Bayesian Gaussian Process Latent Variable Model

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Motivation

- Gaussian processes are used for supervized learning
  - Inputs are fixed/deterministic
- Gaussian process latent variable model (GP-LVM) is trained by optimizing (not marginalizing out) the latent variables

We address the questions:

- How can we train Gaussian process models when inputs are random (e.g. we have uncertain inputs/missing values)?
- How can we marginalize out the latent variables in GP-LVM?

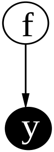
We will introduce a variational Bayes framework that provides approximate Bayesian solutions

Outline

- Variational inference for GPs with random (uncertain/missing/latent) inputs
  - The role of auxiliary parameters
  - The variational lower bound
- Variational inference for GP-LVM
  - Automatic selection of the latent dimensionality with the squared exponential ARD kernel
- Experiments with GP-LVM
- Summary

Gaussian Processes: Deterministic inputs

- Gaussian process (GP) is used as non-parametric prior over some function $f(\mathbf{x})$
- Probability model: Output-input data $(\mathbf{y}, X)$:



$$\begin{aligned} p(\mathbf{y}, \mathbf{f}|X) &= p(\mathbf{y}|\mathbf{f}) \times p(\mathbf{f}|X) \\ \text{Joint} &= \text{Likelihood} \times \text{marginal GP on X} \end{aligned}$$

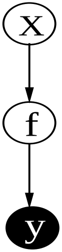
where X is assumed deterministic

But what if the inputs X are random?

Gaussian Processes: Random inputs

- Probability model: As before, but now the inputs X are given a prior (e.g. Gaussian) distribution $p(X)$:

$$p(\mathbf{y}, \mathbf{f}, X) = p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|X)p(X)$$



- The posterior distribution $p(\mathbf{f}, X|\mathbf{y})$ and the marginal likelihood $p(\mathbf{y})$ are intractable
- Approximate inference: Can we apply some standard variational method?

Variational inference: Difficult to apply

- Standard regression with random inputs:

$$p(\mathbf{y}, \mathbf{f}, X) = \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I) p(\mathbf{f}|X) p(X)$$

$$p(\mathbf{y}, \mathbf{f}, X) = \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I) \frac{1}{(2\pi)^{n/2}|K_{NN}|^{1/2}} e^{-\frac{1}{2}\mathbf{f}^T K_{NN}^{-1} \mathbf{f}} p(X)$$

- Applying mean field $q(\mathbf{f}, X) = q(\mathbf{f})q(X)$ is difficult:
  - X appears non-linearly inside the inverse K_{NN}^{-1} and the determinant $|K_{NN}|$
  - Seems impossible to compute the variational bound $\int q(\mathbf{f}, X) \log \frac{p(\mathbf{y}, \mathbf{f}, X)}{q(\mathbf{f}, X)} d\mathbf{f} dX$

Variational inference: Bayesian Linear Regression

Intractability even for the simplest model: Bayesian linear regression

- Standard parameters:

$$\mathbf{y} = X\mathbf{w} + \epsilon, \quad N(\mathbf{w}|\mathbf{0}, \sigma_w^2 I), p(X)$$

  - It is straightforward to apply mean field using $q(\mathbf{w})q(X)$
- Kernelized (non-parametrized):

$$\mathbf{y} = \mathbf{f} + \epsilon, \quad N(\mathbf{f}|\mathbf{0}, \sigma_w^2 XX^T), p(X)$$

  - Variational inference using $q(\mathbf{f})q(X)$ is difficult

Variational inference: Kernelization

- Gaussian processes (kernel methods in general) are somehow marginalized (collapsed)
  - A GP is an exchangeable model:

$$p(f_1, \ldots, f_N) = \int \prod_{n=1}^{N} p(f_n|\mathbf{w}) dP(\mathbf{w})$$

where the underlying (infinite) parameter $\mathbf{w}$ has been integrated out

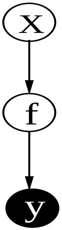
- We need to place back some (approximate) parameters to apply variational inference. We will use extra function values as parameters

Variational inference: The idea

- Initial model:

$$p(\mathbf{y}, \mathbf{f}, X) = \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)p(\mathbf{f}|X)p(X)$$

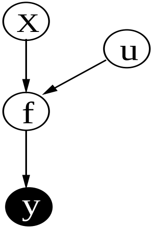
(variational inference in $(\mathbf{f}, X)$ is difficult)



- Augment consistently[a] with extra function values $\mathbf{u} = (f(\mathbf{z}_1), \dots, f(\mathbf{z}_M))$:

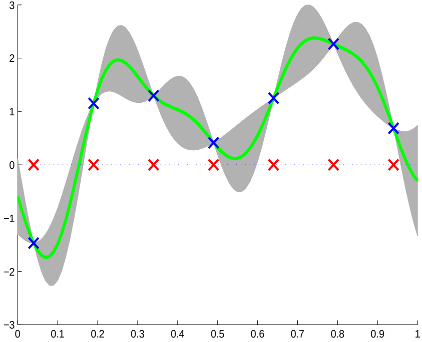
$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}, X) \quad = \quad \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)p(\mathbf{f}|\mathbf{u}, X)p(\mathbf{u})p(X)$$

