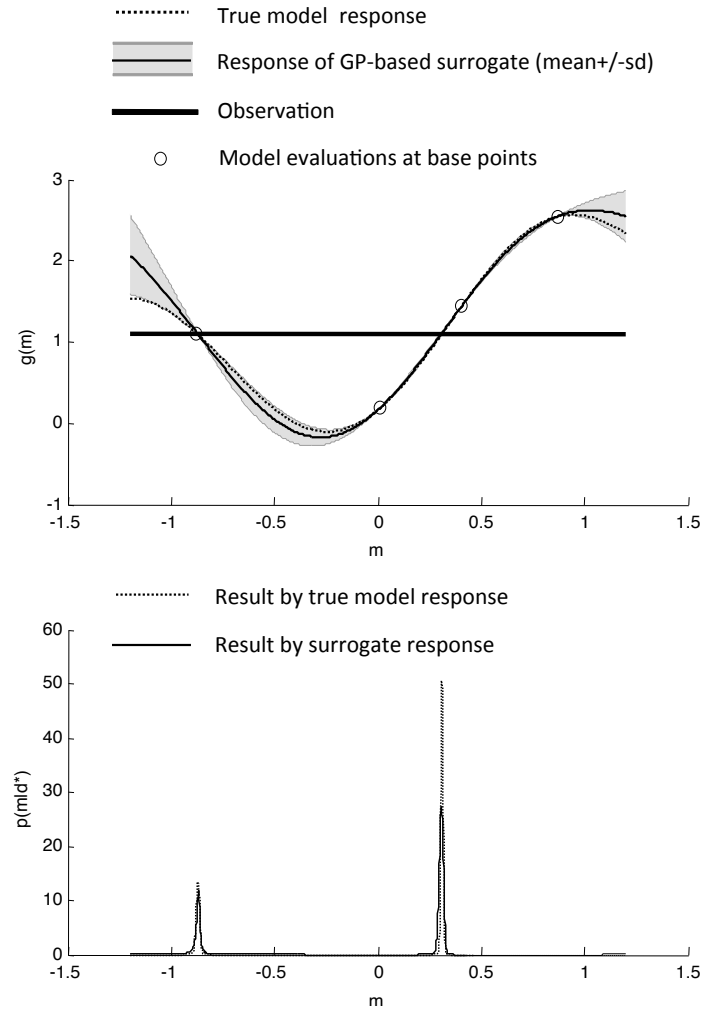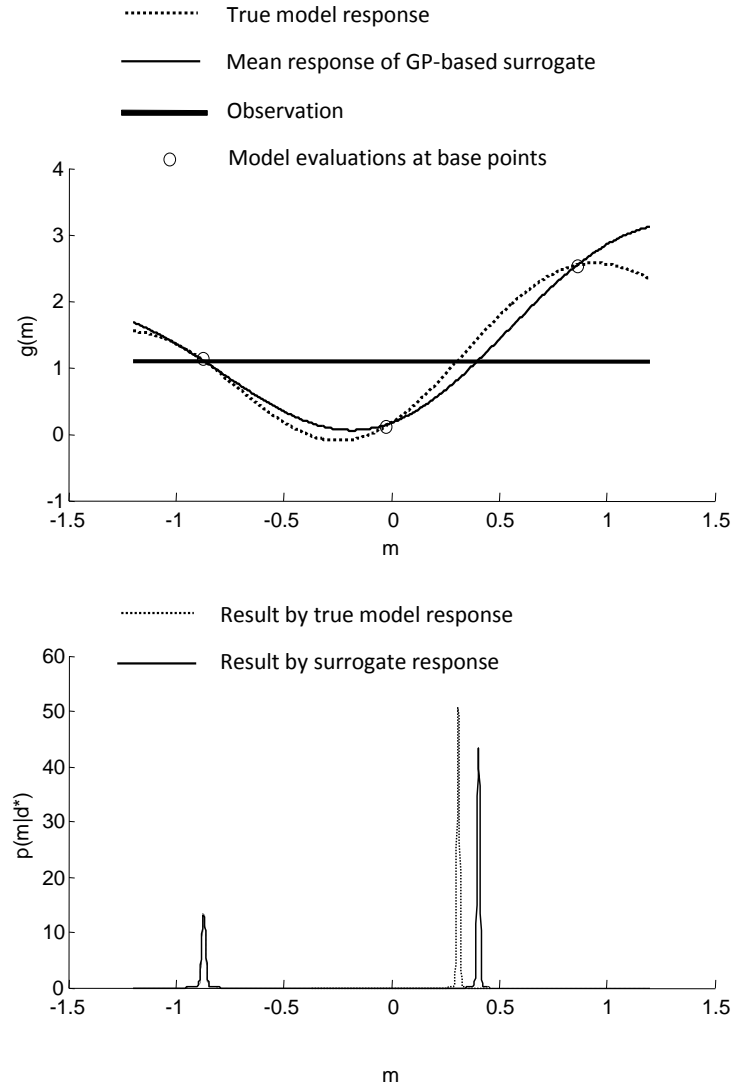
Figure 4.4: Comparison between the true and mean response of the surrogate model, and their corresponding posterior distributions of the model parameter given an observation of the model output. The surrogate is built by a Gaussian process conditioned to model evaluations at three base points. The surrogate error is not considered when computing the posterior distribution.

4.2.2 Selection of Mean and Covariance functions

The properties of a Gaussian process' realizations are determined by the mean and co-variance functions in Eq.(4.4). So the quality of a GP-based surrogate is dependent on the proper selection of these functions according to our prior knowledge about the properties of the model response. The mean function depicts the major trend of the model response. For instance, we can choose from the simplest forms such as a constant function $\mu(\mathbf{m}) = \mu_0$ if we know little about the model response, or more complicate forms such as a linear regression function $\mu(\mathbf{m}) = \mu_0 + \boldsymbol{\beta}^T\mathbf{m}$, where $\boldsymbol{\beta}$ is the coefficients vector. A group of commonly used covariance functions for a model with n_m input parameters take the following form

$$C(\mathbf{m}^{(1)}, \mathbf{m}^{(2)}) = \sigma^2 \exp\left[-\sum_{i=1}^{n_m} \frac{|m_i^{(1)} - m_i^{(2)}|^{\alpha_i}}{\eta_i}\right]. \tag{4.7}$$

Eq.(4.7) assumes that the covariance between $g(\mathbf{m}^{(1)})$ and $g(\mathbf{m}^{(2)})$ depends on the distance separating the two points $\mathbf{m}^{(1)}$ and $\mathbf{m}^{(2)}$. The shorter the distance is, the stronger the correlation is, and a perfect positive correlation is achieved as the distance approaches 0. Such a covariance function is used when we believe the model response is a continuous function. Furthermore the distances along different input dimensions may have different impacts on the correlation, which is controlled by the correlation length parameters η_i and the power parameters α_i. η_i, which is a positive real number, determines the typical correlation length along the ith input dimension, i.e., the distance beyond which two points have relatively weak correlation. On the other hand, α_i, which could be a real number between 1 and 2, controls the smoothness of the realizations. Fig.4.5 shows four GP-based surrogates built on the same three interpolation points but from different covariance func-

tions of the unconditional process. In the first three cases, power parameter α is equal to 2 (known as the Gaussian type correlation function). By comparison among the three posterior processes we see the effect of the correlation length factor η. Large η imposes a strong correlation constraint and tends to underestimate the surrogate error (Fig.4.5c), whereas short η results in an overestimated surrogate error (Fig.4.5b). Only a proper correlation length leads to a good approximation of the true model response (Fig.4.5a). In the fourth case, we change parameter α to 1 (known as the exponential type correlation function). We see that the mean response in this case is less smooth (not differentiable at the interpolation points) comparing with the results of the Gaussian correlation function.

In practice, the mean and covariance functions, or the parameters that determine these functions (e.g. $\mu_0, \boldsymbol{\beta}, \sigma^2, \eta_i, \alpha_i$) could be estimated also from the model evaluations at the base points. For example, we can choose the maximum likelihood estimator (MLE) of the parameters, i.e., the values of the parameters that maximize the joint pdf of the model responses at the n_B base points, which is multi-variate Gaussian $N(\mu(B), C(B, B))$.

To further check the quality of the GP-based surrogate, one could implement a cross validation procedure, which does not incur any extra model evaluations. That procedure is to leave one base point out of the conditioning step and see whether the resulting Gaussian process can predict the true model output at this point. Repeat this process for every base point. Failing in cross validation signals that the surrogate is not reliable. For example, if the predicted mean response deviates from the true model response by as far as three standard deviations of the estimated approximation error, we reject the surrogate and build a new one with some other mean and covariance functions.
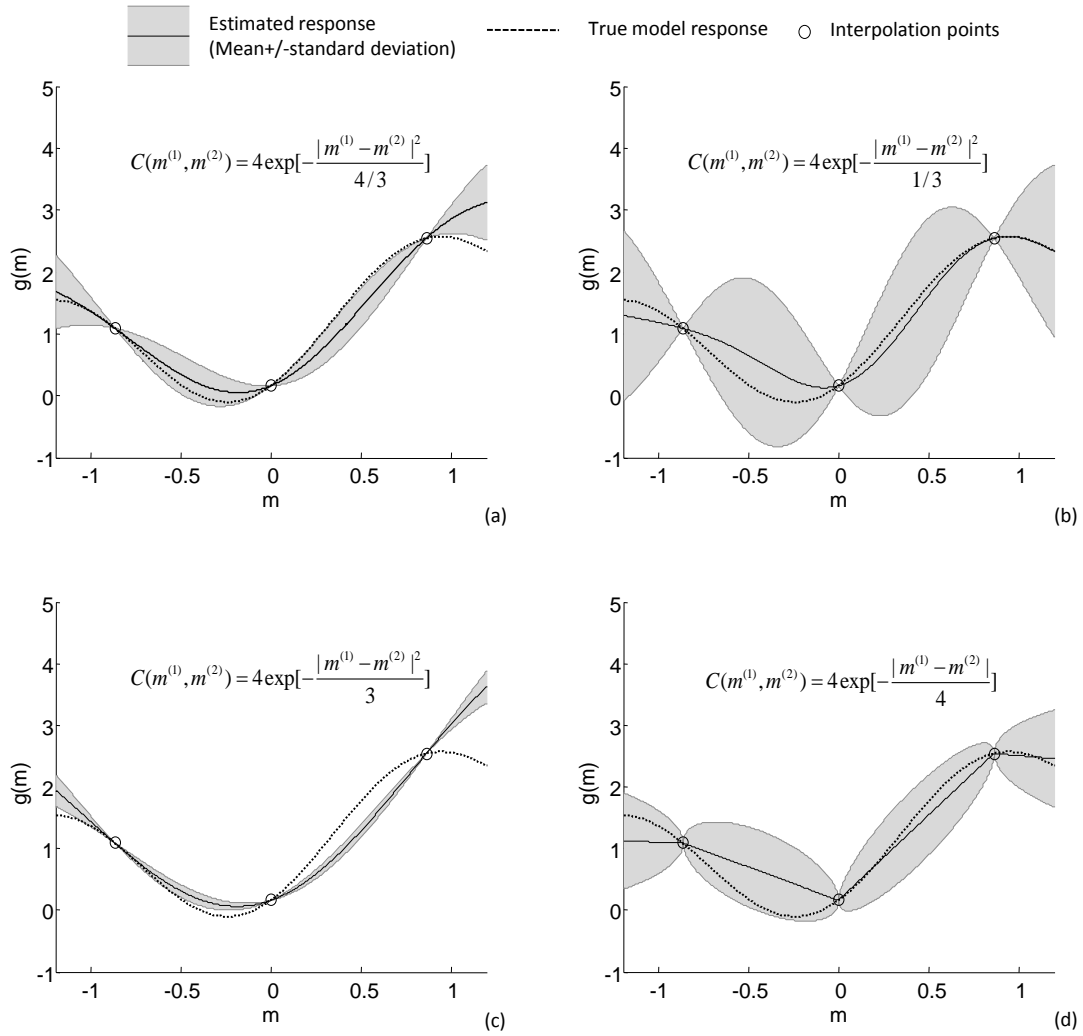
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Figure 4.5: Four GP-based surrogates built on the same base points but with different assumptions of the covariance function.

