Combining Physics-Based Domain Knowledge and Machine Learning using Variational Gaussian Processes with Explicit Linear Prior

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Abstract

Centuries of development in natural sciences and mathematical modeling provide valuable domain expert knowledge that has yet to be explored for the development of machine learning models. When modeling complex physical systems, both domain knowledge and data contribute important information about the system. In this paper, we present a data-driven model that takes advantage of partial domain knowledge in order to improve generalization and interpretability. The presented model, which we call EVGP (Explicit Variational Gaussian Process), uses an explicit linear prior to incorporate partial domain knowledge while using data to fill in the gaps in knowledge. Variational inference was used to obtain a sparse approximation that scales well to large datasets. The advantages include: 1) using partial domain knowledge to improve inductive bias (assumptions of the model), 2) scalability to large datasets, 3) improved interpretability. We show how the EVGP model can be used to learn system dynamics using basic Newtonian mechanics as prior knowledge. We demonstrate that using simple priors from partially defined physics models considerably improves performance when compared to fully datadriven models.

1 Introduction

For centuries, scientists and engineers have worked on creating mathematical abstractions of real world systems. This principled modeling approach provides a powerful toolbox to derive white-box models that we can use to understand and analyze physical systems. However, as the complexity of physical systems grow, deriving detailed principled models becomes an expensive and tedious task that requires highly experienced scientists and engineers. Moreover, incorrect assumptions leads to inaccurate models that are unable to represent the real system.

Data-driven black-box models provide an appealing alternative modeling approach that requires little to none domain knowledge. These models are fit to data extracted from the real system, minimizing the problems derived from incorrect assumptions. However, using data-driven models while completely ignoring domain knowledge may lead to models that do not generalize well and are hard to understand. Completely black-box approaches ignore the structure of the problem, wasting resources [1] and making the model less explainable [2].

Gray-box models combine domain knowledge and data as both provide important and complementary information about the system. Domain knowledge can be used to construct a set of basic assumptions about the system, giving the data-driven model a baseline to build upon. Data can be used to fill the gaps in knowledge and model complex relations that were not considered by the domain expert.

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In this paper, we explore an approach for embedding domain knowledge into a data-driven model in order to improve generalization and interpretability. The presented gray-box model, which we called EVGP (Explicit Variational Gaussian Process), is a scalable approximation of a sparse Gaussian Process (GP) that uses domain knowledge to define the prior distribution of the GP. In this paper domain knowledge is extracted from physics-based knowledge, however the EVGP can be applied to any domain.

The work on this paper has three corner stones (Fig. 1): 1) Gaussian processes are used for learning complex non-linear behavior from data and model uncertainty, 2) Partial domain knowledge is used as prior in order to improve inductive bias, 3) Variational Inference is used to find an approximation that scales well to large datasets. Inductive bias refers to the assumptions made by the model when doing predictions over inputs that have not been observed. The presented approach provides uncertainty estimations which are fundamental in order to avoid the risk associated with overconfidence in unexplored areas [3] and warns the user of possible incorrect estimations [4].

The work in this paper is highly applicable when: 1) modeling physical systems with uncertainty estimations, 2) partial domain knowledge of the system is available, 3) large quantities of data are available. The aim is to help the engineer and take advantage of available knowledge without requiring the derivation of complex and detailed models. Instead, an engineer only has to provide simple, partially formed, models and the EVGP takes care of filling the gaps in knowledge. We show how the EVGP model can be used to learn system dynamics using basic physics laws as prior knowledge.

2 Variational GP using explicit features

The EVGP model is designed to solve regression problems under uncertainty. Given a dataset \( \mathcal{D} = (x^{(i)}, y^{(i)}) \) composed of input/output pairs of samples \((x^{(i)}, y^{(i)})\), we would like to obtain a predictive distribution \( p(y|x, \mathcal{D}) \) that estimates the value of the output \( y \) for a given input \( x \). The EVGP model approximates \( p(y|x, \mathcal{D}) \) using Variational Inference. The EVGP is defined as a distribution \( p(y|x, w) \) where \( w \) are a set of parameters with prior distribution \( p(w) \).

In the following sections we describe in detail: A) the EVGP model, B) the variational loss function used to train the model, C) the predictive distribution that approximates \( p(y|x, \mathcal{D}) \).

2.1 Model Definition

The EVGP model takes the following form:

\[
  y = g(x) + \epsilon_y; \quad g(x) = h(x)^T \beta + f(x)
\]  

where \( f(x) \sim \mathcal{GP}(0, k(x, x')) \) is a Gaussian process with kernel \( k \), \( \epsilon_y \sim \mathcal{N}(0, \Sigma_y) \) is the observation noise and \( g(x) \) is the denoised prediction for the input \( x \). Figure 2 offers a visual representation of the model. The following is the description of the main components of the EVGP model:

- Domain knowledge is embedded in the explicit function \( h(x)^T \beta \), parameterized by \( \beta \). The function \( h(x) \) describes a set of explicit features (hence the name of our method) provided
by the domain expert. $\beta$ is modeled using a normal distribution with a prior that is also extracted from domain knowledge. In this paper, $h(x)\beta$ is derived from partially defined Neutonian mechanics.

- The Gaussian Process $f(x)$ adds the ability to learn complex non-linear relations that $h(x)\beta$ is unable to capture.

Given a dataset $D$, the exact predictive distribution $p(y|x, D)$ for the model in Eq. (1) is described in [5]. For the rest of the paper, we refer to the exact distribution as EGP. Computing the EGP predictive distribution has a large computational cost and does not scale well for large datasets. To alleviate this problem, sparse approximation methods [6] use a small set of $m$ inducing points $(f_m, X_m)$ instead of the entire dataset to approximate the predictive distribution.

