21: Gaussian Process Models

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Introduction

We talk about Gaussian process models in this chapter. Gaussian processes describe random functions, and they can show up in statistical modeling in a few places.

If you would like to dig a little deeper, this is considered a good reference: `http://gaussianprocess.org/gpml/`. We will be using chapter 2 as an additional resource.

Definitions

It's helpful to initially consider $x_i \in \mathbb{R}^p$ where $p = 1$ or $p = 2$.

We say μ follows a **Gaussian process** with mean function m and covariance function k if for any finite set of nonrandom points $x_1, \ldots, x_n$

$$\mu(x_1), \ldots, \mu(x_n) \sim \text{Normal}((m(x_1), \ldots, m(x_n)), K(x_1, \ldots, x_n)).$$

For short, we write $\mu \sim \text{GP}(m, k)$.

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This means $E[\mu(x_i)] = m(x_i)$ and $\text{Cov}(\mu(x_i), \mu(x_j)) = K_{i,j} = k(x_i, x_j)$.

A first example: Gaussian process regression

Let's assume we're regressing univariate y_is on vector-valued x_is. Then we are interested in

$$y_i = \mu(x_i) + \epsilon_i.$$

We could also be interested in the "noiseless" situation, as well.

A first example: Gaussian process regression

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The μ function can be nonlinear and very flexible!

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Picking a prior means we need to pick m and k. We can see that

$$E[y_i \mid x_i] = E[\mu(x_i) \mid x_i] = m(x_i).$$

For m

- can assume $m(x) = 0$ (like assuming regression coefficients have a zero-mean prior)
- can use an informative prior

For k...

A popular choice

Any k function gives you a "similarity" or "nearness" measure for any two pairs of inputs. It needs to be chosen very carefully.

We will often use a **squared exponential kernel**

$$k(x, x') = \tau^2 \exp\left[-\sum_{i=1}^{p} \frac{(x_j - x_j')^2}{2 l_j^2} \right]$$

Each l_j determines the wiggliness in the jth direction of the predictors.

The τ^2 parameter is an overall variance for each $\mu(x)$.

Simulating from the prior

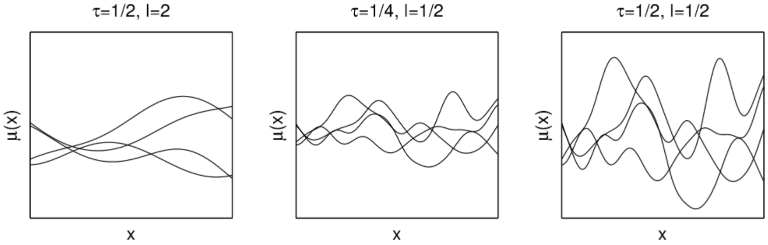

Figure 21.1 *Random draws from the Gaussian process prior with squared exponential covariance function and different values of the amplitude parameter* τ *and the length scale parameter* l.

More to say about kernel choice:
`https://www.cs.toronto.edu/~duvenaud/cookbook/`

Inference: conditional posterior

We will use a lot of properties of Gaussian random vectors when we conduct inference.

If

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \sim \text{Normal}\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \right)$$

then $x_1 \mid x_2$ is also normally distributed with mean vector

$$\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)$$

and covariance matrix

$$\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$$

Inference: conditional posterior

Let's assume the likelihood is $y_i = \mu(x_i) + \epsilon_i$ where $\epsilon_i \sim \text{Normal}(0, \sigma^2)$, and for the prior, $m(x) = 0$.

