S&DS 365 / 665

Intermediate Machine Learning

Nonparametric Bayes: Gaussian Processes

February 11

Yale

Version of 2026/02/10 at 23:50

Reminders

- Assignment 1 due tomorrow
- Assignment 2 is out
- Quiz 3 next Wednesday

For today

- Bayesian inference (redux)
- Gaussian processes
- Examples

Bayesian Inference

The parameter θ 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* $p(\theta \mid \mathcal{D}_n)$.

In machine learning, Bayesian inference is preferred by some researchers as a way of introducing uncertainty

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

Nonparametric Bayes

- In nonparametric Bayesian inference, we replace a finite dimensional model θ 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 π 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?

Nonparametric Bayes procedures may not have coverage and consistency properties of frequentist procedures

Essential methods

We'll explore these questions in a couple of settings

Statistical problem	Frequentist approach	Bayesian approach
regression	kernel smoother	Gaussian process
CDF estimation	empirical cdf	Dirichlet process
density estimation	kernel density estimator	Dirichlet process mixture

NP Bayes

- Nonparametric Bayesian inference can be subtle and technical
- Part of the machine learning toolkit
- Underlying probability theory can be beautiful
- We'll introduce the main techniques to give a flavor
- The notes go into more technical detail

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

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 Ω is a sample space, $\mathcal{F}$ is a σ-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 $\mathbb{E}(\epsilon_i) = 0$.

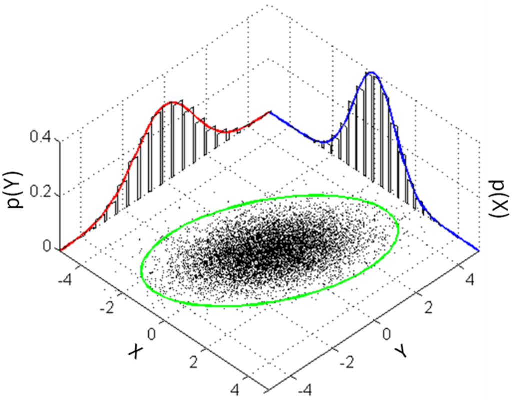
The frequentist kernel estimator for m is

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

where K is a kernel and h is a bandwidth.

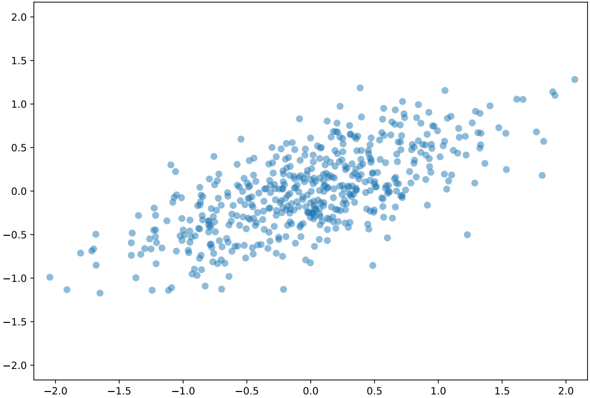
Bayesian version requires prior $\pi(m)$ on regression functions m

Everything boils down to Gaussian marginals and conditionals



https://en.wikipedia.org/wiki/Multivariate_normal_distribution

Starting point: Conditionals of Gaussian



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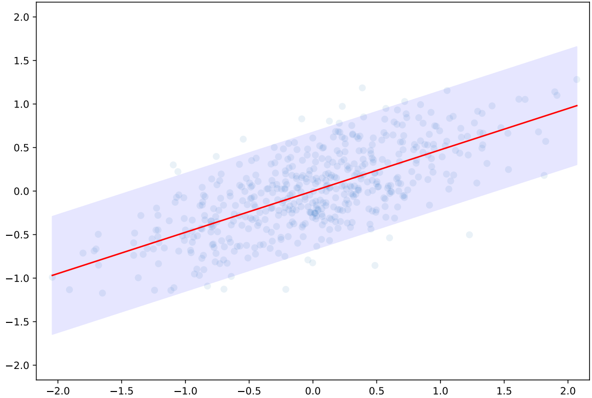


Gaussian conditionals

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

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

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

Gaussian conditionals

If $(X_1, X_2) \in \mathbb{R}^2$ 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

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

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

Note that the variance doesn't depend on x

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 $\mu(x) = (\mu(x_1), \mu(x_2), \ldots, \mu(x_n))$ is a mean function and $K_{ij}(x) = K(x_i, x_j)$ is the Gram matrix of 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

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

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 λ, 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