In order to construct a sparse approximation for the model in Eq. (1), we use a set of $m$ inducing points $(f_m, X_m)$ as parameters that will be learned from data. Given $(f_m, X_m)$ and a set of test points $(g, X)$, the prior distribution of the model can be expressed as follows:

$$\begin{bmatrix} g_m \\ g \end{bmatrix} | \beta \sim N \left( \begin{bmatrix} H_m \beta \\ H_x \beta \end{bmatrix}, \begin{bmatrix} K_{mm} & K_{mx} \\ K_{xm} & K_{xx} \end{bmatrix} \right); \quad H_m = h(X_m); \quad H_x = h(X)
$$

where $X$ denotes the data matrix, where each row represents an individual sample. The rows of $H_x$ represent the value of the function $h()$ applied to the real samples $X$. The rows of $H_m$ represent the value of the function $h()$ applied to the inducing (learned) points $X_m$. Using the conditional rule for multivariate Gaussian distributions, we obtain the definition of the denoised sparse EVGP model:

$$p(g | X, \omega) \sim N \left( H_x \beta + \mu_f(\omega), \Sigma_f(\omega) \right)$$

where $\omega = \{f_m, \beta\}$ are the parameters of our model, $\mu_f(\omega) = K_{xm}K_{mm}^{-1}f_m$, and $\Sigma_f(\omega) = K_{xx} - K_{xm}K_{mm}^{-1}K_{mx}$. Equation (2) defines our scalable EVGP model. In following sections we give prior distributions to the parameters $\omega$ and perform approximate Bayesian inference. Note that Eq. (2) is also conditioned on $X_m$, however we do not indicate this explicitly in order to improve readability.

### 2.2 Variational Loss

In this section we present the loss function that we use to fit our model. In this paper we follow a Variational Bayesian approach (see Appendix A for a brief overview). Given a training dataset $D$ and a prior distribution $p(\omega)$, we wish to approximate the posterior distribution $p(\omega|D)$. The posterior of $\omega$ is approximated using a variational distribution $p_\phi(\omega) \approx p(\omega|D)$ parameterized by $\phi$. For the EVGP parameters $\omega = \{f_m, \beta\}$, we use the following variational posterior distributions:

$$p_\phi(f_m) = N(f_m | a, A); \quad p_\phi(\beta) = N(\beta | \mu_\beta, \Sigma_\beta)$$

The prior-distributions for $\omega$ are also defined as multivariate normal distributions:

$$p(f_m) = N(f_m | 0, K_{mm}); \quad p(\beta) = N(\beta | \mu_\beta, \Sigma_\beta)$$

these prior distributions represent our prior knowledge, i.e. our knowledge before looking at the data.

Given the training dataset $D = (y, X)$, the parameters $\phi$ of $p_\phi(\omega)$ are learned by minimizing the negative Evidence Lower Bound (ELBO). For the EVGP, the negative ELBO takes the following form:

$$\mathcal{L}(\phi) = - \log N \left( y \mid H_x b + K_{xm}K_{mm}^{-1}a, \Sigma_y \right) + \frac{1}{2} \left[ \text{Tr} (M_1 A) + \text{Tr} (M_2 B) + \text{Tr} (\Sigma_y^{-1}\Sigma_f(\omega)) \right] + \mathcal{L}_{KL}$$

where $M_1 = (K_{mm}^{-1}K_{mx})\Sigma_y^{-1}(K_{xm}K_{mm}^{-1})$, and $M_2 = H_x^T\Sigma_y^{-1}H_x$. The term $\mathcal{L}_{KL}$ is the KL-divergence between the posterior and prior distributions for the parameters:

$$\mathcal{L}_{KL} = D_{KL} \left( N(a, A) \mid \mid N(0, K_{mm}) \right) + D_{KL} \left( N(b, B) \mid \mid N(\mu_\beta, \Sigma_\beta) \right)$$

3
A detailed derivation of the variational loss in Eq. (3) is presented in Appendix B. The negative ELBO (Eq. 3) serves as our loss function to learn the parameters \( \phi \) given the training dataset \( y, X \).

In order to scale to very large datasets, the ELBO is optimized using mini-batches (see Appendix C). In our case, the parameters of the variational approximation are: \( \phi = a, A, b, B, X_m \).

### 2.3 Predictive distribution

After learning the parameters \( \phi \), we would like to provide estimations using the approximated variational distribution \( p_\phi(\omega) \). Given a set of test points \( \hat{X} \), the estimated denoised predictive distribution is computed as an expectation of Eq. (2) w.r.t. \( p_\phi(\omega) \):

\[
p_\phi(\hat{y} | \hat{X}) = \mathbb{E}_{p_\phi(\omega)} \left[ p_\phi(\hat{y} | \hat{X}, \omega) \right] ;
\]

\[
= \mathcal{N}\left( \hat{g} | \mu_{\hat{g}|x}, \Sigma_{\hat{g}|x} \right) \quad \text{(4)}
\]

