Unscented Gaussian Process Latent Variable Model: learning from uncertain inputs with intractable kernels

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Abstract
The Gaussian Process (GP) framework flexibility has enabled its use in several data modeling scenarios. The setting where we have unavailable or uncertain inputs that generate possibly noisy observations is usually tackled by the well known Gaussian Process Latent Variable Model (GPLVM). However, the standard variational approach to perform inference with the GPLVM presents some expressions that are tractable for only a few kernel functions, which may hinder its general application. While other quadrature or sampling approaches could be used in that case, they usually are very slow and/or non-deterministic. In the present paper, we propose the use of the unscented transformation to enable the use of any kernel function within the Bayesian GPLVM. Our approach maintains the fully deterministic feature of tractable kernels and presents a simple implementation with only moderate computational cost. Experiments on dimensionality reduction and multistep-ahead prediction with uncertainty propagation indicate the feasibility of our proposal.

1 Introduction
Gaussian Processes (GP) models have been widely used in the machine learning community as a Bayesian approach to nonparametric kernel-based learning, enabling full probabilistic predictions (Rasmussen and Williams, 2006). Due to its flexibility, the GP framework has been applied in several contexts, such as semi-supervised learning (Damianou and Lawrence, 2015), dynamical modeling (Eleftheriadis et al., 2017; Frigola-Alcade et al., 2014; Mattos et al., 2016), variational autoencoders (Casale et al., 2018; Eleftheriadis et al., 2016) and hierarchical modeling (Havasi et al., 2018; Salimbeni and Deisenroth, 2017).

The works above have in common an important building block: the GP Latent Variable Model (GPLVM), proposed by Lawrence (2004) to handle learning scenarios where we have uncertain inputs. GPLVM was extended by Titsias and Lawrence (2010) with a Bayesian training approach (Bayesian GPLVM) and later by Damianou and Lawrence (2013) in a multilayer setting (Deep GPs).

The variational approach by Titsias and Lawrence (2010) for the Bayesian GPLVM presents calculations that are tractable for few choices for the kernel function, such as the radial basis function (RBF) kernel. However, it has been pointed out that the RBF kernel presents limited extrapolation capability (MacKay, 1998). Some authors have been tackling that issue. Duvenaud et al. (2013); Lloyd et al. (2014) pursue a compositional approach to build more expressive kernels from simpler ones. Wilson and Adams (2013) propose the spectral mixture kernel to automatically discover patterns and extrapolate beyond the training data. Al-Shedivat et al. (2017); Wilson et al. (2016a,b) propose the use of deep neural networks to learn kernel functions directly from data. Although those proposals achieve more flexible kernels, they turn some GPLVM expressions intractable.
latent where we were able to analytically integrate out the non-observed (A few authors have already considered the UT in the context of GP models. Ko and Fox (2009); (UGP) model to handle supervised tasks with non-Gaussian likelihoods, such as binary classification. (Julier and Uhlmann, 2004; Menegaz et al., 2015). The UT projects a finite number of sigma points (UT), a deterministic technique to approximate nonlinear mappings of a probability distribution. The remainder of the paper is organized as follows. In Section 2 we present the theoretical background by summarizing the GPLVM framework and the UT approximation. In Section 3 we detail our proposal to apply the UT within the Bayesian GPLVM setting. In Section 4 we present and discuss the obtained empirical results. We conclude the paper in Section 5 and present ideas for further work.

In summary, our main contributions are: (i) an extension to the Bayesian GPLVM using the UT to deterministically handle intractable integrals and enable the use of any kernel; (ii) a set of experiments comparing the proposed approach and alternative approximations using Gauss-Hermite quadrature and Monte Carlo sampling in tasks involving dimensionality reduction and dynamical free simulation. The remainder of the paper is organized as follows. In Section 2 we present the theoretical background by summarizing the GPLVM framework and the UT approximation. In Section 3 we detail our proposal to apply the UT within the Bayesian GPLVM setting. In Section 4 we present and discuss the obtained empirical results. We conclude the paper in Section 5 and present ideas for further work.

