Gaussian Processes for Nonlinear Regression and Nonlinear Dimensionality Reduction

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Probabilistic Machine Learning (CS772A)

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Gaussian Process

- A Gaussian Process (GP) is a distribution over functions
- A random draw from a GP thus gives a function f

$$f \sim \text{GP}(\mu, \kappa)$$

where $\boldsymbol{\mu}$ is the mean function and κ is the covariance/kernel function (the cov. function controls f's shape/smoothness)

- Note: μ and κ can be chosen or learned from data

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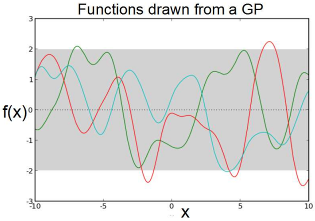

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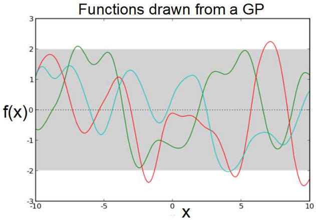

- GP can be used as a nonparametric prior distribution for such functions

Gaussian Process

- A function f is said to be drawn from $\mathrm{GP}(\mu, \kappa)$ if

$$\begin{bmatrix} f(\boldsymbol{x}_1) \\ f(\boldsymbol{x}_2) \\ \vdots \\ f(\boldsymbol{x}_N) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu(\boldsymbol{x}_1) \\ \mu(\boldsymbol{x}_2) \\ \vdots \\ \mu(\boldsymbol{x}_N) \end{bmatrix}, \begin{bmatrix} \kappa(\boldsymbol{x}_1, \boldsymbol{x}_1) \ldots \kappa(\boldsymbol{x}_1, \boldsymbol{x}_N) \\ \kappa(\boldsymbol{x}_2, \boldsymbol{x}_1) \ldots \kappa(\boldsymbol{x}_2, \boldsymbol{x}_N) \\ \vdots \quad \ddots \quad \vdots \\ \kappa(\boldsymbol{x}_N, \boldsymbol{x}_1) \ldots \kappa(\boldsymbol{x}_N, \boldsymbol{x}_N) \end{bmatrix} \right)$$

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- Thus, if f is drawn from a GP then the joint distribution of f's evaluations at a finite set of points $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N\}$ is a multivariate normal

Gaussian Process

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$$\mathbf{f} = \begin{bmatrix} f(\boldsymbol{x}_1) \\ f(\boldsymbol{x}_2) \\ \vdots \\ f(\boldsymbol{x}_N) \end{bmatrix}, \boldsymbol{\mu} = \begin{bmatrix} \mu(\boldsymbol{x}_1) \\ \mu(\boldsymbol{x}_2) \\ \vdots \\ \mu(\boldsymbol{x}_N) \end{bmatrix}, \mathbf{K} = \begin{bmatrix} \kappa(\boldsymbol{x}_1, \boldsymbol{x}_1) \dots \kappa(\boldsymbol{x}_1, \boldsymbol{x}_N) \\ \kappa(\boldsymbol{x}_2, \boldsymbol{x}_1) \dots \kappa(\boldsymbol{x}_2, \boldsymbol{x}_N) \\ \vdots \quad \ddots \quad \vdots \\ \kappa(\boldsymbol{x}_N, \boldsymbol{x}_1) \dots \kappa(\boldsymbol{x}_N, \boldsymbol{x}_N) \end{bmatrix}$$

