Learning Nonlinear Functions via Gaussian Processes (1)

Piyush Rai

Probabilistic Machine Learning (CS772A)

October 17, 2017

Linear Models

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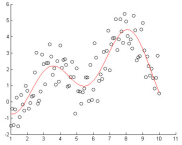
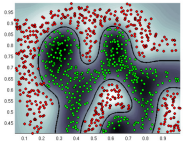
- However, linear models have limited expressive power. Fail to learn highly nonlinear patterns.



Nonlinear Regression



Nonlinear Classification

Linear Regression

- Let's first consider the (probabilistic) linear regression model

$$\begin{aligned} p(\boldsymbol{w}) &= \mathcal{N}(\boldsymbol{w}|\boldsymbol{\mu_0}, \Sigma_0) \qquad \text{(Prior)} \\ p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) &= \mathcal{N}(\boldsymbol{w}^\top \boldsymbol{x}_n, \beta^{-1}) \qquad \text{(Likelihood w.r.t. one obs.)} \end{aligned}$$

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- Thus the joint marginal distr. of $\boldsymbol{y}$ conditioned on $\mathbf{X}$ is the following multivariate normal

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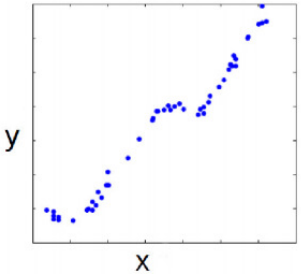
- Note that the cov. matrix above tells us how the different outputs "co-vary" w.r.t. each other

Nonlinear Regression

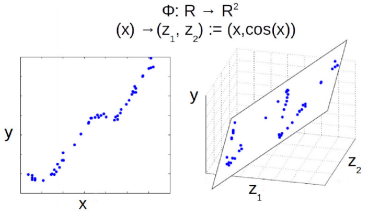
- Consider the following dataset for regression



- Input-output relationship is NOT linear
- A linear model would do badly on such data!

Nonlinear Regression via Mapping Inputs to Higher Dimensions

- Suppose we replace each input $\boldsymbol{x}_n$ by a higher dimensional mapping $\phi(\boldsymbol{x}_n)$



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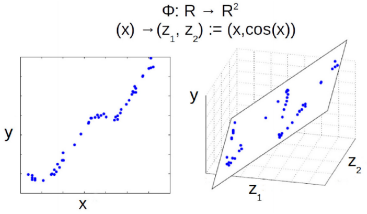

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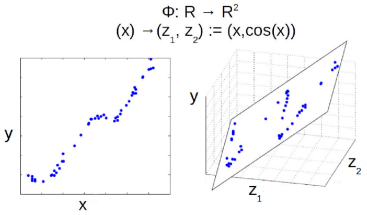

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- The joint distribution $\boldsymbol{y}$ given $\mathbf{X}$ will be the same as the linear case, except that each entry $\boldsymbol{x}_n^\top \boldsymbol{x}_m$ in the covariance matrix is replaced by $\phi(\boldsymbol{x}_n)^\top \phi(\boldsymbol{x}_m)$

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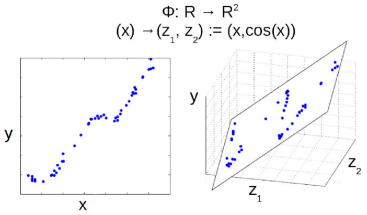

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- Note that $\phi(\boldsymbol{x}_n)^\top \phi(\boldsymbol{x}_m)$ is the Euclidean similarity between $\boldsymbol{x}_n$ and $\boldsymbol{x}_n$ in the high-dim space

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- An example: Radial basis function (RBF) kernel: $\kappa(\boldsymbol{x}_n, \boldsymbol{x}_m) = \exp\left(-\frac{||\boldsymbol{x}_n - \boldsymbol{x}_m||^2}{\gamma}\right)$ where ϕ_n corresponds to an infinite dimensional mapping. Another example: Polynomial kernel

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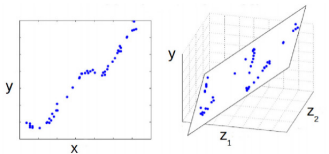
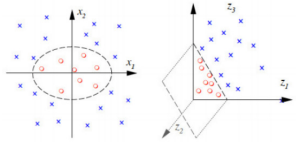


Nonlinear Regression



Nonlinear Classification

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- We saw that, for a nonlin. reg. model with each $\boldsymbol{x}_n$ replaced by a high-dim map $\phi(\boldsymbol{x}_n)$

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Nonlinear Regression

- We saw that, for a nonlin. reg. model with each $\boldsymbol{x}_n$ replaced by a high-dim map $\phi(\boldsymbol{x}_n)$

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- Note: In the noisy case, we only need to add β^{-1} $(=\sigma^2)$ to diagonals of $\mathbf{C}$

Nonlinear Regression

- Assume noisy case. Consider joint distr. of N training outputs $\boldsymbol{y}$ and test output y_* (input $\boldsymbol{x}_*$)

