Bayesian inference of ODEs with Gaussian processes

Pashupati Hegde Çağatay Yıldız Harri Lähdesmäki Samuel Kaski

Markus Heinonen
Department of Computer Science
Aalto University, Finland
first.last@aalto.fi

Abstract

Recent machine learning advances have proposed black-box estimation of unknown continuous-time system dynamics directly from data. However, earlier works are based on approximative ODE solutions or point estimates. We propose a novel Bayesian nonparametric model that uses Gaussian processes to infer posteriors of unknown ODE systems directly from data. We derive sparse variational inference with decoupled functional sampling to represent vector field posteriors. We also introduce a probabilistic shooting augmentation to enable efficient inference from arbitrarily long trajectories. The method demonstrates the benefit of computing vector field posteriors, with predictive uncertainty scores outperforming alternative methods on multiple ODE learning tasks.

1 Introduction

Ordinary differential equations (ODEs) are powerful models for continuous-time non-stochastic systems, which are ubiquitous from physical and life sciences to engineering (Hirsch et al., 2012). In this work, we consider non-linear ODE systems

$$\dot{x}(t) = x_0 + \int_0^t f(x(\tau))d\tau, \quad \dot{x}(t) := \frac{dx(t)}{dt} = f(x(t)),$$

(1)

where the state vector $x(t) \in \mathbb{R}^D$ evolves over time $t \in \mathbb{R}_+$ from an initial state $x_0$, following its time derivative $\dot{x}(t)$. Our goal is to learn the differential function $f : \mathbb{R}^D \rightarrow \mathbb{R}^D$ from state observations, when the functional form $f$ is unknown.

The conventional mechanistic approach involves manually defining the equations of dynamics and optimizing their parameters (Butcher and Goodwin, 2008) or inferring their posteriors (Girolami, 2008) from data. However, the equations are unknown or ambiguous for many systems, such as human motion (Wang et al., 2008). Early seminal works explored fitting unknown ODEs with splines (Henderson and Michailidis, 2014), Gaussian processes (Äijö and Lähdesmäki, 2009) or kernel methods (Heinonen and d’Alché-Buc, 2014) by resorting to biased gradient matching approximations (Varah, 1982). Recently, accurate estimation of free-form non-linear dynamics was proposed using Gaussian processes with sensitivity equations (Heinonen et al., 2018) and neural networks with adjoints (Chen et al., 2018). However, both approaches are restricted to learning point estimates of the dynamics, limiting their uncertainty characterization and generalization.

In this work, we introduce Bayesian learning of unknown, non-linear ODEs. Our contributions are:

- We use Gaussian processes as flexible priors over differentials $f$, and propose stochastic variational inference to learn posteriors over vector fields.
• We adapt decoupled functional sampling to simulate ODEs in linear time from vector field posteriors.
• For the difficult problem of vanishing gradients, which renders straightforward solutions useless on long trajectories, we introduce a novel probabilistic shooting method. It is motivated by the canonical shooting methods from optimal control and makes inference stable and efficient on long trajectories.
• We empirically show the effectiveness of our method even while learning from a limited number of observations. We demonstrate the ability to infer arbitrarily long trajectories efficiently with the shooting extension.

2 Related works

Mechanistic ODE models. In mechanistic modelling the equation \( f_\theta \) is predefined with a set of coefficients \( \theta \) to be fitted (Butcher and Goodwin, 2008). Several works have proposed embedding mechanistic models within Bayesian or Gaussian process models (Calderhead et al., 2008; Dondelinger et al., 2013; Macdonald et al., 2015). Recently both Julia and Stan have introduced support for Bayesian analysis of parametric ODEs (Rackauckas and Nie, 2017; Stan, 2021).

Free-form ODE models. Multiple works have proposed fitting unknown, non-linear and free-form ODE differentials with gradient matching (Ramsay et al., 2007) using splines (Henderson and Michailidis, 2014), Gaussian processes (Äijö and Lähdesmäki, 2009; Äijö et al., 2013; Ridderbusch et al., 2020; Wenk et al., 2020) or kernel methods (Heinonen and d’Alché-Buc, 2014). Recently, Heinonen et al. (2018) proposed accurate maximum a posteriori optimisation of vector fields with sensitivity equation gradients (Kokotovic and Heller, 1967). Neural ODEs (Chen et al., 2018) introduced adjoint gradients (Pontryagin et al., 1962) along with flexible black-box neural network vector fields. Several extensions to learning latent ODEs have been proposed (Yildiz et al., 2019; Rubanova et al., 2019). Bhouri and Perdikaris (2021) proposes a hybrid model combining neural networks and Gaussian processes for sparse ODE system discovery (Brunton et al., 2016).

Discrete-time state-space models. There is a large literature on Markovian state-space models that operate over discrete time increments (Wang et al., 2005; Turner et al., 2010; Frigola et al., 2014). Typically nonlinear state transition functions are model with Gaussian processes and applied to latent state estimation or system identification problems with dynamical systems (Eleftheriadis et al., 2017; Doerr et al., 2018; Ialongo et al., 2019). This paper will focus on continuous-time models and leave the study of discrete vs. continuous formulations for future work.

| Method         | ODE posterior | Freeform dynamics | Exact gradients | Reference                                      |
|----------------|---------------|-------------------|----------------|-----------------------------------------------|
| NeuralODE      | ×             | ✓                 | ✓              | Chen et al. (2018)                            |
| npODE          | ×             | ×                 | ✓              | Heinonen et al. (2018)                         |
| Gradient matching | ×            | ✓                 | ×              | Ramsay et al. (2007); Heinonen and d’Alché-Buc (2014) |
| Mechanistic GM | ✓             | ×                 | ×              | Dondelinger et al. (2013); Wenk et al. (2020)  |
| GPODE          | ✓             | ×                 | ✓              | this work                                     |

Table 1: Related work: for each method, we indicate if it can learn posterior over vector fields, does it assume an unknown system dynamics, and whether the inference is performed directly over the observations or on the empirical gradients.

3 Methods

We consider the problem of learning ODEs (1) and propose a Bayesian model to infer posteriors over the differential \( f(\cdot) \).