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

Calculating the posterior

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

The posterior mean (and mode) is

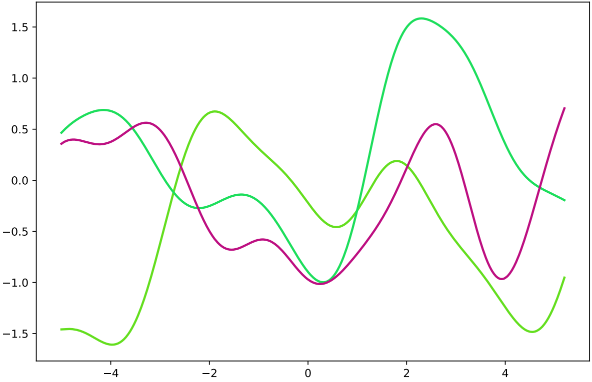
$$\mathbb{E}(\alpha \mid Y) = \left(\mathbb{K} + \sigma^2 I\right)^{-1} Y$$

and thus

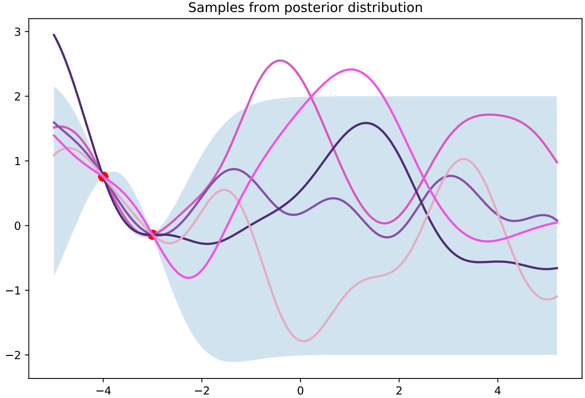
$$\widehat{m} = \mathbb{E}(m \mid Y) = \mathbb{K}\left(\mathbb{K} + \sigma^2 I\right)^{-1} Y.$$

Equivalent to Mercer kernel regression

Samples from prior and posterior



Samples from prior and posterior



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

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

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

All from: Gaussian conditionals

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Let’s look at the notebook demo

(plots from the demo follow)

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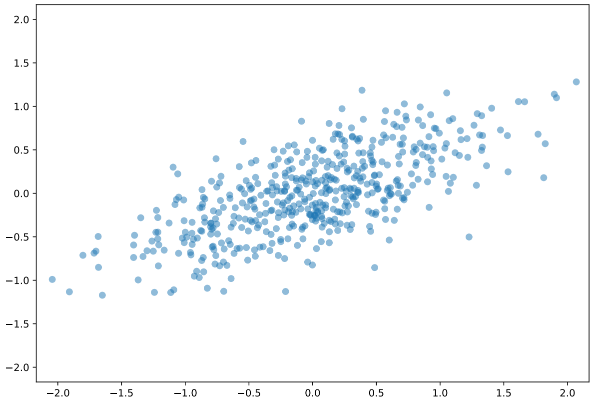

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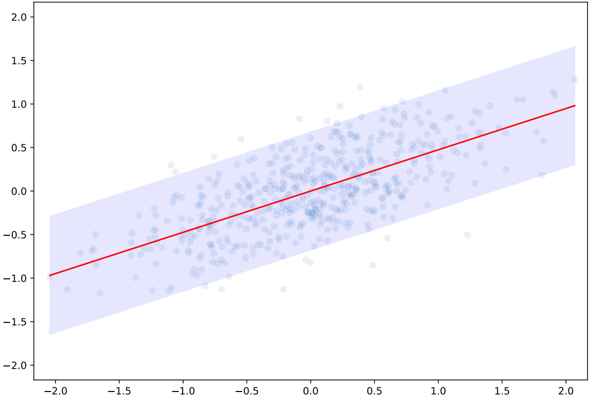

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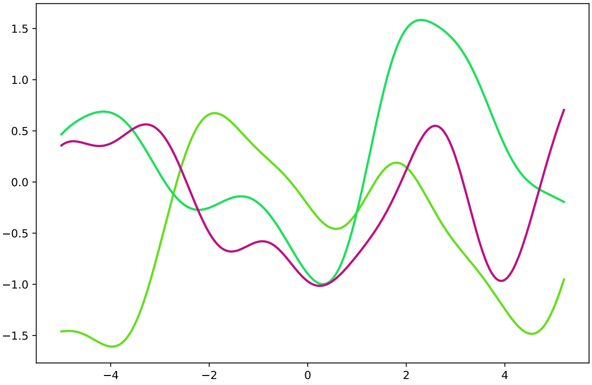
Samples from prior and posterior



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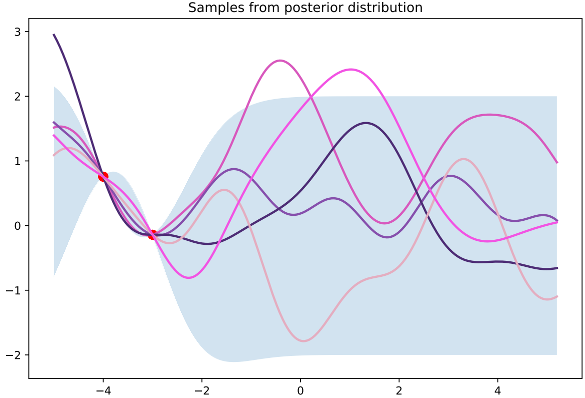
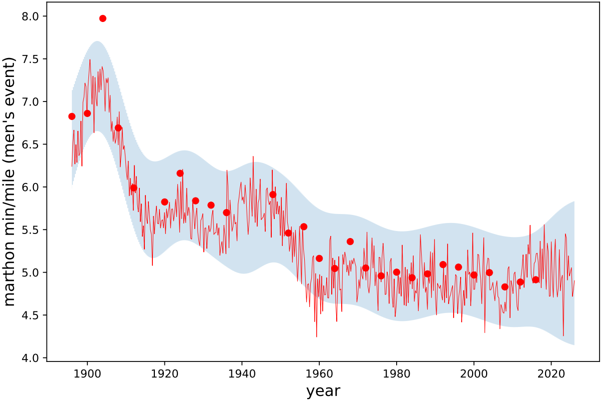


