Gaussian Process for Time Series Analysis

Dr. Juan Orduz

PyData Berlin 2019

Overview

Multivariate Normal Distribution

[Ord19b]

$X = (X_1, \cdots, X_d)$ 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**.

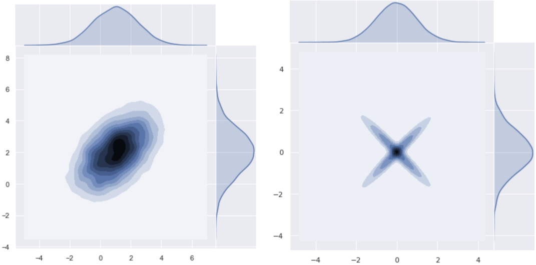


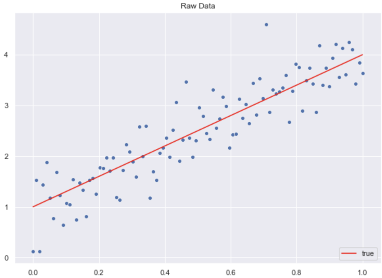
Figure: Left: Multivariate Normal Distribution, Right: Non-Multivariate Normal Distribution

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

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

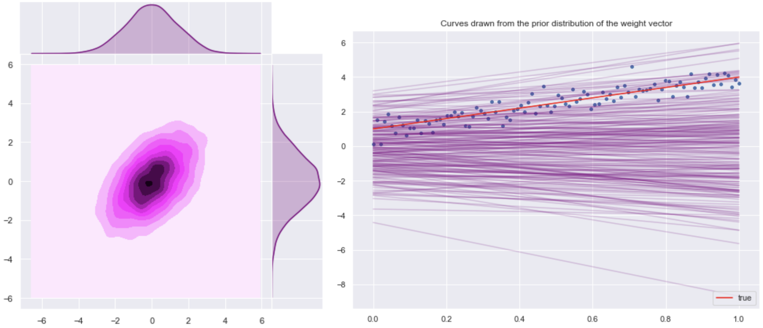


Figure: Prior Distribution

Posterior Distribution Sampling

[SWF16]

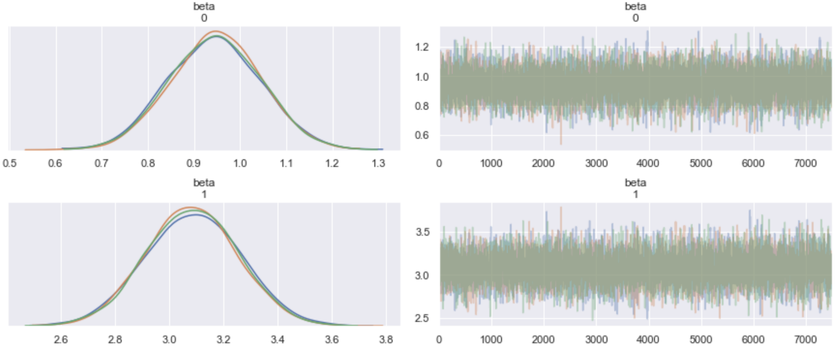


Figure: Posterior distribution beta coefficients MCMC sampling (PyMC3).

Posterior Distribution

[RW05, Chapter 2.1.1]

- Posterior

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

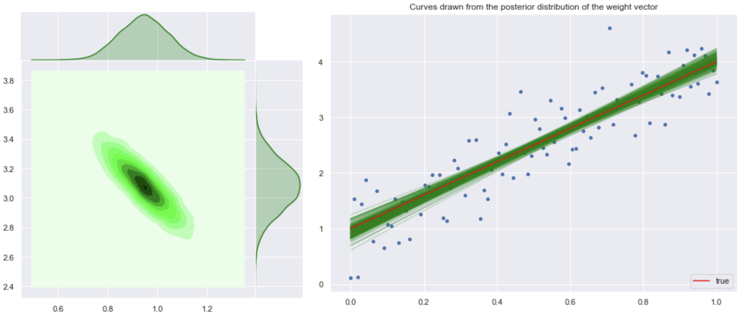


Figure: Posterior Distribution

Predictive Distribution

[RW05, Chapter 2.1.1]