3.1 Bayesian modeling of ODEs using GPs

We assume a sequence of \( N \) observations \( Y = (y_1, y_2, \ldots, y_N)^T \in \mathbb{R}^{N \times D} \), with \( y_i \in \mathbb{R}^D \) representing the noisy observation of the unknown state \( x(t_i) \in \mathbb{R}^D \) at time \( t_i \). We assume a zero
mean vector-valued Gaussian process prior over $f$,

$$f(x) \sim GP(0, K(x, x')),$$  \hspace{1cm} (2)

which defines a distribution of functions $f(x)$ with covariance $\text{cov}[f(x), f(x')] = K(x, x')$, where $K(x, x') \in \mathbb{R}^{D \times D}$ is a matrix-valued kernel (Alvarez et al., 2012).

$$p(U) = \mathcal{N}(U|0, K_{ZZ})$$  \hspace{1cm} (3)

$$p(f|U, Z) = \mathcal{N}(f|\text{vec}(U), K_{XX} - AK_{ZZ}A^T),$$ \hspace{1cm} (4)

where $X = (x_1, x_2, \ldots, x_N)^T \in \mathbb{R}^{N \times D}$ collects all the intermediate state evaluations $x(t_i)$ encountered along numerical approximation of the true continuous ODE integral (1), $f = (f(x_1)^T, \ldots, f(x_N)^T)^T \in \mathbb{R}^{N \times D}$, $K_{XX}$ is a block-partitioned matrix of size $N' \times N'$ with $D \times D$ blocks, so that block $(K_{XX})_{i,j} = K(x_i, x_j)$, and $A = K_{XX}K_{ZZ}^{-1}$. For notational simplicity, we assume that the measurement time points are among the time points of the intermediate state evaluations.

The joint probability distribution follows

$$p(Y, f, U, x_0) = p(Y|f, x_0)p(f, U)p(x_0) = \prod_{i=1}^{N} p(y_i|f, x_0)p(f, U)p(x_0),$$ \hspace{1cm} (5)

where the conditional distribution $p(y_i|f, x_0) = p(y_i|x_i)$ computes the likelihood over ODE state solutions $x_i = x_0 + \int_0^1 f(x(\tau))d\tau$ for a single realization of vector field $f \sim p(f)$ and the initial state $x_0 \sim p(x_0)$.

### 3.2 Variational inference for GP-ODEs

In contrast to earlier approaches that estimate MAP solutions (Heinonen et al., 2018; Ridderbusch et al., 2020), our goal is to infer the posterior distribution $p(f, x_0|Y)$ of the vector field $f$ and initial value $x_0$ from observations $Y$. The posterior is intractable due to the non-linear integration map $x_0 \mapsto x(t)$.

We propose the stochastic variational inference framework (SVI) (Titsias, 2009; Hensman et al., 2013) for sparse GP-based ODE modelling. We introduce a factorized Gaussian posterior approximation for the inducing variables across state dimensions $q(U) = \prod_{d=1}^{D} \mathcal{N}(u_d|m_d, Q_d)$, $u_d \in \mathbb{R}^M$ where $m_d \in \mathbb{R}^M$, $Q_d \in \mathbb{R}^{M \times M}$ are the mean and covariance parameters of the variational Gaussian posterior approximation for the inducing variables. We treat the inducing locations $Z$ as optimized hyperparameters\(^1\). The posterior distribution for the variational approximation is then

$$q(f) = \int p(f|U)q(U) dU$$

$$= \int \mathcal{N}(\text{vec}(U), K_{XX} - AK_{ZZ}A^T) q(U) dU.$$ \hspace{1cm} (6)

The posterior inference goal then translates to estimating the posterior $p(U, x_0|Y)$ of the inducing points $U$ and initial state $x_0$, Under variational inference the learning objective translates into

\(^1\)See Rossi et al. (2021) for discussion on inducing locations inference.
maximizing the evidence lowerbound (ELBO) (Blei et al., 2017),

\[
\log p(Y) \geq \sum_{i=1}^{N} \mathbb{E}_{q(f, x_0)} \log p(y_i | f, x_0) - \text{KL}[q(U) || p(U)] - \text{KL}[q(x_0) || p(x_0)] =: \mathcal{L},
\]

where we also assume posterior approximation \( q(x_0) = \mathcal{N}(\mu_0, \Sigma_0) \) for the initial state \( x_0 \).

### 3.3 Sampling ODEs from Gaussian processes

The Picard-Lindelöf theorem (Lindelöf, 1894) requires valid ODE systems to define unique solutions to the initial value problem (IVP) (1). Our goal is to efficiently sample GP functions \( f(\cdot) \sim q(f) \) (7), such that we can evaluate the sample function \( f(x(t)) \) at arbitrary states \( x(t) \) encountered during ODE forward integration, while accounting for both the inducing and interpolation distributions of Equation (7). Function-space sampling of such GPs has prohibitive cubic complexity (Rasmussen and Williams, 2006; Ustyuzhaninov et al., 2020), while the more efficient weight-space sampling with Fouriers cannot express the posterior (7) non-stationarity (Wilson et al., 2020).

We use the decoupled sampling that decomposes the posterior into two parts (Wilson et al., 2020),

\[
\begin{align*}
\mathbb{E}_{q(f)} f(x) | U &= f(x) + K(x, Z)K(Z, Z)^{-1}(U - f) \\
&\approx \sum_{i=1}^{S} w_i \phi_i(x) + \sum_{j=1}^{M} \nu_j K(x, z_j),
\end{align*}
\]

where we use \( S \) Fourier bases \( \phi_i(\cdot) \) with \( w_i \sim \mathcal{N}(0, I) \) (Rahimi and Recht, 2007; Brault et al., 2016) to represent the stationary prior, and function basis \( K(\cdot, z_j) \) for the posterior update with \( \nu = K(Z, Z)^{-1}(U - \Phi W) \), \( \Phi = \phi(Z) \in \mathbb{R}^{M \times S} \), \( W \in \mathbb{R}^{S \times D} \). By combining these two steps, we can accurately evaluate functions from the posterior (7) in linear time at arbitrary locations. We refer the reader to the supplementary section for more details.

