Explicit Estimation of Derivatives from Data and Differential Equations by Gaussian Process Regression

Hongqiao Wang‡ and Xiang Zhou §

‡School of Mathematics and Statistics
Central South University
Changsha 410083, P.R. China

§School of Data Science and Department of Mathematics
City University of Hong Kong
Kowloon, Hong Kong SAR

Abstract

In this work, we employ the Bayesian inference framework to solve the problem of estimating the solution and particularly, its derivatives, which satisfy a known differential equation, from the given noisy and scarce observations of the solution data only. To address the key issue of accuracy and robustness of derivative estimation, we use the Gaussian processes to jointly model the solution, the derivatives, and the differential equation. By regarding the linear differential equation as a linear constraint, a Gaussian process regression with constraint method (GPRC) is developed to improve the accuracy of prediction of derivatives. For nonlinear differential equations, we propose a Picard-iteration-like approximation of linearization around the Gaussian process obtained only from data so that our GPRC can be still iteratively applicable. Besides, a product of experts method is applied to ensure the initial or boundary condition is considered to further enhance the prediction accuracy of the derivatives. We present several numerical results to illustrate the advantages of our new method in comparison to the standard data-driven Gaussian process regression.

Keywords: Gaussian process, Bayesian inference, Inverse problems

1 Introduction

Differential equations (DEs) which include ordinary differential equation (ODE) and partial differential equation (PDE) are used to model a wide variety of physical phenomena such as heat transfer, electromagnetism, and structural deformations. In physics or chemistry problems, the state, which is the solution of the model, and its derivatives (time derivative or spatial gradient) usually have specific meanings, e.g., location and velocity in
Newton mechanics, electric potential and electric field in electrostatics. In ODE models, often the time derivative of a state variable is of as much interest as the state variable itself [18]. Many physical constitutive laws appear in form of PDEs linking the derivatives to the state variable. In the deterministic PDE, the derivatives are generally computed by numerical differentiation techniques after the solution is computed from numerical methods like finite element method, for instance. In general, the convergence order of errors for such derivatives is one order lower than the convergence rate for the solution itself. In history, this accuracy degradation problem for the gradient is alleviated to certain extent by the mixed finite element method (2), which treats the gradient as an independent variable and constructed an extended system jointly for the solution and its gradient. However, when the PDE models have random or missing parameters/coefficients, the estimate of the solution and the derivatives of the solution becomes a non-trivial task because the numerical solution is typically a random function with uncertainties inherited from the randomness of the PDE or the noisy measurement. Various numerical experiments suggest that a direct numerical difference scheme for the derivative for a random function usually lacks of robustness and the higher order the derivatives, the less accuracy of the estimation.

Our interests of estimating the state function and its derivatives are mainly motivated by the works on data-driven approach to identify or discover the missing information of a DE model, with the available noisy measurement of the state variable only. The missing information can be either a few unknown parameters [8,14,19,20] or even a non-parametric form of all possible terms in a PDE model [3,11,13,15]. In these “inverse” problems, the noisy measurements of the solution are given at randomly drawn or deliberately chosen points and various optimization frameworks are proposed to identify the missing information in the DE. In these optimization problems, the state variables and its all derivatives appearing in the DEs are required as the input information, even though there is no measurement data for the derivatives. For example, to estimate the missing parameters in DE models, a two-stage procedure was proposed (8,10,19), which in the first stage estimates the function and its derivatives from noisy observations using data smoothing methods without considering differential equation models, and then in the second stage estimates of the parameters are obtained by the method of least squares. Many data smoothing methods are applicable in the first stage, such as polynomial interpolation [15], local polynomial regression [8] and spline-based approach [19]. These methods are easy to implement, but the main drawback of the two-stage method is that the underlying differential equation is not utilized at all. In [20] X. Xun et al proposed to incorporate the differential equation as a penalty term in the first stage, where the solution is expressed by B-spline basis functions and the derivatives are based on analytical derivatives of B-splines. This improves the accuracy of estimating parameters, particularly for the parameters associated with derivatives. However, this approach of treating differential equation as a squared penalty gives rise to a difficult optimization problem. The Bayesian approach based on the same idea is even challenging in computation due to the Markov chain Monte Carlo step [20].

Here our aim is for the step of robust estimation of derivatives in the context of differential equations when some measurement data of the state function is given. We propose a new statistical approach based on Gaussian process regression (GPR) to efficiently and robustly predict the derivatives appearing in the differential equations. Compared with
basis-function expansion method and MCMC Bayesian approach, the Gaussian process (GP) models [17] provide a class of flexible and efficient non-parametric fits both for fitting noisy data and solving noisy DEs. The prior knowledge can also be easily encoded by the covariance of the GP. To achieve our goal, we build our method as an extension of some ideas which has been explored in other contexts and applications. Firstly, we treat the state variable and the derivatives appearing in the differential equation jointly as a multi-dimensional GP to leverage the advantage that GP specifies a jointly Gaussian distribution over the function and its derivatives [17]. Secondly, to take account of the differential equation that state and derivatives satisfy, the fact that the residual of the differential operator should be zero is exploited as well as the data of the state variable in order to derive the posterior distributions. This constraint of zero residual is particularly convenient if the differential operator/equation is linear. To generalize our method to non-linear equations, we consider a Picard approximation of linearization in which some non-linear coefficient are approximated by the standard GPR first without using the equation, and the multi-dimensional GP is then updated by the linearized equation. In addition, the linear boundary/initial condition (BC/IC) is also added as one of linear constraints. The product of experts method [1, 4, 9] is used for the boundary and initial conditions (BC/IC) processing. Our method can be applied to the parameter identification problems but it certainly fits in any application which needs a robust scheme of derivative estimation when extra information of differential equation models is available.