2 Theoretical Background

In this section, we summarize the GP and the Bayesian GPLVM models, as well as the UT.

2.1 The Gaussian Process Framework

Let \( N \) inputs \( x_i \in \mathbb{R}^{D_x} \), organized in a matrix \( X \in \mathbb{R}^{N \times D_x} \) be mapped via \( f : \mathbb{R}^{D_x} \rightarrow \mathbb{R}^{D_y} \) to a \( N \) correspondent outputs \( f_i \in \mathbb{R}^{D_y} \), organized in the matrix \( F \in \mathbb{R}^{N \times D_y} \). We observe \( Y \in \mathbb{R}^{N \times D_y} \), a noisy version of \( F \). Considering an observation noise \( \epsilon \sim N(0, \sigma^2 I) \), we have \( f_{id} = f(x_i) + \epsilon \), where \( y_{id} \) denotes the vector comprised of the \( d \)-th component of each observed sample, i.e., the \( d \)-th column of the matrix \( Y \). If we choose a multivariate zero mean Gaussian prior for each dimension of \( F \), we get (Rasmussen and Williams, 2006):

\[
p(Y|X) = \prod_{d=1}^{D_y} N(y_{id}|0, K_f + \sigma^2 I),
\]

where we were able to analytically integrate out the non-observed (latent) variables \( f_{id} \). The elements of the covariance matrix \( K_f \in \mathbb{R}^{N \times N} \) are calculated by \( [K_f]_{ij} = k(x_i, x_j), \forall i, j \in \{1, \cdots, N\} \), where \( k(\cdot, \cdot) \) is the so-called covariance (or kernel) function.
where

Applying Jensen’s inequality to Eq. (2) gives a lower bound to the marginal log-likelihood (Blei et al., 2017; Jordan et al., 1999) to approximately integrate the latent variables. The unscented transformation (UT) is a method for estimating the first two moments of the mapping of a random variable under an arbitrary function. Proposed by Uhlmann (1995) in the context of Kalman filters (KF), the transformation itself is decoupled from the so-called Unscented KF. In the UT, the mean and covariance of the transformed random variable are approximated with a weighted average of transformed sigma points \( s_n \), derived from the first two moments of the original input.

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2.2 The Bayesian Gaussian Process Latent Variable Model

The Gaussian Process Latent Variable Model (GPLVM), proposed by Lawrence (2004), extends the GP framework for scenarios where we do not have the inputs \( X \), which generated the observations \( Y \) via the modeled function. The GPLVM was originally proposed in the context of nonlinear dimensionality reduction, which can be done choosing \( D_x < D_y \). However, the approach has proved to be flexible enough to be used in several other scenarios. For instance, in supervised tasks, the matrix \( X \) can be seen as a set of observed but uncertain inputs (Damianou et al., 2016).

The Bayesian GPLVM, proposed by Titsias and Lawrence (2010), considers a variational approach (Blei et al., 2017; Jordan et al., 1999) to approximately integrate the latent variables \( X \). Inspired by Titsias’ variational sparse GP framework (Titsias, 2009), the Bayesian GPLVM avoids overfitting by considering the uncertainty of the latent space and enables the determination of \( D_x \) by using a kernel function with ARD (automatic relevance determination) hyperparameters.

Following Titsias and Lawrence (2010), we start by including \( M \) inducing points \( z_d \in \mathbb{R}^M \) associated to each output dimension and evaluated in \( M \) pseudo-inputs \( \zeta_j \in \mathbb{R}^{D_x} \), where \( p(z_d) = \mathcal{N}(z_d|0, K_c) \) and \( K_c \in \mathbb{R}^{M \times M} \) is the kernel matrix computed from the pseudo-inputs. The joint distribution of all the variables in the GPLVM is now given by (with omitted dependence on \( \zeta_j \))

\[
p(Y, X, F, Z) = \prod_{d=1}^{D_x} p(y_d|f_d)p(f_d|z_d, X)p(z_d)\, p(X). \tag{2}
\]