### 3.4 Augmenting the ODE model with shooting system

A key bottleneck in ODE modeling is the poor gradient descent performance over long integration times \( x_{0:T} \), which can exhibit vanishing or exploding gradients (Haber and Ruthotto, 2017; Choromanski et al., 2020; Kim et al., 2021). Earlier approaches tackled this issue mainly with more accurate numerical solvers (Zhuang et al., 2020, 2021). The nonlinearity of the integration map \( x_0 \mapsto x_T \) motivates us to instead propose to segment the full integration \( x_{0:T} \) into short segments, which are easier to optimize and can be trivially parallelized (Aydogmus and Tor, 2021). This is denoted as the ‘multiple shooting’ method in optimal control literature (Osborne, 1969; Bock and Plitt, 1984);
We validate the proposed method on Van der Pol (VDP) and FitzHugh–Nagumo (FHN) systems and also on the task of learning human motion dynamics (MoCap). We use 16 inducing points in VDP and FHN experiments and 100 inducing points for the MoCap experiments. We consistently use squared exponential kernel with ARD and optimize kernel lengthscales, signal variance, noise variance, and inducing locations as hyperparameters. For the shooting version of GPODE, we found
the inference of kernel signal variance to be problematic. We identified a constant scaling factor of 0.1 on the inducing KL term in equation 15 to fix this issue, inspired by VAE balancing factors (Alemi et al., 2018).

We use the implicit dopr15 solver with tolerance parameters \( \text{rtol} = 1e^{-5} \) and \( \text{atol} = 1e^{-5} \), and use the adjoint method for computing loss gradients with torchdiffeq\(^2\) package (Chen et al., 2018). We repeat all the experiments 5 times with random initialization and report means and standard errors.

4.1 Learning Van der Pol dynamics

We first illustrate the effectiveness of the proposed method by inferring the vector field posterior on a two-dimensional VDP (see Figure 3),

\[
\dot{x}_1 = x_2, \quad \dot{x}_2 = -x_1 + 0.5x_2(1-x_1^2), \quad x_1(0) = -1.5, \quad x_2(0) = 2.5.
\]

\(^2\)https://github.com/rtqichen/torchdiffeq
We demonstrate the necessity of the shooting formulation for working with long training trajectories. We use the VDP system with four observations per unit of time for $T = (25, 40, 55)$ corresponding to $N = (100, 160, 220)$ observed states. We also vary the observation variance as $\sigma^2 = (0.01, 0.05, 0.1)$. We test the model for forecasting additional 50 time points.

**4.2 Learning with missing observations**

We illustrate the usefulness of learning Bayesian ODE posteriors under missing data with the FHN oscillator

\[
\begin{align*}
    \dot{x}_1 &= 3(x_1 - x_1^3/3 + x_2), \\
    \dot{x}_2 &= (0.2 - 3x_1 - 0.2x_2)/3.
\end{align*}
\] (19)

We generate a training sequence by simulating 25 regularly-sampled time points from $t \in [0, 5]$ with added Gaussian noise with $\sigma^2 = 0.025$. We remove all observations at quadrant $x_1 > 0, x_2 < 0$ and evaluate model accuracy in this region. Figure 4 shows that all models adequately learn smooth forecasts of missing states. The point estimates of npODE and NeuralODE have biases, while the GPODE posterior captures the uncertainty well (See Table 2).

**4.3 Learning long trajectories with the shooting formulation**

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| Task 1: Forecasting | Task 2: Varying $x_0$ |
|---------------------|-----------------------|
| GP gradient matching| MNLL (↓) 1.47 ± 0.02  |
|                     | MSE (↓) 1.27 ± 0.01   |
| NeuralODE           | MNLL (↓) -            |
|                     | MSE (↓) 2.45 ± 0.18   |
| npODE               | MNLL (↓) 7.42 ± 1.88  |
|                     | MSE (↓) 0.29 ± 0.06   |
| GPODE               | MNLL (↓) 0.60 ± 0.03  |
|                     | MSE (↓) 0.13 ± 0.01   |

Table 3: VDP system learning performance on forecasting (task 1) and varying initial state tasks (task 2). We report mean ± standard error over 5 runs from different random initializations, best values bolded. (†): higher is better, (↓) lower is better

Figure 4: Learning FHN with gaps in data (gray region). The GPODE results in a useful posterior under data scarcity, while both NeuralODE and npODE result in some biases.

We simulate a trajectory of 50 regularly-sampled time points inside $t \in [0, 7]$, and add Gaussian noise with $\sigma^2 = 0.05$ to generate the training data. We explore two task scenarios: (1) forecasting the system dynamics between $t \in [7, 14]$, (2) forecasting the system from new initial states. In task 2, we generate new initial states by taking 100 samples from a Gaussian $\mathcal{N}(y_0, 0.04^2 I)$. We compare our GPODE model with npODE (Heinonen et al., 2018), NeuralODE (Chen et al., 2018), and gradient matched GPs (Ridderbusch et al., 2020).

Figure 3(b) shows that GPODE learns a vector field posterior, whose posterior mean closely matches the ground truth with low variance (blue regions) near the observed data. The posterior reduces back to the prior away from data (orange regions), indicating a good uncertainty characterization. The npODE seems to overfit, while the gradient matching GP cannot fit the model adequately. NeuralODE learns an appropriate vector field, but its long-term forecasting is biased. The NeuralODE and npODE models do not represent uncertainty, while the gradient matching GP posterior is poorly fit. A quantitative evaluation of the model fits in Table 3 indicate superior performance of GPODE.

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\] (19)

We generate a training sequence by simulating 25 regularly-sampled time points from $t \in [0, 5]$ with added Gaussian noise with $\sigma^2 = 0.025$. We remove all observations at quadrant $x_1 > 0, x_2 < 0$ and evaluate model accuracy in this region. Figure 4 shows that all models adequately learn smooth forecasts of missing states. The point estimates of npODE and NeuralODE have biases, while the GPODE posterior captures the uncertainty well (See Table 2).

**Table 2: Missing data results on the FHN system.**

|                | MNLL (↓) | MSE (↓) |
|----------------|----------|---------|
| NeuralODE      | -        | 0.18 ± 0.00 |
| npODE          | 6.49 ± 1.49 | 0.08 ± 0.01 |
| GPODE          | **0.09 ± 0.05** | **0.07 ± 0.02** |

We simulate a trajectory of 50 regularly-sampled time points inside $t \in [0, 7]$, and add Gaussian noise with $\sigma^2 = 0.05$ to generate the training data. We explore two task scenarios: (1) forecasting the system dynamics between $t \in [7, 14]$, (2) forecasting the system from new initial states. In task 2, we generate new initial states by taking 100 samples from a Gaussian $\mathcal{N}(y_0, 0.04^2 I)$. We compare our GPODE model with npODE (Heinonen et al., 2018), NeuralODE (Chen et al., 2018), and gradient matched GPs (Ridderbusch et al., 2020).

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Figure 6 demonstrates that vanilla-GPODE and neuralODE fail to fit the data with long sequences on all noise levels. In contrast, inference for the shooting model is successful in all settings. The npODE is remarkably robust to long trajectories. All methods use high-performance gradient matching initialization for a realistic study (see supplementary).