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

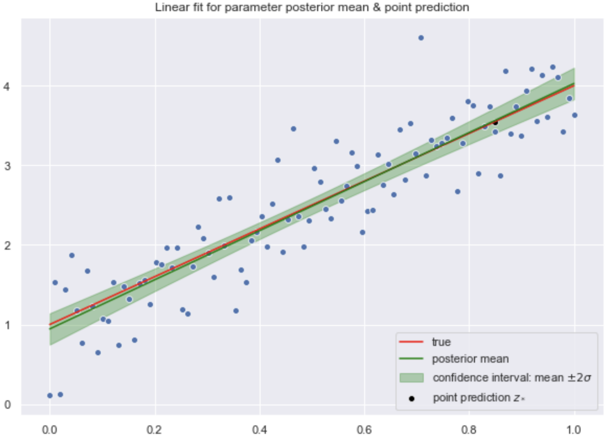


Figure: Prediction Interval

The Kernel Trick

[RW05, 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 $\phi_* = \phi(x_*)$,

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

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

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

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

Gaussian Process

[GCS+13, Chapter 21], [RW05, 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 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 $\mathcal{X}$.

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

Gaussian Process

[GCS+13, Chapter 21], [RW05, 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 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 $k(x, x') = \phi(x)^T \Sigma_p \phi(x')$.

Notation

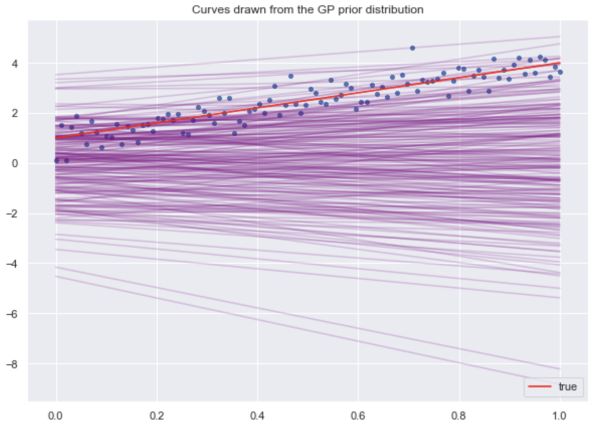
Let $K(X, X)$ denote the matrix the of point-wise kernel images.

Linear Regression - Function Space View

[RW05, Chapter 2.2]

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

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



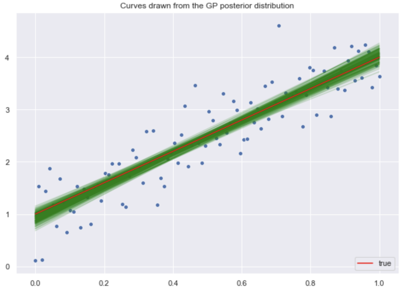
Linear Regression - Function Space View

[RW05, Chapter 2.2]

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



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

$$\text{cov}(f_*) = K(X_*,X_*) - K(X_*,X)(K(X,X) + \sigma_n^2 I)^{-1}K(X,X_*)$$

Kernel Examples

[ROE+], [RW05, Chapter 4.2]

Impose $k : \mathcal{X} \times \mathcal{X} \longrightarrow \mathbb{R}$ to be symmetric and positive semidefinite.

- Squared Exponential

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

- Rational Quadratic

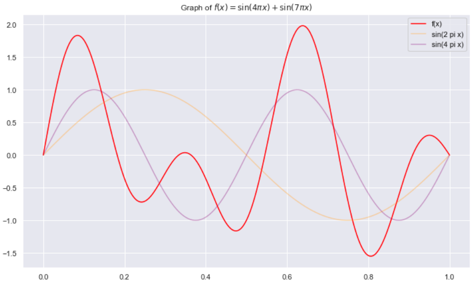
$$k_{RQ}(x, x') = \left(1 + \frac{(x - x')^2}{2\alpha\ell^2}\right)^{-\alpha}$$