In the following part of this section, we review some related works selectively. For the use of GP to solve differential equations, there has been a considerable amount of literature. For example, [7] has used GPs to solve linear differential equations with noisy forcing terms. The use of GPR for inference related to differential equation is intensively studied in the communities of machine learning [1, 16] and statistics [8, 20]. For the idea of exploring the GP for the state function and the state-derivatives jointly rather separately, [4] focused on a Bayesian inference of the parameters in ODE models. [6] used the GP prior in Bayesian method to infer parameters in the ODE models of chemical networks. For recent applications of machine learning techniques to parameter identification, [3, 15] worked on the PDE “discovery” problem by $\ell_0$ or $\ell_1$ optimization to learn the sparsity of a sequence coefficients in PDE. [11, 13] worked with the scarce and noisy measurement of both the state variable and a black-box forcing term in the PDE and the joint GPR model is applied to solve the solution function and infer the forcing-term function. But in existing literature, we have not yet seen a specific method for efficiently and robustly processing the derivative estimation if the differential equation is also given.

The structure of the paper is organized as follows: We first review the problem setup in Section 2. Our Bayesian method for estimating the state and its derivatives is presented in Section 3. A product of experts method for initial or boundary conditions is introduced in Section 4. Numerical examples are presented in Section 5 to demonstrate the effectiveness of the proposed method and the potential extension in nonlinear differential equation problem. Finally, Section 6 offers some closing remarks.
2 Problem setup

In general we formulate the differential equation system as a multidimensional dy-
namic process and view the ordinary differential equation as a one-dimension partial
equation case. The solution function is denoted as \( u(x) \), where \( x = (x_1, \ldots, x_D)^T \in \mathbb{R}^D \).

The PDE is modeled as

\[
\mathcal{F}(x, u, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_p}, \ldots, \frac{\partial^2 u}{\partial x_i \partial x_j}, \ldots) = 0, \tag{2.1}
\]

where the left-hand side of Eq. (2.1) consists of the state \( u(x) \) and its partial derivative
terms \( \left( \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_i \partial x_j}, \ldots \right) \). In practice, we only can directly observe the noisy observation
\( y(x) \) instead the state \( u(x) \).

We assume that \( u(x) \) is observed with measurement error and
specifically, the noisy measurements satisfy

\[
y_i = u(x_i) + \epsilon_i, \tag{2.2}
\]

where \( i = 1, \ldots, n \), is the observation index, each point \( x_i \in \mathbb{R}^D \) and \( \epsilon_i \) is the measurement
error, also called noisy/observation error. Assumption is made that the error \( \epsilon_i \) is an iid
random variable and follows a Gaussian distribution with mean 0 and variance \( \sigma^2_u \).

Our objective is to explicitly estimate the state \( u \) and its derivative terms \( \frac{\partial^k u}{\partial x_i \partial x_j}, \ldots \) from the noisy data \((x_i, y(x_i))\) with the equation (2.1), and
to quantify the uncertainty of our estimations. The estimation problem in linear dynamic
process where \( \mathcal{F} \) in (2.1) is a linear operator is more fundamental and has been serving
as the very start of nonlinear equations [7, 13, 16]. To discuss the linear equation case
first, we use \( \mathcal{L}u(x) \) to denote \( \mathcal{F}(x, u, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial^2 u}{\partial x_i \partial x_j}, \ldots) \) as a function of \( x \) if \( \mathcal{F} \) is a linear
operator.

3 Methodology

The proposed data-driven algorithm for estimating the state and its derivatives, em-

dploys Gaussian process prior that is tailored to the corresponding differential operators.

3.1 Gaussian process regression

Specifically, the method starts by assuming that \( u(x) \) is Gaussian process with the zero
mean and the covariance function \( k_{uu}(x, x'; \gamma) \), which is denoted as

\[
u(x) \sim \mathcal{GP}(0, k_{uu}(x, x'; \gamma)), \tag{3.1}
\]

where \( \gamma \) denotes the hyper-parameters of the kernel function \( k_{uu} \). This means that \( \mathbb{E}[u(x)] \equiv 0 \) and \( \text{Cov}(u(x), u(x')) = k_{uu}(x, x'; \gamma) \). The kernel \( k_{uu} \) allows us to encode any prior knowl-
edge we may have about \( u(x) \), and can accommodate the approximation of arbitrarily
complex functions. The choice of the specific form of \( k_{uu} \) will be discussed later.

The key property of Gaussian process in our favor is that any linear transformation,
such as differentiation and integration, of a Gaussian process is still a Gaussian process.
With the assumption (3.1), we consider the linear differential operator, \(L\), acted on \(u(x)\). Then the function \(Lu(x)\) is also a mean-zero Gaussian process

\[
Lu(x) \sim \mathcal{GP}(0, k_{LL}(x, x'))
\]

(3.2)

where \(k_{LL}(x, x') = \text{Cov}(Lu(x), Lu(x'))\) denotes the covariance function of \(Lu\) between at point \(x\) and at point \(x'\). The following fundamental relationship between the kernels \(k_{uu}\) and \(k_{LL}\) is well-known (see e.g. [7, 17]),

\[
k_{LL}(x, x'; \gamma) = L_x L_{x'} k_{uu}(x, x'; \gamma).
\]

(3.3)