Note that \( \hat{g} \) is just a denoised version of \( \hat{y} \). Eq. (4) approximates \( p(\hat{y}|\hat{x},D) \), using the learned distribution \( p_\phi(\omega) \) (see Appendix B). The result is equivalent to \( \mathcal{N}(\hat{g} | \mu_{\hat{g}|x}, \Sigma_{\hat{g}|x}) \mathcal{N}(\hat{y} | \hat{g}, \Sigma_y) \mathcal{N}(\hat{x} | \mu_{\hat{x}}, \Sigma_{\hat{x}}) = \mathcal{N}(\hat{g} | \mu_{\hat{g}|x}, \Sigma_{\hat{g}|x}) \mathcal{N}(\hat{y} | \hat{g}, \Sigma_y) \mathcal{N}(\hat{x} | \mu_{\hat{x}}, \Sigma_{\hat{x}}) \mathcal{N}(\hat{y} | \hat{g}, \Sigma_y) \mathcal{N}(\hat{x} | \mu_{\hat{x}}, \Sigma_{\hat{x}}) \mathcal{N}(\hat{x} | \mu_{\hat{x}}, \Sigma_{\hat{x}}) \mathcal{N}(\hat{y} | \hat{g}, \Sigma_y) \mathcal{N}(\hat{x} | \mu_{\hat{x}}, \Sigma_{\hat{x}}) \mathcal{N}(\hat{y} | \hat{g}, \Sigma_y) \mathcal{N}(\hat{x} | \mu_{\hat{x}}, \Sigma_{\hat{x}}) \mathcal{N}(\hat{y} | \hat{g}, \Sigma_y) \mathcal{N}(\hat{x

The approximated predictive distribution with observation noise is the following:

\[
p_\phi(\hat{y} | \hat{X}) = \mathcal{N}\left( \hat{g} | \mu_{\hat{g}|x} + \Sigma_{\hat{g}|x} \right) \quad \text{(4)}
\]

where \( p_\phi(\hat{y} | \hat{X}) \approx p(\hat{y} | \hat{x}, D) \). In the next section, we show how Eq. (4) can be used to model system dynamics and predict the next state of a physical system given the control input and current state.

### 3 Embedding physics-based knowledge

In this paper, we apply the EVGP model to learn the dynamics of a physical system. The state \( z_{[t]} \) of the physical system can be modeled as follows:

\[
z_{[t+1]} \sim g(z_{[t]} \oplus u_{[t]})
\]

\[
y_{[t]} \sim z_{[t]} + \epsilon_y
\]

where \( u_{[t]} \) is the control input and \( y_{[t]} \) is the measured output of the system. The symbol \( \oplus \) denotes concatenation and \( x_{[t]} = z_{[t]} \oplus u_{[t]} \) is the input to the EVGP model. For example, in the case of a mechatronic system: \( u_{[t]} \) are the forces applied by the actuators (e.g. electric motors); \( z_{[t]} \) is the position and velocity of the joints; \( y_{[t]} \) is the output from the sensors.

We assume independent EVGP models for each output \( y_{[t]} \) in the equation (5). The function \( g() \) in Eq. (5) is modeled using the EVGP model from Eq. (1) and Eq. (4). In the following sections we present how we can use simple Newtonian mechanics to define useful priors \( h(x)^T \beta \) for the EVGP model.
3.1 Priors from simple Newtonian dynamics

Figure 3a shows a simple example of a single rigid-body link. The simplest model that we can use for this system comes from Newton’s second law \( u = J \ddot{q}_1 \), where \( u \) is the torque applied to the system, \( J \) is the moment of inertia, and \( q_1 \) is the angle of the pendulum. Using Euler discretization method, we obtain the following state-space representation that serves as the prior \( h(x)^T \beta \) for our EVGP model:

\[
\begin{bmatrix}
q_1[t+1] \\
\dot{q}_1[t+1]
\end{bmatrix} = \begin{bmatrix}
1 & Δt \\
0 & 1
\end{bmatrix} \begin{bmatrix}
q_1[t] \\
\dot{q}_1[t]
\end{bmatrix} + \begin{bmatrix}
Δt \\
\Delta t/J
\end{bmatrix} \begin{bmatrix}
q_1[t] \\
\dot{q}_1[t]
\end{bmatrix} + \begin{bmatrix}
\gamma \\
\gamma
\end{bmatrix} \begin{bmatrix}
\text{prior mean } \mu_β \\
h(\pi(x))
\end{bmatrix} \tag{6}
\]

We refer to this prior as IF (inertia+force). \( Δt \) is the discretization time and \( \begin{bmatrix} q_1[t] & \dot{q}_1[t] \end{bmatrix}^T \) is the state \( x(t) \) of the system. The IF prior in Eq. (6) does not include gravitational effects. Gravity pulls the link to the downward position with a force proportional to \( \sin q_1 \). Hence, a prior that considers gravitational forces can be constructed by including \( \sin(q_1[t]) \):

\[
\text{IFG}_{[t+1]} = \begin{bmatrix}
1 & Δt & 0 & 0 \\
0 & 1 & Δt/J & -γ \\
\end{bmatrix} \begin{bmatrix}
q_1[t] \\
\dot{q}_1[t] \\
u[t] \\
\sin(q_1[t])
\end{bmatrix} \tag{7}
\]

we call this prior IFG (inertia+force+gravity). We purposely did not define \( J \) and \( γ \). One of the advantages of the presented approach is that the algorithm can learn the parameters from data if they are not available. If the user does not know the value of \( J \) and \( γ \), a prior with large standard deviation can be provided for these parameters (large \( \Sigma_β \)). Although parameters like \( J \) and \( γ \) are easy to compute for a simple pendulum, for more complex systems they may be hard and tedious to obtain. Our objective is to take advantage of domain knowledge and allow the model to fill in the gaps in knowledge.

For the rest of the paper, priors derived from Eq. (6) are referred as IF priors, while Eq. (7) priors are referred as IFG. In the experiments (section 4), we compare the performance for both priors in order to illustrate how performance can be progressively improved with more detailed priors.

3.2 Simplified priors for Acrobot and Cartpole

In addition to the pendulum, we consider the Acrobot and Cartpole systems in our analysis. For these systems, we consider much simpler priors than the exact dynamic models derived from multi-body dynamics. We use the same principles shown in the previous section in order to get simple priors for the Acrobot and Cartpole.

