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Gaussian functional regression for linear partial differential equations

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Abstract

In this paper, we present a new statistical approach to the problem of incorporating experimental observations into a mathematical model described by linear partial differential equations (PDEs) to improve the prediction of the state of a physical system. We augment the linear PDE with a functional that accounts for the uncertainty in the mathematical model and is modeled as a *Gaussian process*. This gives rise to a stochastic PDE which is characterized by the Gaussian functional. We develop a *Gaussian functional regression* method to determine the posterior mean and covariance of the Gaussian functional, thereby solving the stochastic PDE to obtain the posterior distribution for our prediction of the physical state. Our method has the following features which distinguish itself from other regression methods. First, it incorporates both the mathematical model and the observations into the regression procedure. Second, it can handle the observations given in the form of linear functionals of the field variable. Third, the method is non-parametric in the sense that it provides a systematic way to optimally determine the prior covariance operator of the Gaussian functional based on the observations. Fourth, it provides the posterior distribution quantifying the magnitude of uncertainty in our prediction of the physical state. We present numerical results to illustrate these features of the method and compare its performance to that of the standard Gaussian process regression.

Keywords: Gaussian functionals; Gaussian processes; Regression analysis; Bayesian inference; Data assimilation; Linear PDEs

1. Introduction

Partial differential equations (PDEs) are used to mathematically model a wide variety of physical phenomena such as heat transfer, fluid flows, electromagnetism, and structural deformations. A PDE model of a physical system is typically described by conservation laws, constitutive laws, material properties, boundary conditions, boundary data, and geometry. In practical applications, the mathematical model described by the PDEs is only an approximation to the real physical system due to (i) the deliberate simplification of the mathematical model to keep it tractable (by ignoring certain physics or certain boundary conditions that pose computational difficulties), and (ii) the uncertainty

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of the available data (by using geometry, material property and boundary data that are not exactly the same as those of the physical system). We refer to the PDE model (available to us) as the *best knowledge PDE model* [1] and to its solution as the *best knowledge state*. To assess the accuracy of the best knowledge model in predicting the physical system, the best knowledge state needs to be compared against experimental data, which typically will have some level of noise.

In cases where the discrepancy between the PDE model and the experimental data is beyond an acceptable level of accuracy, we need to improve the current PDE model. There are several approaches to defining a new improved model. *Parameter estimation* [2,3] involves calibrating some parameters in the model to match the data. An alternative approach to obtain an improved model is *data assimilation* [4–8]. Broadly speaking, data assimilation is a numerical procedure by which we incorporate observations into a mathematical model to reflect the errors inherent in our mathematical modeling of the physical system. Although data assimilation shares the same objective as parameter estimation, it differs from the latter in methodology. More specifically, data assimilation does not assume any parameters to be calibrated; instead, data assimilation defines a new model that matches the observations as well as possible, while being as close as possible to the best knowledge model. Another approach is *data interpolation* [9–14] which involves computing a collection of solutions (snapshots) of a parametrized or time-varying mathematical model and reconstructing the physical state by fitting the experimental data to the snapshots.

A widely used technique for obtaining an improved model in parameter estimation and data assimilation is *least squares regression* [15,5,16]. Least squares is a deterministic regression approach that provides an estimate for the physical state which is optimal in least squares sense. However, it does not provide a means to quantify the prediction uncertainty. A recent work [1] poses the least-square regression as a regularized saddle point Galerkin formulation which admits interpretation from a variational framework and permits its extension to *Petrov–Galerkin formulation*. While the Petrov–Galerkin formulation provides more flexibility than the Galerkin formulation, it does not quantify the uncertainty in the prediction either. A popular statistical approach in parameter estimation and data assimilation is *Bayesian inference* [17–20]. In Bayesian inference an estimate of the physical state is described by random variables and the posterior probability distribution of the estimate is determined by the data according to Bayes' rule [18,19]. Therefore, Bayesian inference provides a powerful framework to quantify the prediction uncertainties.

In this paper, we introduce a new statistical approach to the problem of incorporating observations into the best knowledge model to predict the state of a physical system. Our approach has its root in Gaussian process (GP) regression [21–23]. We augment the linear PDE with a functional that accounts for the uncertainty in the mathematical model and is modeled as a *Gaussian process*.[1] This gives rise to a stochastic PDE whose solutions are characterized by the Gaussian functional. By extending the standard GP regression for *functions of vectors* to *functionals of functions*, we develop a *Gaussian functional regression* method to determine the posterior distribution of the Gaussian functional, thereby solving the stochastic PDE for our prediction of the physical state. Our method is devised as follows. We first derive a *functional regression problem* by making use of the adjoint states and the observations. We next solve the functional regression problem by an application of the principle of Gaussian processes to obtain the posterior mean and covariance of the Gaussian functional. Finally, we compute the posterior distribution for our estimate of the physical state. A crucial ingredient in our method is the *covariance operator* representing the *prior* of the Gaussian functional. The bilinear covariance operators considered incorporate a number of free parameters (the so-called *hyperparameters*) that can be optimally determined from the measured data by maximizing a marginal likelihood.

Our Gaussian functional regression method can be viewed as a generalization of the standard GP regression from a finite dimensional vector (input) space to an infinite dimensional function (input) space. GP regression is a well-established technique to construct maps between inputs and outputs based on a set of sample, or training, input and output pairs, but does not offer a direct method to incorporate prior knowledge, albeit approximate, from an existing model relating the inputs and outputs. By combining the best knowledge model with the data, our method can greatly improve the prediction of the physical system.

Furthermore, we introduce a *nonparametric Bayesian inference* method for linear functional regression with Gaussian noise. It turns out that nonparametric Bayesian inference and Gaussian functional regression represent two different views of the same procedure. Specifically, we can think of Gaussian functional regression as defining a

[1] In the cases considered, the physical system is not stochastic but deterministic. The introduction of the Gaussian functional serves to represent uncertainties in the best knowledge model and in the data, *not* in the physical system *per se*.