Here we add the subindex in the linear differential operator \(L\) to specify the differentiation is for \(x\) or \(x'\) variable in the kernel function. \(k_{uu}\) and \(k_{LL}\) share the same hyper-parameter \(\gamma\). Similarly, for the covariance between \(u\) and \(Lu\), \(k_{ul}(x, x') = \text{Cov}(u(x), Lu(x'))\) and \(k_{lu}(x, x') = \text{Cov}(Lu(x)u(x'))\), we have

\[
k_{ul}(x, x'; \gamma) = L_x k_{uu}(x, x'; \gamma), \quad \text{and} \quad k_{lu}(x, x'; \gamma) = L_x k_{uu}(x, x'; \gamma).
\]

(3.4)

Since we shall work on the differential equation \(Lu(x) = 0\), we introduce a random function \(r(x)\) as the residual of the linear differential equation \(Lu = 0\) for convenience:

\[
r(x) := Lu(x).
\]

(3.5)

We refer the original equation as the *equation constraint*, \(r(x) = 0\), and the equation will be interpreted later as the observation of zero values of the function \(r(x)\) at any point \(x\), in a similar way to the observation \(y_i\) of \(u(x)\) at \(x_i\). With the given prior of the GP \(u(x)\), we then have the the prior for the pair \((u(x), r(x))\). The covariances above for \(u\) and \(Lu\) can be rewritten as

\[
\begin{align*}
k_{rr}(x, x'; \gamma) &= L_x L_{x'} k_{uu}(x, x'; \gamma), \\
k_{ur}(x, x'; \gamma) &= L_x k_{uu}(x, x'; \gamma), \\
k_{ru}(x, x'; \gamma) &= L_x k_{uu}(x, x'; \gamma).
\end{align*}
\]

(3.6)

respectively.

So the equation residual \(r(x)\) is also a Gaussian process, whose kernel is related to the derivatives of the kernel of \(u(x)\). Based on the Gaussian assumption and the covariance expression between \(u\) and \(r\) in (3.6), a joint inference framework of Gaussian process regression for the available observation data of \(u\) and \(r\) can be naturally constructed. By interpreting the equation \(r = Lu = 0\) as the constraint of the function \(r\), we refer this approach as *Gaussian Process Regression with Constraint* (GPRC). GPRC will significantly improve the accuracy of estimation of solution and its derivatives due to the additional equation information. The advantages in the comparison with standard Gaussian process regression (without constraint) will be shown in Section 5.

**Remark 1.** The linear differential operator can be easily generalized to an *affine* operator, i.e., the equation \(Lu(x) = f(x)\). Then the linear constraint \(r(x) = 0\) should be modified as \(r(x) = f(x)\). To be concise, we present our ideas and methods only for the linear case \(f(x) = 0\).
The differential equation discussed above is the linear constraint, i.e., \( r = L u \) is a linear mapping of \( u \). For the non-linear differential equation \( \mathcal{F}(u) = 0 \), we propose a linearization strategy to make GPRC applicable to nonlinear problems. To illustrate idea, consider a special case \( \mathcal{F}(u) = L(u) + N(u) \) for example, where \( N \) is the nonlinear part. We apply the standard GPR only from the data \( \{x_i, y_i\} \) to train a GP \( u_0 \), and then apply the GPRC to the affine constraint \( \mathcal{F}_0(u) = L(u) + N(u_0) = 0 \) and the data \( \{x_i, y_i\} \) to train \( u \) as an update of \( u_0 \). This approach can be implemented recursively and is a type of Picard iteration per se. In Section 5.3, we also show how to apply this idea for a nonlinear oscillator equation.

### 3.2 Kernel

As we known the kernel (covariance function) is the crucial ingredient in a Gaussian process predictor, as it encodes our assumptions about the function we wish to learn. Without loss of generality, the Gaussian prior of the solution used in this work is assumed to have a squared exponential covariance function (other kinds of kernels are also suitable in this framework), i.e.,

\[
    k_{uu}(x, x', \gamma) = \gamma_o^2 \exp\left(-\frac{1}{2}||x - x'||_\gamma^2\right) \tag{3.7}
\]

where \( \gamma_o^2 \) is a variance parameter, \( x \) is a \( D \)-dimensional vector that includes spatial and/or temporal coordinates, the norm \( || \cdot ||_{\gamma_i} \) is defined as

\[
    ||v||_{\gamma_i} = (v^T \gamma_i v)^{\frac{1}{2}}, \quad \gamma_i = \text{diag}(\gamma_{i1}, \ldots, \gamma_{iD}). \tag{3.8}
\]

\( \gamma_i \) is the length scale parameter and \( \gamma = (\gamma_o, \gamma_i) \). The squared exponential covariance function chosen above implies smooth approximations. More complex function class can be accommodated by appropriately choosing kernels. For example, non-stationary kernels employing nonlinear warpings of the input space can be constructed to capture discontinuous response. In general, the choice of kernels is crucial and in many cases still remains an art that relies on ones ability to encode any prior information (such as known symmetries, invariant, etc.) into the regression scheme. In our problem here related to the differential operator \( L \), we require that the kernel satisfies the regularity such that the derivatives of the kernel, \( L_x L_x k_{uu}(x, x') \), which is the covariance function of \( Lu \), is at least continuous. Our choice of squared exponential covariance function surely satisfies this requirement.

The kernel \( k_{Lu}(x, x'; \gamma) \) can be easily computed based on (3.7). For instance the kernel of first order derivative term \( \partial_x u(x) \) can be expressed as:

\[
    k_{Lu}(x, x'; \gamma) := \frac{\partial k_{uu}(x, x'; \gamma)}{\partial x} = -k_{uu}(x, x', \gamma)\gamma_i(x - x') \tag{3.9}
\]

The expressions of other kernel for a general linear differential operator, such as \( \frac{\partial^2 k_{uu}(x, x'; \gamma)}{\partial x'^2} \), can be computed similarly.