Figure 5 shows a runtime trace comparison between vanilla GPODE and the shooting variant in wall-clock time for a fixed budget of 2000 optimization steps on VDP system with $N = 100$, $T = 25$ and $\sigma^2 = 0.01$. The shooting model converges approximately 10 times faster. The speedup stems from the parallelization of the shooting ODE solver since the shooting method splits the full IVP problem into numerous short and less non-linear IVPs. In addition, the shooting method relaxes the inference problem with its auxiliary augmentation. This experiment was conducted on a system with Nvidia GeForce GTX 1660S GPU.

Figure 6: Varying sequence length and observation noise: shooting formulation makes GPODE feasible for long sequences, outperforming the non-shooting version and NeuralODE. The optimization for npODE is surprisingly good here. We report the results for different levels of observation noise on the VDP system.

4.4 Learning human motion dynamics

Figure 7: Learning the walking dynamics of subject 39: The true dynamics and predicted dynamics (mean) for the first three components in PCA space are shown in (a). Corresponding trajectories in the observation space for 6 different sensors are shown in (b) (We do not plot the observation noise variance for GPODE and npODE variants)
We learn the dynamics of human motion from noisy experimental data from CMU MoCap database for three subjects 09, 35 and 39. The dataset consists of 50 sensor readings from different parts of the body while walking or running. We follow the preprocessing of Wang et al. (2008) and center the data. The dataset was further split into train, test, and validation sequences (see the supplementary section for details on data size). We observed that both the NeuralODE and npODE models suffer from over-fitting, and we remedy this by applying early stopping by monitoring the validation loss during optimization.

We project the original 50-dimensional data into a 5-dimensional latent space using PCA and learn the dynamics in the latent space (Heinonen et al., 2018). To compute the data likelihood, we project the latent dynamics back to the original data space by inverting the PCA. We divide the experiment into sub-tasks MoCap-short and MoCap-long, based on the length of the sequence considered for model training (see the supplementary section for more details on the experimental setup). We measure the predictive performance on unseen test sequences in both tasks.

| MNLL (\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{\text{
the inference for shooting approximations similar to the works (Ialongo et al., 2019) from discrete domains.

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Supplementary material for Bayesian inference of ODEs with Gaussian processes

Figure 1: Plate diagrams: in the vanilla GPODE formulation (a), the initial state distribution \( x_0 \) is integrated forward in time to match all the observations \( \{ y_1, y_2, \ldots, y_N \} \) forming a full trajectory. The shooting version (b) splits the full trajectory into multiple subintervals. Every subinterval \( i \) starts with an approximated state distribution \( s_i \), which is integrated forward to match the next observation \( y_{i+1} \). In addition, the state evolution from the previous shooting variable is matched to the variational shooting approximation at the current state.

### Inference for the vanilla GPODE model

**The model.** We consider the problem of inferring an ODE system

\[
\begin{align*}
y(t) &= x(t) + \epsilon \\
x(t) &= x_0 + \int_0^t f(x(\tau))d\tau
\end{align*}
\]

from some noisy observations \( y(t) \) of the true system state \( x(t) \in \mathbb{R}^D \), whose evolution over time \( t \in \mathbb{R}_+ \) follows a differential equation vector field

\[
\dot{x}(t) = \frac{dx(t)}{dt} := f(x(t)), \quad f : \mathbb{R}^D \mapsto \mathbb{R}^D
\]

starting from initial state \( x_0 \in \mathbb{R}^D \). Our goal is to learn the underlying ODE vector field \( f \).

We propose a Gaussian process prior for the differential function

\[
\begin{align*}
f(x) &\sim \mathcal{GP}(0, k(x, x')) \\
p(f) &= \mathcal{N}(f|0, K_{xx})
\end{align*}
\]

Following Titsias (2009) for sparse inference of GPs using inducing variables, we augment the full model with inducing values \( U = (u_1, \ldots, u_M)^T \in \mathbb{R}^{M \times D} \) and inducing locations \( Z = (z_1, \ldots, z_M)^T \in \mathbb{R}^{M \times D} \), which results in a low-rank GP

\[
\begin{align*}
p(U) &= \mathcal{N}(U|0, K_{ZZ})
p(f|U) &= \mathcal{N}(f|\text{vec}(U), K_{xx} - AK_{ZZ}A^T),
\end{align*}
\]

where \( X = (x_1, x_2, \ldots, x_N)^T \in \mathbb{R}^{N' \times D} \) collects all the intermediate state evaluations \( x(t_i) \) encountered along numerical approximation of the true continuous ODE integral (2), \( f = (f(x_1)^T, \ldots, f(x_N)^T)^T \in \mathbb{R}^{N'D \times 1} \), \( K_{XX} \) is a block-partitioned matrix of size \( N' D \times N' D \) with \( D \times D \) blocks, so that block \( (K_{XX})_{i,j} = k(x_i, x_j) \), and \( A = K_{xz}K_{zz}^{-1} \).
The joint model. The joint probability of the model is

$$p(Y, f, U, x_0) = \prod_{i=1}^{N} p(y_i|f, x_0)p(f|U)p(U)p(x_0)$$  \hspace{1cm} (9)

$$= \prod_{i=1}^{N} p(y_i|f, x_0) p(f|U) p(U) p(x_0),$$  \hspace{1cm} (10)

where we assume a standard Gaussian prior $p(x_0) = \mathcal{N}(0, I)$ for the unknown initial state $x_0$.

