Gaussian Process for Time Series Analysis

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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**.

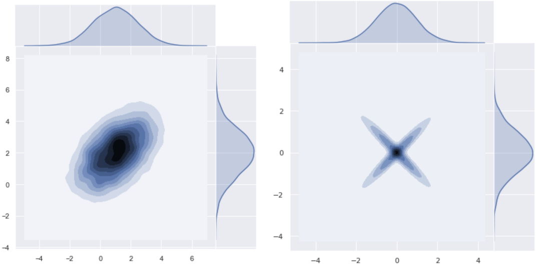


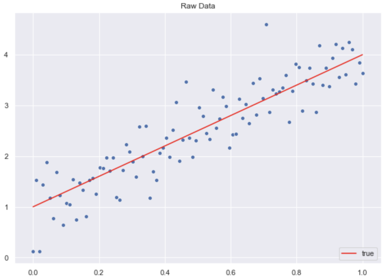
Figure: Left: Multivariate Normal Distribution, Right: Non-Multivariate Normal Distribution

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

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

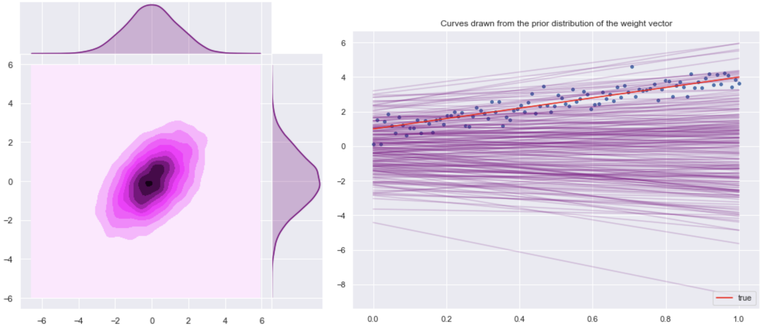
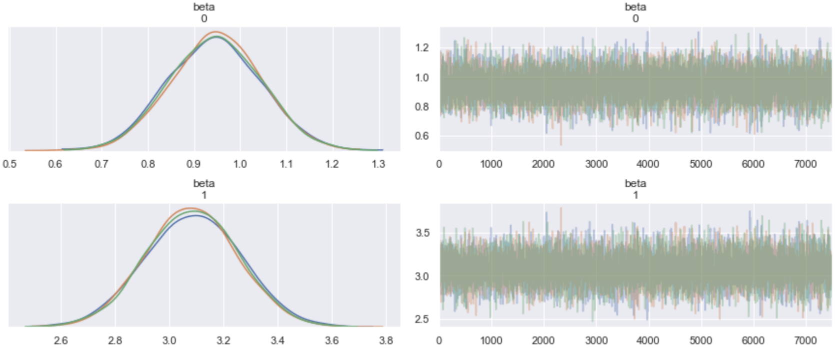


Figure: Prior Distribution

Posterior Distribution Sampling



Posterior Distribution

- Posterior

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

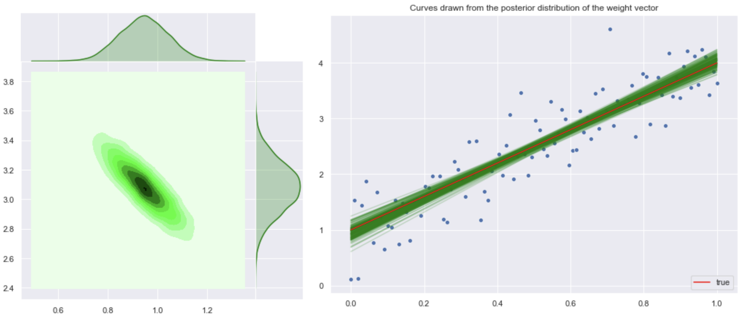


Figure: Posterior Distribution

Predictive Distribution

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

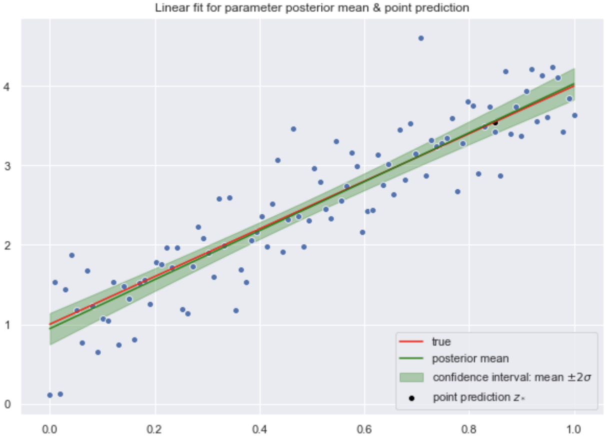


Figure: Prediction Interval

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 $\phi_* = \phi(x_*)$,

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

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

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

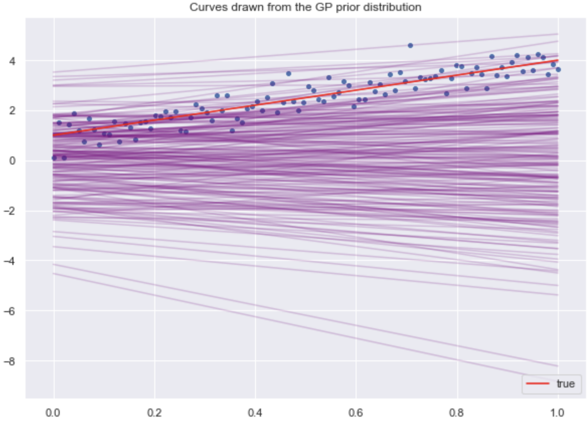
The map $f(x) = \phi(x)^T b$ (with prior $b \sim N(0, \Sigma_p)$) defines a Gaussian process with $m(x) = 0$ and $k(x, x') = \phi(x)^T \Sigma_p \phi(x')$.

Linear Regression - Function Space View

The specification of a covariance function implies a distribution over functions

- Let us consider input points X_* (test set).
- Prior

$$f_* \sim N(0, K(X_*, X_*))$$



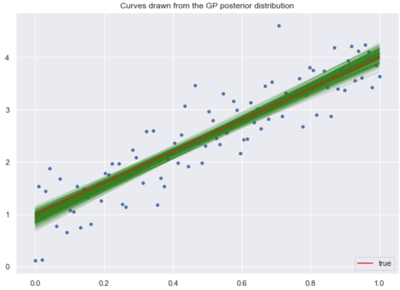
Linear Regression - Function Space View

The specification of a covariance function implies a distribution over functions

- Join Distribution

$$\begin{pmatrix} y \\ f_* \end{pmatrix} \sim N\left(0, \begin{pmatrix} K(X,X)+\sigma_n^2 & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{pmatrix}\right)$$

- Conditional Distribution $f_*|X, y, X_* \sim N(\bar{f}_*, \mathrm{cov}(f_*))$



$$\begin{aligned} \bar{f}_* &= K(X_*,X)(K(X,X)+\sigma_n^2 I)y \\ \mathrm{cov}(f_*) &= K(X_*,X_*) - K(X_*,X)(K(X,X)+\sigma_n^2 I)^{-1}K(X,X_*) \end{aligned}$$

Kernel Examples

The Kernel Space

References

Slides and notebook available at juanitorduz.github.io