The observed data is $\{x_i, y_i\}$, and the parameters are τ, l, σ^2. To find the conditional posterior $p(\mu(x) \mid x, y, \sigma^2, \tau, l)$, we use

$$\begin{pmatrix} y \\ \mu \end{pmatrix} \Bigg| x, \sigma^2, \tau, l \sim \text{Normal}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} K(x,x) + \sigma^2 I & K(x,x) \\ K(x,x) & K(x,x) \end{pmatrix} \right)$$

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By properties of multivariate normal random vectors $\mu \mid x, y, \tau, l, \sigma$ is normally distributed with mean and covariance

$$\begin{aligned} E[\mu \mid x, y, \tau, l, \sigma] &= K(x,x)[K(x,x) + \sigma^2 I]^{-1} y \\ Var[\mu \mid x, y, \tau, l, \sigma] &= K(x,x) - K(x,x)[K(x,x) + \sigma^2 I]^{-1} K(x,x) \end{aligned}$$

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$$E[\mu \mid x, y, \tau, l, \sigma] = K(x,x)[K(x,x) + \sigma^2 I]^{-1} y$$
$$Var[\mu \mid x, y, \tau, l, \sigma] = K(x,x) - K(x,x)[K(x,x) + \sigma^2 I]^{-1} K(x,x)$$

What does this simplify to in the case of "noiseless" regression?

Inference: conditional posterior

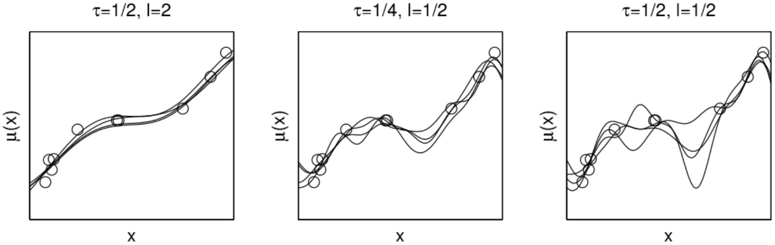


Figure 21.2 *Posterior draws of a Gaussian process $\mu(x)$ fit to ten data points, conditional on three different choices of the parameters τ, l that characterize the process. Compare to Figure 21.1, which shows draws of the curve from the prior distribution of each model. In our usual analysis, we would assign a prior distribution to τ, l and then perform joint posterior inference for these parameters along with the curve $\mu(x)$; see Figure 21.3. We show these three choices of conditional posterior distribution here to give a sense of the role of τ, l in posterior inference.*

Inference: prediction/smoothing at new points

Let's assume the likelihood is $y_i = \mu(x_i) + \epsilon_i$ where $\epsilon_i \sim \text{Normal}(0, \sigma^2)$, and for the prior, $m(x) = 0$.

Call $\tilde{x}$ unseen data, in addition to $\{x_i, y_i\}$. Then

$$\begin{pmatrix} y \\ \tilde{\mu} \end{pmatrix} \Bigg| x, \tilde{x}, \sigma^2, \tau, l \sim \text{Normal}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} K(x,x) + \sigma^2 I & K(x,\tilde{x}) \\ K(\tilde{x}, x) & K(\tilde{x},\tilde{x}) \end{pmatrix} \right)$$

By properties of multivariate normal random vectors, $\tilde{\mu} \mid x, y, \tau, l, \sigma$ is normally distributed with

$$E[\tilde{\mu} \mid x, y, \tau, l, \sigma] = K(\tilde{x}, x)[K(x,x) + \sigma^2 I]^{-1} y$$
$$Var[\tilde{\mu} \mid x, y, \tau, l, \sigma] = K(\tilde{x},\tilde{x}) - K(\tilde{x}, x)[K(x,x) + \sigma^2 I]^{-1} K(x, \tilde{x})$$

Inference: estimating unknown parameters

We need the marginal likelihood for MCMC techniques: $\log p(y \mid \tau, l, \sigma^2)$ equals

$$-\frac{n}{2}\log(2\pi) - \frac{1}{2}\log\det(K(x,x)+\sigma^2 I) - \frac{1}{2}y^T[K(x,x)+\sigma^2 I]^{-1}y$$

We could use this to do Gibbs sampling or some sort of Metropolis-Hastings technique.