4.2.3 Models with Multiple Output Variables

So far we have been discussing the GP-based surrogate for scalar functions. A simple approach to extend this method to models with multiple output variables is to build different GP surrogates for each of them. However, in many subsurface flow models, the outputs are usually temporal and spatial functions and thus high-dimensional, which makes the construction of GP-based surrogates difficult and expensive. But on the other hand, these output variables are often correlated, so we can represent the high-dimensional output with its low-dimensional principal components (Higdon et al., 2008).

$$\mathbf{d} = \mathbf{d}_0 + \mathbf{D}\boldsymbol{\rho}, \tag{4.8}$$

where $\mathbf{d}_0$ is the mean of the output vector $\mathbf{d}$, $\mathbf{D}$ is a matrix whose columns are the principal components of the output vector, and $\boldsymbol{\rho} = [\rho_1, \rho_2, ..., \rho_{n_P}]^T$ is a vector of the corresponding coefficients of each principal components. With this representation we can approximate each element of vector $\boldsymbol{\rho}$ with GP-based surrogates instead of approximating vector $\mathbf{d}$. Not only $\boldsymbol{\rho}$ usually contains much less elements than $\mathbf{d}$, ρ_i are also decorrelated, which makes the mathematical manipulation easier. At any parameter point $\mathbf{m}$, the model output $\mathbf{d}(\mathbf{m})$ is expressed as a multi-variate random vector, with mean

$$\boldsymbol{\mu}_{\mathbf{d}}(\mathbf{m}) = \mathbf{d}_0 + \mathbf{D}\boldsymbol{\mu}_{\boldsymbol{\rho}}(\mathbf{m}) \tag{4.9}$$

and covariance

$$\mathbf{C}_{\mathbf{dd}}(\mathbf{m}) = \mathbf{D}\mathbf{C}_{\boldsymbol{\rho}\boldsymbol{\rho}}(\mathbf{m})\mathbf{D}^T, \tag{4.10}$$

where $\boldsymbol{\mu}_{\boldsymbol{\rho}}(\mathbf{m})$ and $\mathbf{C}_{\boldsymbol{\rho\rho}}(\mathbf{m})$ are the mean vector and covariance matrix of $\boldsymbol{\rho}(\mathbf{m})$ provided by the GP-based surrogates. Similar to the single-output situation, we can write the surrogate model for $\mathbf{d}$ as $\mathbf{d}(\mathbf{m}) = \tilde{\mathbf{g}}(\mathbf{m}) + \mathbf{e}_g(\mathbf{m})$, where $\tilde{\mathbf{g}}(\mathbf{m}) = \mu_{\mathbf{d}}(\mathbf{m})$ provides an approximation of the original model response and $\mathbf{e}_g \sim N\left(\mathbf{0}, \mathbf{C_{dd}}\right)$ reflects the estimation of the approximation error. Substituting this surrogate and its error estimation into Eq.(2.5) or Eq.(2.6) yields the likelihood function for Bayesian inversion.

Moreover, instead of dealing with the original values of the output variables, we normalize each output variable using its corresponding observation error: $\hat{d}_i = d_i/\sigma_{e_i}$. This procedure puts more weights on those output variables with more accurate observation.

4.3 Adaptive Re-sampling and Refinement Algorithm

Sampling from the posterior, even with the help of a surrogate model, is not a trivial task, especially when the posterior is multi-modal and/or covers only a tiny fraction of the prior distribution. In this section, we present an algorithm that adaptively refines the GP-based surrogate and samples from the targeted posterior distribution. The algorithm starts with an initial surrogate and an initial sample of parameter points, and then goes through a series of loops, each consists of a re-sampling step and a refinement step. The re-sampling and refinement steps are implemented alternatively with the assistance of each other and gradually achieve a sample of points that accurately show the targeted posterior.

4.3.1 Initialization

We start by building a GP-based surrogate on n_B initial base points, $B_0 = \{\mathbf{m}_B^{(1)}, ..., \mathbf{m}_B^{(n_B)}\}$, selected according to the prior distribution. In our algorithm the initial base points are generated using the method of latin hyper-cube sampling, which results in a relatively good coverage of the entire prior distribution (McKay et al., 1979). n_B, the number of initial base points and the number of model evaluations needed in this step does not have to be very large because we do not require the surrogate to be globally accurate. The initial surrogate will be adaptively refined in the following steps. Also, we generate an initial sample of parameter points $S_0 = \{\mathbf{m}_{S_0}^{(1)}, \mathbf{m}_{S_0}^{(2)}, ..., \mathbf{m}_{S_0}^{(n_S)}\}$ from the prior distribution. which will shrink to the posterior distribution in the following refinement and re-sampling loops. Note that we could afford to have a much larger number of sample points n_S than the base points since the sampling and re-sampling procedures do not incur simulations of the original model when a surrogate is used instead. After the initialization, we proceed to a series of re-sampling and surrogate refinement loops.

4.3.2 Re-sampling via GP-based Surrogate

In each new loop, say the ith loop, a new sample of points are generated from $p(\mathbf{m}|\mathbf{d}^*, B_{i-1}) = h \cdot p(\mathbf{d}^*|\mathbf{m}, B_{i-1})p(\mathbf{m})$, which is the posterior distribution defined through the surrogate built upon base points B_{i-1} in previous loop. In our algorithm, we choose the method of importance sampling to carry out this step (see section 4.1.2). One of the most challenging parts in importance sampling is the selection of the proposal distribution $q(\mathbf{m})$. Although,

theoretically, any distribution that covers the domain where the targeted distribution exists may be used as the proposal distribution, a properly selected $q(\mathbf{m})$ could greatly improve the qualify of the sample. An ideal proposal distribution should be as close to the targeted distribution as possible. However, in the context of Bayesian inversion, we have no idea of where to construct such a proposal distribution since the target itself, i.e., the posterior, is unknown. Usually, the proposal distribution is chosen as the prior $p(\mathbf{m})$. Note that in most problems the prior has a simple pdf such as uniform or Gaussian, which is easy to sample from. But often the posterior distribution concentrates only on a small portion of the regions covered by the prior distribution. As a result, most of the proposed sample points except a few do not hit the posterior and end up with nearly-zero weights, which causes a large sampling error. This phenomenon is known as "sample degeneracy".

Our algorithm brings a remedy to this issue by using a different proposal distribution that is much closer to the target. Note that the posterior distribution we seek in current loop, $p(\mathbf{m}|\mathbf{d}^*, B_{i-1})$, is not completely unknown because it is an improvement of the posterior we estimated in previous loop, which we have a sample of points $S_{i-1} = \{\mathbf{m}_{S_{i-1}}^{(1)}, \mathbf{m}_{S_{i-1}}^{(2)}, ..., \mathbf{m}_{S_{i-1}}^{(n_S)}\}$ showing its distribution. Inspired by this observation, we choose a proposal $q_i(\mathbf{m})$ in the ith loop such that the points in S_{i-1} are closely incorporated. For the specific form of $q_i(\mathbf{m})$, we use a Gaussian mixture model, which is not only easy to draw sample from, but also flexible enough to fit different distributions of S_{i-1}, including multi-modal distributions induced by strongly nonlinear model $g(\cdot)$. To fit the sample S_{i-1} into a Gaussian mixture model, we first divide the n_S sample points into n_c groups, or clusters, with a clustering method such as K-means (Hartigan and Wong, 1979). Each

cluster of points approximately represents a n_m-dimensional multivariate Gaussian pdf $f_N\left(\mathbf{m}; \boldsymbol{\mu}^{(j)}, \mathbf{C}^{(j)}\right)$, $j = 1, 2, ...n_c$, where the mean $\boldsymbol{\mu}^{(j)}$ and covariance $\mathbf{C}^{(j)}$ are estimated from the jth cluster of points. A Gaussian mixture distribution as the proposal is then constructed

$$q_i(\mathbf{m}) = \sum_{j=1}^{n_c} \frac{n_S^{(j)}}{n_S} f_N\left(\mathbf{m}; \boldsymbol{\mu}^{(j)}, \mathbf{C}^{(j)}\right), \tag{4.11}$$

where $n_S^{(j)}$ is the number of points in the jth cluster. A sample point from this pdf can be obtained simply in two steps: 1) randomly picking a cluster j with probability $n_S^{(j)}/n_S$; and 2) generating a sample point from the Gaussian distribution $f_N\left(\mathbf{m}; \boldsymbol{\mu}^{(j)}, \mathbf{C}^{(j)}\right)$. Fig. 4.6 shows an example of fitting a sample of points into a Gaussian mixture distribution and a new sample regenerated from it.

4.3.3 Refinement of Surrogate Models

After obtaining the new sample in the ith new loop, we check whether further refinement of the surrogate is needed. If so, we refine the surrogate by adding one more base point $\mathbf{m}_B^{(n+i)}$ to the existing ones to form a new set of base points B_i. The selection of the new base point follows two criteria which ensure the efficiency of the refinement scheme. First, the refinement point should be within or close to the regions of posterior distribution; second, the refinement point should not be placed at a location where the surrogate is already accurate enough. Note that the sample points obtained from the previous loop provide an approximate representation of the posterior distribution (though they usually cover a larger region than the true posterior because of the consideration of surrogate error), which
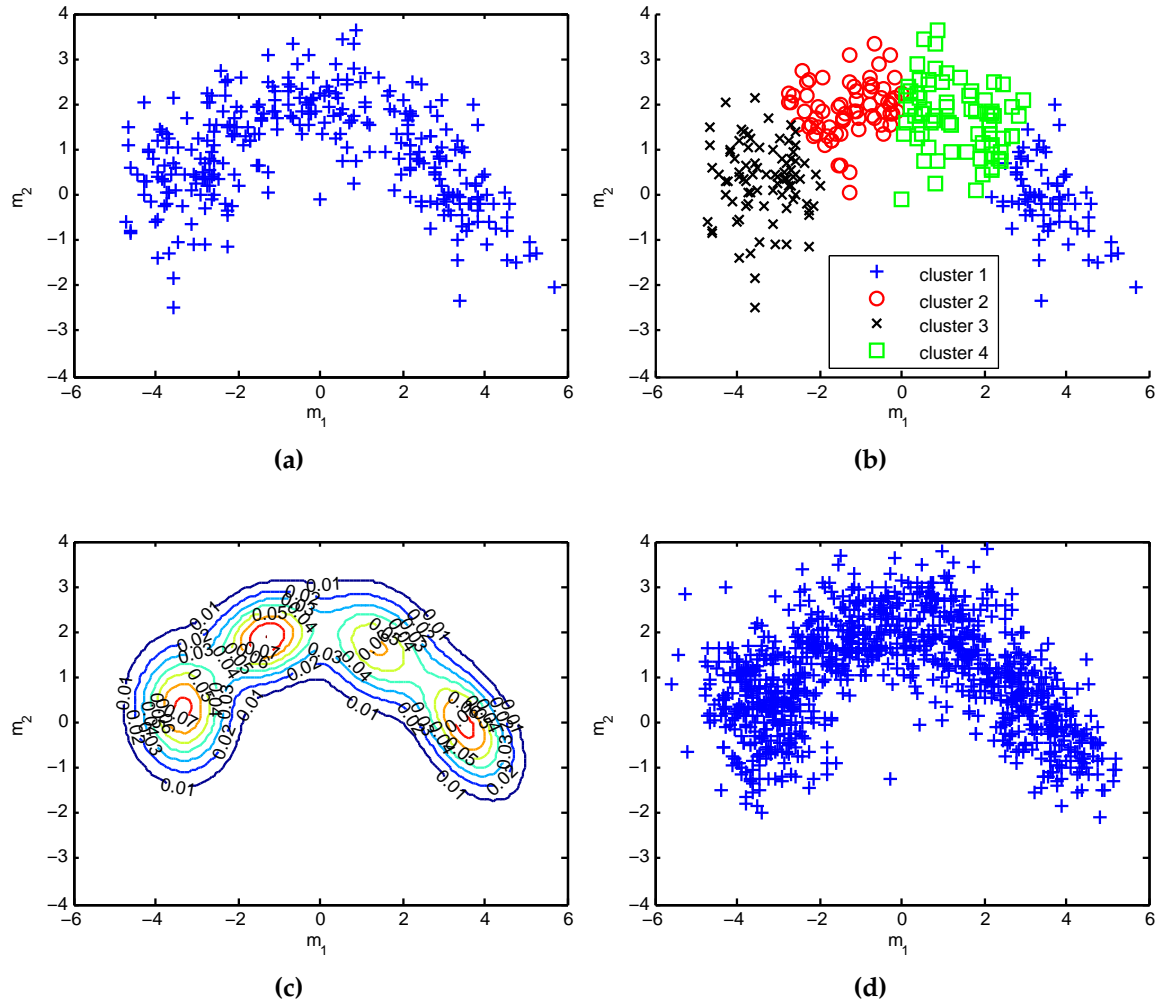
(a)

(b)

(c)

(d)

Figure 4.6: Use a Gaussian mixture distribution as the proposal distribution for importance sampling: an illustrative example. (a) 300 original sample points; (b) clustering of the original sample points; (c) Gaussian mixture distribution fitted from the clusters; (d) 1000 new sample points proposed from the Gaussian mixture distribution.

makes them candidate points meeting the first criterion. So we choose the refinement point to be the point with the largest surrogate error among all the sample points from the previous loop. However, if the surrogate is accurate enough at all candidate points, we stop the refinement loops and report the current sample points as the sample that represent the targeted posterior distribution.