Figure 3c shows a diagram of the Acrobot system. A simple prior for this system can be constructed using the prior in Eq. (6) for each one of the links of the Acrobot:

\[
\text{IF} = \begin{bmatrix}
1 & 0 & Δt & 0 & 0 \\
0 & 1 & 0 & Δt & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & γ_1
\end{bmatrix} : \quad \text{IFG} = \begin{bmatrix}
1 & 0 & Δt & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & Δt & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & -γ_2 & -γ_3 \\
0 & 0 & 0 & 1 & γ_1 & 0 & -γ_4
\end{bmatrix} \begin{bmatrix}
q_1[t] \\
q_2[t] \\
\dot{q}_1[t] \\
\dot{q}_2[t] \\
u[t] \\
\sin_1 \\
\sin_1
\end{bmatrix} \tag{8}
\]

where \( \sin_1 = \sin(q_1[t]) \), and \( \sin_{12} = \sin(q_1[t] + q_2[t]) \). In this case, the input \( u[t] \) only drives the second link. The idea with these priors is to construct an intuitive and simple model from “noisy” Newtonian dynamics. These priors are extremely simple as they do not consider friction or coriolis/centrifugal forces. However, they provide important information about the mechanics of the system. These priors convey the following information:

- The position should increase proportional to the velocity by a factor of \( Δt \).
- The position should stay the same if the velocity is zero.
The velocity should stay the same if no external forces are applied.

For the IFG prior, gravity pulls the links to the downward position proportional to the sine of the angle w.r.t. the horizontal plane. Gravity has no effect when the links are completely down/up.

The objective with these priors is to demonstrate how extremely simplified priors extracted with simple physics can be used to improve performance of data-driven models. The IF and IFG priors for the Cartpole (Figure 3b) are constructed using the same principles:

\[
\begin{align*}
\text{IF} & = \begin{bmatrix}
1 & 0 & \Delta t & 0 & 0 \\
0 & 1 & 0 & \Delta t & 0 \\
0 & 0 & 1 & 0 & \gamma_1 \\
0 & 0 & 0 & 1 & 0
\end{bmatrix}
\begin{bmatrix}
q_1[t] \\
q_2[t] \\
\dot{q}_1[t] \\
\dot{q}_2[t] \\
u[t]
\end{bmatrix},
\\
\text{IFG} & = \begin{bmatrix}
1 & 0 & \Delta t & 0 & 0 \\
0 & 1 & 0 & \Delta t & 0 \\
0 & 0 & 1 & 0 & \gamma_1 \\
0 & 0 & 0 & 1 & 0
\end{bmatrix}
\begin{bmatrix}
q_1[t] \\
q_2[t] \\
\dot{q}_1[t] \\
\dot{q}_2[t] \\
u[t]
\end{bmatrix} - \begin{bmatrix}
\gamma_1 \\
\gamma_2
\end{bmatrix}
\sin(q_2[t]).
\end{align*}
\]

4 Experiments

In order to evaluate the performance of the presented model, we performed experiments on a set of simulated systems: Pendulum, Cartpole and Acrobot. We also performed qualitative tests on a toy-dataset to visualize the performance of the EVGP model.

We used Drake [8] to simulate the Pendulum, Cartpole and Acrobot systems and obtain the control/sensor data used to train and evaluate the EVGP models. We used the squared exponential function for the covariance kernels. The reason for this choice is that all the experiments involve continuous systems. The EVGP model was implemented using Tensorflow and the minimization of the negative ELBO loss was done using the ADAM optimizer [9]. The experiments were run in a computer with a single GPU (Nvidia Quadro P5000) with an Intel(R) Xeon(R) CPU (E3-1505M at 3.00GHz).

4.1 Experiments on Toy Dataset

The toy dataset is intended to serve as an illustration of the behavior of the EVGP model and visualize the qualitative differences between several GP models. We use a modified version of the toy dataset used in [10] [7]. The dataset \( (y, x) \) is modified as follows:

\[(y, x) \leftarrow (6y + 3x, x)\]

The modification is intended to provide a global linear trend to the data (See Figure 4). Figure 4 shows the distribution learned using different versions of a Gaussian Process. Figures 4a and Figure 4c show the exact posterior distributions for a GP and EGP model, respectively. Figures 4b and Figure 4d show the variational approximations obtained with a VGP model and EVGP model. The standard deviation (black line) is used to visualize the uncertainty. The figures show how the uncertainty grows as we move away from the training dataset.

The original dataset is composed of 200 samples, Figure 4 shows that the variational approximations are able to successfully approximate their exact counterparts with as few inducing points as \( m=10 \). The position of the inducing points are shown with green crosses.

In this case, the prior knowledge that we provide to the EVGP is a simple linear function \( h(x, \beta) = x\beta_1 + \beta_2 \). Figure 4d shows how we can use the prior in order to control the global shape of the function. The figure shows how the EGP and EVGP models use the prior knowledge to fit the global behavior of the data (linear) while using the kernels to model the local non-linear behavior.