Applying Jensen’s inequality to Eq. (2) gives a lower bound to the marginal log-likelihood \( \log p(Y) \):

\[
p(Y) = \int p(Y, X, F, Z) \, dX \, dF \, dZ \geq Q \log \left[ \frac{p(Y, X, F, Z)}{Q} \right] \, dX \, dF \, dZ,
\]

where \( Q \) is the variational distribution, chosen to be given by the form \( Q = q(X)q(Z)p(F|Z, X) \), where \( p(F|Z, X) \) is an analytical conditional distribution of Gaussians and the variational distributions \( q(X) = \prod_{i=1}^{n} q(x_i) \) and \( q(Z) = \prod_{j=1}^{D_x} q(z_d) \) respectively approximate the posteriors of the variables \( X \) and \( Z \) by products of multivariate Gaussians.

The final analytical bound derived by Titsias and Lawrence (2010), which may be directly used to perform model selection, depends on the three terms below, named \( \Psi \)-statistics:

\[
\Psi_0 = \sum_{i=1}^{N} \Psi_0^{(i)} \in \mathbb{R}, \quad \text{where} \quad \Psi_0^{(i)} = \int k(x_i, x_i)q(x_i) \, dx_i, \tag{3}
\]

\[
\Psi_1 \in \mathbb{R}^{N \times M}, \quad \text{where} \quad [\Psi_1]_{ij} = \int k(x_i, \zeta_j)q(x_i) \, dx_i \tag{4}
\]

\[
\Psi_2 = \sum_{i=1}^{N} \Psi_2^{(i)} \in \mathbb{R}^{M \times M}, \quad \text{where} \quad [\Psi_2^{(i)}]_{jm} = \int k(x_i, \zeta_j)k(x_i, \zeta_m)q(x_i) \, dx_i. \tag{5}
\]

The above expressions represent convolutions of the kernel function with the variational distribution \( q(X) \) and are tractable only for a few kernel functions, such as the RBF and the linear kernels.

2.3 The Unscented Transformation

The unscented transformation (UT) is a method for estimating the first two moments of the mapping of a random variable under an arbitrary function. Proposed by Uhlmann (1995) in the context of Kalman filters (KF), the transformation itself is decoupled from the so-called Unscented KF. In the UT, the mean and covariance of the transformed random variable are approximated with a weighted average of transformed sigma points \( s_n \), derived from the first two moments of the original input.

Let \( x \sim \mathcal{N}(\mu, \Sigma) \) be a \( D \)-dimensional variable which will pass through an arbitrary transformation \( f: \mathbb{R}^D \rightarrow \mathbb{R}^D \). Given uniform weights for the sigma points, the output moments are computed by:

\[
\mathbb{E}(f(x)) \approx \frac{1}{2D} \sum_{n=1}^{2D} f(s_n) = m, \quad \text{cov}(f(x)) \approx \frac{1}{2D} \sum_{n=1}^{2D} (f(s_n) - m)(f(s_n) - m)^\top.
\]
There are several strategies to select sigma points (see e.g. [Menegaz et al. (2015)]). We follow the original scheme by [Uhlmann (1995)], with uniform weights and sigma points chosen from the columns of the squared root of $D\Sigma$, an efficient way to generate a symmetric distribution of sigma points. Let $\text{chol}(\Sigma)$ be the Cholesky decomposition of the matrix $\Sigma$. Then, the sigma points $s_n$ are defined as:

$$s_n = \mu + [\text{chol}(D\Sigma)]_n, \quad s_{n+D} = \mu - [\text{chol}(D\Sigma)]_n, \quad \forall n \in [1, D],$$

where $[\text{chol}(D\Sigma)]_n$ denotes the $n$-th column of the lower triangular matrix $\text{chol}(D\Sigma)$.

Since only a relatively small number of sigma points is used ($2D$, where $D$ is the dimensionality of the input) and their computation is completely deterministic, the UT presents a viable alternative to other quadrature methods, such as Gauss-Hermite and Monte Carlo sampling.