Note that this algorithm can be easily modified to add multiple refinement base points in each loop, which is particularly useful when the simulations with different parameter points can be run in parallel.

4.3.4 Summary of Work Flow

The implementation procedures of the adaptive sample-refine algorithm are summarized here:

1. **Input to the algorithm**:

   - original model, $g(\cdot)$;

   - prior distribution of model parameters, $p(\mathbf{m})$;

   - observation of model output, $\mathbf{d}^*$, and associated observation errors;

   - number of initial base points, n_B;

   - maximum number of base points, also the maximum number of evaluations of the original model, $\bar{n}_B$;

   - number of sample points used to represent the posterior distribution, n_S;

- surrogate error threshold, $\bar{e}$

2. **Initialization**:

   - generate n_B initial base points $B_0 = \{\mathbf{m}_B^{(1)}, \mathbf{m}_B^{(2)}, ..., \mathbf{m}_B^{(n_B)}\}$ according to $p(\mathbf{m})$ using latin hyper-cube sampling;

   - compute the output values of the original model at the base points: $\mathbf{d}^{(j)} = g\left(\mathbf{m}_B^{(j)}\right), \quad j = 1, 2, ..., n_B$;

   - construct a GP-based surrogate of the original model conditioned to the base points: $G(\mathbf{m}|B_0)$;

   - draw n_S initial sample points $S_0 = \{\mathbf{m}_{S_0}^{(1)}, \mathbf{m}_{S_0}^{(2)}, ..., \mathbf{m}_{S_0}^{(n_S)}\}$ according to the prior distribution $p(\mathbf{m})$.

3. **Re-sampling via surrogate in the ith loop**

   - group the sample points S_{i-1} into clusters with K-means method;

   - construct a proposal distribution $q_i(\mathbf{m})$ using a Gaussian mixture model (Eq.4.11);

   - generate n_S proposed sample points $\{\mathbf{m}_q^{(1)}, \mathbf{m}_q^{(2)}, ..., \mathbf{m}_q^{(n_S)}\}$ from $q_i(\mathbf{m})$, and compute their corresponding weights $\{w_1, w_2, ..., w_{n_S}\}$ using Eq.(4.2) via the surrogate model $G(\mathbf{m}|B_{i-1})$;

   - draw a equal-weight sample $S_i = \{\mathbf{m}_{S_i}^{(1)}, \mathbf{m}_{S_i}^{(2)}, ..., \mathbf{m}_{S_i}^{(n_S)}\}$ from the weighted proposed sample using systematic re-sampling method.

4. **Refine surrogate in the ith loop**

   - check the approximation error of the GP-based surrogate response by calculating its standard deviation $\sigma_{|B}(\mathbf{m})$ using Eq.(4.6) at each sample point of S_i,

locate the point $\mathbf{m}^*$ where the surrogate response has the largest standard deviation;

- if the surrogate error is small enough: $\sigma_{|B}(\mathbf{m}^*) < \bar{e}$, or the maximum number of model evaluation is reached: $n_B + i > \bar{n}_B$, **stop**, and report the sample S_i as the final solution of the inverse problem;

- if the stop criterion is not met, let $\mathbf{m}^*$ be the refinement point $\mathbf{m}_B^{(n+i)}$, add it to current base points, and update the GP-based surrogate use the new set of base points;

- proceed to **step 3: Re-sampling via surrogate** of the next loop.

4.4 Illustrative Examples

4.4.1 Problem 3: Test on an Algebraic Function

To better visualize the surrogate and the adaptive refinement process, we first apply our algorithm to an algebraic model with only 2 input parameters and 1 output variable: $d = g(m_1, m_2) = m_1 m_2$. The prior distributions of m_1 and m_2 are both uniform on [-1,1] and are independent with each other. We have an observation of model output $d^* = 0.4$, which is subject to a normally distributed observation error, $e_o \sim N(0, 0.01^2)$. The objective is to estimate the model parameters from this observation and quantify the remaining uncertainty. Moreover, we assume the analytic expression of $g(\cdot)$ is not known and it can only be evaluated for specific input values, just like a simulator we would encounter in

most inverse problems. We seek a sample of points representing the posterior distribution defined by the Bayes' rule. Even though this model has a simple form, its strong non-linearity results in a spiky and bi-modal posterior, which is extremely difficult to sample from using a classic sampling method.

To start our algorithm, we set the number of initial base points $n_B = 9$, the number of sample points $n_S = 2000$, and the surrogate threshold $\bar{e} = 0.01$, which is equal to the standard deviation of the observation error. The initial surrogate response and the estimation of the approximation error, which are represented by the mean and the standard deviation of the GP-based surrogate, respectively, are shown in Fig. 4.7. We see that the approximation error is pinned down to zero at the base points, but remains relatively large (comparing with the threshold) in some other regions.
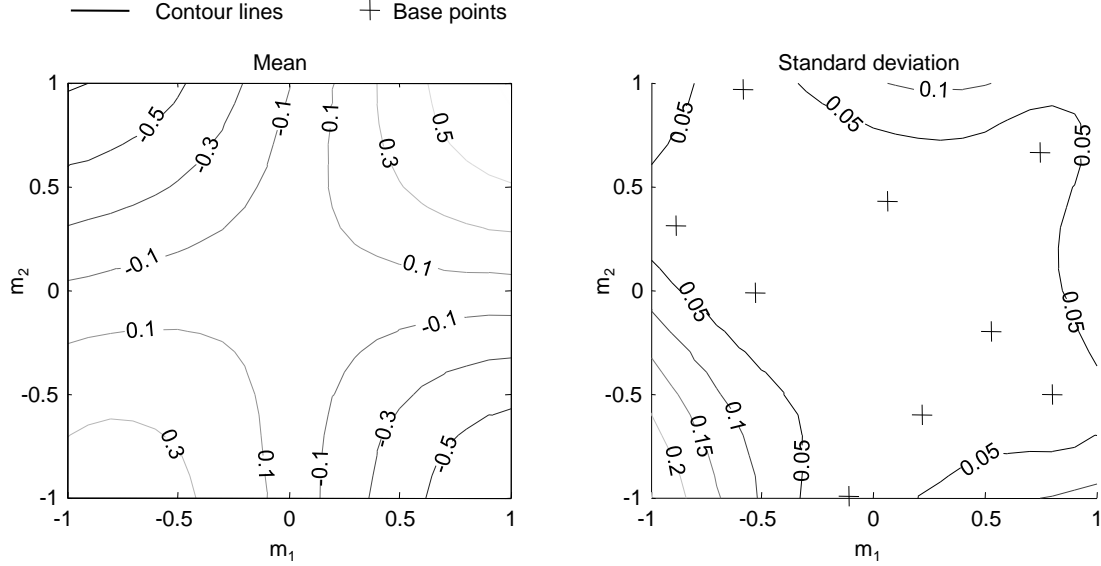

Figure 4.7: Mean and standard deviation of the GP-based surrogate built on 9 initial base points (Problem 3).

The further adaptive refinement process is illustrated in Fig.4.8 and Fig.4.9. We see that in each refinement loop, a sample of points are generated via the surrogate (Fig.4.8). Initially, the sample points are loosely spread around the upper right and lower left corners, which roughly outline the regions of the true posterior but do not provide an accurate representation. In each loop, a new base point is selected among the sample points and is used to improve the local accuracy of the surrogate (Fig.4.9). The stop criterion is met after 6 refinements. Even though the surrogate is still not globally accurate, we see that the adaptive refinement scheme ensures the surrogate accuracy in the regions around the targeted posterior distribution, and as a result, a nice sample of the posterior is obtained. The final sample representing the posterior is achieved at the cost of only 15 model evaluations, including 9 for building the initial surrogate and 6 for adaptive refinement.
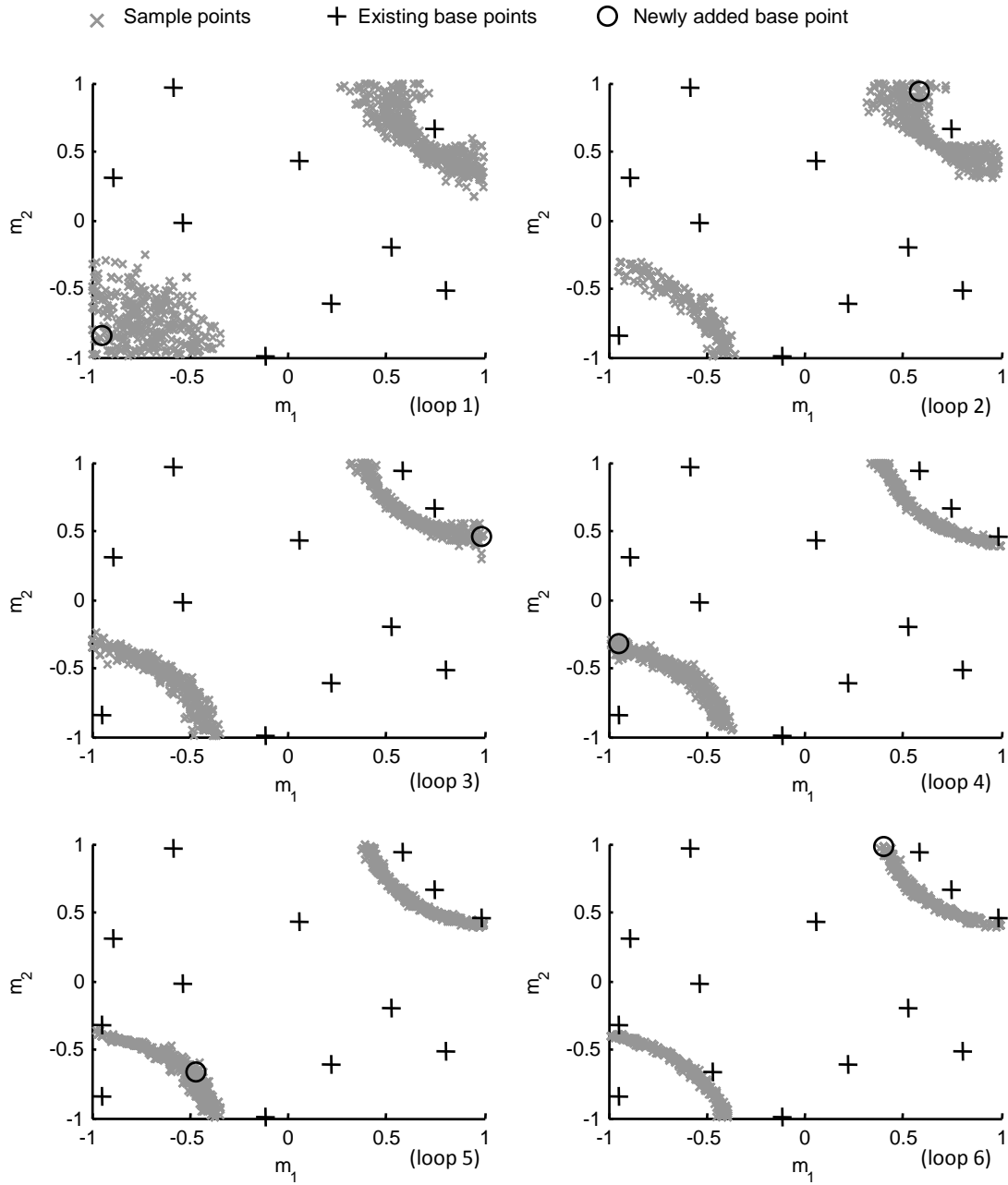
Figure 4.8: Sample points obtained in different re-sampling and refinement loops (Problem 3).

