Gaussian Processes for Time Series Forecasting

Dr. Juan Orduz

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Overview

Aim: Give a better intuition on the notion of Gaussian Process Regression

Multivariate Normal Distribution

[5]

$X = (X_1, \cdots, X_d)$ has a **multinormal distribution** if every linear combination is normally distributed. The joint density has 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**.

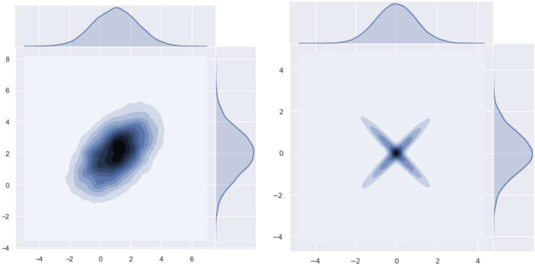

Figure: Left: Multivariate Normal Distribution, Right: Non-Multivariate Normal Distribution

Bayesian Linear Regression

[2], [7, Chapter 2.1]

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.

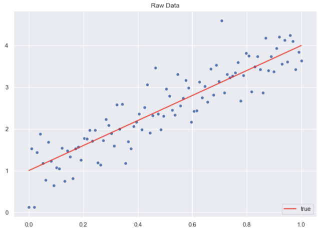

Figure: The true parameters in this example are $b = (1, 3)$ and $\sigma_n = 0.5$

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

- Prior

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

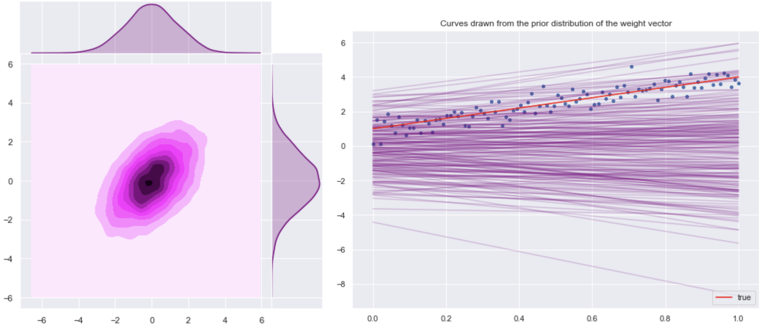

Figure: Prior Distribution, for this example $\Sigma_p = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$.

- Likelihood

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

Posterior Distribution Sampling

[9]

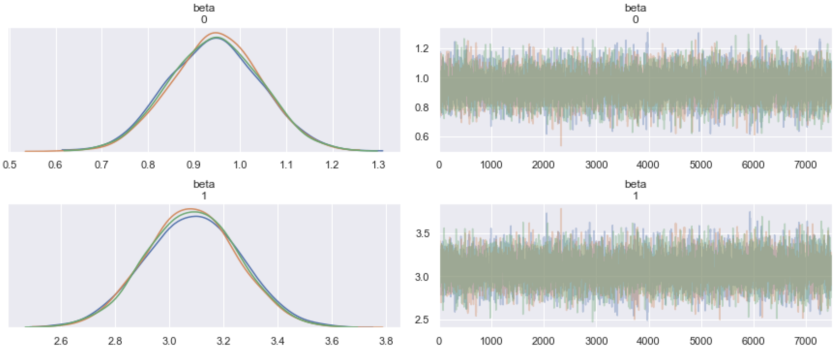

Figure: Posterior distribution of the *b* weight estimation using MCMC sampling (PyMC3). Here we use 3 chains.

Posterior Distribution - Analytical Solution

[7, Chapter 2.1.1]

- Posterior

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

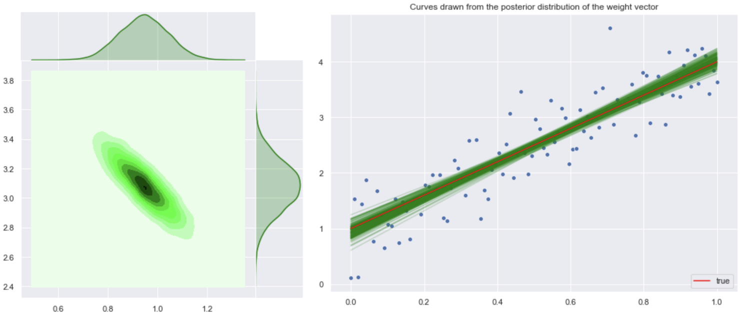

Figure: Posterior Distribution.