Olympic marathon times (men's race)



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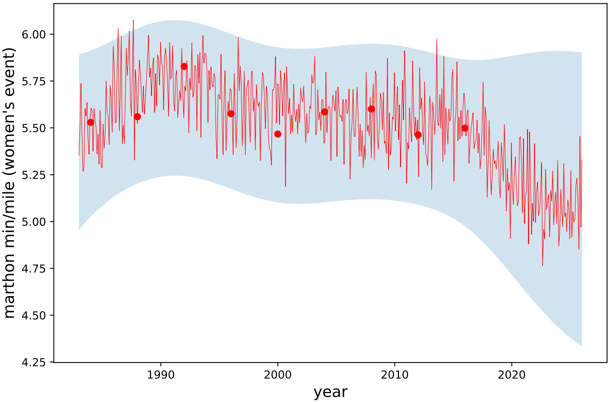

The next few slides give a *very* brief overview of the Dirichlet process.

We won’t ask you about this on an exam, but there could be a quiz question on the definition of the Dirichlet process.

The Dirichlet Process

- The Dirichlet process is analogous to the Gaussian process
- Every partition of sample space has a Dirichlet distribution (more precise shortly)
- GPs are tools for regression functions; DPs are tools for distributions and densities
- DPs finesse the problem of choosing the number of components in a mixture model
    - Example: Number of topics in a topic model

Relation to KDEs

- A DP is a distribution over distributions
- A Dirichlet process mixture is a distribution over mixture models
- DPMs are Bayesian versions of kernel density estimation
- Subject to the curse of dimensionality!

What is a Dirichlet Process?

Recall:

A random function m is distributed according to a Gaussian process if for every $x_1, x_2, \ldots, x_n$ the random vector $m(x_1), \ldots, m(x_n)$ has a multivariate Gaussian distribution

$$N(\mu(x), K(x))$$

What is a Dirichlet Process?

A random distribution F is distributed according to a Dirichlet process $DP(\alpha, F_0)$ if for every partition $A_1, \ldots, A_n$ of the sample space the random vector $F(A_1), \ldots, F(A_n)$ has a Dirichlet distribution

$$\mathrm{Dir}\left(\alpha F_0(A_1), \alpha F_0(A_2), \ldots, \alpha F_0(A_n)\right)$$

where

$$F(A_i) = \mathbb{P}_F(A_i) = \int_{A_i} dF(x)$$

What is a Dirichlet Process?

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where

$$F(A_i) = \mathbb{P}_F(A_i) = \int_{A_i} dF(x)$$

The distribution F_0 and scaling α are hyperparameters of the prior

Analogous to the mean μ and covariance kernel K of the GP prior

Examples

As a special case, if the sample space is the real line we can take the partition to be

$$A_1 = \{z \, : \, z \leq x\}$$
$$A_2 = \{z \, : \, z > x\}$$

then

$$F(x) = \mathbb{P}_F(X \leq x) \sim \text{Beta}\Big(\alpha F_0(x), \alpha(1 - F_0(x))\Big)$$

Examples

As another special case, if the sample space is the real line we can take the partition to be

$$A_1 = (-\infty, -5], \;\; A_2 = (-5, 5], \;\; A_3 = (5, \infty)$$

then $(F(A_1), F(A_2), F(A_3))$ is a random point on the 3-simplex

$$\Delta_3 = \{(p_1, p_2, p_3) : p_i \geq 0, p_1 + p_2 + p_3 = 1\}$$

with distribution

$$(F(A_1), F(A_2), F(A_3)) \sim \text{Dirichlet}\big(\alpha_1, \alpha_2, \alpha_3\big)$$

with $\alpha_1 = \alpha F_0(-5)$, $\alpha_2 = \alpha(F_0(5) - F_0(-5))$, and $\alpha_3 = \alpha(1 - F_0(5))$.

DPs vs GPs

The natural correspondence between the Gaussian process and Dirichlet process is as follows:

Gaussian process	Dirichlet process
points $x_1, \ldots, x_n$	sets $A_1, \ldots, A_n$
prior mean μ	prior mean F_0
prior covariance K	prior scaling α

Big picture

The definition tells us the precise sense in which a DP is an infinite Dirichlet distribution

But this is not concrete

The sticking breaking and “Chinese restaurant processes” give us *algorithms* for working with a DP

See notes for an introduction to these ideas (not required for this course)

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
- Calculation with GPs uses Gaussian conditioning via Schur complements
- Gaussian processes are Bayesian versions of kernel regression; the posterior mean is equivalent to Mercer kernel regression