### 3 Proposed Methodology

From Section 2.2, we can see that the computation of the $\Psi$-statistics in Eqs. (3)-(5) is the only part that prevents the application of the Bayesian GPLVM with arbitrary kernels. Since the $\Psi$-statistics are actually Gaussian expectations of nonlinear functions, we propose to approximate their computation in intractable cases using the UT. We emphasize that the use of the UT to solve the $\Psi$-statistics is convenient since we are often able to limit the dimension of the integrand when learning latent spaces. Furthermore, as noted by [Honkela (2004)], the UT is most suited for Gaussian integrals with lower dimensionality, which is usually the case with the Bayesian GPLVM. A similar result was pointed out by [Zhang et al. (2009)] when comparing UT with other sampling strategies.

Besides enabling the use of non-analytical kernels in the Bayesian GPLVM, our choice of using UT-based approximations in place of, for instance, the Gauss-Hermite (GH) quadrature, brings great computational benefits, due to the number of points that are evaluated to compute the Gaussian integral. Given a $D$-dimensional random variable, the UT requires just a linear number of $2D$ sampled points for evaluation, while the GH quadrature requires $H^D$ points, where $H$ is a user chosen order parameter. Even for $H = 2$ and moderate dimensionality values, e.g. $D = 20$, the GH approach would require at least $2^{20}$ evaluations per approximation, which is infeasible. We also note that the UT and the GH quadrature have similar forms in the single dimension case.

In the Bayesian GPLVM, the amount of sampled points is relevant, since the approximations are computed at each step of the variational lower bound optimization. Thus, the number of times we evaluate the $\Psi$-statistics gives a raw estimate of the chosen approximation computational budget.

To verify how accuracy evolves with dimension when using UT in the context of the Bayesian GPLVM, we computed $\Psi_1$ (see Eq. (4)) considering a RBF kernel on random data of varying dimension. We use both the UT and the GH quadrature. Since we actually compute only a column of the matrix $\Psi_1$, we can measure the approximations accuracies by comparing the error norm between the approximation and the analytical solution, which in this case is feasible.

Fig. 1 indicates that the error norm ratio between the UT and the GH ($E_{UT}/E_{GH}$) presents the tendency of smaller errors for the GH quadrature as the input dimension increases. However, we can see that the UT has slightly better accuracy than the GH on low dimensions ($\leq 8$). Importantly, the UT requires exponentially fewer sample points, as illustrated in the bottom plot of Fig. 1.
4 Experiments

We consider two standard tasks for the GPLVM: dimensionality reduction and free simulation of dynamical models with uncertainty propagation. We compare our UT approach with the Gauss-Hermite (GH) quadrature and the reparametrization trick based Monte Carlo (MC) sampling for computing the $Ψ$-statistics of the Bayesian GPLVM. In the tractable cases, we also consider the analytical expressions. All experiments were implemented in Python using the GPflow framework (Matthews et al., 2017). The implementation can be found at https://github.com/danisson/UnscentedGPLVM.

For the GH experiments, to maintain a reasonable computational cost, we use $2^D$ points, where $D$ is the input dimension. For the MC approximations, we use two different numbers of samples: the same number used by UT and the same number used by GH. Each MC experiment was run ten times, with averages and standard deviations reported. The MC approximation is similar to the one in the doubly stochastic variational framework (Titsias and Lázaro-Gredilla, 2014), but without mini-batch updates.

4.1 Dimensionality Reduction

The dimensionality reduction task is especially suitable for our UT-based approach, since the dimension of the integrand in the $Ψ$-statistics is usually small for the purposes of data visualization.

We used two datasets which were referred by Lawrence (2004) and Titsias and Lawrence (2010), the Oil flow dataset and the USPS digit dataset. In both cases, we compare the analytic Bayesian GPLVM model with the RBF kernel against a kernel with non-analytic $Ψ$-statistics. We have considered the following kernels: Matérn 3/2, the periodic kernel[4] and a Multilayer Perceptron (MLP) composed on a RBF kernel, similar to the manifold learning approach by Calandra et al. (2016).

