Gaussian Process for Time Series Analysis

Dr. Juan Orduz

PyData Berlin 2019

Overview

Multivariate Normal Distribution

$X = (X_1, \cdots, X_d)$ has a **multivariate normal distribution** if every linear combination is normally distributed. In this case it has density of the form

$$p(x|m, K_0) = \frac{1}{\sqrt{(2\pi)^d |K_0|}} \exp\left(-\frac{1}{2}(x-m)^T K_0^{-1}(x-m)\right)$$

where $m \in \mathbb{R}^d$ is the **mean vector** and $K_0 \in M_d(\mathbb{R})$ is the (symmetric, positive definite) **covariance matrix**.

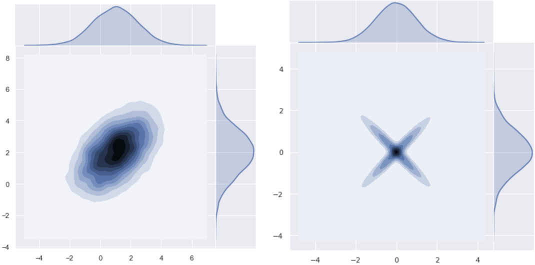


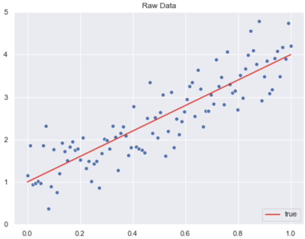
Figure: Left: Multivariate Normal Distribution, Right: Non-Multivariate Normal Distribution

Regularized Bayesian Linear Regression

Let $x_1, \cdots, x_n \in \mathbb{R}^d$ and $y_1, \cdots, y_n$ be a set of observations (data). We want to fit the linear model

$$f(x) = x^T b \quad \text{and} \quad y = f(x) + \varepsilon, \quad \text{with} \quad \varepsilon \sim N(0, \sigma_n^2)$$

where $b \in \mathbb{R}^d$ denotes the parameter vector. Let $X \in M_{d \times n}$ be denote the observation matrix.



We want to compute $p(b|X, y)$ using the Bayes theorem

$$p(b|X, y) = \frac{p(y|X, b)p(b)}{p(y|X)} \propto \text{likelihood} \times \text{prior}$$

Prior Distribution

- Likelihood

$$p(y|X,b) = \prod_{i=1}^{n} p(y_i|x_i,b) = N(X^T b, \sigma_n^2 I)$$

- Prior

$$b \sim N(0, \Sigma_p), \quad \Sigma_p \in M_d(\mathbb{R})$$

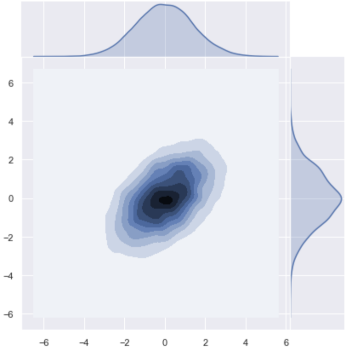


Figure: Prior Distribution

Posterior Distribution

- Posterior

$$p(b|y, X) = N\left(\bar{b} = \frac{1}{\sigma_n^2} A^{-1} Xy, A^{-1}\right)$$

where $A = \sigma_n^{-2} XX^T + \Sigma_p^{-1}$

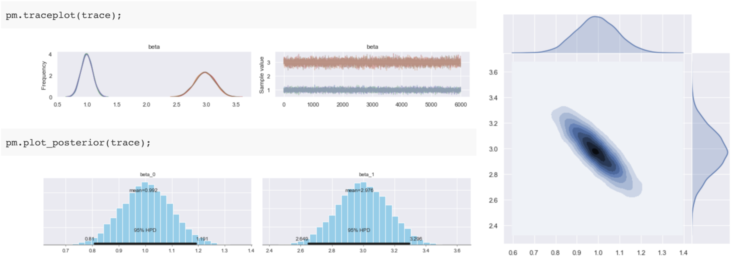


Figure: Posterior Distribution

Predictive Distribution

$$
\begin{aligned}
p(f_*|x_*, X, y) &= \int p(f_*|x_*, b)p(b|X, y)db \\
&= N\left(\frac{1}{\sigma_n^2} x_*^T A^{-1} Xy, x_*^T A^{-1} x_*\right)
\end{aligned}
$$

