STA 437/2005:
Methods for Multivariate Data

Week 4: Gaussian Processes

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Introduction to GPs

Marginal distribution of MVN

Consider the following reformulation of the earlier result:

Suppose $X \sim N_m(\mu, \Sigma)$. Let $T := \{1, \ldots, m\}$ and define

- $m : T \to \mathbb{R}$ such that $m(i) := \mu_i$ (mean function)
- $k : T \times T \to \mathbb{R}$ such that $k(i, j) := \Sigma_{ij}$ (kernel function)

Then for every $A = \{t_1, \ldots, t_n\} \subseteq T$, the vector $X_A = (X_{t_1}, \ldots, X_{t_n})$ is Gaussian with

- The mean μ_A whose i-th entry is $m(t_i)$.
- The covariance matrix Σ_{AA} whose (i, j)-th entry is $k(t_i, t_j)$.

The set T indexes all random variables in the system.

For every $A = \{t_1, \ldots, t_n\} \subseteq T$, $(X_{t_1}, \ldots, X_{t_n})$ is Gaussian.

Gaussian Processes - an immediate generalization

A **Gaussian Process (GP)** is a generalization of the multivariate normal distribution to a collection of random variables indexed by an arbitrary set T.

Definition

A Gaussian Process is a collection of random variables $\{X_t\}_{t \in T}$ such that for any finite set of points $\{t_1, \ldots, t_n\} \subset T$, the corresponding vector $(X_{t_1}, \ldots, X_{t_n})$ follows a multivariate normal distribution.

In what follows we assume $T \subseteq \mathbb{R}^d$ with the Euclidean distance metric.

Often, the correlation between two variables X_s and X_t will depend on the distance $\|t - s\|$.

The mean and the kernel functions

A Gaussian Process is characterized by:

- A **mean function** $m : T \to \mathbb{R}$: $\quad m(t) = \mathbb{E}[X_t]$
- A **kernel function** $k : T \times T \to \mathbb{R}$: $\quad k(t, t') = \mathrm{Cov}(X_t, X_{t'})$

Note that m is pretty much arbitrary (often set to be zero) but k is highly constrained:

Positive semi-definitness:

For any finite set $\{t_1, \ldots, t_n\} \subset T$, the covariance matrix Σ with entries $\Sigma_{ij} = k(t_i, t_j)$ is positive semi-definite.

We can use feature maps $\psi : \mathbb{R}^d \to \mathbb{R}^p$ to define kernels:

$$k(s, t) = \psi(s)^\top \psi(t).$$

Feature maps define kernels but not all kernels are like that (this can be generalized to "infinite dimensional" feature maps).

Common Kernels in GPs

- **Squared Exponential (RBF) Kernel:**

$$k_{\mathrm{E}}(t, t') = \sigma^2 \exp\left(-\frac{\|t - t'\|^2}{2\ell^2}\right).$$

  - Controls smoothness of the functions sampled from the GP.
  - Length scale ℓ: Correlation distance.
  - Signal variance σ^2: Scale of the output.

- **Matérn Kernel:**

$$k_{\mathrm{M}}(t, t') = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\frac{\|t - t'\|}{\ell}\right)^{\nu} K_\nu \left(\sqrt{2\nu}\frac{\|t - t'\|}{\ell}\right).$$

  - ν: Smoothness parameter.
  - More flexible than the RBF kernel for modeling rough functions.

Constructing kernels from kernels

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following kernels will also be valid:

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= c k_1(\mathbf{x}, \mathbf{x}') \quad \text{for } c > 0, \\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') \\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') \\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') \cdot k_2(\mathbf{x}, \mathbf{x}') \\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^\top A \mathbf{x}' \qquad (A \text{ PSD}) \\
k(\mathbf{x}, \mathbf{x}') &= \exp(k_1(\mathbf{x}, \mathbf{x}')) \\
k(\mathbf{x}, \mathbf{x}') &= q(k_1(\mathbf{x}, \mathbf{x}'))
\end{aligned}
$$

where q polynomial with ≥ 0 coefficients.

Modelling with Gaussian processes

Working with Gaussian Processes we fix a kernel function.

Data: Suppose we observed $(X_{t_1}, \ldots, X_{t_n})$ for some $t_1, \ldots, t_n \in T$.

If the kernel function comes with some hyperparameters α, we can learn them maximizing the log-likelihood.

- By definition, $(X_{t_1}, \ldots, X_{t_n})$ is MVN with covariance that depends on α.
- This may be a complicated optimization procedure.

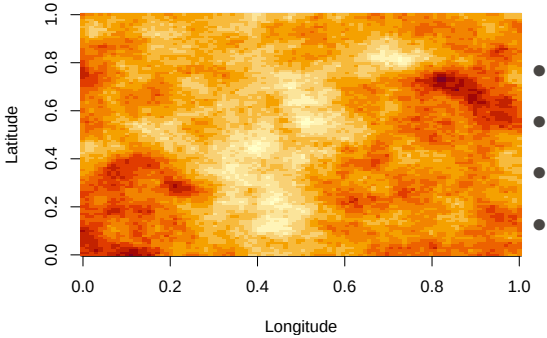
Suppose we want to predict the value of the process at some point t_{n+1}

- By definition $(X_{t_1}, \ldots, X_{t_n}, X_{t_{n+1}})$ is jointly Gaussian so simply compute the conditional distribution: $X_{t_{n+1}} | X_{t_1}, \ldots, X_{t_n}$.
- This gives both the point prodiction (the conditional mean) and uncertainty quantification (conditional variance).

