STAT 576 Bayesian Analysis

Lecture 13: Nonparametric Models

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Prior Assumptions

Given a set of paired data $(x_1, y_1), \ldots, (x_n, y_n)$, we often assume that the expected value of y is a function of x:

$$y_i = \mu(x_i) + \epsilon_i, \quad i = 1, \ldots, n,$$

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- In this lecture, we will discuss nonparametric models, where the prior is placed directly on the function μ within a function space.

Gaussian Process

- A **stochastic process** is a collection of random variables indexed by some set, e.g. time or space.
  - Random walk: r.v.s. indexed by time.
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- A **Gaussian process** is a stochastic process such that any finite collection of r.v.s. has a multivariate normal distribution.
- Specifically, if $\{\mu(x) : x \in \mathcal{X}\}$ is a Gaussian process, then for any finite set of indices $x_1, \ldots, x_n \in \mathcal{X}$, the random vector $(\mu(x_1), \ldots, \mu(x_n))$ has a multivariate normal distribution.
- As a special case, for any $x \in \mathcal{X}$, $\mu(x)$ is a normal random variable.

Gaussian Process

- A Gaussian process is completely specified by its mean function $m(x) = E[\mu(x)]$ and covariance function $k(x, x') = \text{Cov}(\mu(x), \mu(x'))$.
- The process is denoted by $\mu(x) \sim \mathcal{GP}(m, k)$.

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- The joint distribution of $\mu(x_1), \ldots, \mu(x_n)$ is given by

$$\begin{pmatrix} \mu(x_1) \\ \vdots \\ \mu(x_n) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m(x_1) \\ \vdots \\ m(x_n) \end{pmatrix}, K(x_1, \ldots, x_n) \right).$$

where $K(x_1, \ldots, x_n)$ is the covariance matrix with (i, j)-th element $k(x_i, x_j)$.

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  where $K(x_1, \ldots, x_n)$ is the covariance matrix with (i, j)-th element $k(x_i, x_j)$.
- Consistent defintion: the distribution of $\mu(x_1), \ldots, \mu(x_m)$ derived from the joint distribution of $\mu(x_1), \ldots, \mu(x_n)$ is the same for any choice of $x_{m+1}, \ldots, x_n$.
- $K(x_1, \ldots, x_n)$ is positive definite for any choice of $x_1, \ldots, x_n$.

Gaussian Process — Covariance

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Show that the covariance matrix $K(x_1, \ldots, x_n)$ is positive definite.

WLOG, we assume $\tau^2 = l^2 = 1$. To show K is positive definite, we need to show that for any vector $u = (u_1, \ldots, u_n)$, $u^T K u \geq 0$.

- Notice that
$$k(x_i, x_j) = \exp\left(-\frac{1}{2}|x_i - x_j|^2\right) = \mathbb{E}\left[e^{i|x_i - x_j|Z}\right]$$
for $Z \sim \mathcal{N}(0, 1)$.
- Therefore,

$$u^T K u = \sum_{i,j} u_i u_j k(x_i, x_j) = \sum_{i,j} u_i u_j \mathbb{E}\left[e^{i|x_i - x_j|Z}\right] = \mathbb{E}\left[\left(\sum_i u_i e^{ix_i Z}\right)^2\right] \geq 0.$$

Gaussian Process — Basis Functions

The Gaussian Process can also be constructed by basis functions:

$$\mu(x) = \sum_{h=1}^{H} \beta_h b_h(x), \quad \beta = (\beta_1, \ldots, \beta_H) \sim \mathcal{N}(\boldsymbol{\beta}_0, \boldsymbol{\Sigma}_\beta)$$

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Then μ is a Gaussian process with

$$m(x) = \boldsymbol{b}(x)^T \boldsymbol{\beta}_0, \quad k(x, x') = \boldsymbol{b}(x)^T \boldsymbol{\Sigma}_\beta \boldsymbol{b}(x').$$

Gaussian Process — Inference

Suppose, we have observed the data $(x_1, y_1), \ldots, (x_n, y_n)$, and we assume that

$$y_i = \mu(x_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2).$$

Given a new point $\tilde{x}$, we want to estimate the expected value of y at $\tilde{x}$, i.e. $\mu(\tilde{x})$.

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- We assume that μ is a Gaussian process with mean function $m(x) = 0$ and covariance function $k(x, x') = \tau^2 \exp\left(-|x - x'|^2/(2l^2)\right)$.