The means of the variational distribution were initialized based on standard Principal Component Analysis (PCA) and the latent variances were initialized to $0.1$. Also, 30 points from the initial latent space were selected as inducing pseudo-inputs and appropriately optimized during training.

Each scenario was evaluated following two approaches: a qualitative analysis of the learned two-dimensional latent space; a quantitative metric in which we take the known labels from each dataset and find the predictive accuracy of which class a point in the learned latent space should belong to. The method used to that end is a five-fold cross validated 1-nearest neighbor (1-NN). For the quantitative results, we also show the accuracy on the PCA projection as a sanity check.

4.1.1 Oil flow dataset

The multiphase Oil flow dataset consists of 1000 observations with 12 attributes, where each one belongs to one of three classes (Bishop and James, 1993). We apply GPLVM with five latent dimensions and select the two dimensions with the greatest inverse lengthscales.

For the approximations using GH quadrature, we have used $2^5 = 32$ samples in total. This contrasts with the UT, which only uses $2 \times 5 = 10$ samples. We note that we have attempted to follow Titsias and Lawrence (2010) and use ten latent dimensions, but that would require the GH to evaluate $2^{10} = 1024$ samples at each optimization step, which made the method too slow on the used hardware.

In Fig. 2 we can see that independent of the chosen method to solve the $Ψ$-statistics, either the analytic expressions or any approximation yields similar overall qualitative results. Tab. 1 contains the 1-NN predicted accuracy results for all kernels and approximation methods. As expected, all the nonlinear approaches performed better than regular PCA. We can see that the RBF results for the deterministic approaches are all similar, while the Matérn 3/2 kernel with the UT approximation obtained slightly better results overall. However, when using MC sampling with the same amount of points that UT and GH used, the results for all kernels were worse than both UT and GH.

4.1.2 USPS digit dataset

The USPS digit dataset contains 7000 $16 \times 16$ gray-scale images of handwritten numerals from 0 to 9. We considered two scenarios. First, we replicated the same setup by Lawrence (2004), using only 3000 samples from the digits 0 to 4. The second experiment uses all classes and a subset of 5000

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[1]: As defined by MacKay (1998), in Eq. (47).
Figure 2: Two-dimensional projections of the Oil flow and USPS 0-4 digits datasets for GPLVM with different kernels and approximations. The projections shown are the best ones obtained in the crossvalidation steps. 1-NN mislabels are marked in red.

Table 1: Quantitative results for the dimensionality reduction tasks.

| Method      | Kernel   | Oil flow     | 1-NN accuracy % Oil flow | 1-NN accuracy % USPS 0-4 digits | 1-NN accuracy % USPS All digits |
|-------------|----------|--------------|--------------------------|---------------------------------|---------------------------------|
| PCA         | -        | 78.9 ± 6.5   | 65.0 ± 1.3               | 36.8 ± 4.5                      |                                 |
| Analytic    | RBF      | 98.0 ± 2.7   | 72.4 ± 1.5               | 40.8 ± 6.1                      |                                 |
| Gauss-Hermite | Matérn 3/2 | 95.0 ± 6.1   | -                        | -                               |                                 |
| UT          | MLP [2,30,60] | 85.0 ± 2.8   | -                        | -                               |                                 |
|             | RBF      | 98.0 ± 2.7   | 71.2 ± 2.2               | 42.4 ± 6.5                      |                                 |
| UT          | Matérn 3/2 | 100.0 ± 0.0  | -                        | -                               |                                 |
|             | MLP [2,30,60] | -            | -                        | -                               |                                 |
|             | RBF      | 98.0 ± 2.7   | 71.6 ± 2.6               | 40.1 ± 5.9                      |                                 |
| Monte Carlo (10) | Matérn 3/2 | 94.3 ± 0.4   | -                        | -                               |                                 |
|             | MLP [2,30,60] | -            | -                        | -                               |                                 |
|             | RBF      | 93.4 ± 4.5   | 48.4 ± 2.4               | 29.5 ± 3.1                      |                                 |
| Monte Carlo (32) | Matérn 3/2 | 94.7 ± 0.4   | -                        | -                               |                                 |
|             | MLP [2,30,60] | -            | -                        | -                               |                                 |
|             | RBF      | 95.7 ± 0.4   | 49.3 ± 0.4               | 32.5 ± 4.8                      |                                 |

samples. We used a GPLVM with five latent dimensions on all kernels but the MLP kernel, where we use two latent dimensions. We follow the same evaluation methodology previously described.

