

S&DS 365 / 665
Intermediate Machine Learning

Nonparametric Bayes: Gaussian Processes

September 28

For Today

- CNN recap and example
- Review of parametric Bayes
- Introduction to nonparametric Bayes
- Gaussian processes
- Examples

CNN Demo

CNN Demo

Here we illustrate how (dangerously) simple it is to build a convolutional neural network for image classification, using the iconic MNIST dataset. See [this article](#) from last week for greater inspiration!

```
In [1]: import numpy as np
        from tensorflow import keras
        from tensorflow.keras import layers
        import matplotlib.pyplot as plt
```

First, load the MNIST dataset with 60000 training images and 10000 test images.

```
In [2]: num_classes = 10
        input_shape = (28, 28, 1)

        # the data, split between train and test sets
        (x_train, y_train), (x_test, y_test) = keras.datasets.mnist.load_data()
```

Bayesian Inference

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

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

Bayes' Theorem

A simple consequence of conditional probability:

$$\begin{aligned}\mathbb{P}(A|B) &= \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)} \\ &= \frac{\mathbb{P}(B|A) \mathbb{P}(A)}{\mathbb{P}(B)}\end{aligned}$$

Bayes' Theorem

The posterior distribution can be written as

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

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

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

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

Basic Example

Take model $X \sim \text{Bernoulli}(\theta)$.

This is a “coin flip”: $X = 1$ means “heads” and $X = 0$ means “tails.”

Natural prior is $\text{Beta}(\alpha, \beta)$ distribution

$$\pi_{\alpha, \beta}(\theta) \propto \theta^{\alpha-1} (1 - \theta)^{\beta-1}$$

Basic Example

Take model $X \sim \text{Bernoulli}(\theta)$.

Natural prior is $\text{Beta}(\alpha, \beta)$ distribution

$$\pi_{\alpha, \beta}(\theta) \propto \theta^{\alpha-1} (1 - \theta)^{\beta-1}$$

The scaling constant is scary looking:

$$\frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}$$

where $\Gamma(\cdot)$ is the “Gamma function”

$$\Gamma(z) = \int_0^{\infty} x^{z-1} e^{-x} dx$$

Basic Example

$X \sim \text{Bernoulli}(\theta)$ with data $\mathcal{D}_n = \{x_1, \dots, x_n\}$. Prior $\text{Beta}(\alpha, \beta)$ distribution

$$\pi_{\alpha, \beta}(\theta) \propto \theta^{\alpha-1} (1 - \theta)^{\beta-1}$$

Let $s = \sum_{i=1}^n x_i$ be the number of “heads”

Posterior distribution $\theta \mid \mathcal{D}_n$ is another beta distribution!

Specifically, with

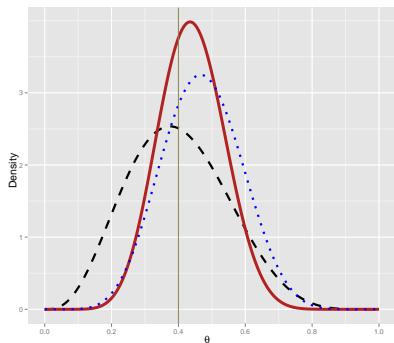
$$\tilde{\alpha} = \alpha + \text{number of heads} = \alpha + s$$

$$\tilde{\beta} = \beta + \text{number of tails} = \beta + n - s$$

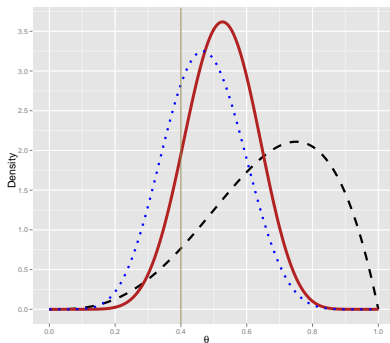
Showing this just uses the simple fact that $\theta^{\alpha-1} \theta^x = \theta^{x+\alpha-1}$

Example

$n = 15$ points sampled as $X \sim \text{Bernoulli}(\theta = 0.4)$, with $s = 7$ heads.



Prior A



Prior B

Prior distribution (black-dashed), likelihood function (blue-dotted),
posterior distribution (red-solid).

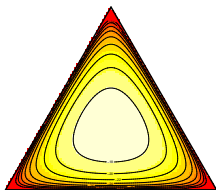
Dirichlet: From coins to dice

Multinomial model with Dirichlet prior is generalization of the Bernoulli/Beta model.