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- The joint distribution of $y = (y_1, \ldots, y_n)$ and $\mu(\tilde{x})$ is given by

$$\begin{pmatrix} y \\ \mu(\tilde{x}) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} K(x,x) + \sigma^2 I & K(x, \tilde{x}) \\ K(\tilde{x}, x) & K(\tilde{x}, \tilde{x}) \end{pmatrix}\right).$$

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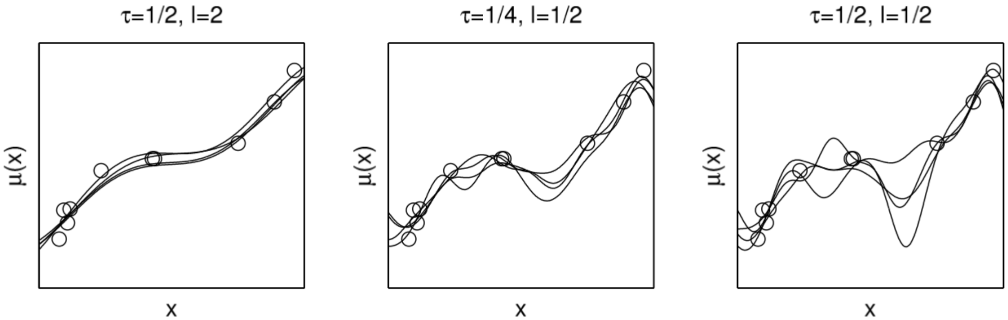
- With the properties of conditional distribution of multivariate normal, we can derive the posterior distribution of $\mu(\tilde{x})$ given y.

$$\begin{aligned} &\mu(\tilde{x}) \mid x, y, \tau^2, \sigma^2, l^2 \\ &\sim \mathcal{N}\left(K(\tilde{x},x)(K(x,x)+\sigma^2 I)^{-1} y, K(\tilde{x},\tilde{x}) - K(\tilde{x},x)(K(x,x)+\sigma^2 I)^{-1} K(x,\tilde{x})\right) \end{aligned}$$

Gaussian Process — Example



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For a Bayesian procedure, we need to specify the prior distributions for the hyperparameters τ^2, σ^2, and l^2.

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For a Bayesian procedure, we need to specify the prior distributions for the hyperparameters τ^2, σ^2, and l^2.
A common choice is

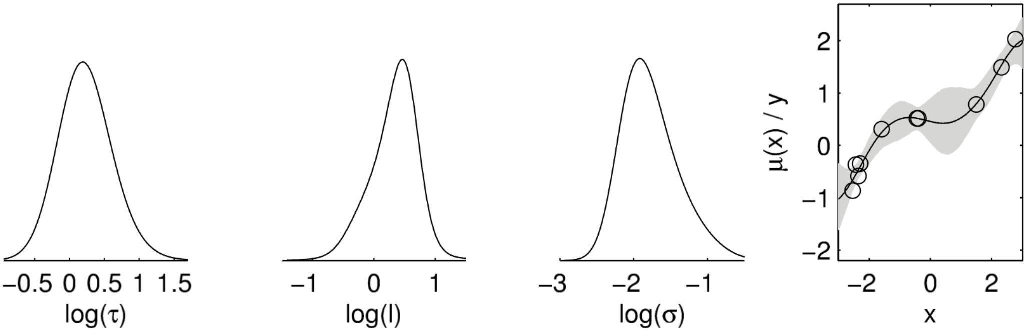
$$p(\log \tau) \propto 1, \quad p(\log \sigma) \propto 1, \quad p(\log l) \propto 1.$$

The log-likelihood is

$$\log p(y \mid x, \tau^2, \sigma^2, l^2) = -\frac{1}{2} y^T (K(x,x) + \sigma^2 I)^{-1} y - \frac{1}{2} \log |K(x,x) + \sigma^2 I| - \frac{n}{2} \log(2\pi).$$

The posterior is now straightforward.

Gaussian Process — Inference



Example — Birth Dates

In this example, we analyze the patterns of birthdays in the United States. The data is the number of births on each day of the year from 1969 to 1988.

- This is a time series data, where the index is the number of days from 1969-01-01.
- The series contains periodic patterns, e.g. yearly and weekly patterns.
- The series also contains long term trends.