Inference. Our primary goal is to learn the vector field $f$ by inferring the model posterior $p(f, U, x_0|y)$, which is intractable. We resort to stochastic variational inference Hensman et al. (2013), and introduce a factorized Gaussian posterior approximation for the inducing variables across state dimensions

$$q(U) = \prod_{d=1}^{D} \mathcal{N}(u_d|m_d, Q_d),$$ \hspace{1cm} (11)

where, $u_d \in \mathbb{R}^d$ and $m_d \in \mathbb{R}^d$, $Q_d \in \mathbb{R}^{M \times M}$ are the mean and covariance parameters of the variational Gaussian posterior approximation for the inducing variables. The Gaussian process posterior process with an inducing approximation can be written as

$$q(f) = \int p(f|U)q(U)dU$$ \hspace{1cm} (12)

$$= \int \mathcal{N}(f|\text{vec}(U), K_{XX} - AK_{ZZ}A^T) q(U)dU.$$ \hspace{1cm} (13)

We also introduce posterior approximation for the initial state variable $x_0$.

$$q(x_0) = \mathcal{N}(x_0|m_0, S_0).$$ \hspace{1cm} (14)

This results in a variational joint posterior approximation

$$q(f, U, x_0) = q(f, U)q(x_0)$$ \hspace{1cm} (15)

$$= p(f|U)q(U)q(x_0),$$ \hspace{1cm} (16)

ELBO. With the above model specification, under variational inference the posterior approximations, the evidence lower bound (ELBO) $\log p(Y) \geq \mathcal{L}$ can be written as,

$$\mathcal{L} = \int \int \int q(f, U, x_0) \log \frac{p(Y, f, U, x_0)}{q(f, U, x_0)} dfdUdx_0$$ \hspace{1cm} (17)

$$= \int \int \int q(f, U, x_0) \log \prod_{i=1}^{N} \frac{p(y_i|f, x_0)}{\mathcal{L}_y} \frac{p(f|U)}{\mathcal{L}_f} \frac{p(U)}{\mathcal{L}_u} \frac{p(x_0)}{\mathcal{L}_{x_0}} dfdUdx_0.$$ \hspace{1cm} (18)

hence the ELBO decomposes into three additive terms

$$\mathcal{L} = \mathcal{L}_y + \mathcal{L}_u + \mathcal{L}_{x_0},$$ \hspace{1cm} (19)

where each term contains the (relevant parts of) expectation over $q(f, U, x_0)$.

Likelihood term. The variational likelihood term $\mathcal{L}_y$ is an expectation of the likelihood wrt the variationally marginalized vectorfield posterior $q(f)$, and the initial state distribution $q(x_0)$,

$$\mathcal{L}_y = \int \int q(f, x_0) \log p(y|f, x_0) df dx_0$$ \hspace{1cm} (20)

$$= \sum_{i=1}^{N} \mathbb{E}_{q(f, x_0)} \log p(y_i|f, x_0).$$ \hspace{1cm} (21)
A sparse GP posterior of the form (31) can be decomposed into two parts using Matheron’s rule (30),

\[ p(y_i | f, x_0) = \int p(y_i | f(x_0)) \, dx_0 \]

where we sum over \( S \) reparameterized samples \( f(x_0) \sim q(f) \) and \( x_0 \sim q(x_0) \).

**Inducing KL.** This term corresponds to the KL divergence between variational posterior and the prior distribution of inducing values. This term can be derived analytically as the KL between multivariate Gaussians.

\[
\mathcal{L}_u = \int q(U) \log \frac{p(U)}{q(U)} \, dU \\
= \sum_{d=1}^{D} \int q(u_d) \log \frac{p(u_d)}{q(u_d)} \, du_d \\
= -\sum_{d=1}^{D} KL[q(u_d) || p(u_d)]
\]

**Initial state KL.** This term corresponds to the KL divergence between variational posterior and the prior distribution of the initial state. With an assumption of Gaussian prior and variational posterior, this term can also be derived analytically.

\[
\mathcal{L}_{x_0} = \int q(x_0) \log \frac{p(x_0)}{q(x_0)} \, dx_0 \\
= -KL[q(x_0) || p(x_0)]
\]

**Complete ELBO.** The full ELBO is then

\[
\mathcal{L} = \sum_{i=1}^{N} \mathbb{E}_q(f, x_0) \log p(y_i | f, x_0) - KL[q(U) || p(U)] - KL[q(x_0) || p(x_0)]
\]

**Decoupled sampling of GPODEs**

In this section we provide details for simulating valid ODE trajectories from a GP vector field posterior of the form

\[
q(u) = \mathcal{N}(m, Q),
\]

\[
q(f) = \int p(f|u)q(u) \, du
\]

\[
= \int \mathcal{N}(f|Au, K_{XX} - AK_{ZZ}A^T) \, q(u) \, du,
\]

where \( A = K_{xz}K_{zz}^{-1} \) and \( m \in \mathbb{R}^M, Q \in \mathbb{R}^{M \times M} \) are the variational mean and covariance parameters of the Gaussian posterior approximation for inducing variables. For simplicity we have considered a scalar valued GP, but it straightforward to extend this approach to vector-valued GPs.

A sparse GP posterior of the form (31) can be decomposed into two parts using Matheron’s rule (Corollary 2 Wilson et al. (2020)),

\[
f(x)|u = f(x) + k(x, Z)K(Z, Z)^{-1}(u - f_Z).
\]
Wilson et al. (2020) propose a decoupled sampling from the prior by using different bases for the prior and update terms. In particular, they propose Fourier basis functions for the prior term and canonical basis for the update term respectively

\[
    f(x) \mid u \approx \sum_{i=1}^{S} w_i \phi_i(x) + \sum_{j=1}^{M} \nu_j K(x, z_j),
\]

where we use \( S \) Fourier bases \( \phi_i(\cdot) \) with \( w_i \sim \mathcal{N}(0, 1) \) (Rahimi and Recht, 2007; Brault et al., 2016) to represent the stationary prior, and function basis \( K(\cdot, z_j) \) for the posterior update with \( \nu = K(Z, Z)^{-1}(u - \Phi w) \), \( \Phi = \phi(Z) \in \mathbb{R}^{M \times S} \), \( w \in \mathbb{R}^S \). We can evaluate functions from the posterior (31) in linear time at arbitrary locations.

For the experimental results presented in the paper, we use squared exponential kernel for which we can compute the feature maps \( \phi_i(x) = \sqrt{\sigma_f^2} (\cos x^T \omega_i, \sin x^T \omega_i) \) where \( \omega_i \) is sampled proportional to the spectral density of the squared exponential kernel \( \omega_i \sim \mathcal{N}(0, \Lambda^{-1}) \), \( \Lambda \) is a diagonal matrix collecting lengthscale parameters of the kernel \( \Lambda = \text{diag}(l_1^2, l_2^2, \ldots, l_D^2) \) and \( \sigma_f^2 \) is the signal variance parameter. In the case of the squared exponential kernel, this results in \( 2S \) feature maps \( \phi(x) \in \mathbb{R}^{2S} \), for which we sample weights \( w \in \mathbb{R}^{2S} \) from the standard Normal \( w_i \sim \mathcal{N}(0, 1) \). By fixing random samples of feature maps \( \phi(\cdot) \), corresponding weights \( w \) and inducing values \( u \) for an ODE integration call, we can sample a unique ODE trajectory from a posterior vector field of the form (31).

