S&DS 365 / 665

**Intermediate Machine Learning**

# Nonparametric Bayes: Gaussian Processes

October 3

Yale

# Reminders

- Assignment 2 posted
- Quiz 3 on Wednesday, Oct 5
- Midterm on Tuesday, October 17 in class
- Practice exam and review next week

# For Today

- Gaussian processes (continued)
- Examples
- Dirichlet process (intro)

# Bayesian Inference

The parameter $\theta$ of a model is viewed as a random variable.
Inference usually carried out as follows:

- Choose a *generative model* $p(x \mid \theta)$ for the data.
- Choose a *prior distribution* $\pi(\theta)$ that expresses beliefs about the parameter before seeing any data.
- After observing data $\mathcal{D}_n = \{x_1, \ldots, x_n\}$, update beliefs and calculate the *posterior distribution* $p(\theta \mid \mathcal{D}_n)$.

---

Please posted notes for a review of some of the basics of Bayesian inference.

# Bayes' Theorem

The posterior distribution can be written as

$$p(\theta \mid x_1, \ldots, x_n) = \frac{p(x_1, \ldots, x_n \mid \theta)\pi(\theta)}{p(x_1, \ldots, x_n)} = \frac{\mathcal{L}_n(\theta)\pi(\theta)}{c_n} \propto \mathcal{L}_n(\theta)\pi(\theta)$$

where $\mathcal{L}_n(\theta)$ is the *likelihood function* and

$$c_n = p(x_1, \ldots, x_n) = \int p(x_1, \ldots, x_n \mid \theta)\pi(\theta)d\theta = \int \mathcal{L}_n(\theta)\pi(\theta)d\theta$$

is the normalizing constant, which is also called *evidence*.

# Nonparametric Bayes

- In nonparametric Bayesian inference, we replace a finite dimensional model $\theta$ with an infinite dimensional model
- This is usually a class of *functions*
- Typically neither the prior nor the posterior have a density; but the posterior is still well defined.

# Core questions

1. How do we construct a prior $\pi$ on an infinite dimensional set $\mathcal{F}$?
2. How do we compute the posterior? How do we draw random samples from the posterior?
3. What are the properties of the posterior?

# Stochastic processes

A stochastic process is a collection of random variables indexed some set (such as time), all defined with respect to a common probability space.

We'll focus on a fundamental stochastic process: The Gaussian process

(We'll also briefly mention the Dirichlet process next time)

---

More technically, a stochastic process $\{X(t)\}_{t \in T}$ is a collection of random variables indexed by a set $T$ and defined on a common probability space $(\Omega, \mathcal{F}, P)$ where $\Omega$ is a sample space, $\mathcal{F}$ is a $\sigma$-algebra, and $P$ is a probability measure.

# Gaussian processes

The nonparametric regression model is

$$Y_i = m(X_i) + \epsilon_i, \quad i = 1, \ldots, n$$

where $\mathbb{E}(\epsilon_i) = 0$.

The frequentist kernel estimator for $m$ is

$$\widehat{m}(x) = \frac{\sum_{i=1}^n Y_i \, K\left(\frac{x - X_i}{h}\right)}{\sum_{i=1}^n K\left(\frac{x - X_i}{h}\right)}$$

where $K$ is a kernel and $h$ is a bandwidth.

Bayesian version requires prior $\pi$ on set of regression functions

# Gaussian process

A stochastic process $m(x)$ indexed by $x \in \mathbb{R}$ is a *Gaussian process* if for each set of points $x_1, \ldots, x_n$ the vector $(m(x_1), m(x_2), \ldots, m(x_n))^T$ is normally distributed:

$$(m(x_1), m(x_2), \ldots, m(x_n))^T \sim N(\mu(x), K(x))$$

where $K_{ij}(x) = K(x_i, x_j)$ is a Mercer kernel.

As before, if $x_1, \ldots, x_n$ are fixed we denote the $n \times n$ matrix with entries $K(x_i, x_j)$ by $\mathbb{K}$.

---

The definition makes sense when indexing by any set $\mathcal{X}$ for an appropriately defined Mercer kernel.

# Gaussian process prior

Let's assume $\mu = 0$, so prior mean function is zero

Density of the Gaussian process prior of $m = (m(x_1), \ldots, m(x_n))$ is

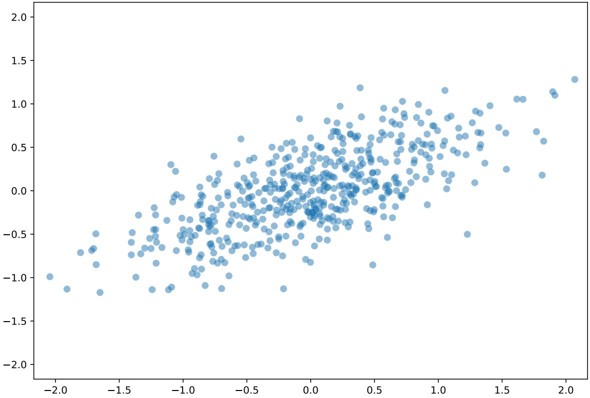
$$\pi(m) = (2\pi)^{-n/2}|\mathbb{K}|^{-1/2} \exp\left(-\frac{1}{2}m^T\mathbb{K}^{-1}m\right).$$