Figure 4.9: Standard deviations of the surrogate errors in different refinement loops (Problem 3).

4.4.2   Problem 4: I-C Fault Model

In the second example, we applied our algorithm to the history matching problem of a reservoir model known as I-C Fault model (Tavassoli et al., 2004; Carter et al., 2006). The model is designed such that the dependent relationship between the production history and the uncertain model parameters is strongly nonlinear, which results in a complex multi-modal posterior. In the original study of (Tavassoli et al., 2004), the authors thoroughly explored the three-dimensional parameter space with the simulations of 159,645 randomly generated realizations. But, the realization that best matched the production history did not reflect the true geological properties of the reservoir and yielded a wrong prediction of future production. In a following research paper, Christie et al. (2006) studied the quantification of the posterior uncertainty by sampling from the posterior distribution. Machine learning algorithms including Genetic Algorithms and Artificial Neural Network were used to reduce the computational burden. However, thousands of model simulations were still needed to achieve a satisfying sample.

We give a brief review of the I-C Fault model, while more details may be found in the above cited references. The I-C Fault model represents the 2-D vertical cross section of an oil reservoir that consists of six layers of alternating high- and low-permeable sand (Fig.4.10). The reservoir is 1000 ft wide and 60 ft thick, where the thickness of the six layers is an arithmetic progression from the bottom (7.5 ft) to the top (12.5ft). The reservoir is divided into two parts by a fault in the middle. A water injection well and a production well are located at the left and right boundaries, respectively, both operating at constant pressures. The upper and lower boundaries are bounded by no flow boundary conditions.
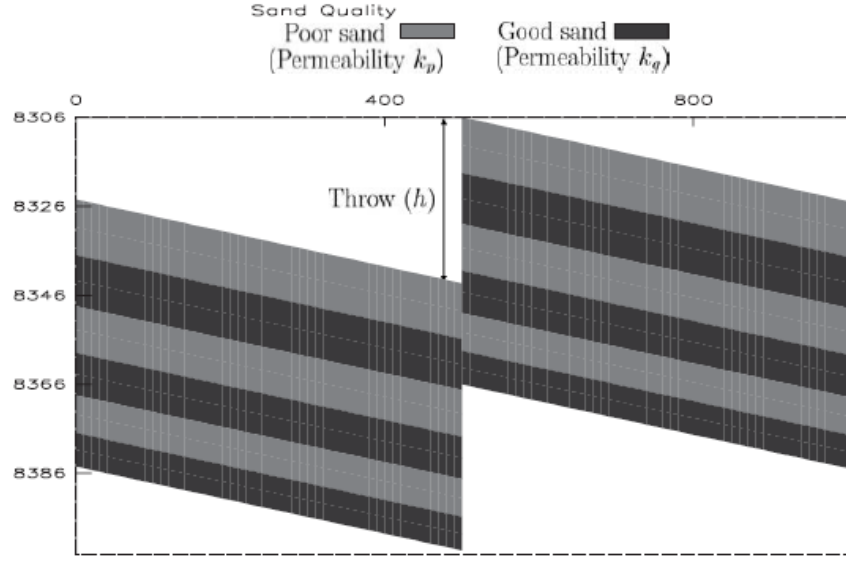
Figure 4.10: I-C Fault model (Carter et al., 2006), distances are measured in feet (Problem 4).

The model has three uncertain input parameters with independent and uniform prior distributions: the fault throw ($h \in [0, 60]$ft), the permeability of the good-quality sand ($k_g \in [100, 200]$md), and the permeability of the poor-quality sand ($k_p \in [0, 50]$md). For each realization sampled from the parameter space, the corresponding production history (water cut and oil production rate in this problem) could be simulated from the model. Fig.4.11 shows the simulation results from an ensemble of input realizations drawn from the prior distribution. It is seen that the variations of the input parameters cause a large uncertainty in the simulation results. To reduce the uncertainty, we calibrate the input parameters to the observations of the "synthetic true" production history, which are recorded every month in the first three years of production. The observed data are generated from the simulation based on a reference parameter point ($h_0 = 10.4$ft, $k_{g0} = 131.6$md,

$k_{p0} = 1.3$md), and are perturbed randomly according to the observation errors, which we assume are normally distributed, with zero means and standard deviations equal to 5% of the predicted standard deviations (prior uncertainty) of the simulation results.
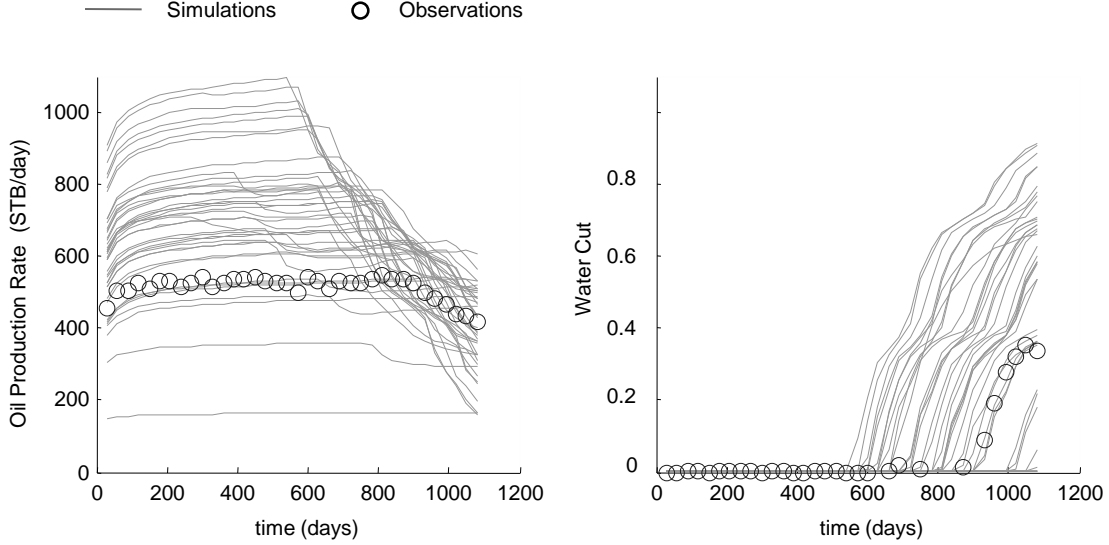

Figure 4.11: Simulation results of the I-C Fault model based on the parameter points sampled from prior distribution (Problem 4).

Our algorithm starts by building an initial GP-based surrogate with 40 initial base points selected from the prior distribution using latin hyper-cube sampling. Note that the simulation results of this model are two time sequences, which make a high-dimensional output and may be represented with the principal components method. Similar to the one-dimensional output case, the surrogate returns an approximate model output and an error estimation for each input parameter point. The surrogate responses at some input points are plotted in Fig.4.12 with error estimations. The simulation results of the original model are also shown in the same plots for comparison. With only 40 model evaluations,

we did not obtain an perfect approximation of the original model. However, at most input parameter points, the true outputs fall into the confidence intervals (mean +/- 2 standard deviations) provided by the surrogate. An initial sample of parameter points are drawn from the posterior via the surrogate (Fig.4.13). Again, this sample does not accurately show the true posterior distribution but outlines a region for further refinement.

After 40 adaptive re-sampling and refinement loops, we obtained the final sample of parameter points as shown in Fig.4.14. Although this sample distributes within a much smaller region comparing with the initial sample, the parametric uncertainty is not completely eliminated. Especially, the fault throw is not identifiable from the observation of the production history. To verify the history matching results, we run the original model at some parameter points picked randomly from the final sample and compare the simulation results with the observations (Fig.4.15). It is seen that all the simulations and the observations are in good agreement.

To further check the quality of the final sample obtained from our algorithm, we generate another sample (Fig.4.16) from the large number (159645) of Monte Carlo simulations of the original model provided by the creators of the model. Through the comparison, we see the two samples are very close to each other. However, our algorithm employs only 80 simulations of the original model.

The final objective of history matching is to predict the quantities of our interest using the calibrated model. Moreover, we are able to quantify the uncertainty in the prediction using the multiple solutions obtained with our algorithm. In this example, we predict the cumulative oil production for the next seven years after the observed history. We im-
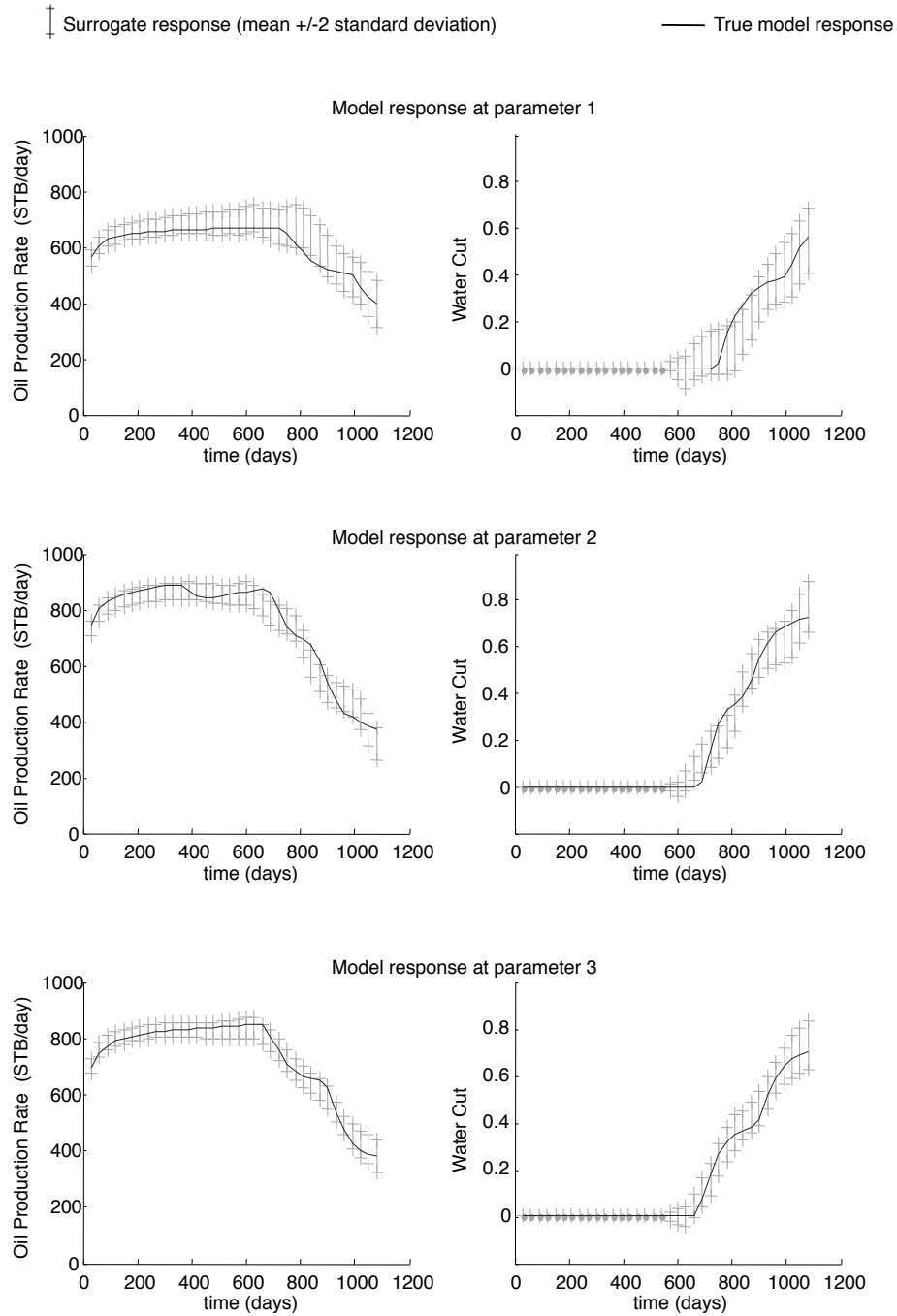
Figure 4.12: Comparison between original I-C Fault model responses and surrogate responses evaluated at three randomly selected parameter points. The responses of the GP-based surrogate are shown with error estimation (mean +/- 2 standard deviations), (Problem 4).
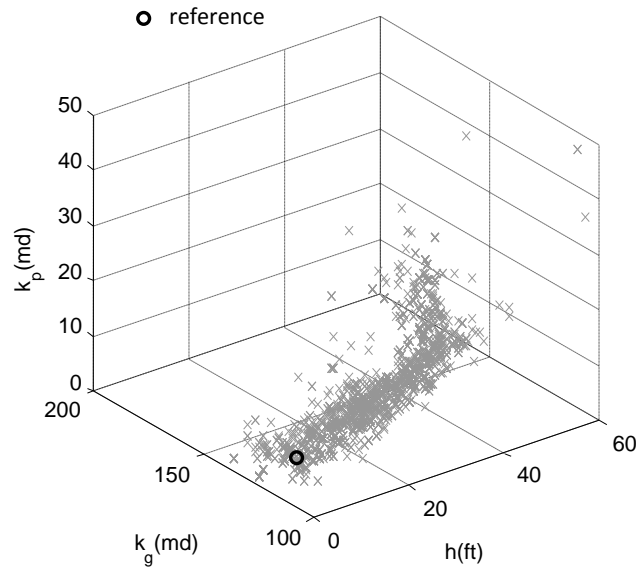
Figure 4.13: Sample from the posterior distribution of the I-C Fault model parameters via the GP-based surrogate built on 40 initial base points (Problem 4).
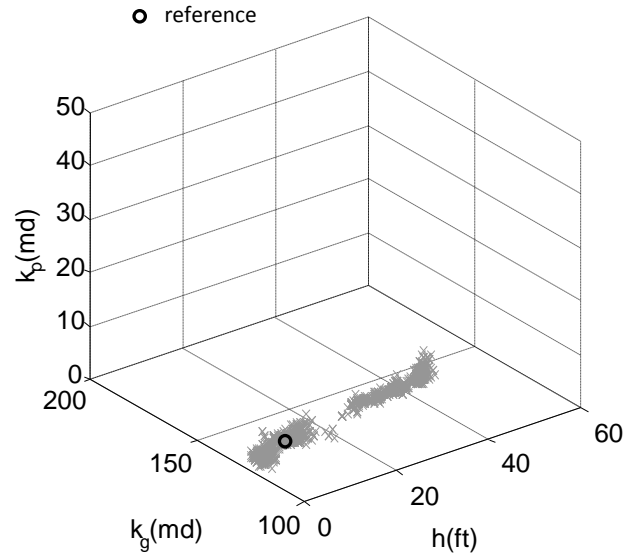
Figure 4.14: Sample from the posterior distribution of the I-C Fault model parameters via the GP-based surrogate built on 40 initial and 45 refinement base points (Problem 4).