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

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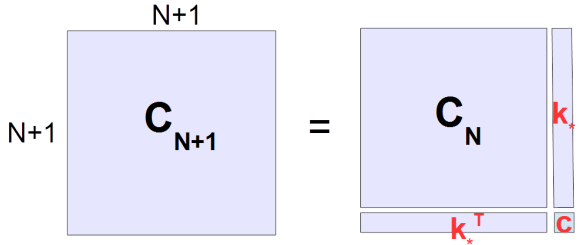

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  - Such models are called "nonparametric" models (model's complexity depends on the data)
  - A downside: Making predictions gets slower

Learning Nonlinear Functions via Gaussian Processes (what we just saw, but in a more formal way)

Gaussian Process

- Recall that our kernel version of probabilistic linear regression (noiseless case) had

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- Note: A slightly general version would be with nonzero mean

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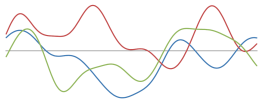

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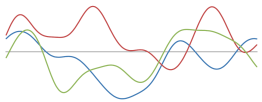

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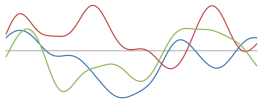

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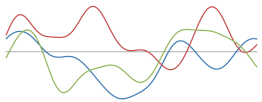

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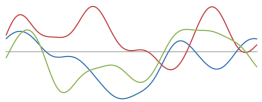

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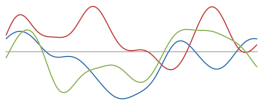

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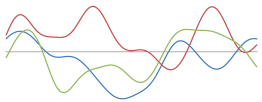

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- GP can therefore be used as a flexible prior distribution over functions

Gaussian Process Prior

- f is said to be drawn from a $\mathcal{GP}(\mu, \kappa)$ if its finite dim. version is the following joint Gaussian

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

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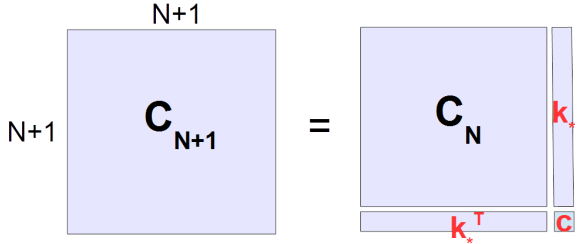

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- The desired predictive posterior will be (using conditional from joint property of Gaussian)

$$\begin{aligned} p(y_*|\boldsymbol{y}) &= \mathcal{N}(y_*|\mu_*, \sigma_*^2) \\ \mu_* &= \mathbf{k}_*^\top \mathbf{C}_N^{-1} \boldsymbol{y} \\ \sigma_*^2 &= \kappa(\boldsymbol{x}_*, \boldsymbol{x}_*) + \sigma^2 - \mathbf{k}_*^\top \mathbf{C}_N^{-1} \mathbf{k}_* \end{aligned}$$

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$$p\left(\begin{bmatrix} \boldsymbol{y} \\ y_* \end{bmatrix}\right) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{y} \\ y_* \end{bmatrix} \middle| \begin{bmatrix} \mathbf{0} \\ 0 \end{bmatrix}, \begin{bmatrix} \mathbf{C}_N & \mathbf{k}_* \\ \mathbf{k}_*^\top & c \end{bmatrix}\right)$$

- The desired predictive posterior will be (using conditional from joint property of Gaussian)

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- Note: The test time cost

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  - .. just like kernel SVM or nearest neighbor methods
  - However, unlike kernel SVM or nearest neighbor methods, GP also gives us the variance σ_*^2

GP Regression: Interpreting GP Predictions

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

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- Two interpretations for the mean prediction μ_*
  - A kernel SVM like interpretation

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    where $\boldsymbol{\alpha}$ is akin to the weights of support vectors

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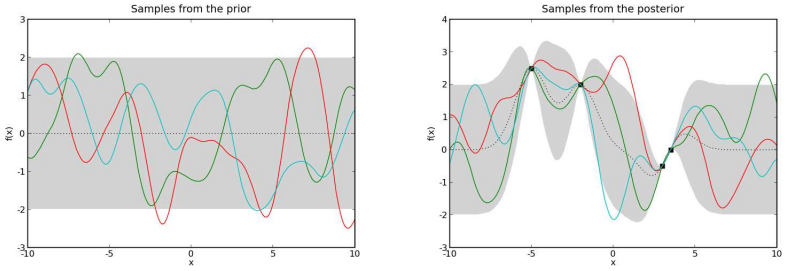
  - A nearest neighbors interpretation

$$\mu_* = \mathbf{k}_*{}^\top \mathbf{C}_N^{-1} \boldsymbol{y} = \boldsymbol{w}^\top \boldsymbol{y} = \sum_{n=1}^{N} w_n y_n$$

    where $\boldsymbol{w}$ is akin to the weights of the neighbors

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

Summary

- Gaussian Process is a very powerful framework for modeling nonlinear input-output relationships
- Can think of it as Bayesian kernel methods
- Can learn the kernel hyperparameters (big advantage)
- Can use kernels that can be compositions of many kernels

Next Class

- Other examples/applications of GPs
- Inference and other issues
- Gaussian Process Latent Variable Models