Due to the irreducible measure noise in \( \mathcal{Q}_2 \), the covariance matrix in the prior of \( u(x) \), \( k_{uu} \) usually needs to be added a noise kernel \( \sigma_u^2 I \), \( I \) is identity matrix and the variance parameter of noise \( \sigma_u^2 \) can be optimized with the kernel parameters \( \gamma \) which will be introduced in Section 5.3. In a similar style, we can also introduce a small parameter \( \sigma_r^2 I \), for the residual function \( r(x) \).
3.3 Training

The training process is to find the optimal hyper-parameters \( \gamma \) by maximum likelihood estimation (MLE). Since all GPs appearing above share the same set of hyper-parameters \( \gamma \), this helps reduce computational burden.

Given \( n \) noisy observations of \( u \) and \( r \) at \( n \) points \( \{x_i : 1 \leq i \leq n\} \), we denote the state vector \( y \equiv [y_1, y_2, \ldots, y_n]^T \in \mathbb{R}^{n \times 1} \), the constraint vector \( r \equiv [r_1, r_2, \ldots, r_n]^T \in \mathbb{R}^{n \times 1} \) and the training point matrix \( X \equiv [x_1, x_2, \ldots, x_n]^T \in \mathbb{R}^{n \times D} \). Let \( Y = \begin{bmatrix} y \\ r \end{bmatrix} \in \mathbb{R}^{2n} \). Then the negative log marginal likelihood of \( p(Y|\gamma, \sigma_u^2) \) has the following expression

\[
-\log p(Y|\gamma, \sigma_u^2) = \frac{1}{2} \log(\det K) + \frac{1}{2} Y^T K^{-1} Y + \frac{n}{2} \log 2\pi, \tag{3.10}
\]

where the \( 2n \times 2n \) matrix \( K \) is defined by

\[
K = \begin{bmatrix}
K_{uu} + \sigma_u^2 I & K_{ur} \\
K_{ru} & K_{rr} + \sigma_r^2 I
\end{bmatrix},
\]

The matrices \( K_{uu}, K_{ur}, K_{ru} \) and \( K_{rr} \) correspond to, respectively, the kernel functions \( k_{uu}, k_{ur}, k_{ru} \) and \( k_{rr} \) in (3.7) and (3.6), evaluated at the \( n \) points \( \{x_i\} \). \( \sigma_u^2 \) and \( \sigma_r^2 \) are two parameters which has the contribution to regularization.

To compute the optimal kernel hyperparameters \( \gamma \) and observation noise variance \( \sigma_u^2 \), a Quasi-Newton optimizer L-BFGS is employed to minimize the negative log marginal likelihood (3.10). \( \sigma_u^2 \) is preset as a very small constant. Cholesky factorization of \( K \) is used to compute both the inverse and the determinant.

3.4 Prediction

After the hyper-parameters in the GPR are computed, the prediction of the function \( u(x) \) or its derivatives of interest, denoted as a function \( l(x) \) (e.g., \( l(x) = \partial_x u(x) \)), at a new test point \( x_* \) is described below. The covariance function of the GP \( l(x) \) is denoted by \( k_l(x, x') \) by the convention.

With a given point \( x_* \), the differential equation provides the fact \( r(x_*) = 0 \), which is a useful observation to incorporate the Bayesian inference. To enhance this condition, we actually consider a small neighbourhood around \( x_* \) and choose \( m \) points in this neighbourhood. We refer the collection of these \( m \) points as the extended set \( \chi := \{x^*_j : 1 \leq j \leq m\} \) and by the differential equation, we have the equation constraints in this extend set, i.e., \( r_\chi = 0 \). The best selection of points in the extend set \( \chi \) for each test point \( x_* \) is related to the length scale parameter, the complexity of constraint process’s kernel, the data sparsity and noise level. In practice, just a few number of \( m \) in each dimension is sufficient and we will give some details in Section 5.

Let \( u_* \) and \( l_* \) represent the state and its derivative at the test point \( x_* \), respectively. Adding the equation constraint vector \( r_\chi \) at the points in the extend set \( \chi \), we have the joint distribution for the Gaussian priors

\[
\begin{bmatrix}
y \\ r_\chi \\ u_* \\ l_*
\end{bmatrix} = \mathcal{N}(0, \begin{bmatrix}
K_{uu} & K_{ul} \\
K_{lu} & K_{ll}
\end{bmatrix}), \tag{3.11}
\]
where

\[ \widehat{K}_{ux} = \begin{bmatrix} K_u & K_{ur}^T \\ K_{ur} & K_r \end{bmatrix} \in \mathbb{R}^{(n+m)\times(n+m)}, \]

\[ K_u = K_{uu} + \sigma_u^2 I_u \in \mathbb{R}^{n\times n}, \]

\[ K_{ur} = K_{ur} + \sigma_r^2 I_r \in \mathbb{R}^{n\times m}, \]

other matrices, e.g., \( K_{uu}, K_{ur}, K_{ur,r} \) are defined similarly via the kernels \( k_{uu}, k_{ur}, k_{ur} \). As mentioned above, \( r = L \mathbf{u}(\chi) \) is actually known as a zero vector since the differential equation \( Lu = 0 \) holds everywhere. So, based on the Bayesian formula