Figure 4.15: Simulation results of the I-C Fault model based on the parameter points sampled from posterior distributions obtained using the final GP-based surrogate (Problem 4).

Figure 4.16: Sample from the posterior distribution of the I-C Fault model parameters using a large number of Monte Carlo simulations (Problem 4).
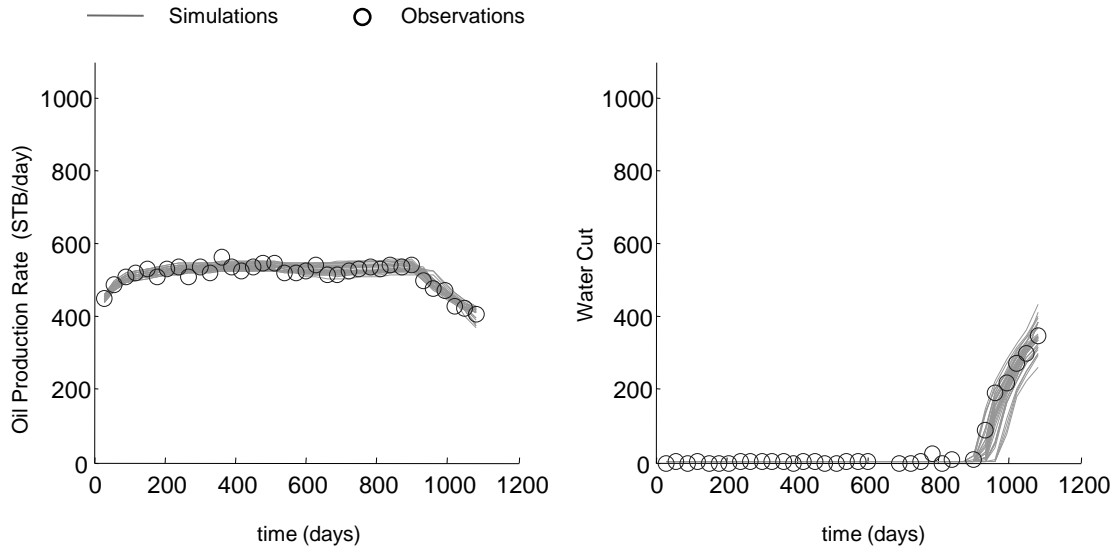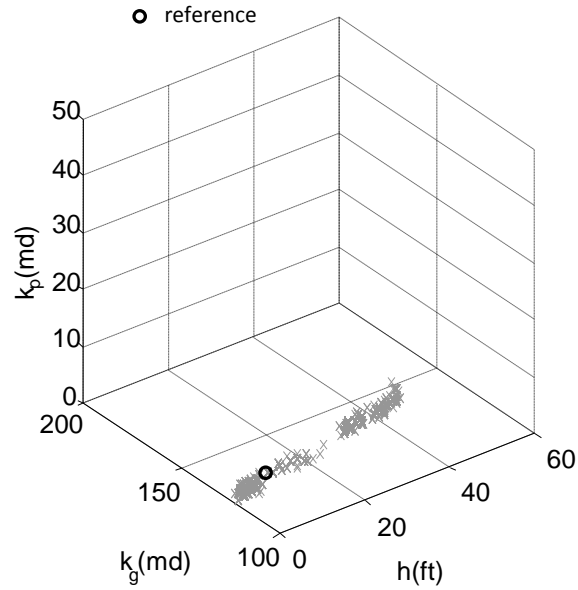
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plement two sets of simulations, which are based on the sample points before and after the history matching, respectively (Fig.4.17). It is seen from the figure that matching the production history significantly improves the accuracy of prediction. The calibrated simulations are reliable in the near future, with little prediction uncertainty. Nevertheless, as the simulation time moves forward, the prediction uncertainty gradually increases, showing that a single simulation matching the first three years of production history does not necessarily provide a reliable prediction over a long-time period.
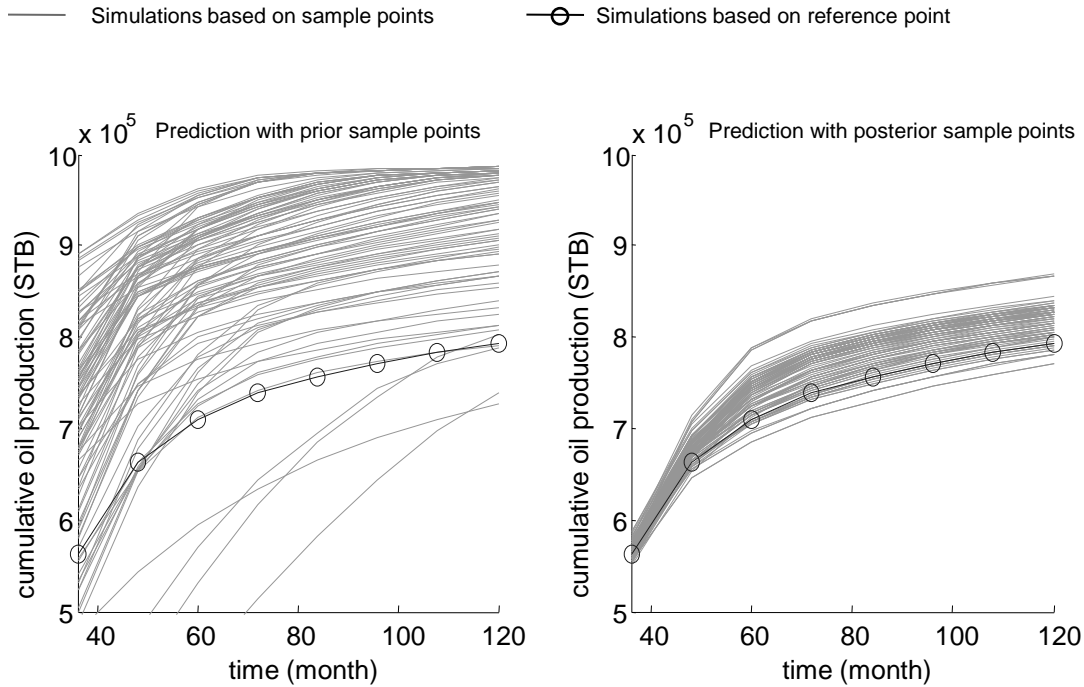

Figure 4.17: Predictions of cumulative oil production for the next 7 years after the first three years of observed production history. Simulations are based on 1) sample parameter points from the prior distribution and 2) sample parameter points obtained from the posterior distribution using G-P based surrogate (Problem 4).

4.4.3 Problem 5: Solute Transport with Groundwater

Now we apply the algorithm to a problem of conservative solute transport in a confined aquifer as shown in Fig. 4.18. The standard mathematical model for this problem computing the concentration of the solute C in the time and space is the advection dispersion equation:

$$\frac{\partial(\phi C)}{\partial t} = -\nabla \cdot (\phi C \mathbf{v} - \phi \mathbf{D} \nabla C), \tag{4.12}$$

where ϕ is effective porosity, $\mathbf{D}$ is the dispersion tensor with the longitudinal and transverse components being $D_L = \alpha_L|\mathbf{v}|$ and $D_T = \alpha_T|\mathbf{v}|$, respectively. α_L and α_T are longitudinal and transverse dispersivities. The linear velocity of water flux $\mathbf{v}$ is determined by the continuity equation:

$$\nabla \cdot (\phi \mathbf{v}) = 0, \tag{4.13}$$

and the Darcy's law:

$$\mathbf{v} = -\frac{1}{\phi}\mathbf{K}\nabla h, \tag{4.14}$$

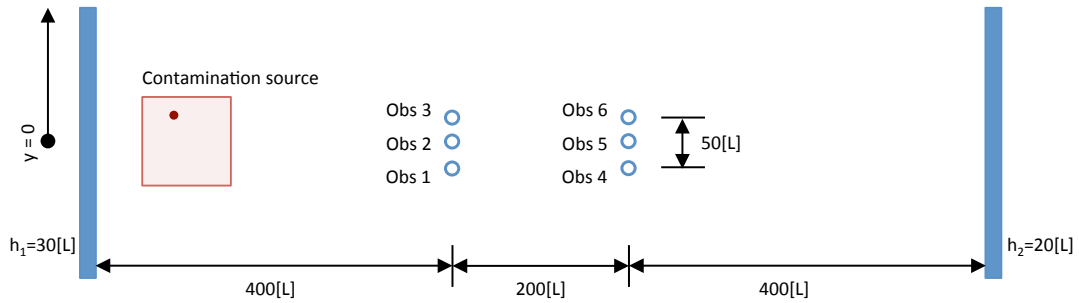where $\mathbf{K}$ is the tensor of hydraulic conductivity.

Figure 4.18: Schematic representation of the solute transport model (Problem 5).