Example — Birth Dates

We model the time series as an additive model:

$$y(t) = f_1(t) + f_2(t) + f_3(t) + f_4(t) + f_5(t) + \epsilon_t,$$

- Long-term trend:

$$f_1(t) \sim \mathcal{GP}(0, k_1), \quad k_1(t, t') = \sigma_1^2 \exp\left(-\frac{|t - t'|^2}{2l_1^2}\right)$$

- Short-term trend:

$$f_2(t) \sim \mathcal{GP}(0, k_2), \quad k_2(t, t') = \sigma_2^2 \exp\left(-\frac{|t - t'|^2}{2l_2^2}\right)$$

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- Weekly pattern:

$$f_3(t) \sim \mathcal{GP}(0, k_3), \quad k_3(t, t') = \sigma_3^2 \exp\left(-\frac{2\sin^2(\pi(t-t')/7)}{l_{3,1}^2}\right) \exp\left(-\frac{|t-t'|^2}{2l_{3,2}^2}\right)$$

- Yearly pattern:

$$f_4(t) \sim \mathcal{GP}(0, k_4), \quad k_4(t, t') = \sigma_4^2 \exp\left(-\frac{2\sin^2(\pi(t-t')/365.25)}{l_{4,1}^2}\right) \exp\left(-\frac{|t-t'|^2}{2l_{4,2}^2}\right)$$

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$$y(t) = f_1(t) + f_2(t) + f_3(t) + f_4(t) + f_5(t) + \epsilon_t,$$

- Special days and its interaction with weekends:

  $$f_5(t) = I_{s.d.}(t)\beta_a + I_{s.d.}(t)I_{w.e.}(t)\beta_b$$

  where $I_{s.d.}(t)$ is an indicator function for special days (13 holidays), and $I_{w.e.}(t)$ is an indicator function for weekends.
- $\epsilon_t \sim \mathcal{N}(0, \sigma^2)$ is the residual.

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- The model can be fit through a standard GP inference.
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- The model can be further extended by considering weekdays v.s. weekends. See textbook Ch. 21.2.

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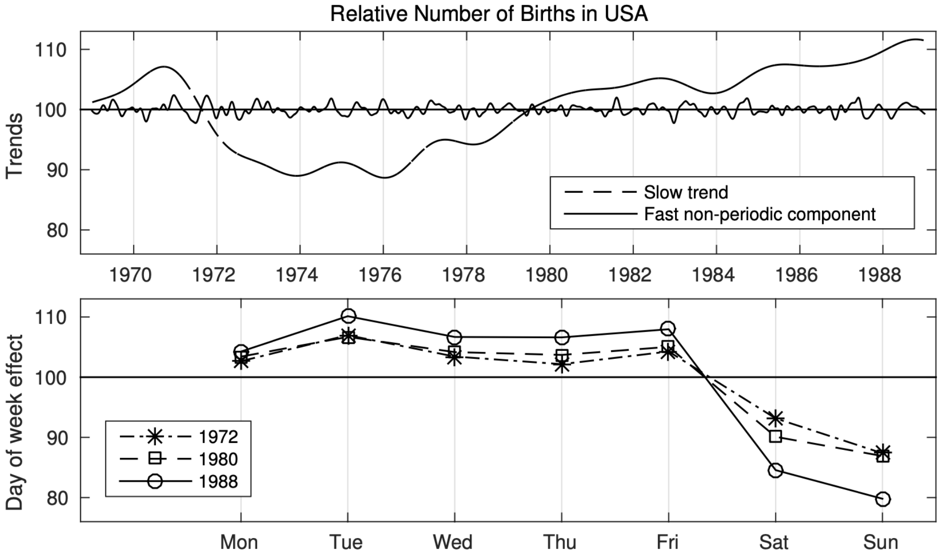

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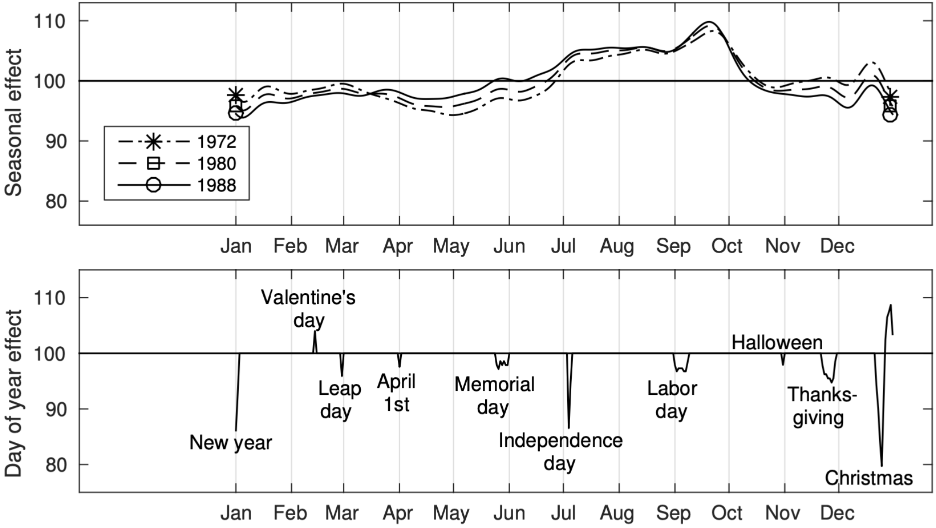

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- In defining Gaussian process, we considered the joint distribution of the function values at any finite number of points.
- For the distribution space, we consider probabilites of any finite partitions of the sample space.