Birthdays and Birthdates example

$$y(t) = \mu(t) + \epsilon_t$$

with

$$\mu(t) = f_1(t) + f_2(t) + f_3(t) + f_4(t) + f_5(t).$$

Birthdays and Birthdates example

Slow and fast trends:

$$f_1(t) \sim GP(0, k_1)$$

$$k_1(t, t') = \sigma_1^2 \exp\left[-\frac{(t - t')^2}{2l_1^2}\right]$$

and

$$f_2(t) \sim GP(0, k_2)$$

$$k_2(t, t') = \sigma_2^2 \exp\left[-\frac{(t - t')^2}{2l_2^2}\right].$$

There is an identifiability concern. They mention that they put log-t priors on l_1 and l_2 and log-uniform priors on σ_1 and σ_2^2, but they do not give specifics.

Birthdays and Birthdates example

A quasi-periodic weekly effect:

$$f_3(t) \sim GP(0, k_3)$$

$$k_3(t, t') = \sigma_3^2 \exp\left[-\frac{2\sin^2(\pi[t-t']/7)}{l_{3,1}^2}\right] \exp\left[-\frac{(t-t')^2}{2l_{3,2}^2}\right].$$

The kernel k_3 is “high” only when both baby kernels are “high.”

Also note $2\sin^2(\pi[t-t']/7) = 1 - \cos\left(\frac{2\pi[t-t']}{7}\right)$ by “product identity.”

Birthdays and Birthdates example

A quasi-periodic yearly effect:

$$f_4(t) \sim GP(0, k_4)$$

$$k_4(t, t') = \sigma_4^2 \exp\left[-\frac{2\sin^2(\pi[t - t']/365.25)}{l_{4,1}^2}\right] \exp\left[-\frac{(t - t')^2}{2l_{4,2}^2}\right].$$

Birthdays and Birthdates example

Regular regression parameters

$$f_5(t) = I_{\text{special day}}\beta_a + I_{\text{special day and weekend}}\beta_b$$

where $I_{\text{special day}} = (I_{\text{New Year's Day}}, I_{\text{Valentine's Day}}, \ldots, I_{\text{Christmas}})'$.

$$k_5(t, t') = ?$$

Birthdays and Birthdates example

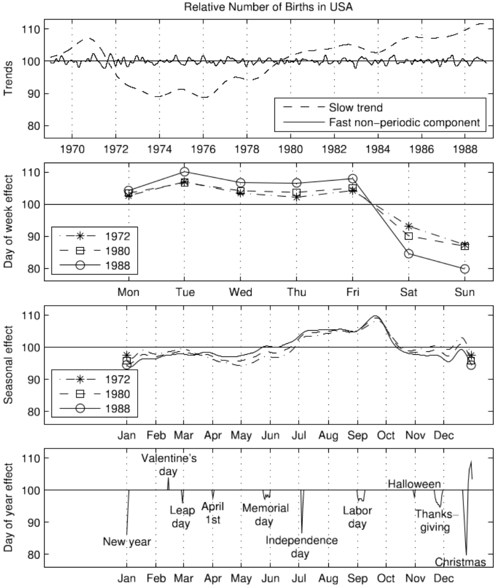
This means

$$\mu(t) = f_1(t) + f_2(t) + f_3(t) + f_4(t) + f_5(t) \sim GP(0, k)$$

where

$$k(t, t') = k_1(t, t') + k_2(t, t') + k_3(t, t') + k_4(t, t') + k_5(t, t').$$

Birthdays and Birthdates example



The Catch

All of this seems easy. We're just using normal-normal conjugacy, right?

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Yes, but there are computational difficulties. For large data sets with more than several thousand rows, naively inverting $K(x, x) + \sigma^2 I$ is going to be brutal.

Density estimation example

So far we have discussed Gaussian processes as prior distributions for a function controlling the location and potentially the shape parameter of a parametric observation model.

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So far we have discussed Gaussian processes as prior distributions for a function controlling the location and potentially the shape parameter of a parametric observation model.

To get more flexibility we would like to model also the conditional observation model as nonpara- metric.