In this 2-D illustrative problem, we assume the aquifer has homogeneous and isotropic conductivity K, and is bounded by two rivers with constant head at the left ($h_1 = 30[L]$) and the right ($h_2 = 20[L]$) boundaries, respectively, which results in a uniform background flow from left to right. Suppose an amount Q_0 of contaminant is accidentally released (instantaneously) into the aquifer at a point (x_0, y_0) and time t_0. The solute concentration is measured at some observation wells downstream of the contamination source, and is used for model calibration. Consider the following cases of inverse modeling problems listed in Table 4.1.

Table 4.1: List of case studies of Problem 5 with different parameter and observation settings.

Parameters	Case 1	Case 2	Case 3
x_0 [L]	[50,150]	[50,150]	[50,150]
y_0 [L]	[-50,50]	[-50,50]	[-50,50]
Q_0 [M]	$[0.5,1.5] \times 10^6$	$[0.5,1.5] \times 10^6$	$[0.5,1.5] \times 10^6$
t_0 [T]	0	0	[0,60]
ϕ	0.2	0.2	[0.15,0.25]
K [LT^{-1}]	20	20	[15,25]
α_L [L]	2	2	[1.5,2.5]
α_T [L]	0.8	0.8	[0.6,1]
Observations	Case 1	Case 2	Case 3
obs 2	CH*	CH	CH
obs 1, obs 3	NA	CH	CH
obs 4 - obs 6	NA	NA	CH

*CH: 3 characteristics—maximum concentration, 1st and 2nd moments—of the breakthrough curve observed at the well; NA: not available.

In case 1, we assume the data available are the concentration values/breakthrough curve measured at observation well #2 ($x = 400$[L], $y = 0$[L]). The objective is to infer the location (x_0, y_0) of contamination source and the total released mass (Q_0), which all have uniform prior distributions, whereas other parameters are of known deterministic values (see Table 4.1). We first construct an initial GP surrogate from 30 base points sampled from the prior distribution using latin hyper-cube sampling. The simulated breakthrough curves at 10 of the initial points are plotted in Fig. 4.19 in comparison with the observation. The initial simulation results reveal great variability and hardly match the observation. We see that although the output in this problem is a time series $C(t)$ (hence high-dimensional), it is a bell-shaped curve that can be characterized with three quantities: cumulative concentration $I_0 = \int_{t=0}^{\infty} C(t)dt$, the 1st normalized moment: $I_1 = \frac{1}{I_0} \int_{t=0}^{\infty} tC(t)dt$, which shows the approximate arrival time of the peak concentration; and the 2nd normalized moment: $I_2 = \frac{1}{I_0} \int_{t=0}^{\infty} (t - I_1)^2 C(t)dt$, which reflects the length of the time period in which a significant solute concentration is seen at the well. This implies that we can conveniently represent the model output with only three variables instead of a high-dimensional time series. We then proceed to the adaptive re-sampling and refinement loops. After adding 8 refinement points, the algorithm stops with a sample shown in Fig. 4.20a. The histograms of three parameters are also shown in Fig. 4.20b-d. Clearly, the observations in this problem are deficient to determine a single solution, but instead lead to a non-Gaussian, bimodal posterior. x_0 is the only parameter that is identified with high resolution. Because of the symmetry of the concentration pattern, an initial contamination at (x_0, y_0) would induce the same breakthrough curve at well #2 as induced by a source at (x_0, $-y_0$) with the same released amount Q_0. As a result, two distinct possibilities of the value of y_0 are seen in the

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posterior. Finally, the posterior provides little information about the true value of Q_0. This is because the effect of a larger/smaller Q_0 on the observation is easily compensated with a larger/smaller distance between the observation well and the path of the center of the contaminant slug, which is determined by y_0. Simulations from the posterior sample are shown in Fig. 4.21, where we see a great agreement with the observed curve.

Figure 4.19: Concentration breakthrough curves at well *obs2* simulated using prior sample points (Case 1, Problem 5).

To gain more information about the contamination source, we measure the breakthrough curves at two more wells #1 ($x = 400$[L], $y = -25$[L]) and #3 ($x = 400$[L], $y = 25$[L]) in the second case study. Again, we start with the initial GP surrogate built from 30 base points. But this time, the adaptive sampling algorithm stops after adding only two refinement points. The posterior sample is shown in Fig. 4.22 with the histograms of each
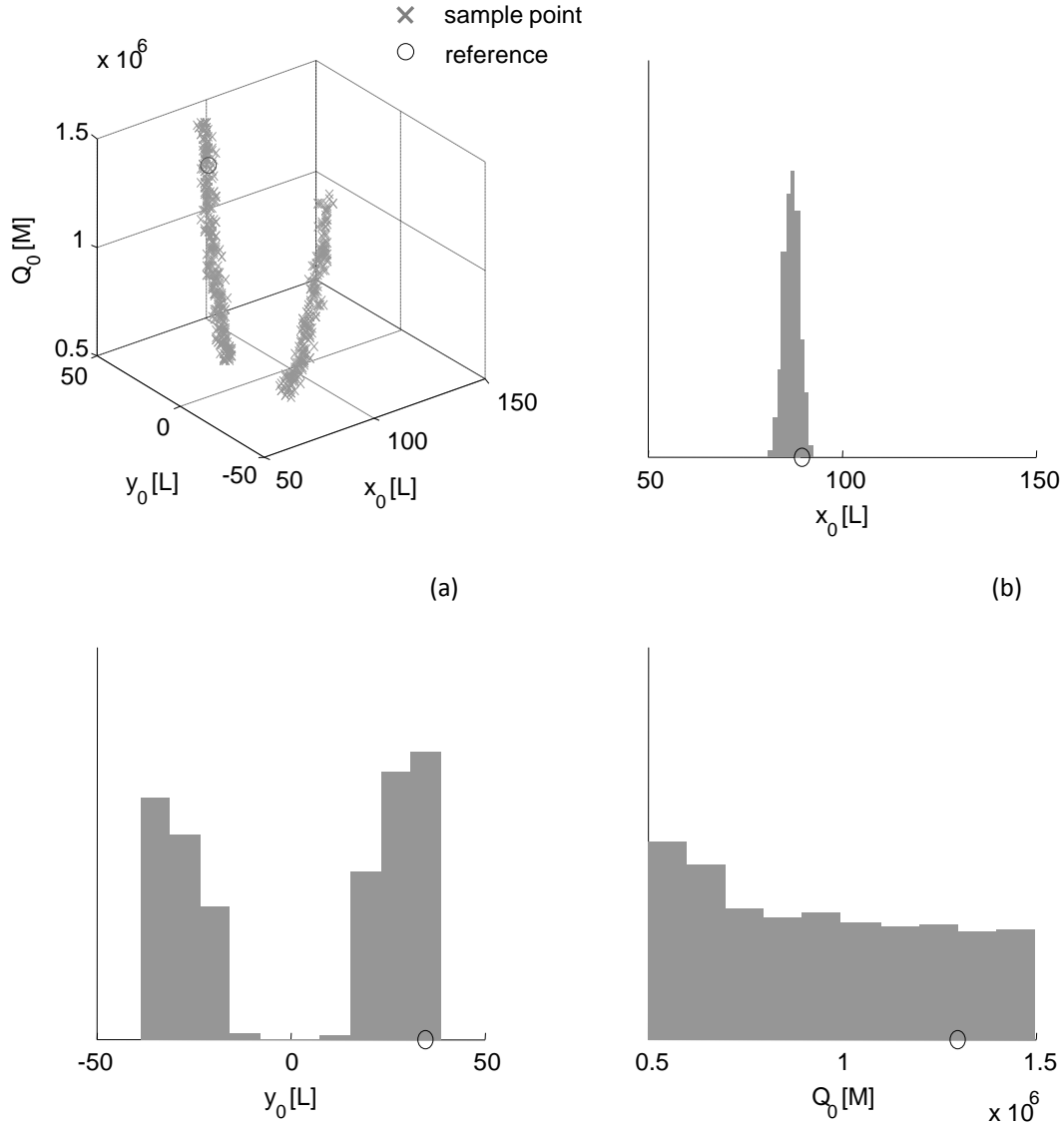
Figure 4.20: Estimated posterior distribution (Case 1, Problem 5); (a) posterior sample points; (b-d) posterior histograms for each uncertain parameter.
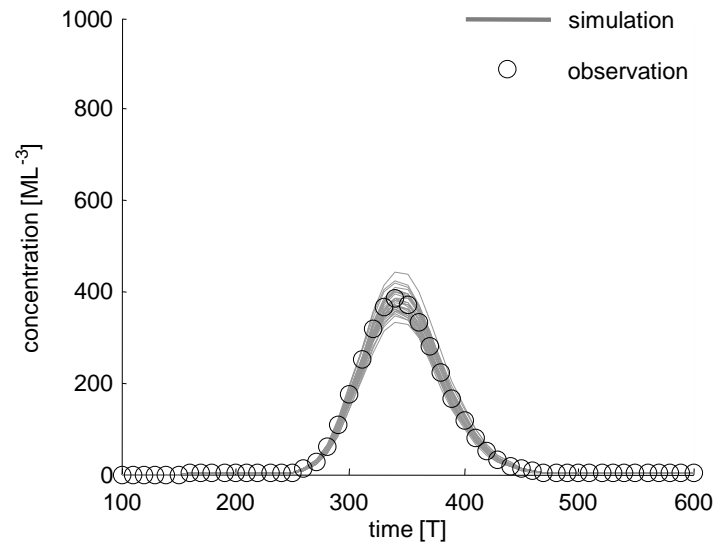
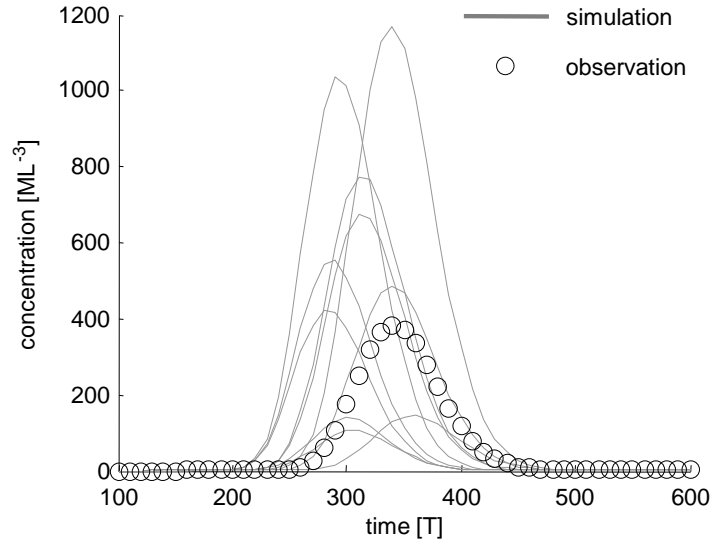**Figure 4.21:** Concentration breakthrough curves at well *obs2* simulated using posterior sample points (Case 1, Problem 5).

parameter. In this case the posterior sample points converge to a small region around the reference parameter point, showing that all three parameters are accurately estimated with little remaining uncertainty. Again, the simulations from the posterior match the observed breakthrough curves well (Fig. 4.23). Note that our adaptive sampling method requires fewer (original) model evaluations, and thus less computational cost, for case 2 than for case 1. This is because the added observations in case 2 restrict the posterior distribution within a much smaller region, in which the refinement of the GP-based surrogate is much easier.

We further test our algorithm with a more challenging case (Case 3, Table 4.1) , in which we infer all 8 uncertain parameters with uniform prior distributions from the breakthrough curves observed at 6 wells. Comparing with cases 1 and 2, the parameter space to be explored in Case 3 is much larger because of an increased number of uncertain parameters. A posterior sample is obtained using a GP surrogate based on 40 initial and 48 refinement base points. The simulation results from prior and posterior samples are shown in Fig. 4.25. As a result of more uncertain parameters, the prior results reveal a greater variability. Nevertheless, the posterior given by our algorithm achieves a good match to the observations. Fig. 4.24 presents the (posterior) histograms of the parameters. We see that the reference values of all parameters are correctly incorporated within the posterior distributions. However, significant parameter uncertainty remains, showing that different combinations of the input parameters may all yield the observed breakthrough curves.