4.2 Learning system dynamics

We evaluated the performance of the EVGP model in learning system dynamics using data obtained from simulations of the Pendulum, Cartpole and Acrobot systems. Concretely, we evaluated the accuracy of the EVGP model with IF and IFG priors in predicting the next state of the system given the current control inputs and state.

\[\text{Obrained from http://www.gatsby.ucl.ac.uk/~snelson/SPGP_dist.tgz}\]
Table 1: Parameters used to collect training and testing data

| System  | $\alpha$   | $\eta$ | $H$ | $|D|$ |
|---------|------------|--------|-----|------|
| Pendulum| $[\pi, 0.5]$ | 1.0    | 48  | 4800 |
| Cartpole| $[1.0, \pi, 0.5, 0.5]$ | 100.0  | 48  | 4800 |
| Acrobot | $[\pi, 1.0, 0.5, 0.5]$ | 0.5    | 93  | 9300 |

Table 2: Number of inducing points and hidden units

| System  | Pendulum | Cartpole | Acrobot |
|---------|----------|----------|---------|
| VGP     | 40       | 100      | 250     |
| RES-VGP | 40       | 100      | 250     |
| RES-DBNN| $[15, 15]$| $[50, 50]$| $[60, 60]$ |
| EVGP-IF | 10       | 60       | 150     |
| EVGP-IFG| 10       | 60       | 150     |

**Data:** to evaluate the difference in generalization, we sampled two different datasets for each system: one for training and one for testing. The datasets were sampled by simulating the system using random initial states $z_{[0]} \sim \alpha U(-1, 1)$ and random control inputs $u_{[t]} \sim \eta N(0, 1)$ drawn from uniform and normal distributions, respectively. Table 1 shows the values of the scales ($\alpha, \eta$) that were used to sample the trajectories. These values were chosen in order to cover at least the range $(-\pi, \pi)$ for the angles on the systems. In Table 1, $H$ refers to the number of sampled trajectories, $|D|$ refers to the total number of samples. All trajectories were sampled for 100 time steps and $\Delta t = 0.03s$.

**Baseline:** we compare the EVGP model with a standard VGP model, a residual VGP (RES-VGP), and a residual Deep Bayesian Neural Network (RES-DBNN). The VGP model is based on [11] and uses a zero mean prior. The residual VGP and DBNN models assume the system can be approximated as $z_{[t+1]} = z_{[t]} + g_r(z_{[t]} \oplus u_{[t]})$. Approximating residuals is a common approach used to simplify the work for GP and DBNN models [12] [13] [14]. The RES-DBNN model is trained using the local reparameterization trick presented in [15] with Normal variational distributions for the weights. For these set of experiments, we did not consider the exact GP and EGP models given the large number of samples in the training datasets.

Table 2 shows the number of inducing points (m) used for the VGP and EVGP models. The table also shows the number of hidden units for the DBNN model, where $[15, 15]$ means a two-layer network with 15 units in each layer. We used the LeakyRelu activation function.

Table 3: Complexity comparison

| Model   | Space  | Time   |
|---------|--------|--------|
| VGP     | $O(mn)$| $O(mn^3)$ |
| DBNN    | $O(Ln^2)$| $O(Ln^3)$ |
| EVGP    | $O(mn)$| $O(mn^3)$ |
| System   | Model  | CR-1  | CR-2  | CR-3  | Error | # Param. |
|----------|--------|-------|-------|-------|-------|----------|
| Pendulum | VGP    | 0.327 | 0.576 | 0.716 | 0.484 | 407      |
|          | RES-VGP| 0.471 | 0.762 | 0.880 | 0.216 | 407      |
|          | RES-DBNN| 0.515 | 0.846 | 0.955 | 0.081 | 634      |
|          | EVGP-IF| 0.745 | 0.962 | 0.987 | 0.075 | 119      |
|          | EVGP-IFG| 0.704 | 0.957 | 0.996 | 0.064 | 123      |
| Cartpole | VGP    | 0.591 | 0.856 | 0.913 | 0.265 | 2813     |
|          | RES-VGP| 0.592 | 0.888 | 0.946 | 0.131 | 2813     |
|          | RES-DBNN| 0.440 | 0.827 | 0.921 | 0.041 | 6008     |
|          | EVGP-IF| 0.843 | 0.961 | 0.983 | 0.023 | 1733     |
|          | EVGP-IFG| 0.901 | 0.979 | 0.995 | 0.010 | 1741     |
| Acrobot  | VGP    | 0.625 | 0.818 | 0.895 | 0.812 | 7013     |
|          | RES-VGP| 0.690 | 0.850 | 0.912 | 0.684 | 7013     |
|          | RES-DBNN| 0.555 | 0.803 | 0.897 | 0.500 | 8408     |
|          | EVGP-IF| 0.793 | 0.910 | 0.956 | 0.135 | 4253     |
|          | EVGP-IFG| 0.737 | 0.899 | 0.952 | 0.121 | 4269     |

Table 3 shows the space and time complexity of the models considered in this paper. In this table, \( m \) is the number of inducing points, \( o \) is the number of outputs, \( L \) is the number of hidden layers, and \( n \) is the number of hidden units in each layer. To simplify the analysis, we assume all hidden layers of the DBNN have the same number of hidden units. The table shows that the complexity of the VGP and EVGP models are governed by the matrix inversion \( K^{-1} \). Because we assume completely independent VGP and EVGP models for each output of the system, their complexity also depends on the number of outputs \( o \). The complexity of the DBNN model is governed by the matrix-vector product between the weight matrices and the hidden activation vectors. All models have constant space complexity w.r.t. the training dataset size \( |D| \). Furthermore, all models have linear time complexity w.r.t. \( |D| \) if we assume that training requires to visit each sample in \( D \) at least once.

**Metrics:** for comparison, we used two metrics: 1) prediction error, 2) containing ratios (CR). Prediction error is computed as the difference between sampled values \( (y) \) and the expected estimated output \( (\hat{y}) \):

\[
\text{Error} = \frac{1}{|D|} \sum_{i=1}^{|D|} \left\| y^{(i)} - E\left[\hat{y}^{(i)}\right]\right\|
\]

where \( |D| \) is the number of samples in the respective dataset. The expected output \( E\left[\hat{y}^{(i)}\right] \) for the EVGP model is equal to \( \mu_{\hat{y}|\hat{x}} \) in Eq. (4). For the DBNN model, the expectation is estimated using Monte-Carlo.