Dirichlet Process

Consider a finite partition of the sample space:

$$\Omega = B_1 \cup B_2 \cup \cdots \cup B_k, \text{ and } B_i \cap B_j = \varnothing \; \forall \; i \neq j$$

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Let P be a probaility measure on Ω with density function f. The probability measures of the partitions are

$$(P(B_1), \dots, P(B_k)) = \left(\int_{B_1} f(y)dy, \dots, \int_{B_k} f(y)dy \right)$$

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with

$$\sum_{i=1}^{k} P(B_i) = 1.$$

Dirichlet Process

A natural probability measure on $(P(B_1), \dots, P(B_k))$ is the Dirichlet distribution:

$$(P(B_1), \dots, P(B_k)) \sim \text{Dirichlet}\,(\alpha P_0(B_1), \dots, \alpha P_0(B_k))$$

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Now we assume P is a random measure, and the distribution of P is the **Dirichlet process**, denoted by $\mathcal{DP}(\alpha P_0)$ if:

for any finite partition $B_1, \ldots, B_k$ of Ω, the probability measures $(P(B_1), \ldots, P(B_k))$ follows the Dirichlet distribution with parameters $(\alpha P_0(B_1), \ldots, \alpha P_0(B_k))$.

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To check the consistency of the defition of a Dirichlet process, consider two partitions $B_1, \ldots, B_k$ and $B'_1, \ldots, B'_{k-1}$ with

$$B_i = B'_i \text{ for } 1 \leq i \leq k-2, \text{ and } B'_{k-1} = B_{k-1} \cup B_k$$

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- On the one hand, the distribution of $(P(B_1), \ldots, P(B_k))$ is Dirichlet with parameters $(\alpha P_0(B_1), \ldots, \alpha P_0(B_k))$. Therefore, the distribution of $(P(B_1)', \ldots, P(B'_{k-1}))$ is Dirichlet with parameters

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- On the other hand, the distribution of $(P(B_1)', \ldots, P(B'_{k-1}))$ is Dirichlet with parameters

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$$(\alpha P_0(B'_1), \ldots, \alpha P_0(B'_{k-2}), \alpha P_0(B'_{k-1})).$$
- They are equal because
$$B_i = B'_i \text{ for } 1 \leq i \leq k-2, \text{ and } P_0(B'_{k-1}) = P_0(B_{k-1}) + P_0(B_k)$$

Dirichlet Process

Let B be a measurable subset of Ω. Then its probability measure follows a Dirichlet process:

$$(P(B), P(\Omega \setminus B)) \sim \mathrm{Dirichlet}(\alpha P_0(B), \alpha(1 - P_0(B))) \sim \mathrm{Beta}(\alpha P_0(B), \alpha(1 - P_0(B)))$$

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$$Var[P(B)] = \frac{\alpha P_0(B)\alpha(1 - P_0(B))}{(\alpha P_0(B) + \alpha(1 - P_0(B))^2)(\alpha P_0(B) + \alpha(1 - P_0(B)))} = \frac{P_0(B)(1 - P_0(B))}{\alpha + 1}$$

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Therefore, in the Dirichlet process, P_0 controls the mean measure and α controls the variance.

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In the special case that $\alpha = 0$, we have

$$P \mid y \sim \mathcal{DP}\left(\sum_i \delta_{y_i}\right)$$

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It is easy to verify that:

$$\sum_{h=1}^{\infty} \pi_h = 1$$

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- Repeat the process.

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Polya urn model:

- We start with a urn with x red balls and y blue balls.
- At each step, we draw a ball from the urn and put it back with an additional ball of the same color.

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- The number of customers at each table follows a Polya urn model.
- The process is exchangeable.

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Then the model is a hierarchical model. The posterior distribution of α can be derived through MCMC.

- See marginal Gibbs sampling and block Gibbs sampling in textbook Ch. 23.3.