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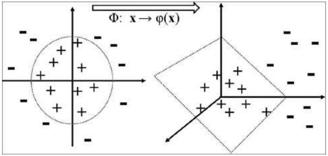
- Often, we assume the mean function to be zero. Thus $\mathbf{f} \sim \mathcal{N}(\mathbf{0}, \mathbf{K})$
- Covariance/kernel function κ measures similarity between two inputs
  - $\kappa(\boldsymbol{x}_n, \boldsymbol{x}_m) = \exp\left(-\frac{||\boldsymbol{x}_n - \boldsymbol{x}_m||^2}{\gamma}\right)$: RBF kernel
  - $\kappa(\boldsymbol{x}_n, \boldsymbol{x}_m) = v_0 \exp\left\{-\left(\frac{|\boldsymbol{x}_n - \boldsymbol{x}_m|}{r}\right)^\alpha\right\} + v_1 + v_2\delta_{nm}$

Kernel Functions

- Covariance/kernel function κ measures similarity between two inputs
- Corresponds to implicitly mapping data to a higher dimensional space via a feature mapping ϕ ($\boldsymbol{x} \rightarrow \phi(\boldsymbol{x})$) and computing the dot product that space

$$\kappa(\boldsymbol{x}_n, \boldsymbol{x}_m) = \phi(\boldsymbol{x}_n)^\top \phi(\boldsymbol{x}_m)$$

- Popularly known as the kernel trick (used in kernel methods for nonlinear regression/classification/clustering/dimensionality reduction, etc.)
- Allows extending linear models to nonlinear problems



Today's Plan

Gaussian Processes for two problems

- Nonlinear Regression: Gaussian Process Regression
- Nonlinear Dimensionality Reduction: Gaussian Process Latent Variable Models (GPLVM)

Gaussian Process Regression

Gaussian Process Regression

- Training data $\mathcal{D}$: $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$. $\boldsymbol{x}_n \in \mathbb{R}^D$, $y_n \in \mathbb{R}$
- Assume the responses to be a noisy function of the inputs

$$y_n = f(\boldsymbol{x}_n) + \epsilon_n = f_n + \epsilon_n$$

- Don't *a priori* know the form of f (linear/polynomial/something else?)

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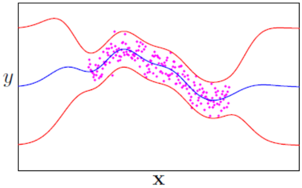

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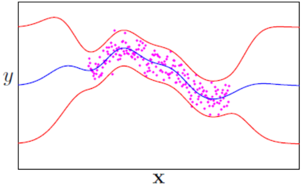

- We'll use GP prior on f and use Bayes rule to get the posterior on f

$$p(f|\mathcal{D}) = \frac{p(f)p(\mathcal{D}|f)}{p(\mathcal{D})}$$

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- Assume a zero-mean Gaussian error: $\epsilon_n \sim \mathcal{N}(\epsilon_n | 0, \sigma^2)$

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- Thus the likelihood model

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- We will assume a zero mean Gaussian Process prior on f, which means:

$$p(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mathbf{0}, \mathbf{K})$$

Gaussian Process Regression

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- The marginal distribution of the training data responses $\boldsymbol{y}$

$$p(\boldsymbol{y}) = \int p(\boldsymbol{y}|\mathbf{f})p(\mathbf{f})d\mathbf{f} = \mathcal{N}(\boldsymbol{y}|\mathbf{0}, \mathbf{K} + \sigma^2\mathbf{I}_N) = \mathcal{N}(\boldsymbol{y}|\mathbf{0}, \mathbf{C}_N)$$

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$$p(y_*) = \mathcal{N}(y_*|0, \kappa(\boldsymbol{x}_*, \boldsymbol{x}_*) + \sigma^2)$$

- But what we actually want is the predictive distribution $p(y_*|\boldsymbol{y})$

Making Predictions

- Let's consider the joint distr. of N training responses $\boldsymbol{y}$ and test response y_*

$$p\left(\begin{bmatrix} \boldsymbol{y} \\ y_* \end{bmatrix}\right) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{y} \\ y_* \end{bmatrix} \middle| \begin{bmatrix} \boldsymbol{0} \\ 0 \end{bmatrix}, \mathbf{C}_{N+1}\right)$$

where the $(N+1) \times (N+1)$ matrix $\mathbf{C}_{N+1}$ is given by

$$\mathbf{C}_{N+1} = \begin{bmatrix} \mathbf{C}_N & \mathbf{k}_* \\ \mathbf{k}_*^\top & c \end{bmatrix}$$