The containing ratios (CR) are the percentage of values covered by the estimated distribution \( \hat{y} \). We consider containing ratios for one, two and three standard deviations (CR-1, CR-2, and CR-3 respectively).

**Results:** Table 4 shows the prediction error and CR scores obtained in the testing dataset. EVGP-IF and EVGP-IFG refers to the use of an IF or IFG prior, respectively. We can observe a considerable improvement on the testing error and CR-3 scores when using EVGP models. We also see a progressive improvement on the testing error when using more detailed priors. Using IFG prior results in lower prediction errors when compared with the IF prior. Also, the residual models have a lower error than the standard VGP model. The EVGP-IFG model provided the estimations with the lowest prediction error and CR-3 scores close to 100%.

Table 4 also shows that the EVGP model required the lowest number of parameters. This translates into lower training and inference times with lower memory cost.

Figure 5 shows a comparison of the prediction error on the test dataset as we increase the number of training samples. For this experiment, we kept the testing dataset fixed while samples were progressively aggregated into the training dataset. The figure shows the mean, max and min values obtained for four independent runs. Figure 5a shows a comparison that includes all models. As expected, the prediction error is reduced as we increase the size of our training dataset. The figure shows that the EVGP provides the most accurate predictions while requiring less number of samples.
Figure 5: Prediction error on testing dataset for increasing number of training samples. The EVGP model provides the most accurate predictions while requiring less number of samples. Note that the number of training samples is in the order of thousands.

Figure 5a also shows how the performance of VGP and RES-VGP plateaus, struggling to take advantage of larger datasets. Although the RES-DBNN performs poorly with small training datasets, the high capacity of the RES-DBNN model allows it to take advantage of large datasets and improve accuracy, reducing the performance gap w.r.t. the EVGP models as more data is available. Thanks to the lower computational time-cost of the RES-DBNN (see Table 3), this model can use a larger set of parameters without incurring in excessive training times.

Figure 5b shows a scaled version that only considers the EVGP model with different priors. This figure shows that the IFG prior provides more accurate predictions when compared to the IF prior. In the case of the pendulum, the IFG prior provides a highly accurate model of the system, requiring only a small number of training samples. Figure 5b also shows how as training data is aggregated, the accuracy gap between IF and IFG priors is reduced.

The priors that we use are extremely simple, they are ignoring friction and coriolis/centrifugal effects. Nonetheless, we observe a considerable performance improvement after providing our data-driven model basic information with the IF and IFG priors.

Understanding the learned model: one of the advantages of incorporating domain knowledge is that the learned model is easy to interpret by the domain expert. For example, in the case of the Acrobot, the value of the parameter $\beta$ can be visualized to understand and debug what the model has learned. Figure 6 shows the value of $b$ learned with the IF (Fig. 6a) and IFG priors (Fig. 6b).

We observe in Figure 6 that the learned parameters follow a similar structure given by the prior (see Eq. 8). In our experiments, we did not enforce the sparse structure from the priors, i.e. zero parameters in the prior are allowed to have non-zero values in the posterior.

Figure 6: Visualization of the learned value of $b$ for the Acrobot.
Figure 6a shows that when using the IF prior, the EVGP model compensates for the missing gravity information by assigning negative values to $(\dot{q}_1, q_1)$ and $(\dot{q}_2, q_2)$. The reason for this behavior is that $q_1 \approx \sin q_1$ for small $q_1$, however this approximation is no longer valid for large $q_1$. When using IFG priors (Fig. 6b), we observe that the model no longer assigns negative values to $(\dot{q}_1, q_1)$ and $(\dot{q}_2, q_2)$. The reason is that IFG provides the values of $\sin(q_1)$ and $\sin(q_1 + q_2)$ which help to model the effect of gravity more accurately.

5 Related work

Incorporating prior scientific knowledge in machine-learning algorithms is an ongoing effort that has recently gained increased attention. Convolutional neural networks (CNNs) have been used in modeling and simulation applications such as forecasting of sea surface temperature [16] and efficient simulation of the Navier-Stokes equations [17]. Gaussian Processes (GP) provide a general purpose non-parametric model that has been used for system identification and control under uncertainty [12] [18]. Previous work has explored using GPs to include partial model information [19]. In [20] a GP model is used to correct a highly simplified physics model and improve accuracy. Our work is based on the GP model with explicit features presented in [5]. Variations of this model are commonly used in calibration of computer models [21] [22].

Despite the advantages of GP models for modeling complex non-linear relations with uncertainty, GPs are computationally expensive. A large bulk of research has focused on improving the computational requirements of GPs. Sparse GP approximation methods are some of the most common approaches for reducing GP computation cost [6]. Bayesian approximation techniques such as Variational Inference provide a rich toolset for dealing with large quantities of data and highly complex models [23] [7]. Variational approximations of a sparse GP have been explored in [7] [11]. In [3] a variational GP model is presented for nonlinear state-space models. In [13] [14], Deep Bayesian Neural Networks (DBNNs) are proposed as an alternative to GPs in order to improve scalability in reinforcement learning problems. Given the popularity of GP models and Variational Inference, there is an increased interest on developing automated variational techniques for these type of models [24] [25].

6 Conclusion

In this paper, we presented the EVGP model, a variational approximation of a Gaussian Process which uses domain knowledge to define the mean function of the prior. We compared the performance of the EVGP model against purely data-driven approaches and demonstrated improved accuracy and interpretability after incorporating simple priors derived from Neutonian mechanics. The EVGP also provided higher accuracy with smaller training datasets. The priors provided a rough but simple approximation of the mechanics, informing the EVGP of important structure of the real system.