(variational inference in $(\mathbf{f}, \mathbf{u}, X)$ is tractable)



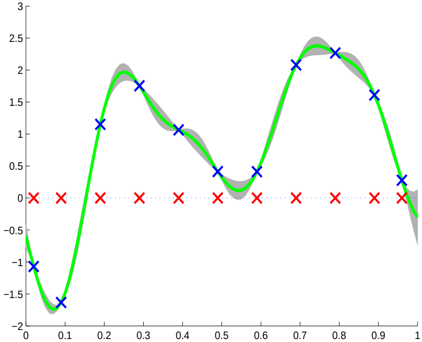
[a] $\int p(\mathbf{f}|\mathbf{u}, X)p(\mathbf{u})d\mathbf{u} = p(\mathbf{f}|X)$, for any value of inputs Z

Visualization



- Blue Xs: extra function points $\mathbf{u}$
- Red Xs: inputs of extra function points
- Green curve: function $\mathbf{f}$ drawn from $p(\mathbf{f}|\mathbf{u}, X)$
- **Shaded area:** conditional GP prior $p(\mathbf{f}|\mathbf{u}, X)$

Visualization

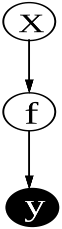


- You can think of $\mathbf{u}$ as a parameter that specifies the function $\mathbf{f}$
- When I use more points in $\mathbf{u}$, $p(\mathbf{f}|\mathbf{u}, X)$ becomes more certain, i.e. the parameter $\mathbf{u}$ is more informative
- If the kernel is linear, 2 points (u_1, u_2) fully specify an 1-D function ($p(\mathbf{f}|\mathbf{u}, X)$ becomes the delta function)

Variational inference

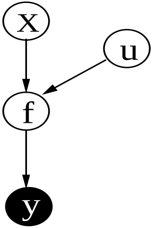
- Initial model:

$$p(\mathbf{y}, \mathbf{f}, X) = \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)p(\mathbf{f}|X)p(X)$$



- Augmented model:

$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}, X) \quad = \quad \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)p(\mathbf{f}|\mathbf{u}, X)p(\mathbf{u})p(X)$$



We apply variational inference in the space of $(\mathbf{f}, \mathbf{u}, X)$

Variational inference

- Variational distribution:

$$q(\mathbf{f}, \mathbf{u}, X) = p(\mathbf{f}|\mathbf{u}, X)\phi(\mathbf{u})q(X)$$

  - $q(X) = \mathcal{N}(\boldsymbol{\mu}, \Sigma)$: Gaussian distribution
  - $\phi(\mathbf{u})$: unrestricted (turns out to be Gaussian)
  - $p(\mathbf{f}|\mathbf{u}, X)$: conditional GP prior (**trick**)

- Maximize the lower bound

$$\log \int \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)p(\mathbf{f}|\mathbf{u}, X)p(X)d\mathbf{f}d\mathbf{u}\mathbf{X} \geq$$

$$\int p(\mathbf{f}|\mathbf{u}, X)\phi(\mathbf{u})q(X) \log \frac{\mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)p(\mathbf{f}|\mathbf{u}, X)p(\mathbf{u})p(X)}{p(\mathbf{f}|\mathbf{u}, X)\phi(\mathbf{u})q(X)} d\mathbf{f}d\mathbf{u}\mathbf{X}$$

where $p(\mathbf{f}|\mathbf{u}, X)$s inside the log cancel

This is now tractable. Matrix inverses containing X are gone

Variational inference

$$\int p(\mathbf{f}|\mathbf{u}, X)\phi(\mathbf{u})q(X)\log\frac{\mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)p(\mathbf{u})p(X)}{\phi(\mathbf{u})q(X)}d\mathbf{f}\,d\mathbf{u}\,d\mathbf{X}$$

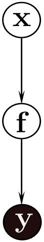
- The lower bound is analytically tractable for linear kernels, squared exponential, exponential, polynomial kernels and possibly others
- It is maximized jointly over variational parameters and model hyperparameters

Gaussian process latent variables model (Lawrence, 2005)

- Latent variable model:

$$\mathbf{y} = \mathbf{f}(\mathbf{x}) + \epsilon$$

  - $\mathbf{y} \in \mathbb{R}^D$: observed variable
  - $\mathbf{x} \in \mathbb{R}^Q$ $(Q \ll D)$: latent variable
  - $\mathbf{f} : \mathbb{R}^Q \rightarrow \mathbb{R}^D$: latent mapping
  - GP-LVM: GP priors on the latent mapping