\[ p(\mathbf{y}, \mathbf{r}_x) = \frac{p(\cdot, \mathbf{y}, \mathbf{r}_x)}{p(\mathbf{y}, \mathbf{r}_x)}, \]

and the Gaussian process priors assumption of \( p(\cdot, \mathbf{y}, \mathbf{r}_x) \) and \( p(\mathbf{y}, \mathbf{r}_x) \), we can get an explicit estimation \( p(\mathbf{y}, \mathbf{r}_x) \) as below:

\[ p(u(x))|\mathbf{y}, \mathbf{r}_x) = \mathcal{N}(\bar{u}(x), S_u(x)), \]

\[ p(l(x))|\mathbf{y}, \mathbf{r}_x) = \mathcal{N}(\bar{l}(x), S_l(x)), \]

with

\[ \bar{u}(x) = K_{u,\bullet} \widehat{K}_{ux}^{-1} \begin{bmatrix} \mathbf{y} \\ \mathbf{r}_x \end{bmatrix}, \]

\[ S_u(x) = K_{uu}(x, x) - K_{u,\bullet} \widehat{K}_{ux}^{-1} K_{u,\bullet}^T, \]

\[ \bar{l}(x) = K_{l,\bullet} \widehat{K}_{ur}^{-1} \begin{bmatrix} \mathbf{y} \\ \mathbf{r}_x \end{bmatrix}, \]

\[ S_l(x) = K_{ll}(x, x) - K_{l,\bullet} \widehat{K}_{ur}^{-1} K_{l,\bullet}^T, \]

where \( K_{u,\bullet} = [K_{u,uu}, K_{u,ur}] \in \mathbb{R}^{1\times(n+m)} \) and \( K_{l,\bullet} = [K_{l,uu}, K_{l,ur}] \in \mathbb{R}^{1\times(n+m)} \). The posterior variances \( S_u(x) \) and \( S_l(x) \) can be used as good indicators of how confident the predictions are. The above results can be easily generalized to multiple test points and multiple output of different derivates.

Then the estimation of posterior of state \( p(u(x))|\mathbf{y}, \mathbf{r}_x) \) and its derivative \( p(l(x))|\mathbf{y}, \mathbf{r}_x) \) include the data and differential equation information. Furthermore, such built-in quantification of uncertainty encoded in the posterior variances is a direct consequence of the Bayesian approach adopted in this work. Although not pursued here, this information is very useful in designing a data acquisition plan, often referred to as active learning, which can be used to optimally enhance our knowledge about the parametric linear equation under consideration.

## 4 Initial and Boundary Conditions (IC/BC)

The Gaussian process regression method may have a poor prediction near the initial stage or boundary which is caused by imbalance data there. To improve the predictions by a given IC/BC, we employ a Product of Experts method which has been widely used \cite{1,4,9}, to correct the posteriors of state and its derivatives. We define a normal distribution \( p(u|x, IC/BC) \) which contains the IC/BC information, whose mean is the state value at
the point \( x_0 \) (the nearest initial or boundary point to \( x \)) and whose variance increases as \( x \) moves away from \( x_0 \). The notation \( IC/BC \) represents the initial and boundary condition information. The formula of Product of Experts links the statistical models \( p(u,|x, y, r_x) \) in (3.12) and the normal distribution \( p(u,|x, IC/BC) \) by

\[
p(u,|x, y, r_x, IC/BC) \\
\propto p(u,|x, y, r_x) \cdot p(u,|x, IC/BC),
\]

(4.1)

where \( p(u,|x, y, r_x, IC/BC) \) is the posterior both considering the equation constraint and the IC/BC. We propose the following Gaussian assumption for \( p(u,|x, IC/BC) \)

\[
p(u,|x, IC/BC) = N(\tilde{u}_{IC/BC}(x), S_{IC/BC}(x)),
\]

(4.2)

where

\[
\tilde{u}_{IC/BC}(x) = u(x_0), \quad S_{IC/BC}(x) = \exp(||x_0 - x_0||^2_\gamma) - 1.
\]

Here \( x_0 \) is an initial or boundary point closest to \( x \) and \( \gamma \) is the same kernel hyper-parameters as in \( k_{uw} \). Then the posterior distribution \( p(u,|x, y, r_x, IC/BC) \) in (4.1) is also a Gaussian distribution with the density function

\[
p(u,|x, y, r_x, IC/BC) = C_c(x) \cdot p_N(u; u_c(x), S_c(x)),
\]

(4.3)

where \( p_N(\cdot; \mu, \Sigma) \) refers to the probability density function for the Gaussian distribution with mean \( \mu \) and covariance \( \Sigma \), and

\[
C_c(x) = p_N(\tilde{u}; \tilde{u}_{IC/BC}, (S_u + S_{IC/BC})),
\]

\[
u_c(x) = (S_u^{-1} + S_{IC/BC}^{-1}S_u^{-1}\tilde{u} + S_{IC/BC}^{-1}\tilde{u}_{IC/BC}),
\]

\[
S_c(x) = (S_u^{-1} + S_{IC/BC}^{-1})^{-1}.
\]

\( \tilde{u} \) is defined by (3.14) and \( S_u \) is defined by (3.15).

The formulation of (4.1), (4.2) and (4.3) can also be extended to the estimation of derivative terms for satisfying the initial and boundary conditions if we knew the IC/BC of the derivatives in concern from the given differential equation.