GPs for Spatial Data

Example: Modeling Spatial Data with GPs

GPs are widely used in spatial statistics, e.g. temperature across a grid of locations.



- Grid of 100^2 points.
- Fix the exponential kernel $\exp\{-\frac{1}{2}\|\mathbf{x} - \mathbf{x}'\|\}$
- Compute the $100^2 \times 100^2$ covariance matrix
- Get 1 sample from the corresponding distr.

Handling a 10000-dimensional Gaussian comes with its own computational challenges.

Spatial GP: Prediction

We explained how to make a prediction for $X_{t_{n+1}}$. This easily generalizes.

Suppose we observed the mean zero GP over some locations $\mathbf{x}_{\text{train}}$.

Our goal is to make predictions over some other points $\mathbf{x}_{\text{test}}$

1. Combine training and test locations.
2. Compute the covariance matrix using the kernel function.
3. Use Gaussian conditioning formulas:

$$\mathbb{E}[\mathbf{x}_{\text{test}}|\mathbf{x}_{\text{train}}] = \Sigma_{\text{test,train}}\Sigma_{\text{train,train}}^{-1}\mathbf{x}_{\text{train}},$$
$$\text{Cov}(\mathbf{x}_{\text{test}}|\mathbf{x}_{\text{train}}) = \Sigma_{\text{test,test}} - \Sigma_{\text{test,train}}\Sigma_{\text{train,train}}^{-1}\Sigma_{\text{test,train}}.$$

Nonparametric Regression with GPs

Nonparametric Regression

GPs can be used for nonparametric regression:

$$y_i = f(\mathbf{x}_i) + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2), \quad i = 1, \ldots, n.$$

Prior over $f : \mathbb{R}^d \to \mathbb{R}$: GP defined by $m(\mathbf{x})$ and $k(\mathbf{x}, \mathbf{x}')$.

- In this sense GP defines a distribution over (random) functions $f : \mathbb{R}^d \to \mathbb{R}$.

We have $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)) \sim N_n(\mu, \Sigma)$

- $\mu_i = m(\mathbf{x}_i)$
- $\Sigma_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$

Say $d = 1$. Given $m(x)$ and $k(x, x')$, how would you plot random samples of the corresponding random functions on $\mathbb{R}$?

Nonparametric Regression

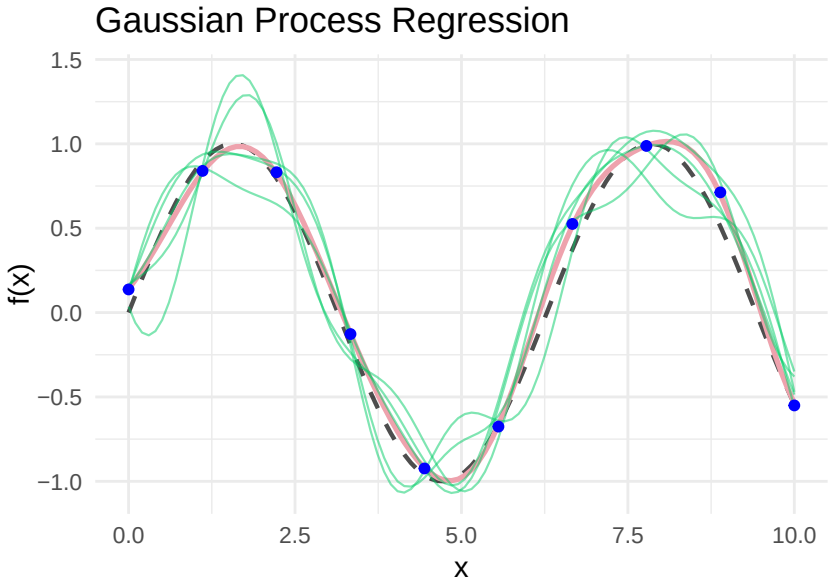
Note that $\mathbf{y} = (y_1, \ldots, y_n) = (f(\mathbf{x}_1) + \varepsilon_1, \ldots, f(\mathbf{x}_n) + \varepsilon_n)$.

Consider the underlying Gaussian Process $y(\mathbf{x})$:

- The mean is $m(\mathbf{x})$.
  - $\mathbb{E}[y(\mathbf{x}_i)] = \mathbb{E}[f(\mathbf{x}_i) + \varepsilon_i] = m(\mathbf{x}_i)$.
- The kernel is $k(\mathbf{x}, \mathbf{x}') + \sigma^2 \mathbf{1}\{\mathbf{x} = \mathbf{x}'\}$.
  - $\text{cov}[y(\mathbf{x}_i), y(\mathbf{x}_j)] = \text{cov}(f(\mathbf{x}_i) + \varepsilon_i, f(\mathbf{x}_j) + \varepsilon_j) = k(\mathbf{x}_i, \mathbf{x}_j) + \sigma^2 \mathbf{1}\{\mathbf{x}_i = \mathbf{x}_j\}$.

Given data $(y_1, \mathbf{x}_1)$, $\ldots$, $(y_n, \mathbf{x}_n)$ we can now easily predict y at any other point $\mathbf{x}$.

Illustration



Summary

- Gaussian Processes are a versatile tool for regression and spatial modeling.
- Key components:
  - Mean function.
  - Kernel function.
- Takeaway: Conceptually it is not harder than MVNs and the same formulas apply.
- Computational issues can be significant.