### Probabilistic shooting derivation for GPODE

**The model.** We consider the problem of inferring an ODE system

\[
    y(t) = x(t) + \epsilon
\]

\[
    x(t) = x_0 + \int_{0}^{t} f(x(\tau)) d\tau,
\]

from some noisy observations \( y(t) \) of the true system state \( x(t) \in \mathbb{R}^D \), whose evolution over time \( t \in \mathbb{R}_+ \) follows a differential equation

\[
    \dot{x}(t) = \frac{dx(t)}{dt} := f(x(t)), \quad f: \mathbb{R}^D \mapsto \mathbb{R}^D
\]

starting from initial state \( x_0 \in \mathbb{R}^D \). Our goal is to learn the underlying ODE vector field \( f \).

**Shooting augmentation.** We propose an augmented ‘shooting’ ODE system

\[
    y(t_i) = x(t_i) + \epsilon
\]

\[
    x(t_i) = s_{i-1} + \int_{t_{i-1}}^{t_i} f(x(\tau)) d\tau
\]

\[
    s(t_i) = s_{i-1} + \int_{t_{i-1}}^{t_i} f(s(\tau)) d\tau,
\]

where we introduce an additional shooting ODE \( s(t) \) and segment the state function into \( N \) pieces that branch from the shooting model, while both models follow the same differential \( f \). The augmented system is equivalent to the original ODE system since the differential is shared.

**Gaussian process ODE.** We propose a Gaussian process prior for the differential function

\[
    f(x) \sim \mathcal{GP}(0, k(x, x'))
\]

\[
    p(f) = \mathcal{N}(f|0, K_{xx}).
\]

In addition, we augment the full model with inducing values \( U = (u_1, \ldots, u_M)^T \in \mathbb{R}^{M \times D} \) and inducing locations \( Z = (z_1, \ldots, z_M)^T \in \mathbb{R}^{M \times D} \), which results in a low-rank GP

\[
    p(U) = \mathcal{N}(U|0, K_{ZZ})
\]

\[
    p(f|U) = \mathcal{N}(f|\text{Avec}(U), K_{xx} - \text{AK}_{ZZ}A^T),
\]

where \( A = K_{xz}K_{zz}^{-1} \).
The joint model. The joint probability of the model is

\[
p(Y, X, S, f, U) = \prod_{i=1}^{N} p(y_i|x_i)p(x_i|s_{i-1}, f) \prod_{i=1}^{N-1} p(s_i|s_{i-1}, f)p(s_0)p(f|U)p(U)
\]

(44)

\[
= \prod_{i=1}^{N} p(y_i|x_i)p(x_i|s_{i-1}, f) \prod_{i=1}^{N-1} p(s_{i-2}|s_{i-1}, f)p(s_0)p(f|U)p(U),
\]

(45)

where \( X = (x_1, x_2, \ldots, x_N)^T \in \mathbb{R}^{N \times D} \) collects all the state distributions \( x(t_i) \) at observation times and \( S = (s_0, s_1, \ldots, s_{N-1})^T \in \mathbb{R}^{N \times D} \) collects all shooting variables.

We also note that observations are at indices \( 1, \ldots, N \), while the shooting variables are always one behind the observations at \( 0, \ldots, N - 1 \) (see plate diagram 1 (b)).

Inference. Our primary goal is to learn the vector field \( f \) by inferring the model posterior \( p(X, X, f, U|Y) \), which is intractable. In a similar way to non-shooting GPODEs, we introduce a factorized Gaussian posterior approximation for the inducing variables across state dimensions

\[
q(U) = \prod_{d=1}^{D} \mathcal{N}(u_d|m_d, Q_d),
\]

(46)

where, \( u_d \in \mathbb{R}^M \) and \( m_d \in \mathbb{R}^M, Q_d \in \mathbb{R}^{M \times M} \) are the mean and covariance parameters of the variational Gaussian posterior approximation for the inducing variables. The Gaussian process posterior process with an inducing approximation can be written as

\[
q(f) = \int p(f|U)q(U)dU = \int \mathcal{N}(f|\text{vec}(U), K_{XX} - AK_{zz}A^T) q(U)dU.
\]

(47)

(48)

Next, we introduce a factorized Gaussian posterior approximations for the shooting variables \( S \) as well,

\[
q(S) = \prod_{i=0}^{N-1} q(s_i) = \prod_{i=0}^{N-1} \mathcal{N}(s_i|a_i, \Sigma_i).
\]

(49)

where, \( a_i \in \mathbb{R}^D \) and \( \Sigma_i \in \mathbb{R}^{D \times D} \) are the mean and covariance parameters of the variational Gaussian posterior approximation for the shooting variables.

This results in a variational joint posterior approximation

\[
q(X, S, f, U) = q(X, S|f)q(f, U)
\]

(50)

\[
= \prod_{i=1}^{N} p(x_i|s_{i-1}, f) \prod_{i=0}^{N-1} q(s_i)p(f|U)q(U).
\]

(51)

ELBO. Under variational inference the posterior approximations \( q \) are optimised to match the true posterior in the KL sense,

\[
\arg\min_q \text{KL} \left[ q(X, S, f, U) \ || \ p(X, S, f, U|Y) \right].
\]

(52)

This is equivalent to maximizing the evidence lower bound (ELBO) \( \log p(Y) \geq \mathcal{L} \),

\[
\mathcal{L} = \int \int \int \int q(X, S, f, U) \log \frac{p(Y, X, S, f, U)}{q(X, S, f, U)} dX dS dU df
\]

(53)

\[
= \int \int \int \int q(X, S, f, U) \log \left\{ \prod_{i=1}^{N} \left[ \frac{p(y_i|x_i)}{p(y_i|x_i)} \left[ \frac{p(x_i|s_{i-1}, f)}{p(x_i|s_{i-1}, f)} \right] \right] \right\} dX dS dU df
\]

(54)

\[
= \prod_{i=1}^{N-1} \left[ \frac{p(s_i|s_{i-1}, f)}{q(s_i)} \right] \left[ \frac{p(s_0)}{q(s_0)} \right] \left[ \frac{p(U)}{q(U)} \right] \left[ \frac{p(f|U)}{q(f|U)} \right] \left[ \frac{p(U)}{q(U)} \right] dX dS dU df.
\]
Two ratios cancel out, which results the ELBO decomposing into three additive terms

\[ \mathcal{L} = \mathcal{L}_y + \mathcal{L}_s + \mathcal{L}_0 + \mathcal{L}_u, \]  
(55)

where each term contains the (relevant parts of) expectation over \( q(X, S, f, U) \).