5 Numerical examples

5.1 Linear ordinary differential equation

In this example \( u \) is a function of time and \( u, u', u'' \) refer to the state, the first order and second order derivative functions respectively. The linear ODE here is

\[
u''(t) + bu'(t) + cu(t) = 0,
\]

(5.1)

where \( b = 1 \) and \( c = 3 \). The initial condition is given \( u(0) = \pi - 0.1, u'(0) = 0 \), then the second order derivative can be computed directly by (5.1), \( u''(0) = 0.3 - 3\pi \). We assume the prior of the state function \( u \) is a zero-mean Gaussian process expressed in (3.1). As discussed in Section 3 the equation constraint \( r = u'' + bu' + cu \) is also a Gaussian process,
Figure 1: The posterior of the state function $u$. The black triangles represent the 21 observation data. The black solid curve represents the true solution computed by ODE solver. The blue dash-dot/green dotted traces are the inferred posterior means by GPRC and GPR methods, respectively. The confidence bounds of one posterior standard deviation are also shown.

$r \sim \mathcal{GP}(0, k_{rr}(x, x'; \gamma))$. With the property of covariance, the covariance between $r$ and $u$ can be expanded as

$$
\text{Cov}(r, u) = \text{Cov}(u'' + bu' + cu, u) = \text{Cov}(u'', u) + b\text{Cov}(u', u) + c\text{Cov}(u, u).
$$

So, $k_{ru} = k_{u'u} + bk_{u'1} + ck_{u, u}$. Similarly, the kernel functions corresponding to covariances $\text{Cov}(r, u'), \text{Cov}(r, u'')$ and $\text{Cov}(r, r)$ are expressed as

$$
\begin{align*}
    k_{rr} &= k_{u'u'} + b^2 k_{u'1} + c^2 k_{u, u}, \\
    k_{ru} &= k_{u'u} + b k_{u'1} + c k_{u, u}, \\
    k_{ru'} &= k_{u'u'} + b^2 k_{u'1} + 2bk_{u'1} + 2ck_{u, u} + 2bck_{u, u}.
\end{align*}
$$

By Section 3.4, the posterior distributions $p(u, r_y) = \mathcal{N}(m_{u\cdot}, \Sigma_{u\cdot})$, $p(u', r_y) = \mathcal{N}(m_{u'\cdot}, \Sigma_{u'\cdot})$ and $p(u''(y, r_y) = \mathcal{N}(m_{u''\cdot}, \Sigma_{u''\cdot})$ are given below

$$
\begin{align*}
    m_u &= K_{\star u}^T \tilde{\Sigma}_{u\cdot}^{-1} Y, \quad \Sigma_{u\cdot} = K_{u\cdot} - K_{\star u}^T \tilde{\Sigma}_{u\cdot}^{-1} K_{\star u}, \\
    m_{u'} &= K_{\star u}^T \tilde{\Sigma}_{u'\cdot}^{-1} Y, \quad \Sigma_{u'\cdot} = K_{u'\cdot} - K_{\star u}^T \tilde{\Sigma}_{u'\cdot}^{-1} K_{\star u'}, \\
    m_{u''} &= K_{\star u}^T \tilde{\Sigma}_{u''\cdot}^{-1} Y, \quad \Sigma_{u''\cdot} = K_{u''\cdot} - K_{\star u}^T \tilde{\Sigma}_{u''\cdot}^{-1} K_{\star u''},
\end{align*}
$$

where $Y = [y, r_y]^T$. This is the posterior estimation of state and derivative functions without considering initial condition. Then (4.3) is applied for the initial conditions for $u, u'$ and $u''$.

In our experiment, there are 21 observations contaminated by the Gaussian noise with zero-mean and variance $\sigma_u^2 = 0.01$. We set the parameter for the equation constraint $\sigma_r^2 = 0.1$. In the prediction, for each $t$, the extended set $\chi$ is chosen as 20 points equally spaced in its neighbour $[t - 1, t + 1]$. Figure 1 and 2 show the posteriors of the state and its derivatives in comparison between GPRC and GPR methods. The numerical solution from the ODE solver is regarded as the true solution. The results show that the estimations of all three functions from the GPRC method are much closer to the true solution than the
traditional GPRC and demonstrate a great ability to correct the model from the noisy observations with the consideration of equation information. Besides, the GPRC gives a greater extent to the variance reduction of the posteriors estimation since the additional observations from the equation constraint $r$ and $r_x$ are used.

To examine the effectiveness of our method of incorporating the equation, Figure 3 shows the residual function $r(t) = Lu(t)$ where all derivatives in $Lu$ are the mean function of the estimations from GPRC and GPR. We see from this figure that the GPRC with the Product of Experts method in Section 4 show an overall smallness for the residuals. For a quantitative comparison, Table 1 presents the Root Mean Square (RMS) values computed by the posterior mean functions of $u$, $u'$, $u''$ and $r$. This confirms the better accuracy of GPRC method. In addition, we tested two difference choices of $\sigma_r^2$ in GPRC method in this table. The slack parameter $\sigma_r^2$ is used as a regularization matrix $\sigma_r^2 I_r$ for the covariance matrix $K_r$ of the residual $r$. Although the equation constraint is strict, the performance of GPRC is actually worse if $\sigma_r^2$ is too small, probably due to the intrinsic noise in the observation data of $u$. In practice, the use of a non-zero $\sigma_r^2$ is a beneficial regularization technique.