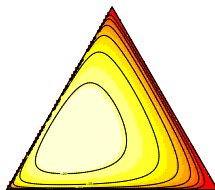
$$\text{Dirichlet}_{\alpha}(\theta) \propto \theta_1^{\alpha_1-1} \theta_2^{\alpha_2-1} \dots \theta_K^{\alpha_K-1}$$

where $\alpha = (\alpha_1, \dots, \alpha_K) \in \mathbb{R}_+^K$ is a non-negative vector.

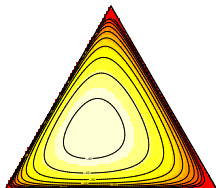
Example



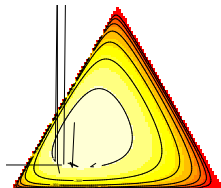
prior with Dirichlet(6,6,6)



likelihood function with $n = 20$



posterior distribution with $n = 20$



posterior distribution with $n = 200$

Parametric Bayes demo

Demo code for Bayesian analysis

In this notebook we illustrate some of the basic models and priors for Bayesian inference. These concepts will be important for our discussions about "topic models."

First, we illustrate the situation where the parameter θ that we are modeling is a Bernoulli parameter. This can be thought of as the probability that flipping a certain coin comes up heads. The most commonly used prior distribution for this model is a beta distribution. Under a beta prior, the posterior distribution is again a beta distribution.

This is illustrated in the following simulation. The prior distribution is a beta distribution. As the sample size increases, the posterior distribution becomes concentrated on the true parameter. But as the variance of the prior decreases, the posterior distribution becomes more concentrated on the true parameter.

```
In [5]: import os, gzip
import numpy as np
import matplotlib.pyplot as plt
```

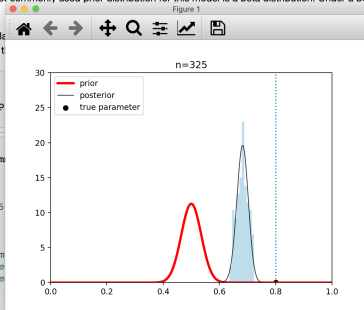
```
In [*]: %matplotlib qt
from scipy.special import gamma
from scipy import random
from scipy.stats import beta

theta = np.linspace(0,1,num=5)
fig = plt.figure(1)
plt.ion()

# The following are the parameters
# variance of the prior decreases
# the posterior to be centered

scale = 100
a0 = scale*1
b0 = scale*1

sample_size = 100
```



Nonparametric Bayes

- Bayesian inference for infinite-dimensional spaces
- Alternative to classical/frequentist approaches
- Caution required with interpretation

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?

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

Before diving in...

- Nonparametric Bayesian inference can be subtle and technical
- Part of the machine learning toolkit
- 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 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 (Ω, \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

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

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

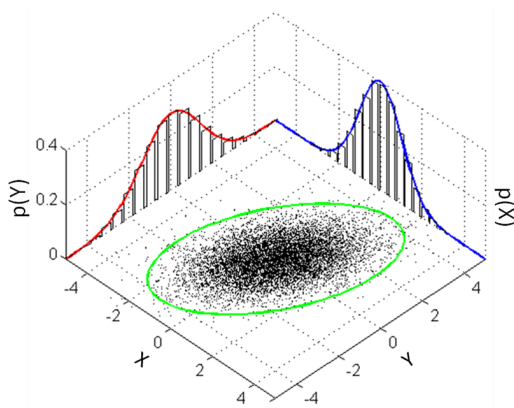
The frequentist kernel estimator for m is

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

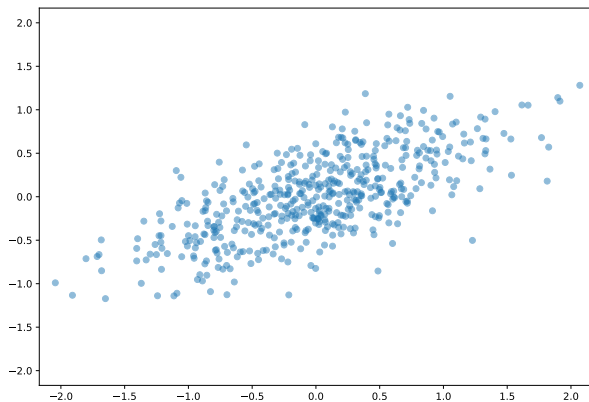
where K is a kernel and h is a bandwidth.