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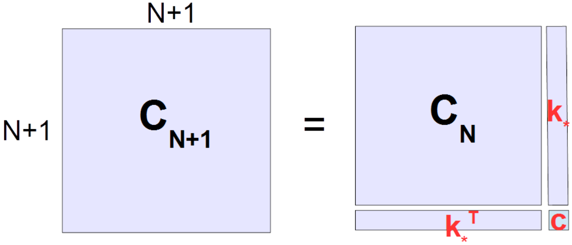

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- The predictive distribution will be

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- Follows readily from property of Gaussians (lecture 2 and PRML 2.94-2.96)

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- Test time cost

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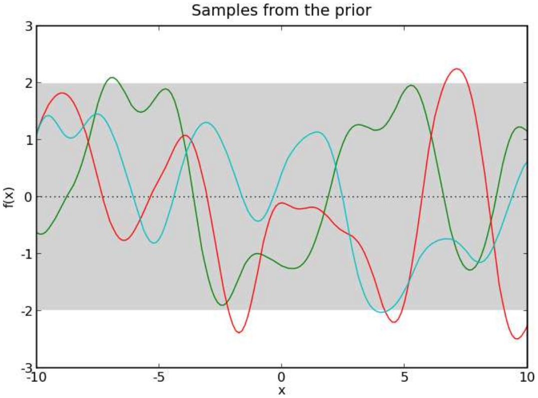
- Test time cost is $\mathcal{O}(N)$: linear in the number of training examples (just like kernel SVM or nearest neighbor methods)

GP Regression: Pictorially

A GP with squared-exponential kernel function



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

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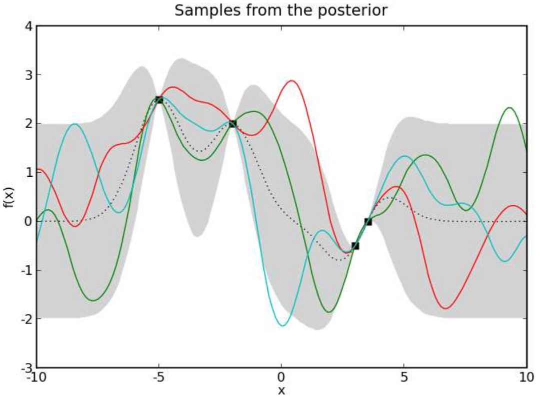
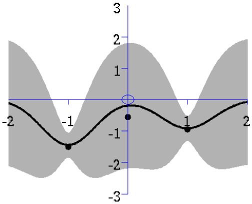


Shaded area denotes twice the standard deviation at each input

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

GP Regression: Pictorially



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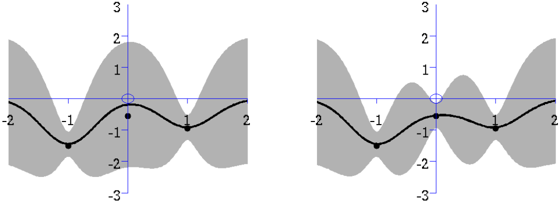

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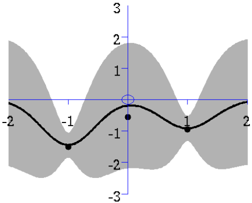