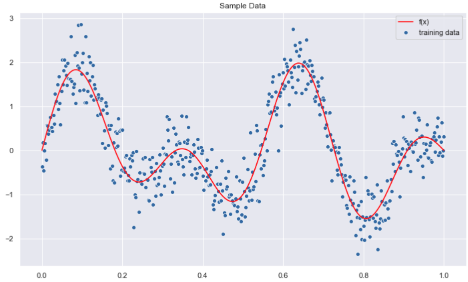
- Exp-Sine-Squared

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

Example: Non-Linear Function ([Ord19a])

$n = 500$



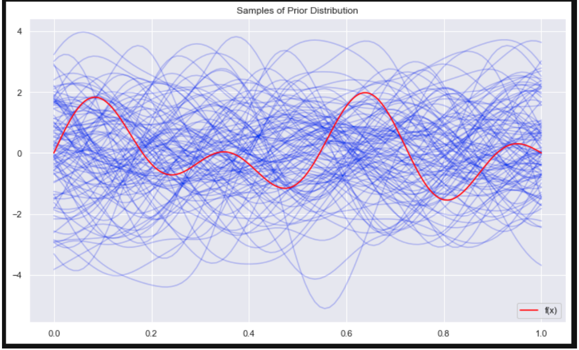


Prior Distribution

$n_* = 100$

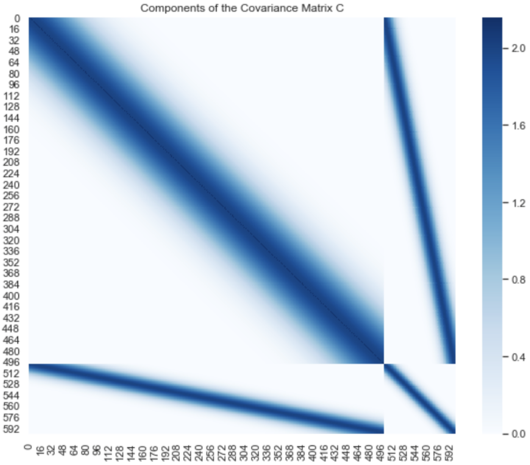
$$f \sim N(0, K(X_*, X_*))$$

```
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');
```



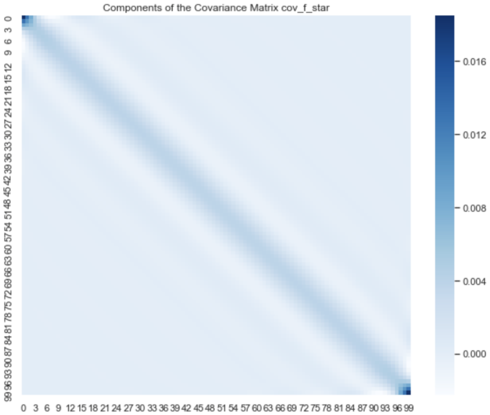
Join Distribution

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



Conditional Distribution

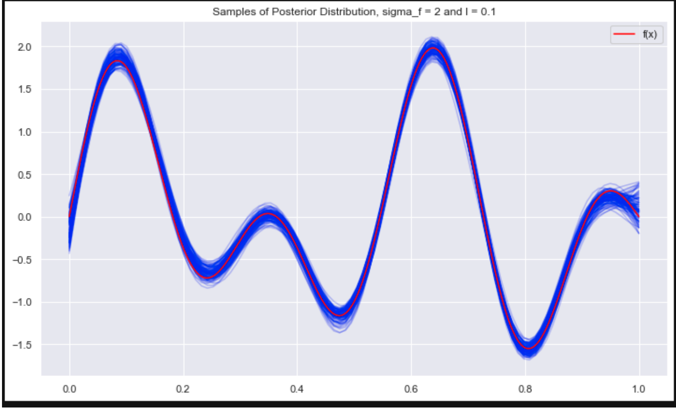
$$f_*|X, y, X_* \sim N(\bar{f}_*, \text{cov}(f_*))$$



