Gaussian Processes for Learning Nonlinear Functions

Piyush Rai

Topics in Probabilistic Modeling and Inference (CS698X)

Jan 28, 2019

Announcements

- Discussion session on project topics/ideas: Tomorrow 7pm-8pm (KD-101)

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- HW1 out now. Due on Feb 8, 11:59pm. Please start early.

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- Quiz 1 on Jan 31, 7pm-8pm (RM-101)

Recap: Bayesian Generative Classification

- Recall generative classification $p(y=k|x) = \frac{p(y=k)p(x|y=k)}{\sum_{k=1}^{K} p(y=k)p(x|y=k)}$

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- Eq (1) is the posterior predictive distribution of test output y_* given input $\boldsymbol{x}_*$
  - Note that we have done posterior averaging for all the parameters
- In contrast, for gen. class with MLE/MAP, $p(y_* = k|\boldsymbol{y}) \approx \pi_k$ and $p(\boldsymbol{x}_*|\mathbf{X}^{(k)}) \approx p(\boldsymbol{x}_*|\theta_k)$

Gaussian Processes (GP)

(GP = Bayesian Modeling + Kernel Methods)

(Goal: learning **nonlinear** discriminative models $p(y|\boldsymbol{x})$)

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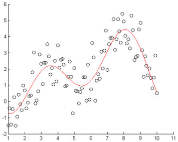
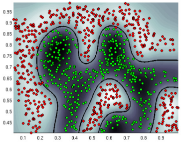
- However, linear models have limited expressive power. Unable to learn highly nonlinear patterns.


Nonlinear Regression


Nonlinear Classification

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  - Gaussian Processes (a Bayesian approach to kernel based nonlinear learning; today)

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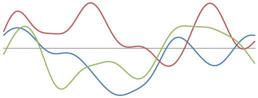

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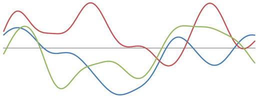

- Mean function μ models the "average" function f from $\mathcal{GP}(\mu, \kappa)$

$$\mu(\boldsymbol{x}) = \mathbb{E}[f(\boldsymbol{x})]$$

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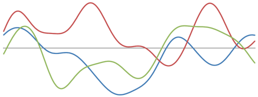

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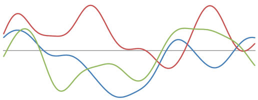

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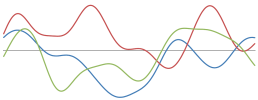

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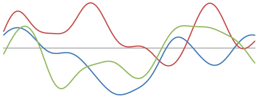

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Gaussian Process

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A Perspective from Bayesian Linear Regression

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

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\begin{aligned}
p(\boldsymbol{w}) &= \mathcal{N}(\boldsymbol{w}|\boldsymbol{\mu_0}, \Sigma_0) \qquad &\text{(Prior)} \\
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- A "function space" view of linear regression as opposed to "weight space" view (both equivalent)

GP for Regression and Classification

(Note that GP only defines the score $f(\boldsymbol{x})$ but $y = f(\boldsymbol{x}) +$ "noise")

("noise" may be Gaussian, sigmoid-Bernoulli, or something else)

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- Let's choose zero mean Gaussian Process prior $\mathcal{GP}(0, \kappa)$ on f, which is equivalent to

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

where $K_{nm} = \kappa(\boldsymbol{x}_n, \boldsymbol{x}_m)$.

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

- We now need a prior on the function f that enables us to model a nonlinear f
- Let's choose zero mean Gaussian Process prior $\mathcal{GP}(0, \kappa)$ on f, which is equivalent to

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

where $K_{nm} = \kappa(\boldsymbol{x}_n, \boldsymbol{x}_m)$. For now, assume κ is a known function with fixed hyperparameters.

GP Regression

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GP Regression

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- What's the posterior predictive $p(y_*|\boldsymbol{x}_*, \boldsymbol{y}, \mathbf{X})$ or $p(y_*|\boldsymbol{y})$ (skipping $\mathbf{X}, \boldsymbol{x}_*$ from the notation)?

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

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

GP Regression

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- Using the same result, the marginal distribution $p(y_*) = \mathcal{N}(y_*|0, \kappa(\boldsymbol{x}_*, \boldsymbol{x}_*) + \sigma^2)$

GP Regression: Making Predictions

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

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

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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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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\mu_* = \mathbf{k}_*{}^\top \mathbf{C}_N^{-1} \boldsymbol{y} = \mathbf{k}_*{}^\top \boldsymbol{\alpha} = \sum_{n=1}^{N} k(\boldsymbol{x}_*, \boldsymbol{x}_n) \alpha_n
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where $\boldsymbol{\alpha}$ is akin to the weights of support vectors

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  - A nearest neighbors interpretation

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\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

Next Class

- Properties of GP based models, choice of kernels, etc
- Learning hyperparameters in GP based models
- GP for classification and GLMs
- Making GP models scalable
- Some recent advances in GP