References

[1] C. Szegedy, W. Liu, Y. Jia, P. Sermanet, S. Reed, D. Anguelov, D. Erhan, V. Vanhoucke, and A. Rabinovich, “Going deeper with convolutions,” in Proceedings of the IEEE conference on computer vision and pattern recognition, 2015, pp. 1–9.

[2] A. Adadi and M. Berrada, “Peeking inside the black-box: A survey on explainable artificial intelligence (xai),” IEEE Access, vol. 6, pp. 52 138–52 160, 2018.

[3] R. Frigola, Y. Chen, and C. E. Rasmussen, “Variational gaussian process state-space models,” in Advances in Neural Information Processing Systems, 2014, pp. 3680–3688.

[4] D. Marino, K. Amarasinghe, M. Anderson, N. Yancey, Q. Nguyen, K. Kenney, and M. Manic, “Data driven decision support for reliable biomass feedstock preprocessing,” in Resilience Week (RWS), 2017. IEEE, 2017, pp. 97–102.

[5] C. E. Rasmussen, “Gaussian processes in machine learning,” in Advanced lectures on machine learning. Springer, 2004, pp. 27–29.

[6] J. Quiñonero-Candela and C. E. Rasmussen, “A unifying view of sparse approximate gaussian process regression,” Journal of Machine Learning Research, vol. 6, no. Dec, pp. 1939–1959, 2005.
[7] M. Titsias, “Variational learning of inducing variables in sparse gaussian processes,” in Artificial Intelligence and Statistics, 2009, pp. 567–574.

[8] R. Tedrake and the Drake Development Team, “Drake: A planning, control, and analysis toolbox for nonlinear dynamical systems;” 2016. [Online]. Available: https://drake.mit.edu

[9] D. P. Kingma and J. Ba, “Adam: A method for stochastic optimization,” arXiv preprint arXiv:1412.6980, 2014.

[10] E. Snelson and Z. Ghahramani, “Sparse gaussian processes using pseudo-inputs,” in Advances in neural information processing systems, 2006, pp. 1257–1264.

[11] J. Hensman, N. Fusi, and N. D. Lawrence, “Gaussian processes for big data,” arXiv preprint arXiv:1309.6835, 2013.

[12] M. Deisenroth and C. E. Rasmussen, “Pilco: A model-based and data-efficient approach to policy search,” in Proceedings of the 28th International Conference on machine learning (ICML-11), 2011, pp. 465–472.

[13] Y. Gal, R. T. McAllister, and C. E. Rasmussen, “Improving pilco with bayesian neural network dynamics models,” in Data-Efficient Machine Learning workshop, 2016.

[14] D. Marino and M. Manic, “Modeling and planning under uncertainty using deep neural networks,” IEEE Transactions on Industrial Informatics, pp. 1–1, 2019.

[15] D. Kingma, T. Salimans, and M. Welling, “Variational dropout and the local reparameterization trick,” in Advances in Neural Information Processing Systems, 2015, pp. 2575–2583.

[16] E. de Bezenac, A. Pajot, and P. Gallinari, “Deep learning for physical processes: Incorporating prior scientific knowledge,” arXiv preprint arXiv:1711.07970, 2017.

[17] J. Tompson, K. Schlachter, P. Sprechmann, and K. Perlin, “Accelerating eulerian fluid simulation with convolutional networks,” in Proceedings of the 34th International Conference on Machine Learning-Volume 70. JMLR. org, 2017, pp. 3424–3433.

[18] H. Bijl, T. B. Schönh, J.-W. van Wingerden, and M. Verhaegen, “System identification through online sparse gaussian process regression with input noise,” IFAC Journal of Systems and Control, vol. 2, pp. 1–11, 2017.

[19] J. Hall, C. Rasmussen, and J. Maciejowski, “Modelling and control of nonlinear systems using gaussian processes with partial model information,” in 2012 IEEE 51st IEEE Conference on Decision and Control (CDC). IEEE, 2012, pp. 5266–5271.

[20] F. M. Gray and M. Schmidt, “A hybrid approach to thermal building modelling using a combination of gaussian processes and grey-box models,” Energy and Buildings, vol. 165, pp. 56–63, 2018.

[21] M. C. Kennedy and A. O’Hagan, “Bayesian calibration of computer models,” Journal of the Royal Statistical Society: Series B (Statistical Methodology), vol. 63, no. 3, pp. 425–464, 2001.

[22] W. Li, S. Chen, Z. Jiang, D. W. Apley, Z. Lu, and W. Chen, “Integrating bayesian calibration, bias correction, and machine learning for the 2014 sandia verification and validation challenge problem,” Journal of Verification, Validation and Uncertainty Quantification, vol. 1, no. 1, p. 011004, 2016.

[23] D. P. Kingma and M. Welling, “Auto-encoding variational bayes,” arXiv preprint arXiv:1312.6114, 2013.

[24] T. V. Nguyen and E. V. Bonilla, “Automated variational inference for gaussian process models;” in Advances in Neural Information Processing Systems, 2014, pp. 1404–1412.

[25] A. Kucukelbir, D. Tran, R. Ranganath, A. Gelman, and D. M. Blei, “Automatic differentiation variational inference,” The Journal of Machine Learning Research, vol. 18, no. 1, pp. 430–474, 2017.