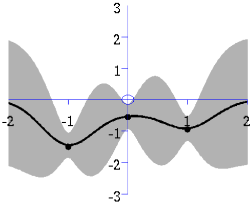

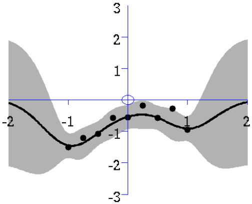

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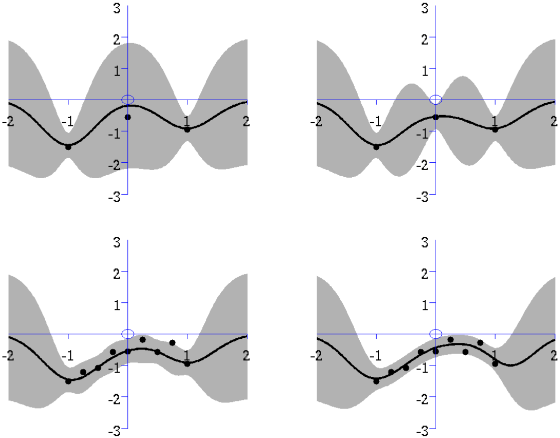

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- Let's look at the predictions made by GP regression

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Inferring Hyperparameters

- There are two hyperparameters in GP regression models
  - Variance of the Gaussian noise σ^2
  - Hyperparameters θ of the covariance function κ, e.g.,

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- We will revisit one such example (GP for binary classification) later during the semester

GP vs (Kernel) SVM

- The objective function of a soft-margin SVM looks like

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- Negative log-posterior $\log p(\boldsymbol{y}|\mathbf{f})p(\mathbf{f})$ of a GP can be written as

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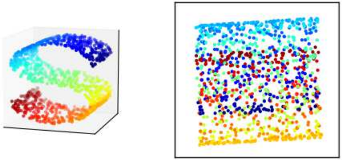
  - Learning compositions of kernels for more flexible modeling

$$\mathbf{K} = \mathbf{K}_{\theta_1} + \mathbf{K}_{\theta_2} + \ldots$$

Nonlinear Dimensionality Reduction using Gaussian Process (GPLVM)

Why Nonlinear Dimensionality Reduction?

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



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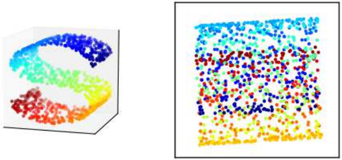

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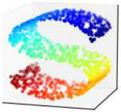

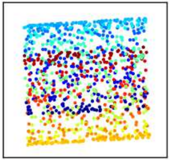

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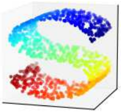

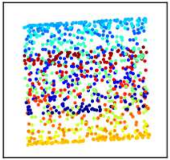

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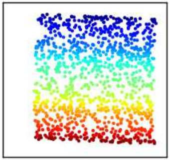

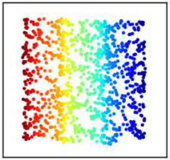

Recap: Probabilistic PCA

- Given: $N \times D$ data matrix $\mathbf{X} = [\boldsymbol{x}_1^\top, \ldots, \boldsymbol{x}_N^\top]^\top$, with $\boldsymbol{x}_n \in \mathbb{R}^D$
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- 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 $\mathbf{Z} = [\boldsymbol{z}_1^\top, \ldots, \boldsymbol{z}_N^\top]^\top$, $\boldsymbol{z}_n \in \mathbb{R}^K$
- Assume the following generative model for each observation $\boldsymbol{x}_n$

$$\boldsymbol{x}_n = \mathbf{W}\boldsymbol{z}_n + \epsilon_n \qquad \text{with } \mathbf{W} \in \mathbb{R}^{D \times K},\ \epsilon_n \sim \mathcal{N}(0, \sigma^2)$$

- The conditional distribution

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- The marginal distribution of $\boldsymbol{x}_n$ (after integrating out latent variables $\boldsymbol{z}_n$)

$$\begin{aligned} p(\boldsymbol{x}_n|\mathbf{W}, \sigma^2) &= \mathcal{N}(\mathbf{0}, \mathbf{W}\mathbf{W}^\top + \sigma^2\mathbf{I}_D) \\ p(\mathbf{X}|\mathbf{W}, \sigma^2) &= \prod_{n=1}^{N} p(\boldsymbol{x}_n|\mathbf{W}, \sigma^2) \end{aligned}$$