Predictive Distribution - Analytical Solution

[7, Chapter 2.1.1]

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

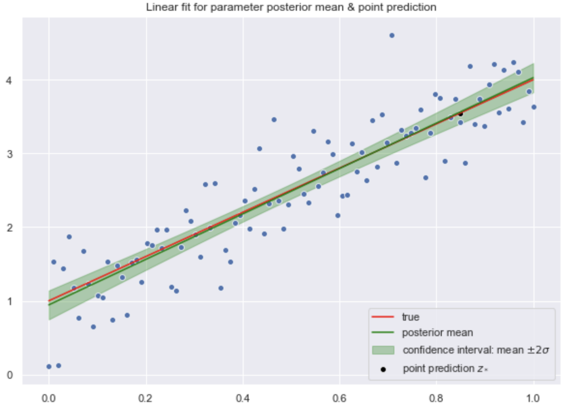

Figure: Prediction Interval.

The Kernel Trick

[7, Chapter 2.1.2]

Let us consider a map $\phi : \mathbb{R}^d \longrightarrow \mathbb{R}^N$ and 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 $\phi_* = \phi(x_*)$,

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

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

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

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

Gaussian Process

[1, Chapter 21], [7, Chapter 2.2]

Main Idea

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

Gaussian Process

- A **Gaussian Process** is a collection of random variables, any finite number of which have a joint multinormal 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 $\mathcal{X}$.

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

Gaussian Process

[1, Chapter 21], [7, Chapter 2.2]

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

Notation

Let $K(X, X)$ denote the matrix of the point-wise kernel images.

Linear Regression - Function Space View

[7, Chapter 2.2]

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

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

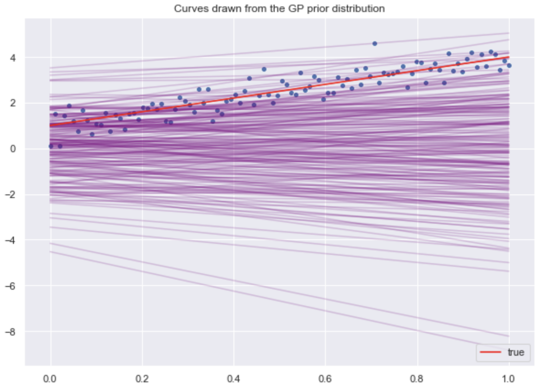


Figure: We sample from the prior space of functions by plotting their realization on $n_* = 80$ points.

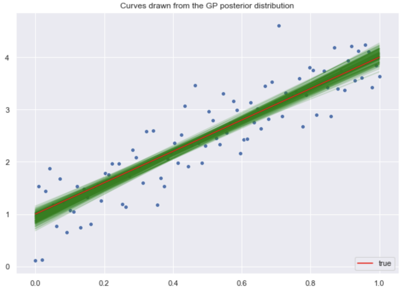
Linear Regression - Function Space View

[7, Chapter 2.2]

- Joint 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

[8], [7, Chapter 4.2]

Symmetric and positive semi-definite functions $k : \mathcal{X} \times \mathcal{X} \longrightarrow \mathbb{R}$.

- Dot Product

$$k_{DOT}(x, x') = (\sigma_0^2 + x^T \Sigma_p x')^m$$

- Squared Exponential

$$k_{SE}(x, x') = \exp\left(-\frac{(x - x')^2}{2\ell^2}\right)$$

- Rational Quadratic

$$k_{RQ}(x, x') = \left(1 + \frac{(x - x')^2}{2\alpha\ell^2}\right)^{-\alpha}$$

- Exp-Sine-Squared

$$k_{ESS}(x, x') = \exp\left(-2\left(\frac{\sin(\pi(x - x')/T)}{\ell}\right)^2\right)$$

Example: Non-Linear Function

[4]

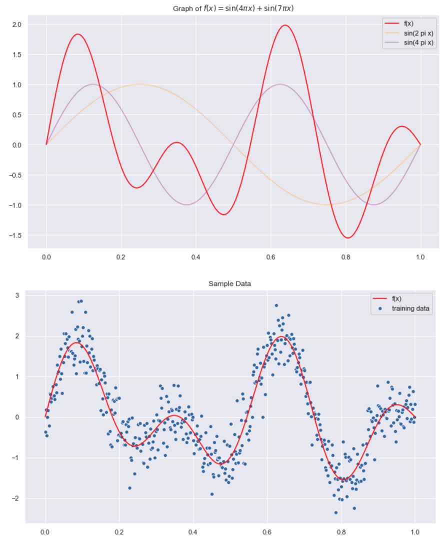


Figure: Non-Linear Example with $n = 500$ training points.

