Learning Nonlinear Functions via Gaussian Processes (2)

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Probabilistic Machine Learning (CS772A)

October 24, 2017

Today's Plan

- Recap of GP and GP regression

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  - Deep Gaussian Processes

Linear to Nonlinear Regression..

- For linear model $y_n = \boldsymbol{w}^\top \boldsymbol{x}_n$, marginal distribution of responses $\boldsymbol{y} = [y_1, \ldots, y_N]$

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- Straightforward to compute the response y_* for a new input $\boldsymbol{x}_*$ (simple Gaussian manipulations)

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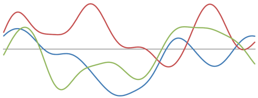

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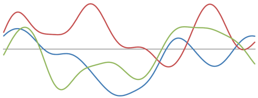

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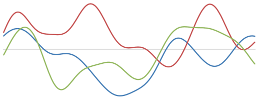

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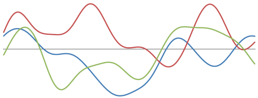

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.. i.e., the finite dimensional marginal of f is a multivariate Gaussian distribution

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- We can now compute things such as posterior $p(\mathbf{f}|\boldsymbol{y})$, posterior predictive $p(y_*|\boldsymbol{x}_*, \boldsymbol{y}, \mathbf{X})$, marginal likelihood $p(\boldsymbol{y}|\theta)$ where θ are model's hyperparams (e.g., of GP mean/covar function, noise var.)

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- General approach shown below (the practical shortcut for regression shown on next slide)
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  - Still important to understand the above general procedure. For "hard" problems (e.g., when the above integrals are not tractable), we'd need to follow it to get the posterior, posterior predictive, etc.

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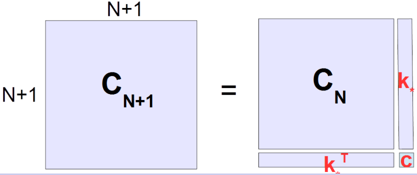

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- Note: A huge amount of work on scaling up GPs (recent methods can predict in $\mathcal{O}(1)$ time)

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- Let's look at the predictions made by GP regression

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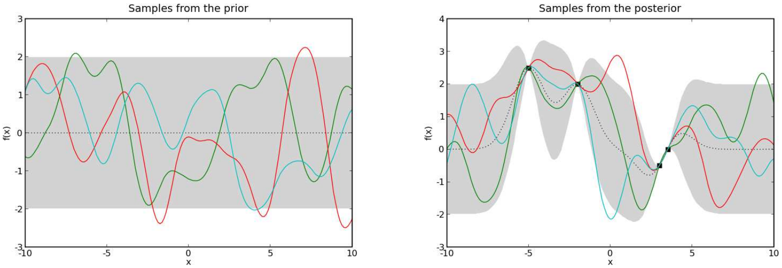
GP Regression: Pictorially

A GP with a squared-exponential kernel function



Left: Samples of f from the prior $\mathcal{GP}(0, \kappa)$
Right: Samples of f from the posterior of f after 4 observations

Picture courtesy: https://pythonhosted.org/infpy/gps.html

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- MLE-II for GP regression maximizes the log marginal likelihood w.r.t. the hyperparameters

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where θ_j is the j^{th} hyperparam. of the kernel, and $\boldsymbol{\alpha} = \mathbf{K}_y^{-1}\mathbf{y}$

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GP Regression: Learning Hyperparameters

- The (log) marginal likelihood

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GP for Problems other than Regression

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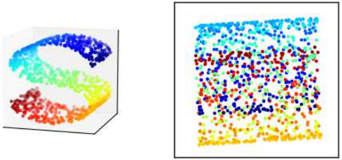
- Designing deep learning models: Deep Gaussian Processes

GP for Unsupervised Learning (Nonlinear Dimensionality Reduction)

Why Nonlinear Dimensionality Reduction?

- Embeddings learned by PCA (left: original data, right: PCA)



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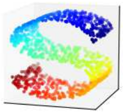

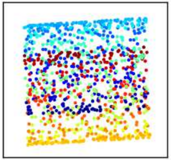

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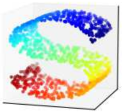

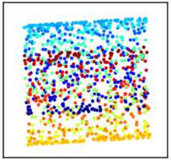

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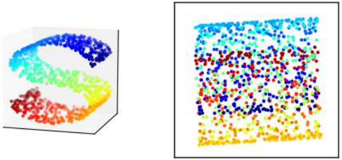

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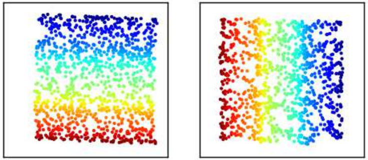
  - Uses Euclidean distances; learns linear projections which doesn't preserve nonlinear distances
- An ideal nonlinear embedding that we desire to learn for such data