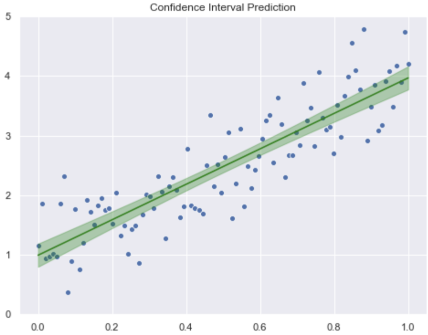


Figure: Left: Join Posterior Distribution, Right: Prediction + Confidence Interval

The Kernel Trick

Let us consider a map $\phi : \mathbb{R}^d \longrightarrow \mathbb{R}^N$ and consider the model

$$f(x) = \phi(x)^T b \quad \text{and} \quad y = f(x) + \varepsilon, \quad \text{with} \quad \varepsilon \sim N(0, \sigma_n^2).$$

It is easy to verify that the analysis for this model as analogous to the standard linear model replacing X with $\Phi := \phi(X)$. Set $\phi_* = \phi(x_*)$,

$$p(f_*|x_*, X, y) = N\left(\overbrace{\frac{1}{\sigma_n^2}\phi_*^T A^{-1}\Phi y}^{(1)}, \underbrace{\phi_*^T A^{-1}\phi_*}_{(2)}\right)$$

$$(1) = \phi_*^T \Sigma_p \Phi(\Phi^T \Sigma_p \Phi + \sigma_n^2 I)^{-1} y$$
$$(2) = \phi_* \Sigma_p \phi_* - \phi_*^T \Sigma_p \Phi(\Phi^T \Sigma_p \Phi + \sigma_n^2 I)^{-1} \Phi^T \Sigma_p \phi_*$$

This motivates the definition of the **covariance function** or **kernel**

$$k(x, x') := \phi(x)^T \Sigma_p \phi(x')$$

Gaussian Process

- A **Gaussian Process** is a collection of random variables, any finite number of which have a joint Gaussian distribution.
- A Gaussian process $f \sim \mathcal{GP}(m, k)$ is completely specified by its mean function $m(x)$ and covariance function $k(x, x')$. Here $x \in \mathcal{X}$ denotes a point on the index set $\mathcal{X}$.

$$m(x) = E[f(x)] \quad \text{and} \quad k(x, x') = E[(f(x) - m(x))(f(x') - m(x'))]$$

Example: The map $f(x) = \phi(x)^T b$ (with prior $b \sim N(0, \Sigma_p)$) defines a Gaussian process with $m(x) = 0$ and $k(x, x') = \phi(x)^T \Sigma_p \phi(x)$.

The specification of a covariance function implies a distribution over functions.

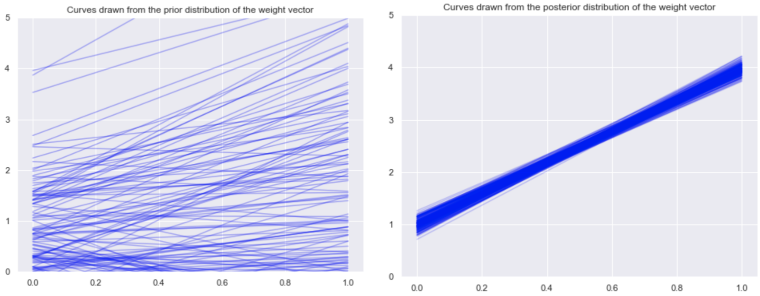


Figure: Prior (left) and posterior (right) distribution for linear model.

References

Slides and notebook available at juanitorduz.github.io