Prior Distribution

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

```
fig, ax = plt.subplots()

for i in range(0, 100):
    # Sample from prior distribution.
    z_star = np.random.multivariate_normal(mean=np.zeros(n_star), cov=K_star2)
    # Plot function.
    sns.lineplot(x=x_star, y=z_star, color='blue', alpha=0.2)

# Plot "true" linear fit.
sns.lineplot(x=x, y=f_x, color='red', label='f(x)')
ax.set(title='Samples of Prior Distribution')
ax.legend(loc='lower right');
```

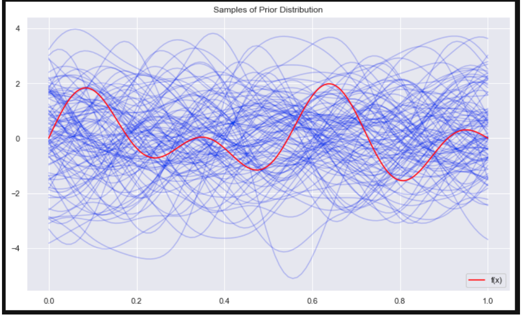
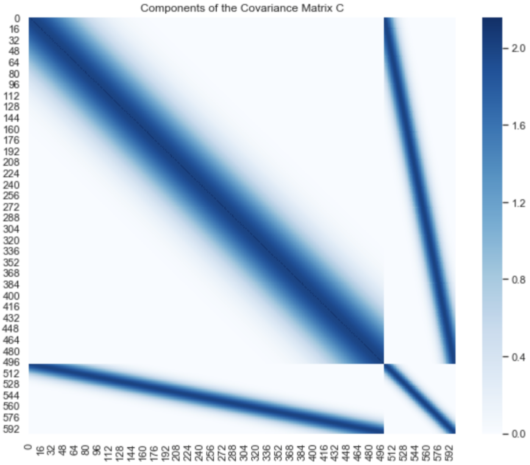


Figure: We sample from the prior space of functions by plotting their realization on $n_* = 100$ points.

Joint 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

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

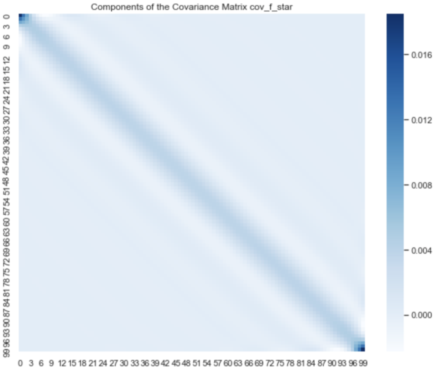


Figure: Covariance matrix of the posterior (conditional) distribution.

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

Posterior Distribution

```python
fig, ax = plt.subplots()

for i in range(0, 100):
    # Sample from posterior distribution.
    z_star = np.random.multivariate_normal(mean=f_bar_star.squeeze(), cov=cov_f_star)
    # Plot function.
    sns.lineplot(x=x_star, y=z_star, color="blue", alpha=0.2);

# Plot "true" linear fit.
sns.lineplot(x=x, y=f_x, color='red', label = 'f(x)')
ax.set(title='Samples of Posterior Distribution, sigma_f = {} and l = {}'.format(sigma_f, l))
ax.legend(loc='upper right');
```

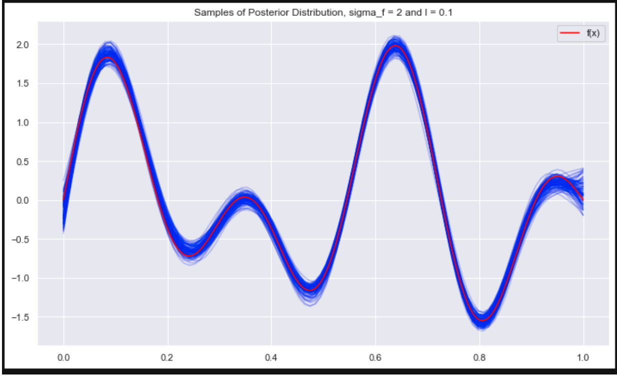


Figure: We sample from the posterior space of functions by plotting their realization on $n_* = 100$ points.