Figure 3: The constraint value computed with posterior means by GPR (green dotted line) and GPRC (blue dash-dot line) method respectively.
Table 1: RMS of the posterior mean of state, first derivative, second derivative and constraint computed by GPR and GPRC respectively.

|        | \(u\) | \(u'\) | \(u''\) | \(r\) |
|--------|-------|-------|--------|------|
| GPR    | 0.36  | 0.93  | 3.32   | 2.09 |
| GPRC(\(\sigma_r^2 = 1e^{-3}\)) | 0.28  | 0.39  | 0.75   | 0.69 |
| GPRC(\(\sigma_r^2 = 1e^{-1}\)) | 0.15  | 0.20  | 0.44   | 0.38 |

5.2 Poisson equation

Poisson equation describes the spatial variation of a potential function for given source terms and have important applications in electrostatics and fluid dynamics. Our setting of Poisson equation is as follows

\[
\nabla^2 u(x) = g(x),
\]

\[
g(x) = \exp(-x_1)(x_1 - 2 + x_2^3 + 6x_2),
\]

with Dirichlet boundary conditions

\[
u(0, x_2) = x_2^3,
\]

\[
u(1, x_2) = (1 + x_2^3)\exp(-1),
\]

\[
u(x_1, 0) = x_1 \exp(-x_1),
\]

\[
u(x_1, 1) = (x_1 + 1) \exp(-x_1),
\]

and the domain is \([0, 1] \times [0, 1]\). The analytic solution is

\[
u(x) = \exp(-x_1)(x_1 + x_2^3).
\]

This PDE corresponds to the constraint \(r := \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} = g\). Assume the state is a Gaussian process as (3.1), and then the constraint is also a Gaussian process which is written as \(r(x) \sim N(0, k_r)\), where \(k_r = k_{u''u''} + k_{u''u''} + k_{u''u''} + k_{u''u''}\). The boundary conditions of \(u\) and \(\frac{\partial^2 u}{\partial x_2^2}\) can be easily obtained by Poisson equation (5.2) and Dirichlet BCs (5.3).

15 observations of \(u\) at 15 locations in the square domain were measured as shown in Figure 4 with additive noise with the variance \(\sigma_u^2 = 0.01\). Here we set the slack parameter \(\sigma_r^2 = 0.3\). The extended set \(\chi\) in the neighbourhood of a test point \(x^*\) is composed of \(5 \times 5\) points equally spaced in square domain \([x_1 - 0.33, x_1 + 0.33] \times [x_2 - 0.33, x_2 + 0.33]\). Figure 4 also shows the posterior mean functions of the state \(u\) estimated by GPRC and GPR, respectively. Figure 5 shows the posterior mean functions of the second order derivatives \(\frac{\partial^2 u}{\partial x_1^2}\) and \(\frac{\partial^2 u}{\partial x_2^2}\), respectively. The predictions of these derivatives by GPRC are much better than the ones by the GPR method.

5.3 Van der Pol equation

Van der Pol equation is a typical nonlinear ODE which may generate shock wave solution. It is defined as

\[
d^2 u \quad dt^2 - \mu(1 - u^2) \frac{du}{dt} + u = 0,
\]

(5.4)
Figure 4: A: The black triangles represent the positions of the observation data and the contour plot of the true solution $u(x)$. B and C show the posterior mean of state computed by GPRC and GPR, respectively.

Figure 5: The first and second rows represent the estimation of $\frac{\partial^2 u}{\partial x_1 \partial x_2}$ and $\frac{\partial^2 u}{\partial x_2^2}$, respectively. A and D show the analytical solutions. B and E represent the posterior means estimated by GPRC. C and F represent the posterior means estimated by GPR.
where $\mu = 1$ and the initial conditions are $u(0) = 2, u'(0) = 0$. We can’t directly make use of GPRC method to formulate the equation information in (5.4) as a aforementioned Gaussian variable $r$, since the product of two Gaussian process is not a Gaussian process anymore. Here we proposed a kind of linearization method for this kind of nonlinear equation, which is motivated from the Picard iteration method [5]. Assume we have an initial guess of the solution $u_0$, then we can rewrite the equation (5.4) as:

$$\frac{d^2u}{dt^2} - \mu(1 - u_0^2)\frac{du}{dt} + u = 0,$$

where the original $u$ in the nonlinear coefficient term is replaced by the approximation $u_0$. Now the Eq. (5.5) is a linear equation of $u$ and GPRC can be easily applied for estimating the solution $u$ and its derivatives $u', u''$. The constraint variable is expressed as $r = \frac{d^2u}{dt^2} - \mu(1 - u_0^2)\frac{du}{dt} + u$ and the corresponding value is 0. This is a quite straightforward linearization strategy and can be easily applied in most non-linear differential equations. The initial solution guess $u_0$ can be rough estimated by classical Gaussian process regression or any other basis-function expansion method from observations.

Table 2: RMS of constraint computed by the posterior mean function of GPRC with observation contaminated by different noise levels.

| $\sigma_u^2$ | 0.10  | 0.05  | 0.01  |
|-------------|-------|-------|-------|
| RMS        | 0.0128| 0.0094| 0.0079|

40 observations are measured with equal space in the time interval [0, 20], contaminated by Gaussian noise with variance $\sigma^2_{u} = 0.01$. The extend set $\chi$ for each test point $x_i$ is chosen as 4 points equally spaced in $[x_i - 0.2, x_i + 0.2]$ and the slack parameter $\sigma_r^2 = 0.1$. Figure 6 shows the result of estimation by GPR, GPRC and traditional ODE solver. Both GPRC and GPR method perform well on the estimation of state and the first order derivative function. Whereas for the estimation of second order derivative, the GPRC method gives a more precise posterior than the one estimated by GPR method due to the inclusion of equation constraint in GPRC. Although we give a general solution $u_0$ for linearization in (5.5), the constraint line computed by ‘GPRC mean’ shows a much small fluctuation than the one calculated by ‘GPR mean’, which means the linearization method works well. The RMS (Root Mean Square) of constraint with different observation noise variances are summarized in Table 2 and illustrates the trend of convergence of the GPRC algorithm.