Under change of variables $m = \mathbb{K}\alpha$, we have $\alpha \sim N(0, \mathbb{K}^{-1})$ and

$$\pi(\alpha) = (2\pi)^{-n/2}|\mathbb{K}|^{1/2} \exp\left(-\frac{1}{2}\alpha^T\mathbb{K}\alpha\right).$$

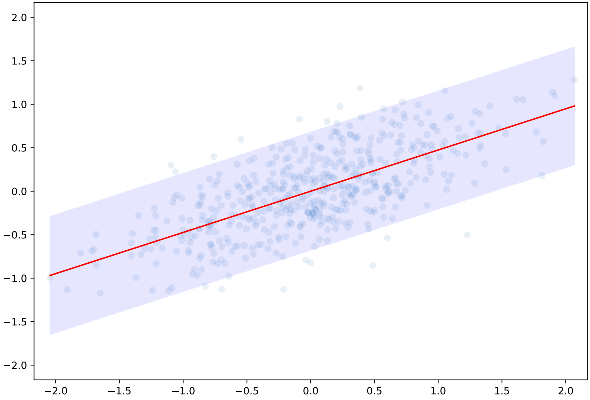
# Conditionals of Gaussian

Posterior is calculated using Gaussian conditionals



# Conditionals of Gaussian

Posterior is calculated using Gaussian conditionals



# Gaussian conditionals

If $(X_1, X_2)$ are jointly Gaussian with distribution

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim N\left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} \right)$$

then the conditional distributions are also Gaussian and given by

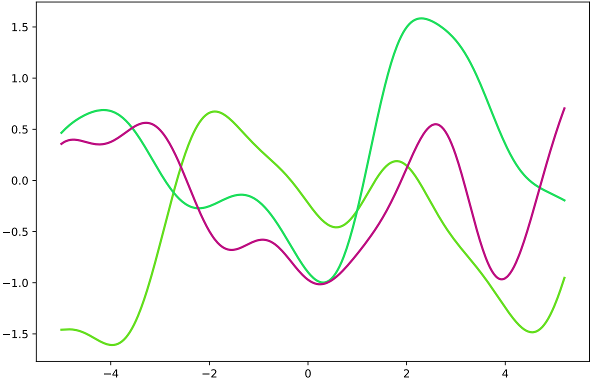
$$X_1 \mid x_2 \sim N\left( \frac{K_{12}}{K_{22}} x_2,\ K_{11} - \frac{K_{12}^2}{K_{22}} \right)$$

$$X_2 \mid x_1 \sim N\left( \frac{K_{12}}{K_{11}} x_1,\ K_{22} - \frac{K_{12}^2}{K_{11}} \right)$$

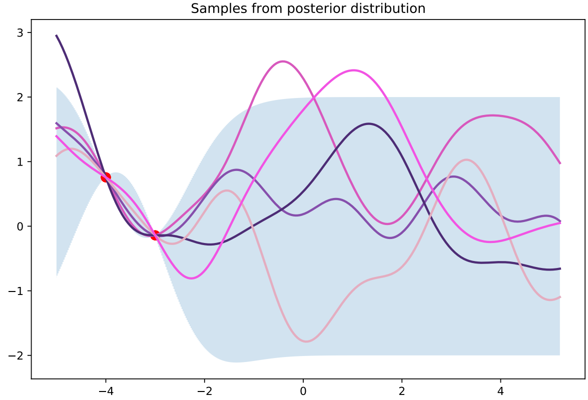
Let’s look at the notebook demo

(plots from the demo follow)

# Samples from prior and posterior



# Samples from prior and posterior



# Gaussian processes prior

What functions have high probability according to the Gaussian process prior?

The prior favors $m^T \mathbb{K}^{-1} m$ being small. If $v$ is an eigenvector of $\mathbb{K}$, with eigenvalue $\lambda$, then

$$\frac{1}{\lambda} = v^T \mathbb{K}^{-1} v$$

- Eigenfunctions of the Mercer kernel $K$ with *large* eigenvalues are favored by the prior
- These correspond to smooth functions; the eigenfunctions that are very wiggly correspond to small eigenvalues

# Using the likelihood

We observe $Y_i = m(x_i) + \epsilon_i$ where $\epsilon_i \sim N(0, \sigma^2)$. So, log-likelihood is

$$\log p(Y \mid m) = -\frac{1}{2\sigma^2} \sum_i (Y_i - m(x_i))^2 + C$$

where $C = -\log(\sqrt{2\pi\sigma^2})$.