We expected the MLP kernel to fare better than the RBF kernel. This is due to the well known capabilities of neural networks to find lower dimensional representations of higher dimensional structured data [Wilson et al., 2016a]. As seen in Tab. [1] this was indeed the case. Bayesian GPLVM with a neural network in the kernel function obtained the best results. Fig. [2] shows a comparison between the analytic solution with RBF versus the approximate solutions using a MLP kernel with a single hidden layer and [2, 30, 60] neurons (input, hidden and output, respectively). For the experiment with all digits, we can see in Tab. [1] that the difference between kernels was even higher.

Tab. [1] also presents that all the MC experiments were worse performing than PCA for this specific task. We conjecture that such weakness was due to the dimensionality of the optimization surface, as well as noisy approximations of the objective function and its gradients, which can misdirect the optimization. This problem shines a light on the potential weakness of non-deterministic approximations when used to optimize the model kernel hyperparameters and variational parameters.
Table 2: Summary of the free simulation results for the Air passengers dataset. Note that the MC experiments with 24 samples presented numerical issues and could not be completed.

| Model       | Method        | Kernel                  | NLPD | RMSE  |
|-------------|---------------|-------------------------|------|-------|
| GP-NARX     | RBF+Linear    | 21.82                   | 69.39|       |
|             | Periodic+RBF+Linear | 14.00               | 44.99|       |
| GPLVM       | Analytic      | RBF+Linear              | 13.23| 68.92 |
|             |               | RBF+Linear              | 13.22| 68.88 |
| Gauss-Hermite|               | Periodic+RBF+Linear     | 9.49 | 45.03 |
| UT          |               | RBF+Linear              | 13.23| 68.88 |
|             |               | Periodic+RBF+Linear     | 9.59 | 45.28 |
| Monte Carlo | (4096)        | RBF+Linear              | 13.30±0.24 | 68.70±0.27 |
|             |               | Periodic+RBF+Linear     | 9.50±0.17 | 45.50±0.27 |
| Monte Carlo | (24)          | RBF+Linear              | -    | -     |
|             |               | Periodic+RBF+Linear     | -    | -     |

4.2 Dynamical Free Simulation

Free simulation, or multistep-ahead prediction, is a task that consists in forecasting the values of a dynamical system arbitrarily far into the future based on past predicted values. In most simple models, such as the GP-NARX model (Kocijan et al., 2005), each prediction does not depend on the uncertainty of past predictions, but only past mean predicted values. To propagate the uncertainty of each prediction to the next implies to perform predictions with uncertain inputs. This task has been approached before, for instance by Girard et al. (2003), but for GP models using the RBF kernel.

In this section, we first train a GP-NARX without considering uncertain inputs, following the regular NARX approach (Kocijan et al., 2005). Then, we apply the same optimized kernel hyperparameters in a GPLVM, selecting all the training inputs as pseudo-inputs. Finally, the GPLVM is used to perform a free simulation with uncertain inputs formed by the past predictive distributions. Since we apply approximations for computing the \( \Psi \)-statistics in the predictions, we can choose any valid kernel.

4.2.1 Airline passenger dataset

We consider the Airline passenger numbers dataset, which was recorded monthly from 1949 to 1961 (Hyndman, 2018). The first four years were used for training and the rest was left for testing. We chose an autoregressive lag of 12 past observations as input. After the GP-NARX kernel hyperparameters are optimized, as previously mentioned, we choose the variance of the variational distribution in the GPLVM to be equal to the optimized noise variance. We perform a free simulation from the beginning of the training set until the end of the test set, using past predicted variances as variational variances of the uncertain inputs, which enables approximate uncertainty propagation during the simulation.