Hyperparameter Estimation

[7, Chapter 2.3, 5]

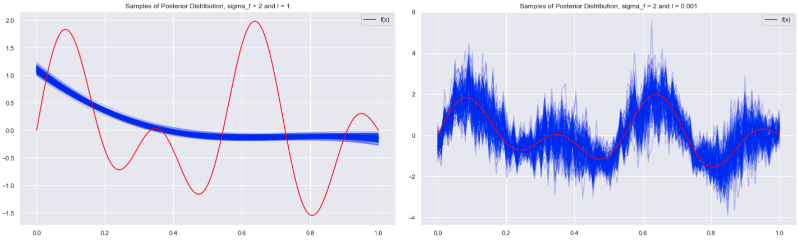


Figure: Samples from two gaussian processes with different scale parameters (left: $\ell = 1$ and right: $\ell = 0.001$).

Methods

- Marginal Likelihood (θ = parameter vector)

$$\log(p(y|X,\theta)) = -\frac{1}{2}y^T(K+\sigma_n^2 I)^{-1}y - \frac{1}{2}\log|K+\sigma_n^2 I| - \frac{n}{2}\log(2\pi)$$

- Cross Validation

The Kernel Space

[8], [7, Chapter 4]

Let $k_1, k_2 : \mathcal{X} \times \mathcal{X} \longrightarrow \mathbb{R}$ be two kernels, then the following are also kernels

- $k_1 + k_2$
- $k_1 \times k_2$
- $k_1 * k_2$ (convolution)

If $k : \mathcal{X}_1 \times \mathcal{X}_1 \longrightarrow \mathbb{R}$ and $h : \mathcal{X}_2 \times \mathcal{X}_2 \longrightarrow \mathbb{R}$ are two kernels, then the following are also kernels (on $\mathcal{X}_1 \times \mathcal{X}_2$)

- $k_1 \oplus k_2$
- $k_1 \otimes k_2$

Remark ([7, Chapter 4.3])

There is a rich theory of spectral theory for kernels by considering the integral operator $T_k : L^2(\mathcal{X}, \mu) \longrightarrow L^2(\mathcal{X}, \mu)$ (where $(\mathcal{X}, \mu)$ is a finite measure space and $k \in L^\infty(\mathcal{X} \times \mathcal{X}, \mu \times \mu)$).

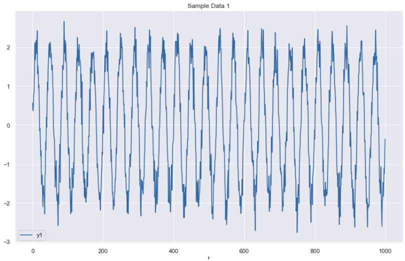
$$(T_k\phi)(x) = \int_{\mathcal{X}} k(x, x')\phi(x')d\mu(x')$$

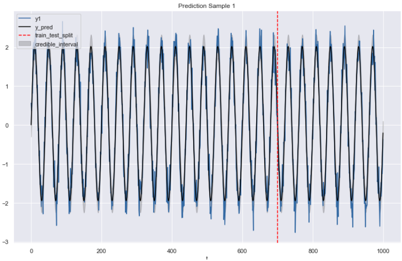
Example: Periodic Component I ([3])

[6, Section 1.7. Gaussian Processes]

```python
from sklearn.gaussian_process.kernels import WhiteKernel, ExpSineSquared, ConstantKernel

k0 = WhiteKernel(noise_level=0.3**2, noise_level_bounds=(0.1**2, 0.5**2))

k1 = ConstantKernel(constant_value=2) * ExpSineSquared(length_scale=1.0, periodicity=40, periodicity_bounds=(35, 45))

kernel_1  = k0 + k1
```

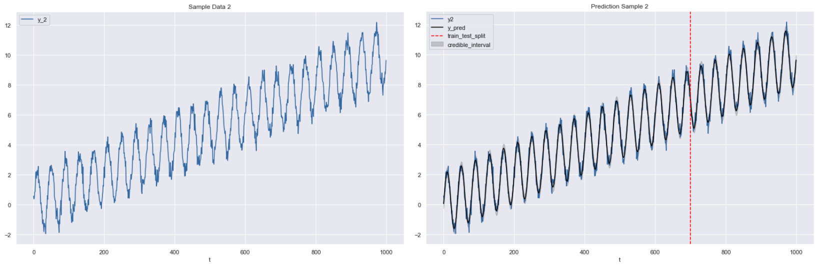
```python
from sklearn.gaussian_process import GaussianProcessRegressor

gp1 = GaussianProcessRegressor(
    kernel=kernel_1,
    n_restarts_optimizer=10,
    normalize_y=True,
    alpha=0.0
)
```