Log-posterior is

$$\begin{aligned} \log p(Y \mid m) + \log \pi(m) &= -\frac{1}{2\sigma^2} \|Y - \mathbb{K}\alpha\|_2^2 - \frac{1}{2}\alpha^T \mathbb{K}\alpha + C' \\ &= -\frac{1}{2\sigma^2} \|Y - \mathbb{K}\alpha\|_2^2 - \frac{1}{2}\|\alpha\|_K^2 + C' \end{aligned}$$

---

$C'$ is just another constant.

# Calculating the posterior

In Bayesian *maximum a posteriori (MAP)* inference, one estimates the mode of the posterior.

The posterior mean (and mode) is

$$\mathbb{E}(\alpha \mid Y) = \left(\mathbb{K} + \sigma^2 I\right)^{-1} Y$$

and thus

$$\widehat{m} = \mathbb{E}(m \mid Y) = \mathbb{K}\left(\mathbb{K} + \sigma^2 I\right)^{-1} Y.$$

Equivalent to Mercer kernel regression

# Gaussian conditionals

If $(X_1, X_2)$ are jointly Gaussian with distribution

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim N\left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}\right)$$

then the conditional distributions are also Gaussian and given by

$$\begin{aligned} X_1 \mid x_2 &\sim N\left(\mu_1 + CB^{-1}(x_2 - \mu_2),\ A - CB^{-1}C^T\right) \\ X_2 \mid x_1 &\sim N\left(\mu_2 + C^T A^{-1}(x_1 - \mu_1),\ B - C^T A^{-1} C\right) \end{aligned}$$

The matrix $A - CB^{-1}C^T$ is called the *Schur complement* of $B$.

# Predicting at a new point

How do we predict $Y_{n+1} = m(x_{n+1}) + \epsilon_{n+1}$?

Let $k$ be the vector

$$k = (K(x_1, x_{n+1}), \ldots, K(x_n, x_{n+1})).$$

Then $(Y_1, \ldots, Y_{n+1})$ are jointly Gaussian with covariance

$$\begin{pmatrix} \mathbb{K} + \sigma^2 I & k \\ k^T & K(x_{n+1}, x_{n+1}) + \sigma^2 \end{pmatrix}.$$

# Predictive distribution

Using above expression for Gaussian conditionals:

The posterior mean and variance are

$$\begin{aligned}\mathbb{E}(Y_{n+1} \mid x_{1:n}, Y_{1:n}) &= k^T(\mathbb{K} + \sigma^2 I)^{-1} Y \\ \mathrm{Var}(Y_{n+1} \mid x_{1:n}, Y_{1:n}) &= K(x_{n+1}, x_{n+1}) + \sigma^2 - k^T(\mathbb{K} + \sigma^2 I)^{-1} k\end{aligned}$$

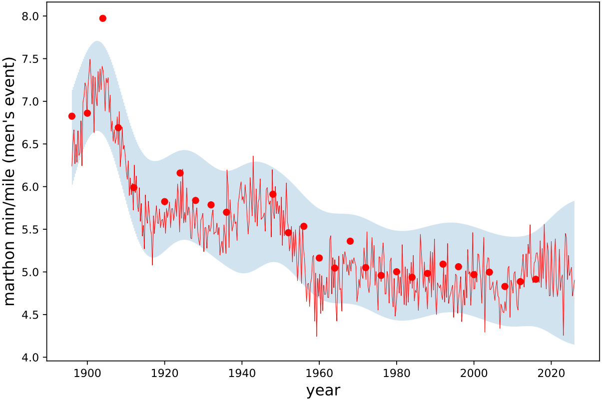
# Predictive distribution

- Note that the mean is identical to what we saw for Mercer kernel regression
- But now we get a measure of uncertainty (the variance), which comes from the Gaussian process assumption

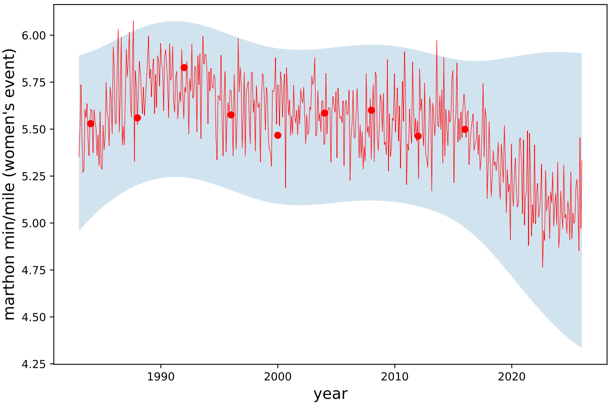
Let’s return to the notebook demo

(plots from the demo follow)

# Olympic marathon times (men's race)



# Olympic marathon times (women's race)



# Summary

- In a Bayesian approach, the parameters are random, and the data are fixed.
- In nonparametric Bayes, the "parameters" are functions
- A Gaussian process is a stochastic process $m$ where each collection of random variables $m(x_1), m(x_2), \ldots, m(x_n)$ is jointly Gaussian
- Gaussian processes are Bayesian versions of kernel regression; the posterior mean is equivalent to Mercer kernel regression