We used the following kernels: a mixture of a RBF kernel with a linear kernel; a mixture of periodic, RBF and linear kernels. The latter combination of kernels was chosen due to our prior knowledge that airplane ticket sales follow a periodic trend and have an overall upward tendency because of the popularity increase and decrease in the tickets prices. We emphasize that the choice of such a flexible combination of kernels would not be possible without the use of approximate methods when considering the uncertain inputs scenario and the GPLVM framework.

Quantitative evaluation is done by computing the root mean squared error (RMSE), given by

\[
\text{RMSE} = \sqrt{\frac{1}{N^*} \sum_{i=1}^{N^*} (y_i - \hat{\mu}_i)^2} \]

where \( N^* \) is the number of test samples, \( y_i \) is the true output and \( \hat{\mu}_i \) is the predicted mean output. We also compute the average negative log-predictive density (NLPD), given by

\[
\text{NLPD} = \frac{1}{2} \log 2\pi + \frac{1}{2N^*} \sum_{i=1}^{N^*} \left[ \log \hat{\sigma}_i^2 + \frac{(y_i - \hat{\mu}_i)^2}{\hat{\sigma}_i^2} \right]
\]

where \( \hat{\sigma}_i^2 \) is the \( i \)-th predicted variance.

We note that both metrics are “the lower, the better” and are computed only for the test set.

Tab. 2 presents the obtained results. Although with similar RMSE, all GPLVM variants presented better NLPD values when compared to their standard GP-NARX counterparts. That is expected, since the uncertainty of each prediction is being approximately propagated to the next predictions.

Since this experiment deals with 12-dimensional inputs, following the discussion in Section 3, the GH approximation might have better accuracy than the UT approximation. However, even using...
![Graphs showing data and prediction for different models](image)

(a) GP-NARX, RBF + Linear.  
(b) GPLVM, RBF + Linear.  
(c) GPLVM, Periodic + RBF + Linear (GH).  
(d) GPLVM, Periodic + RBF + Linear (UT).  
(e) GPLVM, Periodic + RBF + Linear (MC(4096)).  
(f) GPLVM, Periodic + RBF + Linear (MC(24)).

**Figure 3:** Illustration of the results obtained in the dynamical free simulation experiments. Best obtained runs are shown. Note that the MC run with 24 samples presented numerical issues and could not be completed.

only $2 \times 12 = 24$ points against GH’s $2^{12} = 4096$ points, the difference between UT’s and GH’s accuracies is negligible, given that predictions using UT runs much faster. As shown in Fig. 3, visual difference between the two methods is subtle. The results obtained by the MC approximation with the same amount of samples as the GH quadrature (4096) are similar, but when using the same quantity as the UT (24 samples), the model presents numerical issues and do not obtain meaningful outputs.

### 5 Conclusion

In this work, we have considered the problem of learning GP models from unavailable or uncertain inputs within the Bayesian GPLVM framework. We have tackled the intractabilities that arise in the original variational methodology by [Titsias and Lawrence, 2010] when non-RBF and nonlinear kernels are used by proposing the use of the unscented transformation.

We have performed computational experiments on two tasks: dimensionality reduction and free simulation of dynamical models with uncertainty propagation. In both cases, our UT-based approach scaled much better than the compared Gauss-Hermite quadrature, while obtaining a similar overall approximation. The UT results were also more stable and consistent than the ones obtained by Monte Carlo sampling, which may also require a larger number of samples. Importantly, our method is simple to implement and does not impose any stochasticity, maintaining the deterministic feature of the standard Bayesian GPLVM variational framework.

For future work we aim to evaluate the UT in more scenarios where inference with GP models falls into intractable integrals. For instance, we intend to tackle intractable expressions that arise with hierarchical GP models and GP-based Bayesian optimization with uncertain inputs.
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