**Likelihood term.** The variational likelihood term \( \mathcal{L}_y \) is an expectation of the likelihood wrt the variationally marginalized state distributions \( q(x_i) \),

\[ \mathcal{L}_y = \iiint q(X, S, f, U) \log p(Y|X) dS df dU \]  
(56)

\[ = \int q(x_1) \cdots q(x_N) \log \prod_{i=1}^{N} p(y_i|x_i) dX \]  
(57)

\[ = \sum_{i=1}^{N} \mathbb{E}_{q(x_i)} \log p(y_i|x_i) \]  
(58)

with marginalized state distributions

\[ q(x_i) = \iiint q(x_i, s_{i-1}, f, U) ds_{i-1} df dU \]  
(59)

\[ = \int p(x_i|s_{i-1}, f)q(s_{i-1})q(f) ds_{i-1} df \]  
(60)

\[ = \int q_{\to}(x_i|f)q(f) df \]  
(61)

\[ = q_{\to}(x_i) \]  
(62)

which are “short” continuous-time normalizing flows \( q_{\to}(\cdot) \) from the previous shooting states \( q(s_{i-1}) \) and marginalised over vector fields \( q(f) \). We only need samples \( x_i \sim q_{\to}(x_i) \) for the Monte Carlo integration of the expected likelihood term. By taking reparameterized samples from the posteriors of the starting point \( q(s_i) \) and the vector field \( q(f) \), we can approximate the likelihood term as

\[ \mathcal{L}_y \approx \frac{1}{S} \sum_{s=1}^{S} \sum_{i=1}^{N} \log p(y_i|x_i^{(s)}), \]  
(63)

where we sum over \( S \) reparameterized samples

\[ x_i^{(s)} = s_{i-1}^{(s)} + \int_{t_{i-1}}^{t_i} f^{(s)}(s(\tau)) d\tau, \]  
(64)

and \( f^{(s)} \sim q(f), s_{i-1}^{(s)} \sim q(s_{i-1}) \).
**Shooting KL term.** The shooting term $\mathcal{L}_s$ is a variational expectation over the log ratio between the true shooting state evolution $p_{\to}^s (s(t_i))$ against the point-wise approximations $q(s_i)$,

\[
\mathcal{L}_s = \int \int \int q(X, S, f, U) \log \frac{\prod_{i=1}^{N-1} p(s_i|s_{i-1}, f)}{q(s_i)} dX dS df dU \\
= \int q(s_{N-1}) \cdots q(s_1) q(s_0) q(f) \log \frac{p(s_{N-1}|s_{N-2}, f) \cdots p(s_1|s_0, f)}{q(s_{N-1}) \cdots q(s_1)} dS df \\
= \sum_{i=1}^{N-1} \left[ \int q(f) q(s_i) q(s_{i-1}) \log p(s_i|s_{i-1}, f) ds_{i-1} ds_i df - \int q(s_i) \log q(s_i) ds_i \right] \\
= \sum_{i=1}^{N-1} \left[ \int q(f) q(s_i) \left( \int q(s_{i-1}) \log p(s_i|s_{i-1}, f) ds_{i-1} \right) ds_i df - \int q(s_i) \log q(s_i) ds_i \right] \\
= \sum_{i=1}^{N-1} \int q(s_i) \log q_{\to} (s_i) ds_i - \int q(s_i) \log q(s_i) ds_i \\
= - \sum_{i=1}^{N-1} \text{KL} \left[ q(s_i) \middle| q_{\to} (s_i) \right],
\]

where the $q_{\to} (s_i | f)$ is a change of density of a multivariate Gaussian $q_{i-1} (s_{i-1})$ through a realization of a non-linear ODE $f$ in (39), resulting in density of $s_i$. We can evaluate this density through the instantaneous change of variables formula (Chen et al., 2018),

\[
\log q_{\to} (s_i | f) = \log q_{i-1} (s_{i-1}) + \int_{t_{i-1}}^{t_i} \text{tr} \left( \frac{\partial f}{\partial s(t)} \right) dt \tag{72}
\]

\[
\tilde{s}_{i-1} = s_i + \int_{t_i}^{t_{i-1}} f(s(\tau)) d\tau. \tag{73}
\]

This procedure entails first integrating $s_i \sim q(s_i)$ at time $t_i$, backwards-in-time to find the originating value $\tilde{s}_{i-1}$ at time $t_{i-1}$. We can then evaluate the transformed density by computing $q_{i-1} (\tilde{s}_{i-1})$ and adjusting it with the density change.

Equivalently, we can compute the above term by doing the following forward integration

\[
\log q_{\to} (s_i | f) = \log q_i (\tilde{s}_i) + \int_{t_{i-1}}^{t_i} \text{tr} \left( \frac{\partial f}{\partial s(t)} \right) dt \tag{74}
\]

\[
\tilde{s}_i = s_{i-1} + \int_{t_{i-1}}^{t_i} f(s(\tau)) d\tau. \tag{75}
\]

In this procedure, we first sample the originating value $s_{i-1} \sim q(s_{i-1})$ at time $t_{i-1}$ and solve the system forward-in-time to generate $\tilde{s}_i$ at time $t_i$. We then evaluate the transformed density by computing $q_i (\tilde{s}_i)$ at time $t_i$ and adjusting it with the density change term. This is more efficient in practice, since it avoids the additional backward ODE solve.

The shooting KL term (71) can be decomposed a cross-entropy term an entropy term (70). The cross-entropy term involves the continuos-time normalizing flow and can be evaluated with Monte Carlo
intergration. The entropy term can be simplified analytically as entropy of multivariate Gaussians.

\[
L_s = - \sum_{i=1}^{N-1} \text{KL} \left[ q(s_i) \mid \mid q(s_i) \right] 
\]

\[
= \sum_{i=1}^{N-1} \left[ \int q(s_i) \log q(s_i) ds_i - \int q(s_i) \log q(s_i) ds_i \right] 
\]

\[
\approx \sum_{i=1}^{N-1} \left[ \frac{1}{S} \sum_{s=1}^{S} \log q(s_i) [q(s_i) | f(s)] - \int q(s_i) \log q(s_i) ds_i \right] 
\]

where we take \( S \) reparameterized samples \( s_i^{(s)} \sim q(s_i) \) and \( f(s) \sim q(f) \).