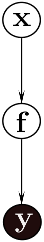
GP-LVM is trained by optimizing (not marginalizing out) the latent variables

- Not proper density in the latent space
- Cannot select the latent dimensionality Q
- It may overfit since it is not fully Bayesian

Bayesian Gaussian process latent variables model

- Latent variable model:

$$\mathbf{y} = \mathbf{f}(\mathbf{x}) + \epsilon$$



- Bayesian training: Integrate out both the latent mapping and the latent space
  - Exact Bayesian inference is intractable
  - But variational Bayesian inference is tractable

The variational method is applied as before. The only difference is that now we have D latent functions (one for each observed output) and not just one

Bayesian Gaussian process latent variables model

Automatic selection of the latent dimensionality

- Squared exponential ARD kernel

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{1}{2}\sum_{q=1}^{Q} \alpha_q (x_q - x_q')^2\right)$$

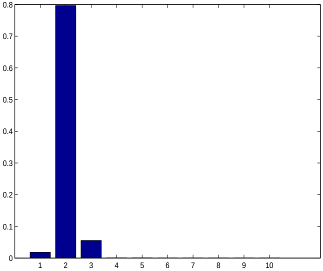
- Maximizing the variational lower bound w.r.t. α_qs allows to remove redundant latent dimensions

Experiments: Visualization

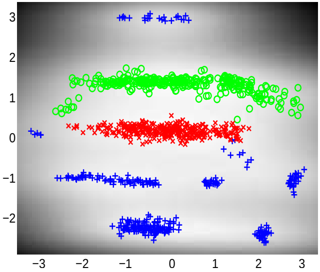
- Oil flow data: 1000 training; 12 dimensions; 3 known classes
- Compare:
  - Bayesian GP-LVM
  - Standard sparse GP-LVM
  - Probabilistic PCA

Experiments: Visualization

Oil flow data



(α_qs)

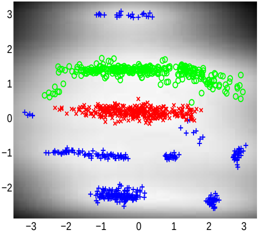


(Bayesian GP-LVM)

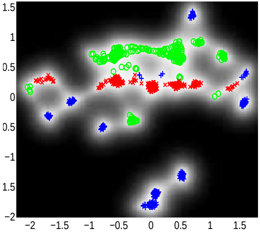
- Bayesian GP-LVM runs with 10 latent dimensions
- The red, green and blue points are the predicted means for the latent variables labeled with the known class
- 7 out 10 latent dimensions are shrunk to zero
- Visualization is shown for the dominant (with the largest inverse lengthscales) latent dimensions

Experiments: Visualization

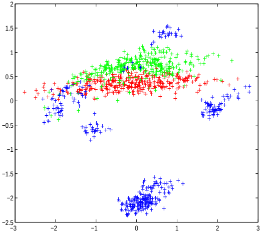
Oil flow data



(Bayesian GP-LVM)



(GP-LVM)

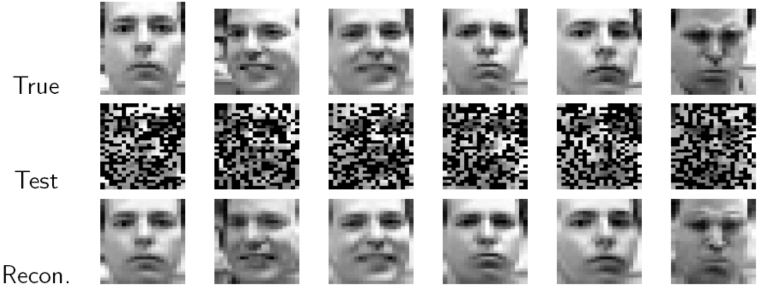


(PPCA)

GP-LVM and Bayesian GP-LVM are both initialized based on PCA

Experiments: Predict missing values

Frey faces: 1965 images; $28 \times 20 = 560$ dimensions; 1000 for training; 965 for testing



- Bayesian GP-LVM is trained with 30 latent dimensions, mean absolute reconstruction error: 7.4003
- Standard sparse GP-LVM is trained with several latent dimensions: $Q = 2, 5, 10, 30$. Errors: $10.5748, 9.7284, 19.6949, 19.6961$

Experiments: Generative classification

- USPS digits dataset: 16×16 images for all 10 digits, 7291 training examples and 2007 test examples
- Run 10 Bayesian GP-LVMs: one for each digit
- Compute Bayesian class conditional densities in the test data of the form $p(\mathbf{y}_* | Y, \text{digit})$

Results: From 2007 test images we have 95 incorrectly classified digits, i.e. 4.73% error

Summary/Future work

Summary:

- Variational framework to approximately integrate out inputs in GPs
- Allows for Bayesian training of GP-LVM

Future work:

- Speed up optimization of the variational lower bound
- Learn non-parametric/non-linear dynamical systems using GPs and variational Bayes