Bayesian version requires prior π on set of regression functions

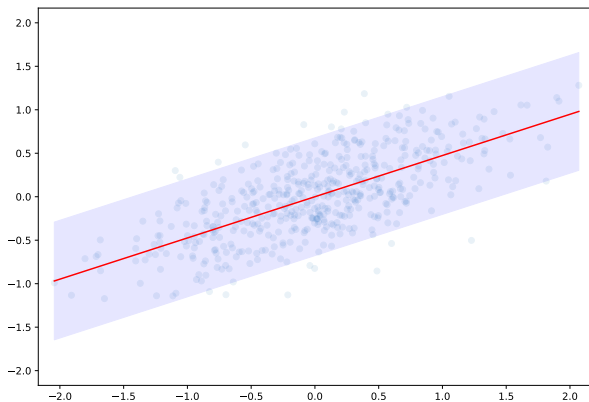
Gaussian marginals and conditionals



Starting point: Conditionals of Gaussian



Starting point: Conditionals of Gaussian



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

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

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

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, \dots, x_n the vector $(m(x_1), m(x_2), \dots, m(x_n))^T$ is normally distributed:

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

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

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

Gaussian process prior

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

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

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

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

Log-posterior is

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

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

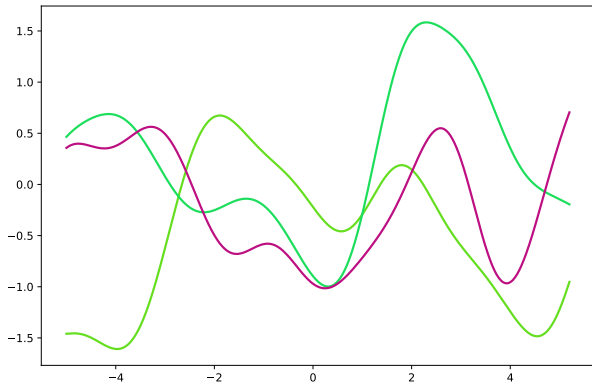
$$\mathbb{E}(\alpha \mid Y) = \left(\mathbb{K} + \sigma^2 I \right)^{-1} Y$$

and thus

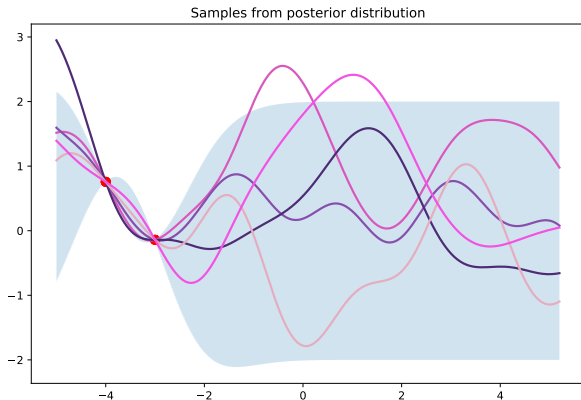
$$\hat{m} = \mathbb{E}(m \mid Y) = \mathbb{K} \left(\mathbb{K} + \sigma^2 I \right)^{-1} Y.$$

Equivalent to Mercer kernel regression

Samples from prior and posterior



Samples from prior and posterior



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

$$X_1 | x_2 \sim N \left(\mu_1 + CB^{-1}(x_2 - \mu_2), A - CB^{-1}C^T \right)$$

$$X_2 | x_1 \sim N \left(\mu_2 + C^T A^{-1}(x_1 - \mu_1), B - C^T A^{-1}C \right)$$

Predicting at a new point

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

Let k be the vector

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

Then (Y_1, \dots, 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

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

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

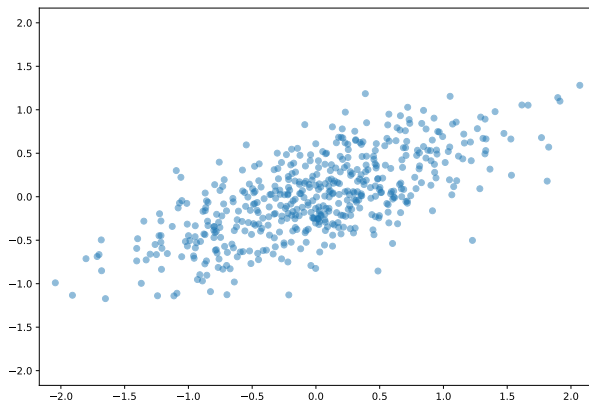
Predictive distribution

- 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

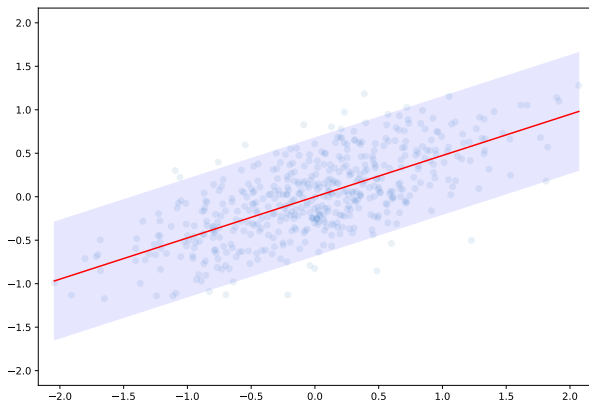
Let's look at the notebook demo

(plots from the demo follow)