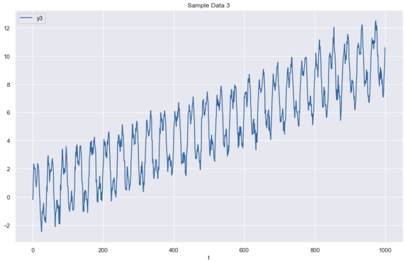
Example: Add Linear Trend

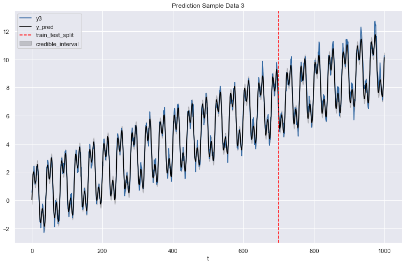
```
from sklearn.gaussian_process.kernels import RBF

k0 = WhiteKernel(noise_level=0.3**2, noise_level_bounds=(0.1**2, 0.5**2))

k1 = ConstantKernel(constant_value=2) * ExpSineSquared(length_scale=1.0, periodicity=40, periodicity_bounds=(35, 45))

k2 = ConstantKernel(constant_value=10, constant_value_bounds=(1e-2, 1e3)) * RBF(length_scale=100.0, length_scale_bounds=(1, 1e4))

kernel_2  = k0 + k1 + k2
```



Example: Add Periodic Component II

```
k0 = WhiteKernel(noise_level=0.3**2, noise_level_bounds=(0.1**2, 0.5**2))

k1 = ConstantKernel(constant_value=2) * ExpSineSquared(length_scale=1.0, periodicity=40, periodicity_bounds=(35, 45))

k2 = ConstantKernel(constant_value=10, constant_value_bounds=(1e-2, 1e3)) * RBF(length_scale=100.0, length_scale_bounds=(1, 1e4))

k3 = ConstantKernel(constant_value=1) * ExpSineSquared(length_scale=1.0, periodicity=12, periodicity_bounds=(10, 15))

kernel_3  = k0 + k1 + k2 + k3
```





Computational Challenges

- Calculating the posterior mean and covariance matrix requires $\mathcal{O}(n^3)$ computations.
- A practical implementation of Gaussian process regression is described in [7, Algorithm 2.1], where the Cholesky decomposition is used instead of inverting the matrices directly.
- There are remarkable approximation methods for Gaussian processes to speed up the computation ([1, Chapter 20.1])

References I

[1] A. Gelman, J.B. Carlin, H.S. Stern, D.B. Dunson, A. Vehtari, and D.B. Rubin.
Bayesian Data Analysis, Third Edition.
Chapman & Hall/CRC Texts in Statistical Science. Taylor & Francis, 2013.

[2] Juan Orduz.
Bayesian regression as a gaussian process.
https://juanitorduz.github.io/reg_bayesian_regression/, Apr 2019.

[3] Juan Orduz.
Gaussian processes for time series forecasting.
https://juanitorduz.github.io/gaussian_process_time_series/, Oct 2019.

[4] Juan Orduz.
An introduction to gaussian process regression.
https://juanitorduz.github.io/gaussian_process_reg/, Apr 2019.

[5] Juan Orduz.
Sampling from a multivariate normal distribution.
https://juanitorduz.github.io/multivariate_normal/, Mar 2019.

References II

[6] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay.
Scikit-learn: Machine learning in Python.
Journal of Machine Learning Research, 12:2825–2830, 2011.

[7] Carl Edward Rasmussen and Christopher K. I. Williams.
Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning).
The MIT Press, 2005.

[8] S. Roberts, M. Osborne, M. Ebden, S. Reece, N. Gibson, and S. Aigrain.
Gaussian processes for timeseries modelling.
Philosophical Transactions of the Royal Society.

[9] John Salvatier, Thomas V. Wiecki, and Christopher Fonnesbeck.
Probabilistic programming in python using PyMC3.
PeerJ Computer Science, 2:e55, apr 2016.