Recap: Probabilistic PCA

- Given: $N \times D$ data matrix $\mathbf{X} = [\boldsymbol{x}_1^\top, \ldots, \boldsymbol{x}_N^\top]^\top$, with $\boldsymbol{x}_n \in \mathbb{R}^D$
- Goal: Find a lower-dim. rep., an $N \times K$ matrix $\mathbf{Z} = [\boldsymbol{z}_1^\top, \ldots, \boldsymbol{z}_N^\top]^\top$, $\boldsymbol{z}_n \in \mathbb{R}^K$

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- Limitation: $\boldsymbol{z}_n$ to $\boldsymbol{x}_n$ mapping is linear (defined by $\mathbf{W}$)

Gaussian Process Latent Variable Model (GPLVM)

- Consider the same model $\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n$, $\mathbf{W} \in \mathbb{R}^{D \times K}$, $\epsilon_n \sim \mathcal{N}(0, \sigma^2)$
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&= (2\pi)^{-DN/2} |\mathbf{K}_z|^{-D/2} \exp\left(-\frac{1}{2} \text{tr}(\mathbf{K}_z^{-1} \mathbf{X}\mathbf{X}^\top) \right) \quad \text{(verify)}
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  - How? By defining $\mathbf{K}_z = \mathbf{K} + \sigma^2 \mathbf{I}$ (with $\mathbf{K}$ being some appropriately defined kernel matrix over $\mathbf{Z}$)

Gaussian Process Latent Variable Model (GPLVM)

- With $\mathbf{K}_z = \mathbf{K} + \sigma^2\mathbf{I}$, we can write $p(\mathbf{X}|\mathbf{Z}, \sigma^2)$ as a product of D GPs ($\mathbf{Z}$ to $\mathbf{X}_{:,d}$, $d = 1, \ldots, D$)

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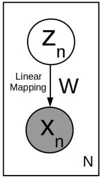
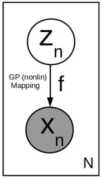
- But with $\mathbf{K}_z = \mathbf{K} + \sigma^2\mathbf{I}$ (for some nonlinear covariance/kernel function) will give nonlinear dimensionality reduction



Probabilistic PCA



GPLVM

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- Can also impose a prior on $\mathbf{Z}$ and do MAP (or fully Bayesian) estimation

Deep Gaussian Processes

- GPs can be "stacked" to construct deep learning models (both supervised and unsupervised)

"Deep Gaussian Processes", Damianou and Lawrence (AISTATS 2013)

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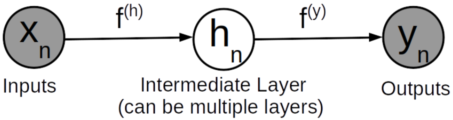

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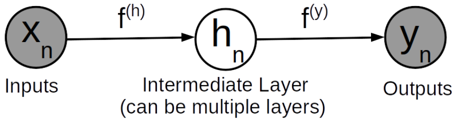

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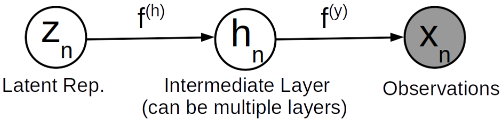

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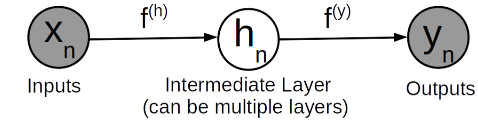

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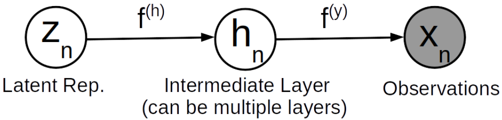

- With no intermediate layers, the above models reduce to the standard GP based models

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- Readily provides estimates of the variance in the predictions
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- Can use kernels that can be compositions of many kernels
- Many other applications - pretty much any problem that requires estimating an unknown function from (especially small amounts of) data, e.g., Bayesian Optimization, Active Learning, etc.

Some Useful Resources on Gaussian Process

- Some MATLAB/Python Packages: Useful to play with, build applications, extend existing models and inference algorithms for GPs (both regression and classification)
  - GPML: `http://www.gaussianprocess.org/gpml/code/matlab/doc/`
  - GPStuff: `http://research.cs.aalto.fi/pml/software/gpstuff/`
  - pyGPs: `https://github.com/marionmari/pyGPs`
  - GP in tensorflow: `https://github.com/GPflow/GPflow`
  - All these toolboxes allow using different types of likelihood function, different types of mean and covariance functions, and inference procedures, including hyperparameter estimation, etc.