**Initial state KL.** This term corresponds to the KL divergence between variational posterior and the prior distribution of the initial state. With the assumption of Gaussian prior and variational posterior, this term can also be derived analytically,

\[
L_0 = \int q(s_0) \log \frac{p(s_0)}{q(s_0)} ds_0 
\]

\[
= - \text{KL} \left[ q(s_0) \mid \mid p(s_0) \right] 
\]

**Inducing KL.** This term corresponds to the KL divergence between variational posterior and prior distribution of inducing values. This term can also be derived analytically as the KL between multivariate Gaussians.

\[
L_u = \int q(U) \log \frac{p(U)}{q(U)} dU 
\]

\[
= \sum_{d=1}^{D} \int q(u_d) \log \frac{p(u_d)}{q(u_d)} du_d 
\]

\[
= - \sum_{d=1}^{D} \text{KL} \left[ q(u_d) \mid \mid p(u_d) \right] 
\]

**Complete ELBO.** The full ELBO is then

\[
\mathcal{L} = \sum_{i=1}^{N} \mathbb{E}_{q_{-i}(x_i)} \log p(y_i | x_i) - \sum_{i=1}^{N-1} \text{KL} \left[ q(s_i) \mid \mid q(s_i) \right] 
\]

\[
- \text{KL}[q(s_0) \mid \mid p(s_0)] - \text{KL}[q(u) \mid \mid p(u)] 
\]

**Experiments**

**Optimization setup**

We use Adam (Kingma and Ba, 2014) optimizer and jointly train all the variational parameters and hyperparameters. The complete list of optimized parameters, along with additional method-specific details, are given below.

**Vanilla GPODE model.** We use ‘whitened’ representation for inducing variables and optimize following parameters against the evidence lowerbound.

- Variational posterior parameters for inducing variables \( q(U) \) and initial states \( q(x_0) \) - mean and covariance parameters of the Gaussian approximation.
- Inducing locations \( Z \).
- Likelihood parameters - noise variance parameter in case of Gaussian likelihood.
- Kernel parameters - lengthscales and signal variance parameters in case of squared exponential kernel.
**Shooting GPODE model.** We use ‘whitened’ representation for inducing variables and optimize the following parameters against the evidence lower bound.

- Variational posterior parameters for inducing variables $q(U)$ and shooting states $q(S)$ - mean and covariance parameters of the Gaussian approximation.

- Inducing locations $Z$.

- Likelihood parameters - noise variance parameter in case of Gaussian likelihood.

- Kernel parameters - length scales and signal variance parameters in case of the squared exponential kernel.

**npODE model.** We use ‘whitened’ representation for inducing variables, maximum a posteriori (MAP) objective, and optimize following parameters:

- Inducing values $U$ and locations $Z$.

- Likelihood parameters - noise variance parameter in case of Gaussian likelihood.

- Kernel parameters - length scales and signal variance parameters in case of the squared exponential kernel.

**NeuralODE model.** We use tanh activation and a fully connected block with one hidden layer having 32 units in Van der Pol/ Fitz-Hugh Nagumo experiments and 64 hidden units in CMU MoCap experiments. All the network parameters were optimized against L1 loss.

**Gradient initialization strategy**

In case of sparse Gaussian process model with inducing variables, we initialize the vector field with empirical gradients from the observed data. We first initialize inducing locations $Z$ as $k$means cluster centers of observations $\hat{Y}$. Next we compute empirical gradient estimates, $\tilde{Y} = (y_2 - y_1, y_3 - y_2, \ldots, y_N - y_{N-1})$ at locations $\tilde{Y} = (y_1, y_2, \ldots, y_{N-1})$ and initialize inducing values $U$ as the GP mean interpolation of empirical gradients at inducing locations.

$$U = \Delta t \cdot K(Z, \hat{Y}) K(\hat{Y}, \hat{Y})^{-1} \hat{Y},$$

where $\Delta t$ is the time difference between two consecutive observations in the dataset.

**CMU MoCap dataset**

The dataset used in this experiment was obtained from [http://mocap.cs.cmu.edu/](http://mocap.cs.cmu.edu/). The database consists of sensor recordings for different activities in .amc files. We use data for three subjects 09, 35, and 39. The action sequences considered for train, validation and test purposes are given in table 1. The training sequences and their lengths were selected to include at least one full cycle of the dynamics while learning the model.
Table 1: For each subject (a), we report the activity considered for the experiment (b), the data split train/validation/test (c), the number of sequences considered for the corresponding split (d), and the files used in the corresponding split (e).

| Subject | Activity | Split  | # Sequences | Files |
|---------|----------|--------|-------------|-------|
| 09      | running  | train  | 6           | 05.amc, 06.amc, 07.amc, 08.amc, 09.amc, 11.amc |
|         |          | validation | 2        | 01.amc, 02.amc |
|         |          | test     | 2           | 03.amc, 04.amc |
| 35      | walking  | train  | 16          | 01.amc, 02.amc, 03.amc, 04.amc, 05.amc, 06.amc, 07.amc, 08.amc, 09.amc, 10.amc, 11.amc, 12.amc, 13.amc, 14.amc, 15.amc, 16.amc |
|         |          | validation | 3        | 28.amc, 29.amc, 30.amc |
|         |          | test     | 4           | 31.amc, 32.amc, 33.amc, 34.amc |
| 39      | walking  | train  | 6           | 01.amc, 02.amc, 07.amc, 08.amc, 09.amc, 10.amc |
|         |          | validation | 2        | 03.amc, 04.amc |
|         |          | test     | 2           | 05.amc, 06.amc |

Table 2: For each subject (a), we report the experiment type (b), the data split train/validation/test (c), and the number of observations considered for the corresponding split (d).

| Subject | Experiment Type | Split  | Sequence Length |
|---------|----------------|--------|-----------------|
| 09      | short          | train  | 50              |
|         |                | validation | 120          |
|         |                | test     | 120             |
|         | long           | train  | 100             |
|         |                | validation | 120          |
|         |                | test     | 120             |
| 35      | short          | train  | 50              |
|         |                | validation | 300          |
|         |                | test     | 300             |
|         | long           | train  | 250             |
|         |                | validation | 300          |
|         |                | test     | 300             |
| 39      | short          | train  | 100             |
|         |                | validation | 300          |
|         |                | test     | 300             |
|         | long           | train  | 250             |
|         |                | validation | 300          |
|         |                | test     | 300             |