[26] Y. Gal and Z. Ghahramani, “Dropout as a bayesian approximation: Representing model uncertainty in deep learning,” in international conference on machine learning, 2016, pp. 1050–1059.
Appendix A  Variational Inference

In a Bayesian learning approach, we model the parameters $\omega$ of our model $p(y \mid x, \omega)$ using probability distributions. The parameters are given a prior distribution $p(\omega)$ that represents our prior knowledge about the model before looking at the data. Given a dataset $D$, we would like to obtain the posterior distribution of our parameters following the Bayes rule:

$$p(\omega | D) = \frac{p(D | \omega)p(\omega)}{p(D)}$$

Variational Inference (VI) provides a tool for approximating the posterior $p(\omega | D)$ using a variational distribution $p_\phi(\omega)$ parameterized by $\phi$. In other words, with VI we find the value of $\phi$ such that $p_\phi(\omega) \approx p(\omega | D)$. The parameters $\phi$ of the distribution $p_\phi(\omega)$ are found by maximizing the Evidence Lower Bound (ELBO) between the approximate and real distributions:

$$\phi \leftarrow \arg \max_{\phi} \mathbb{E}_{p_\phi(\omega)} \left[ \log p(D | \omega) \right] - D_{KL}(p_\phi(\omega) \mid \mid p(\omega))$$

Maximizing the ELBO is equivalent to minimizing the KL divergence between the variational distribution and the real distribution.

Having obtained the variational approximation $p_\phi(\omega)$, we can approximate the predictive distribution $p(y | x, D)$ as follows:

$$p(y | x, D) = \mathbb{E}_{p(\omega | D)} [p(y | x, \omega)]$$

$$\approx \mathbb{E}_{p_\phi(\omega)} [p(y | x, \omega)]$$

which is the approximated variational predictive distribution $p_\phi \left( \hat{y} \mid \hat{X} \right)$ (see section 2.3):

$$p_\phi \left( \hat{y} \mid \hat{X} \right) = \mathbb{E}_{p_\phi(\omega)} \left[ p \left( \hat{y} \mid \hat{X}, \omega \right) \right]$$

Appendix B  ELBO

Given the training dataset $D = (y, X)$, the parameters $\phi$ of $p_\phi(\omega)$ are learned by minimizing the negative Evidence Lower Bound (ELBO). For the EVGP, the negative ELBO takes the following form:

$$\mathcal{L}_1(\phi) = - \mathbb{E}_{p_\phi(\omega)} \left[ \ln \mathbb{E}_{g|\omega} [p(y | g)] \right] + \mathcal{L}_{KL}$$

(10)

where $\mathcal{L}_{KL}$ denotes the KL divergence between the variational posterior and the prior $\mathcal{L}_{KL} = D_{KL}(p_\phi(\omega) \mid \mid p(\omega))$. Note that the inner expectation in Eq. (10) is taken w.r.t. $g | \omega$, presented in Eq. (2). Following a similar approach than [11], we apply Jensen’s inequality in the inner expectation of Eq. (10):

$$\log \mathbb{E}_{g|\omega} [p(y | g)] \geq \mathbb{E}_{g|\omega} \left[ \log p(y | g) \right]$$

$$\mathbb{E}_{g|\omega} \left[ \log p(y | g) \right] = \log \mathcal{N} \left( y \mid \mu_{g|\omega}, \Sigma_y \right) - \frac{1}{2} \text{Tr} \left( \Sigma_y^{-1} \Sigma_{g|\omega} \right)$$

where $\mu_{g|\omega} = H_x \beta + \mu_{f|\omega}$, $\Sigma_{g|\omega} = \Sigma_{f|\omega}$. This allows us to express the ELBO in a way that simplifies the computation of the expectations w.r.t. the parameters $\omega$. Now, the variational loss in Eq. (3) can be obtained by simply computing the expectation w.r.t. the model parameters:

$$\mathcal{L}(\phi) = \mathbb{E}_{p_\phi(\omega)} \left[ \mathbb{E}_{g|\omega} \left[ - \log p(y | g) \right] \right] + \mathcal{L}_{KL}$$

$$= - \mathbb{E}_{p_\phi(\omega)} \left[ \log \mathcal{N} \left( y \mid \mu_{g|\omega}, \Sigma_y \right) - \frac{1}{2} \text{Tr} \left( \Sigma_y^{-1} \Sigma_{g|\omega} \right) \right] + \mathcal{L}_{KL}$$

$$= - \log \mathcal{N} \left( y \mid H_x \beta + K_x n \Sigma_{f|\omega}, \Sigma_y \right)$$

$$+ \frac{1}{2} \left[ \text{Tr} \left( M_1 A \right) + \text{Tr} \left( M_2 B \right) + \text{Tr} \left( \Sigma_y^{-1} \Sigma_{f|\omega} \right) \right]$$

$$+ \mathcal{L}_{KL}$$
where $M_1 = (K_{mm}^{-1} K_{mx}) \Sigma_y^{-1} (K_{xm} K_{mm}^{-1})$, and $M_2 = H_x^T \Sigma_y^{-1} H_x$. The value of the KL-divergence is simply the sum of the divergence for both parameters:

$$\mathcal{L}_{KL} = D_{KL}(\mathcal{N}(a, A) || \mathcal{N}(0, K_{mm})) + D_{KL}(\mathcal{N}(b, B) || \mathcal{N}(\mu_\beta, \Sigma_\beta))$$

**Appendix C  Mini-batch optimization**

In order to make the model scalable to very large datasets, the ELBO can be optimized using mini-batches. Following [26], assuming the samples are i.i.d., the loss for a mini-batch $(y, X)$ composed of $|X|$ number of samples can be expressed as follows:

$$\mathcal{L} (\phi) = -\frac{1}{|X|} \mathbb{E}_{p(w)} \left[ \ln (p(Y | X, w)) \right] + \frac{1}{|D|} \mathcal{L}_{KL}$$

where $|D|$ is the total number of samples in the training dataset.