6 Conclusions

In this work, we have shown how to improve the accuracy and robustness for the numerical estimation of derivatives from the noisy state data by our new method of Gaussian process regression with constraint (GPRC) for linear and nonlinear differential equations. Explicit posteriors with uncertainty information are obtained in the Bayesian framework for the joint multi-dimensional GPR. For nonlinear differential equations, a strategy of linearization method motivated from the Picard iteration is applied. From the perspective
Figure 6: Van der Pol equation. A B and C: The triangles represent the observed data-points of the noisy output process. The black trace shows the solution computed by ODE solver. The blue dash-dot/green dotted traces are the inferred posterior means by GPRC and GPR method with ± posterior standard deviation tubes around them. D: The black trace shows the approximation linearization equation constraint values in (5.5). The blue dash-dot/green dotted traces are real nonlinear equation constraint in (5.4) computed by the posterior means.
of incorporating the differential equations into the Gaussian process regression (GPR), our work is a kind of physics-informed Gaussian process regression, compatible with the recent awareness of the importance of combining the observations of solution data and the underlying physical model [12]. The method developed here may have a potential application for the more complication problems like parameter identification [15].

So far, the equations we have considered are deterministic with all known coefficients, though we find the introduction of a non-zero slack parameter $\sigma^2_r$ is beneficial in practice to allow some prior distribution for the zero residual. For the stochastic differential equations with random coefficients, one may include this uncertainty of equation into the likelihood function in the same Bayesian framework; however with the restriction of Gaussian assumption, the approach of GPR may not be applicable except in some special cases in [13].

References

[1] David Barber and Yali Wang. Gaussian processes for bayesian estimation in ordinary differential equations. In International Conference on Machine Learning, pages 1485–1493, 2014.

[2] F. Brezzi. A survey of mixed finite element methods. In D. L. Dwoyer, M. Y. Hussaini, and R. G. Voigt, editors, Finite Elements, pages 34–49, New York, NY, 1988. Springer New York.

[3] Steven L. Brunton, Joshua L. Proctor, J. Nathan Kutz, and William Bialek. Discovering governing equations from data by sparse identification of nonlinear dynamical systems. Proc. Natl. Acad. Sci. U. S. A., 113(15):3932–3937, 2016.

[4] Ben Calderhead, Mark Girolami, and Neil D Lawrence. Accelerating Bayesian Inference over Nonlinear Differential Equations with Gaussian Processes. In Advances in Neural Information Processing Systems, 2009.

[5] Earl A Coddington and Norman Levinson. Theory of ordinary differential equations. Tata McGraw-Hill Education, 1955.

[6] Pei Gao, Antti Honkela, Magnus Rattray, and Neil D. Lawrence. Gaussian process modelling of latent chemical species: Applications to inferring transcription factor activities. In Bioinformatics, 2008.

[7] Thore Graepel. Solving noisy linear operator equations by gaussian process: Application to ordinary and partial differential equations. In International Conference on Machine Learning, pages 234–241, 2003.

[8] Hua Liang and Hulin Wu. Parameter estimation for differential equation models using a framework of measurement error in regression models. Journal of the American Statistical Association, 103(484):1570–1583, 2008.

[9] Guy Mayraz and Geoffrey E Hinton. Recognizing hand-written digits using hierarchical products of experts. In Advances in neural information processing systems, pages 953–959, 2001.
[10] AA Poyton, M Saeed Varziri, Kim B McAuley, P James McLellan, and Jim O Ramsay. Parameter estimation in continuous-time dynamic models using principal differential analysis. *Computers & chemical engineering*, 30(4):698–708, 2006.

[11] Maziar Raissi and George Em Karniadakis. Hidden physics models: Machine learning of nonlinear partial differential equations. *Journal of Computational Physics*, 357:125–141, 2018.

[12] Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378:686–707, 2019.

[13] Maziar Raissi, Paris Perdikaris, and George Em Karniadakis. Machine learning of linear differential equations using gaussian processes. *Journal of Computational Physics*, 348:683–693, 2017.

[14] J. O. Ramsay, G. Hooker, D. Campbell, and J. Cao. Parameter estimation for differential equations: A generalized smoothing approach. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 69(5):741–796, 2007.

[15] Samuel H Rudy, Steven L Brunton, Joshua L Proctor, and J Nathan Kutz. Data-driven discovery of partial differential equations. *Science Advances*, 3(4):e1602614, 2017.

[16] Simo Särkkä. Linear operators and stochastic partial differential equations in gaussian process regression. In *International Conference on Artificial Neural Networks*, pages 151–158. Springer, 2011.

[17] Matthias Seeger. Gaussian processes for machine learning. *International journal of neural systems*, 14(02):69–106, 2004.

[18] Peter S Swain, Keiran Stevenson, Allen Leary, Luis F Montano-Gutierrez, Ivan BN Clark, Jackie Vogel, and Teuta Pilizota. Inferring time derivatives including cell growth rates using gaussian processes. *Nature communications*, 7:13766, 2016.

[19] James M Varah. A spline least squares method for numerical parameter estimation in differential equations. *SIAM Journal on Scientific and Statistical Computing*, 3(1):28–46, 1982.

[20] Xiaolei Xun, Jiguo Cao, Bani Mallick, Arnab Maity, and Raymond J Carroll. Parameter estimation of partial differential equation models. *Journal of the American Statistical Association*, 108(503):1009–1020, 2013.