Note that for this simple solute transport problem, we actually have an analytic solu-
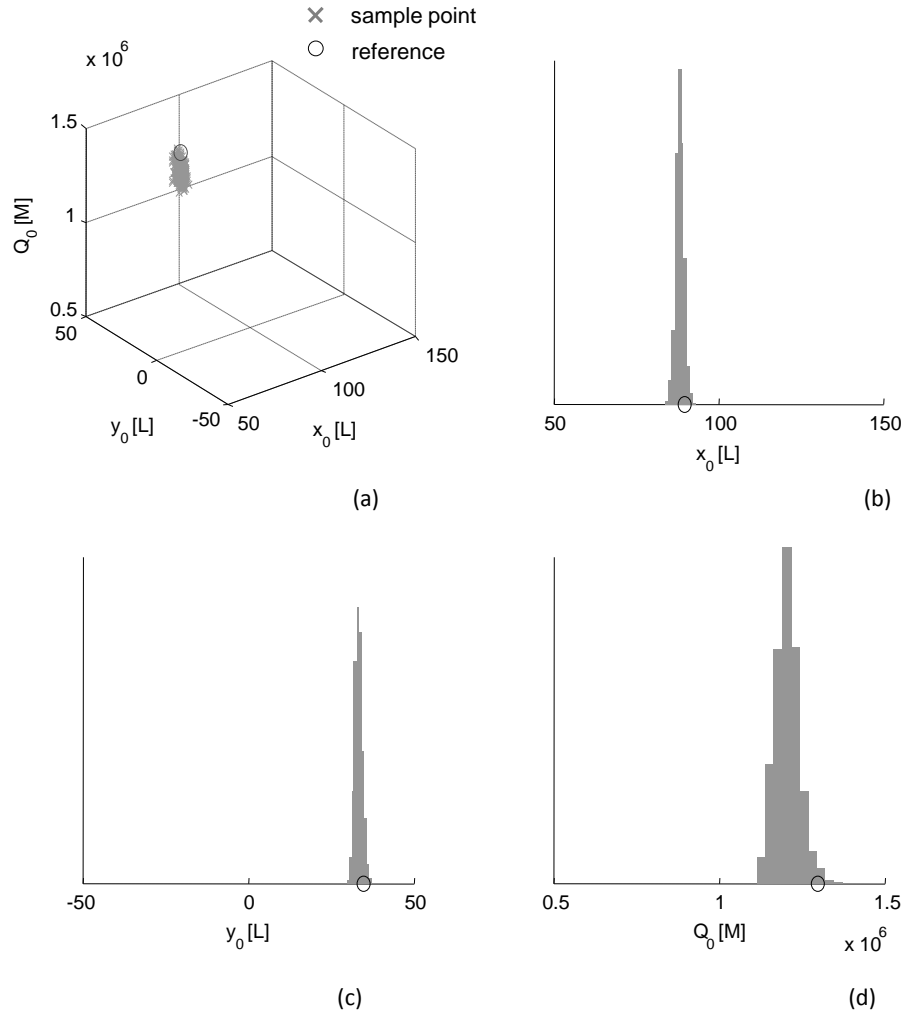
Figure 4.22: Estimated posterior distribution (Case 2, Problem 5); (a) posterior sample points; (b-d) posterior histograms for each uncertain parameter.
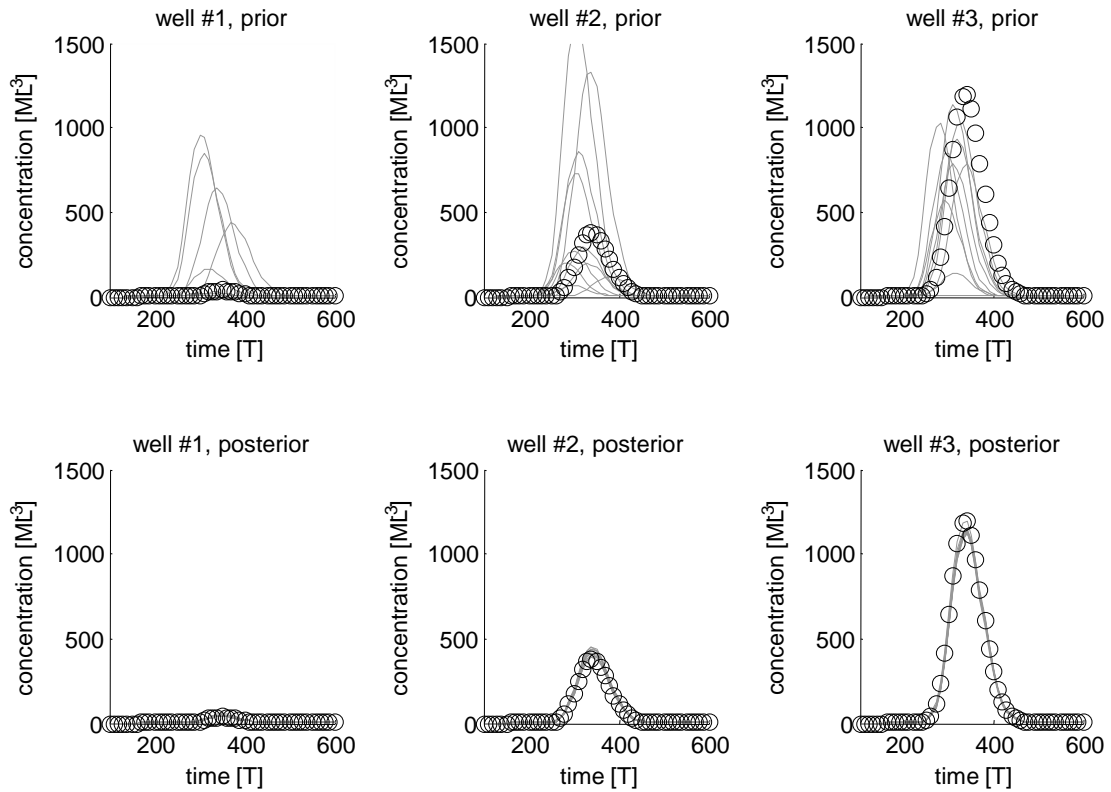
Figure 4.23: Concentration breakthrough curves at wells *obs1, obs2, obs3*, simulated using prior and posterior sample points (Case 2, Problem 5).
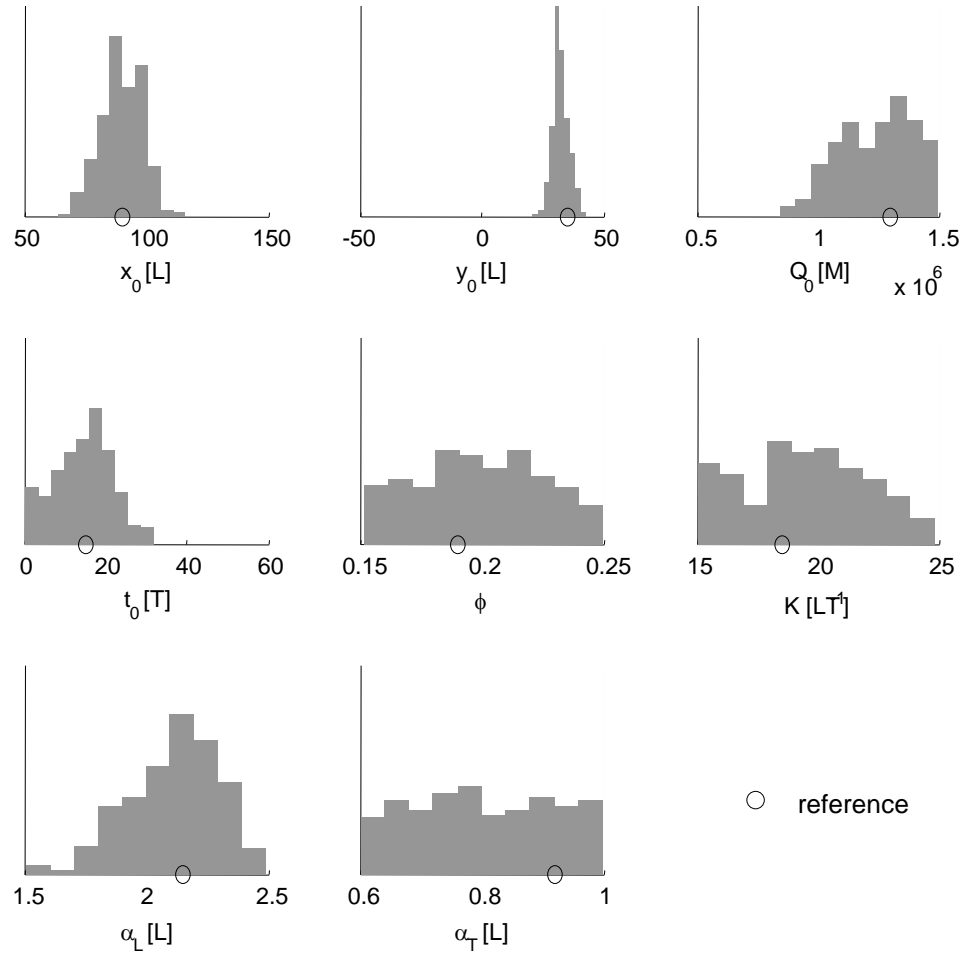
Figure 4.24: Estimated posterior histograms for each uncertain parameter (Case 3, Problem 5).
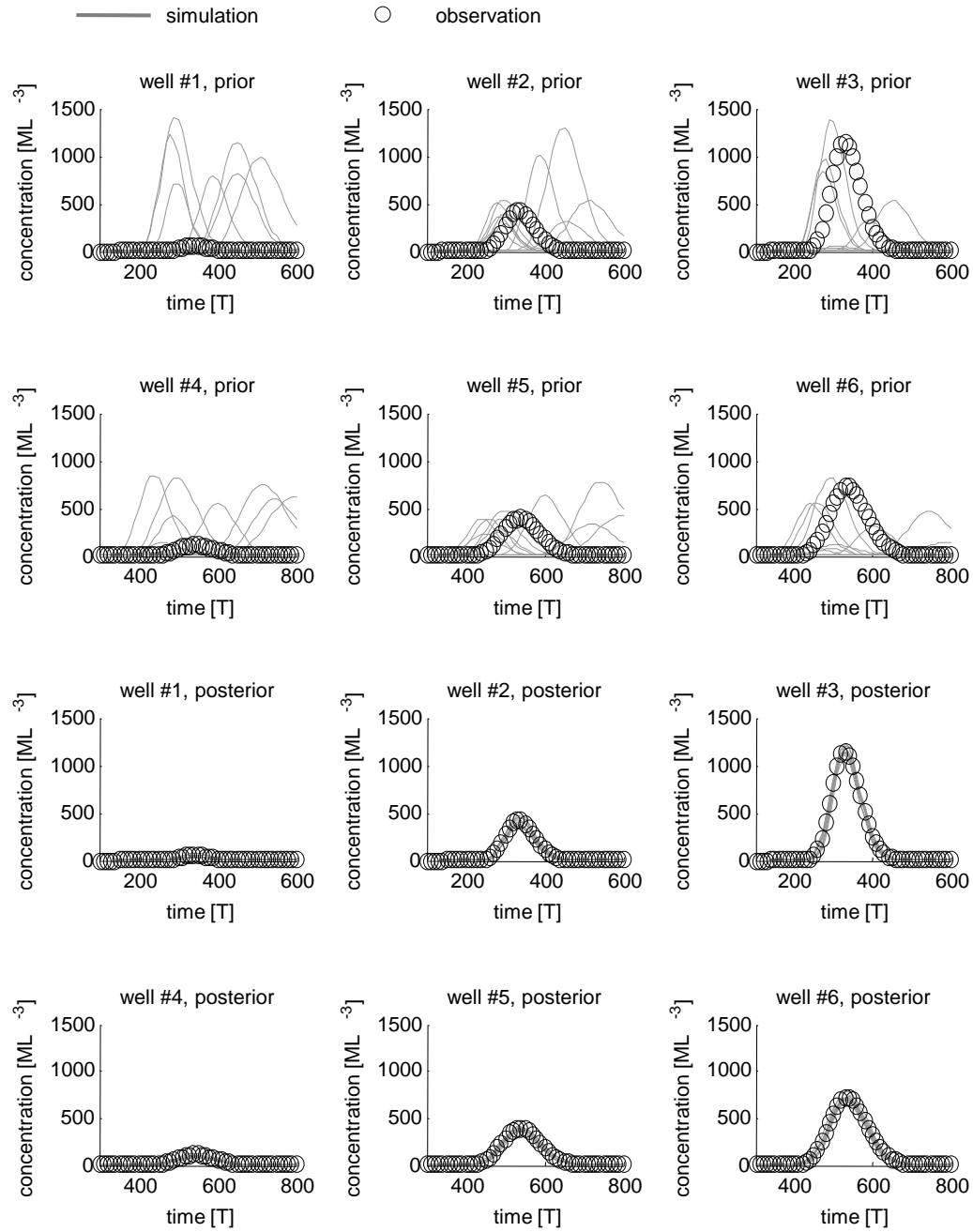
Figure 4.25: Concentration breakthrough curves at wells *obs1-obs6*, simulated using prior and posterior sample points (Case 3, Problem 5).