Gaussian Process Latent Variable Model (GPLVM)

- Consider the same model

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$$\begin{aligned} p(\mathbf{X}|\mathbf{Z},\sigma^2) &= \prod_{d=1}^{D} \mathcal{N}(\mathbf{X}_{:,d}|\mathbf{0},\mathbf{Z}\mathbf{Z}^\top + \sigma^2\mathbf{I}_D) \\ &= (2\pi)^{-DN/2}|\mathbf{K}_z|^{-D/2}\exp\left(-\frac{1}{2}\text{tr}(\mathbf{K}_z^{-1}\mathbf{X}\mathbf{X}^\top)\right) \end{aligned}$$

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- Note that we can think of $\mathbf{X}_{:,d}$ modeled by a GP regression model

$$\mathbf{X}_{:,d} \sim \mathcal{N}(\mathbf{0}, \mathbf{Z}\mathbf{Z}^\top + \sigma^2\mathbf{I}_D)$$

- There are a total of D such GPs (one for each column of $\mathbf{X}$)

GPLVM

- $p(\mathbf{X}|\mathbf{Z},\sigma^2)$ is now a product of D GPs (one per column of data matrix $\mathbf{X}$)

$$
\begin{aligned}
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\end{aligned}
$$

- Using $\mathbf{K}_z = \mathbf{Z}\mathbf{Z}^\top + \sigma^2\mathbf{I}$ and doing MLE will give the same solution for $\mathbf{Z}$ as linear PCA (note that $\mathbf{Z}\mathbf{Z}^\top$ is a linear kernel over $\mathbf{Z}$, the low-dim rep of data)
- But with $\mathbf{K}_z = \mathbf{K} + \sigma^2\mathbf{I}$ (with $\mathbf{K}$ being some appropriately defined kernel matrix over $\mathbf{Z}$) will give nonlinear dimensionality reduction

MLE for GPLVM

- Log-likelihood is given by

$$\mathcal{L} = -\frac{D}{2}\log|\mathbf{K}_z| - \frac{1}{2}\mathrm{tr}(\mathbf{K}_z^{-1}\mathbf{X}\mathbf{X}^\top)$$

where $\mathbf{K}_z = \mathbf{K} + \sigma^2\mathbf{I}$ and $\mathbf{K}$ denotes the kernel matrix of our low-dim rep. $\mathbf{Z}$

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$$\frac{\partial \mathcal{L}}{\partial Z_{nk}} = \frac{\partial \mathcal{L}}{\partial \mathbf{K}_z}\frac{\partial \mathbf{K}_z}{\partial Z_{nk}}$$

  where $\frac{\partial \mathcal{L}}{\partial \mathbf{K}_z} = \mathbf{K}_z^{-1}\mathbf{X}\mathbf{X}^\top\mathbf{K}_z^{-1} - D\mathbf{K}_z^{-1}$ and $\frac{\partial \mathbf{K}_z}{\partial Z_{nk}}$ will depend on the kernel function used (note: hyperparameters of the kernel can also be learned just as we did it in the GP regression case)

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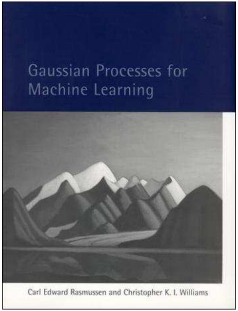
- Can also impose a prior on $\mathbf{Z}$ and do MAP (or fully Bayesian) estimation

Resources on Gaussian Processes

- Book: Gaussian Processes for Machine Learning (freely available online)



- MATLAB 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/`
  - GPLVM: `https://github.com/lawrennd/gplvm`