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

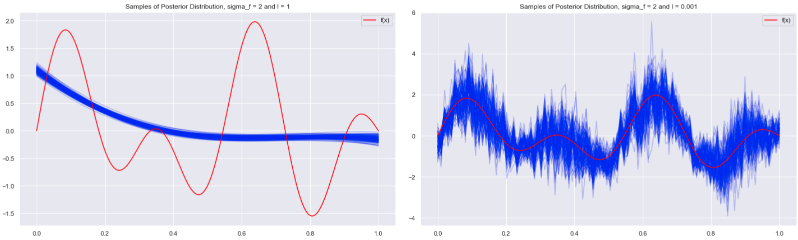
Posterior Distribution

```
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');
```



Hyperparameter Estimation

[RW05, Chapter 2.3, 5]



Methods

- Marginal Likelihood

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

- Cross Validation

The Kernel Space

[ROE+], [RW05, 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

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 $k \in L^\infty(\mathcal{X} \times \mathcal{X}, \mu \times \mu)$).

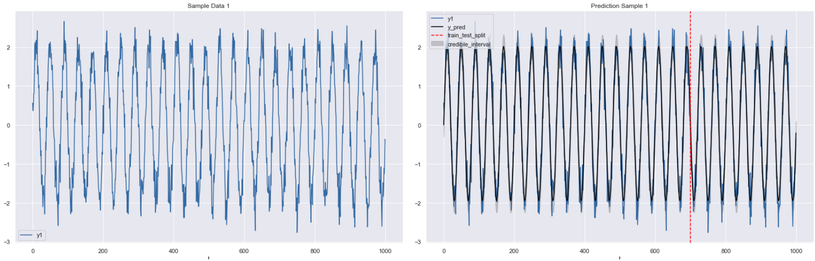
$$(T_k \phi)(x) = \int_{\mathcal{X}} k(x, x') \phi(x') d\mu(x')$$

Example: Periodic Component I ([?])

[PVG+11, Section 1.7. Gaussian Processes]

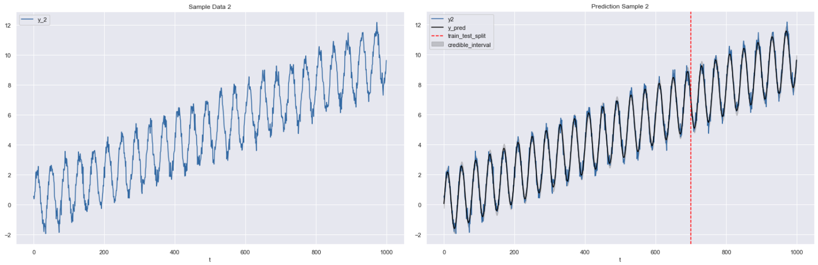
```python
from sklearn.gaussian_process.kernels import WhiteKernel, ExpSineSquared, ConstantKernel

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
)
```



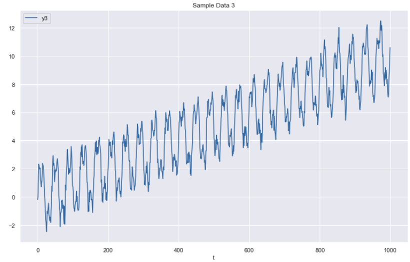
Example: Add Linear Trend

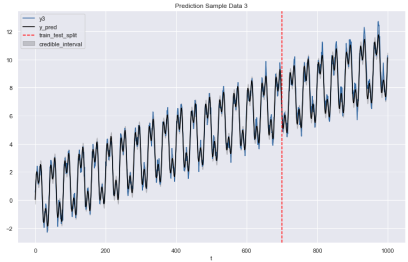
```
from sklearn.gaussian_process.kernels import RBF

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

- A practical implementation of Gaussian Process Regression is described in [RW05, Algorithm 2.1], where the Cholesky decomposition is used instead of inverting the matrices directly.
- Calculating the posterior mean and covariance matrix requires $\mathcal{O}(n^3)$ computations.

References I

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.

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

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

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.

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

References II

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

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