Starting point: Conditionals of Gaussian



Starting point: Conditionals of Gaussian



Gaussian conditionals

If (X_1, X_2) are jointly Gaussian with distribution

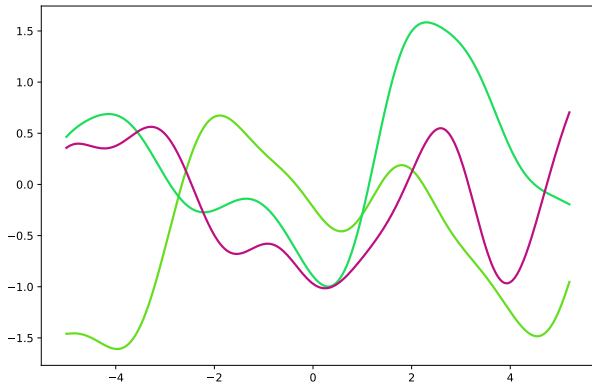
$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim N \left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} \right)$$

then the conditional distributions are also Gaussian and given by

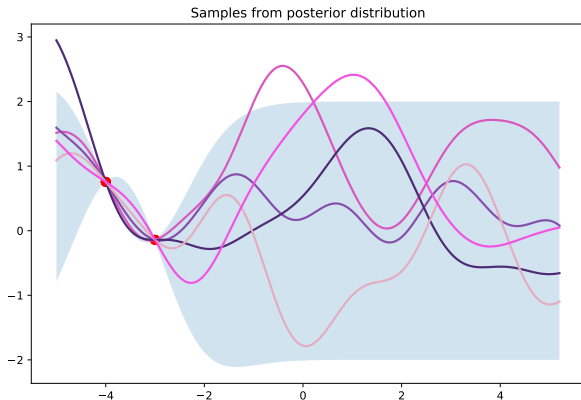
$$X_1 | x_2 \sim N \left(\frac{K_{12}}{K_{22}} x_2, K_{11} - \frac{K_{12}^2}{K_{22}} \right)$$

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

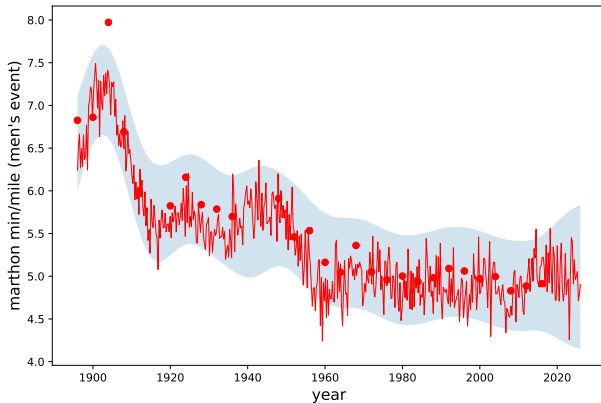
Samples from prior and posterior



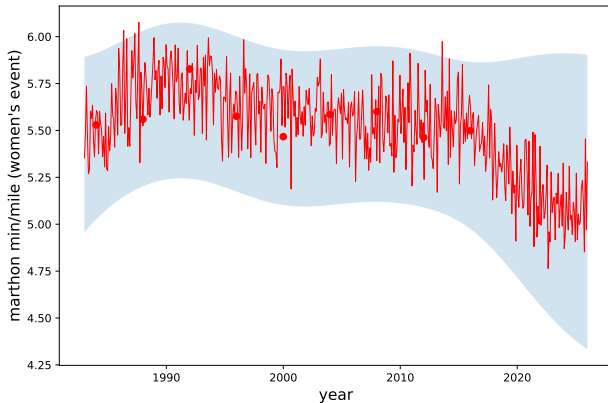
Samples from prior and posterior



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 $m(x_1), m(x_2), \dots, m(x_n)$ is jointly Gaussian
- Gaussian processes are Bayesian versions of kernel regression; the posterior mean is equivalent to Mercer kernel regression