tion to the forward model. The concentration at any time and location is given by

$$C(x, y, t) = \frac{Q_0}{4\pi(t - t_0)\phi\sqrt{D_L D_T}} \exp\left[-\frac{(x - x_0 - v(t - t_0))^2}{4D_L(t - t_0)} - \frac{(y - y_0)^2}{4D_T(t - t_0)}\right]. \quad (4.15)$$

The analytic solution makes it plausible to sample without using a surrogate. To verify the accuracy of our algorithm, we solve Case 3 again by applying the importance sampling with a large number (10^5) of evaluations of the true model. The estimated posterior histograms of every uncertain parameter are shown in Fig. 4.26. From the comparison between Fig. 4.24 and Fig. 4.26, we see that the results obtained via the GP-based surrogate are really close to that obtained using the true model.
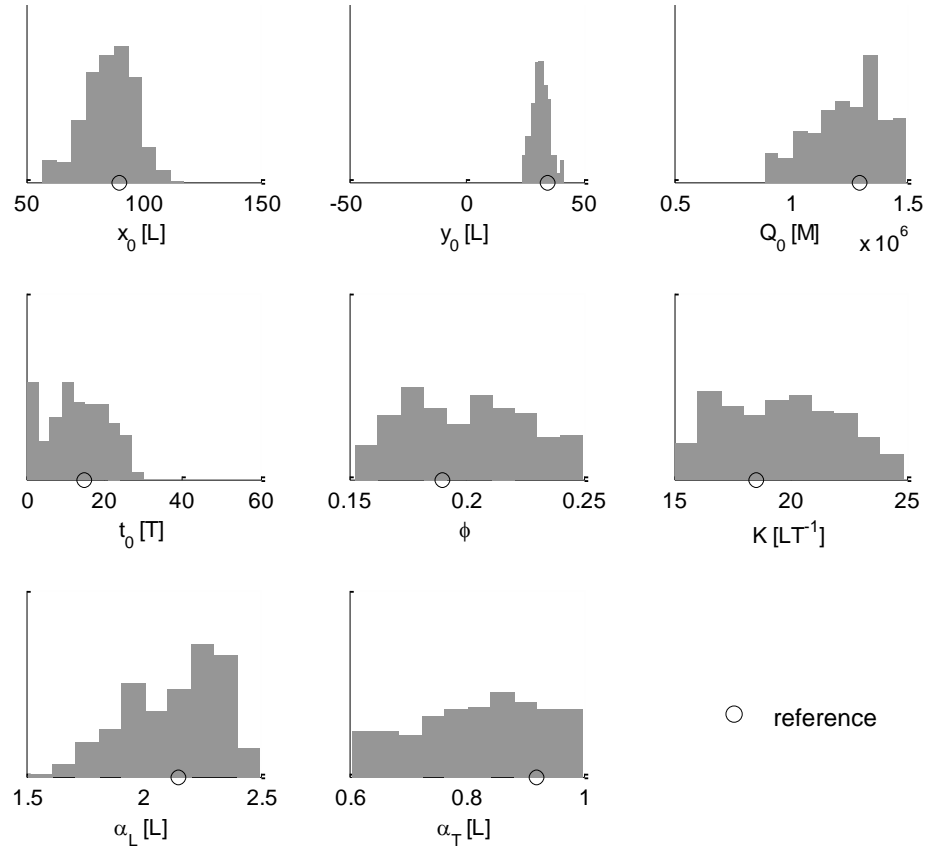
Figure 4.26: Posterior histograms for each uncertain parameter estimated by sampling via the true model (Case 3, Problem 5).

4.5 Discussions

In this chapter we present an adaptive sampling algorithm for general nonlinear inverse modeling and UQ problems. The four major ingredients of this algorithm are: 1) a GP surrogate for simulation acceleration; 2) an adjustment of the posterior according to the estimated surrogate error, which consistently reflects the uncertainty associated with the unknown true model response; an importance sampler using Gaussian mixture proposal distribution, which tackles the issue of sample deficiency; 4) an adaptive refinement scheme, which keeps the number of (original) model evaluations at a minimum level. In the illustrative examples, the algorithm demonstrates its capability to handle strongly nonlinear models and accurately capture the multi-modal posterior distribution with a relatively low computational cost.

Chapter 5

Conclusion, Discussions, and Future Work

5.1 Conclusion

By assimilating observed data from the real world, inverse modeling is a critical technique to estimate uncertain model parameters and to improve the fidelity of simulations and predictions. Often the inverse modeling problems are ill-posed and have non-unique solutions. Although capturing non-unique solutions (probabilistic inversion) is much more challenging than finding a single best match (deterministic inversion), it allows quantifying the remaining uncertainty and yields more reliable predictions.

This study has developed two new inversion algorithms, i.e., the "adaptive ANOVA-

based PCKF" and "adaptive sampling via GP-based surrogates", and applied them to different flow in porous media problems. The values of the new approaches are: 1) both approaches quantify the remaining uncertainty by incorporating different possible parameter points in the solutions; 2) each approach results in a significant efficiency improvement comparing with the related existing inversion methods; 3) both approaches apply to nonlinear models, although they deal with different levels of complexity. The former method works for mildly nonlinear models with approximately Gaussian posterior distributions, whereas the latter is able to catch complex non-Gaussian, multi-modal posterior resulted from strong nonlinearity.

5.2 Discussions

Some more points are discussed below:

1) The inversion approaches presented here are not limited to flow in porous media models and may be applied to inverse modeling and UQ problems in other fields.

2) An automatic and universally optimal inversion approach is impossible. We need our intuition and understanding of the system being studied to choose the proper approach. For example, knowing the properties about the true model response (nonlinearity, continuity, etc.) could help us select an appropriate surrogate model.

3) The presented inversion approaches have limitations in handling extremely nonlinear or high dimensional models, as well as models with fundamental modeling errors.

Both extreme nonlinearity and high input dimensionality make the input-output relationship difficult and costly to detect and to approximate. Also, a severe modeling error associated with the (original) forward model, such as an unrecognized geological structure, would result in a posterior distribution far from the reality.

5.3 Future work

In the future, this research work can be furthered along the following directions:

1) Input dimension reduction by inverse regression. Besides the dimension reduction procedures previously used in inverse modeling, a technique that has been successfully implemented in many other applications is the sliced inverse regression (Li, 1991). This method reduces the input dimension based on a nonlinear "inverse regression" of the input variables against the output variables. It takes advantage of the fact that in many problems the "true input dimension" is much lower than the actual number of input parameters, because some parameters have little individual or combining effect on the observable output variable and hence may be excluded from inverse modeling. A potential research topic would be the combination of this method with the developed inversion approaches.

2) Different types of surrogate models other than GPs. A critical step in the adaptive sampling approach is the construction of a surrogate model. Any surrogate model may fit in this role, though it has to provide a practical means of error estimation. The selection of the surrogate depends on the specific model being studied. A proper choice is expected to balance the needs for accuracy and efficiency. It is worth devoting more research work on

studying and testing different types of statistically and physically based surrogate models.

3) Software tools development. User friendly software tools implementing the presented inversion approaches are expected to be developed and made available to related research communities. So these methods can be easily applied to and tested with different problems.

Nomenclature

α power parameter characterizing the covariance function of a Gaussian process

$\boldsymbol{\beta}$ vector of regression coefficients

$\boldsymbol{\mu}$ mean/expectation

$\boldsymbol{\theta}$ anchor point

$\boldsymbol{\xi}$ vector of random variables with know pdfs, used for PCE representation

$\delta(\cdot)$ Dirac-delta function

δ_{ij} Kronecker delta function

ϵ threshold for 2nd-order active dimension selection

η correlation length characterizing the covariance function of a Gaussian process

γ acceptance probability in M-H sampling algorithm

λ_i the ith eigenvalue

$\mathbb{R}$ set of real numbers

$\mathbf{C}$ covariance matrix

$\mathbf{c}_i$ deterministic coefficient of the ith PCE term

$\mathbf{d}^*$ observed values output variables

$\mathbf{D}$ matrix with columns being the principal components of $\mathbf{d}$

$\mathbf{d}$ vector of observable output variables

$\mathbf{e}_g$ modeling error

$\mathbf{e}_o$ observation error

$\mathbf{G}$ transformation matrix mapping input parameters to output variables when model $g(\cdot)$ is linear

$\mathbf{K}$ Kalman gain

$\mathbf{m}$ vector of model parameters

$\mathbf{m}_i$ the ith eigenvector of $\mathbf{m}$

ψ_i basis function of the ith PCE term

ρ_i coefficients of the principal components of $\mathbf{d}$

σ^2 variance

τ temperature

$\tilde{\mathbf{K}}$ modified gain used in EnSRF

$\tilde{g}(\cdot)$ surrogate of forward model $g(\cdot)$

A set of active dimensions

B set of base points for building a GP surrogate

$C(\cdot, \cdot)$ covariance function of a Gaussian process

$d\pi(\boldsymbol{\xi})$ integration measure of $\boldsymbol{\xi}$

e total error, sum of observation and modeling errors

$E(\cdot)$ expectation operator

Err error caused by the truncation of ANOVA components

$f(\cdot)$ function mapping random vector $\boldsymbol{\xi}$ to model output $\mathbf{d}$

f_e pdf of error

G Gaussian process as a surrogate of $g(\cdot)$

$g(\cdot)$ original forward model that simulates observable output variables from input parameters

h normalizing constant in Bayes' rule

k maximum polynomial degree in a PCE representation

N	normal/Gaussian distribution
n_ψ	number of perturbation terms in PCE, total number of PCE terms is $n_\psi + 1$
n_A	number of ANOVA components
n_B	number of initial base points for building a GP surrogate
n_e	number of realizations in an ensemble
n_m	number of uncertain input parameters
n_P	number of principal components
n_S	number of sample points
n_ξ	number of random variables used in a PCE representation
p	probability density function
q	proposal distribution
S_i	sample set in the ith re-sampling and refinement loop
T	transpose of a vector/matrix
U	uniform distribution
u	uniform random variable
w_i	weights

Abbreviations

ANOVA analysis of variance. 27, 28, 35, 41, 50, 68

BHP bottom hole pressure. 82

EGO efficient global optimization. 33

EKF extended Kalman filter. 24, 44

EnKF ensemble Kalman filter. 24–26, 28, 45–49

EnSRF ensemble square root filter. 46

GP Gaussian process. 15, 16, 32–35, 92, 93, 101, 131, 132, 135, 140, 142, 144, 145

KLE Karhunen-Loève expansion. 63

MCMC Markov chain Monte Carlo. 29, 93–96

OPR oil production rate. 82

PCA principal component analysis. 63, 68

PCE polynomial chaos expansion. 15, 25–28, 30, 35, 47–50

PCKF probabilistic collocation Kalman filter. 15, 26, 27, 35, 41, 47–50, 144

PCM probabilistic collocation method. 26

UQ uncertainty quantification. 15, 18, 24, 26, 27, 35, 36, 50, 142, 144

WPR water production rate. 82

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