

Gaussian Processes for Time Series Forecasting

Dr. Juan Orduz

The Fields Institute

Second Symposium on Machine Learning and Dynamical Systems

Overview

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

Introduction

Bayesian Linear Regression

The Kernel Trick

Gaussian Process Regression

Kernel Examples

Non-Linear Example (RBF)

The Space of Kernels

Example: Time Series

Multivariate Normal Distribution

[5]

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

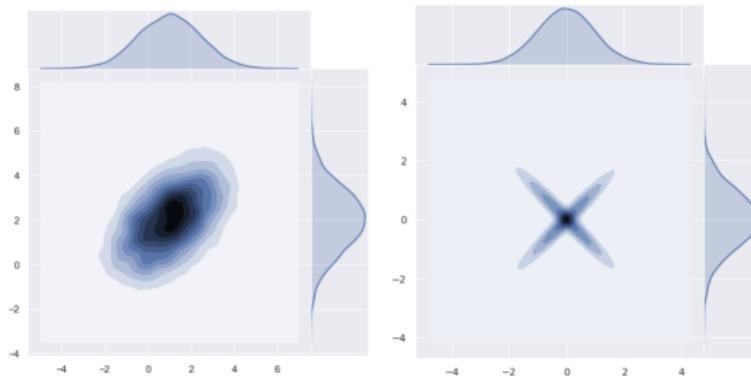


Figure: Left: Multivariate Normal Distribution, Right: Non-Multivariate Normal Distribution

Bayesian Linear Regression

[2], [7, Chapter 2.1]

Let $x_1, \dots, x_n \in \mathbb{R}^d$ and y_1, \dots, 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.

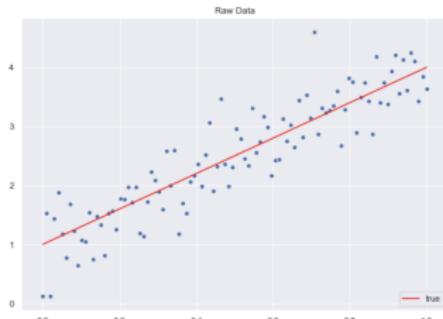


Figure: The true parameters in this example are $b = (1, 3)$ and $\sigma_n = 0.5$

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

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

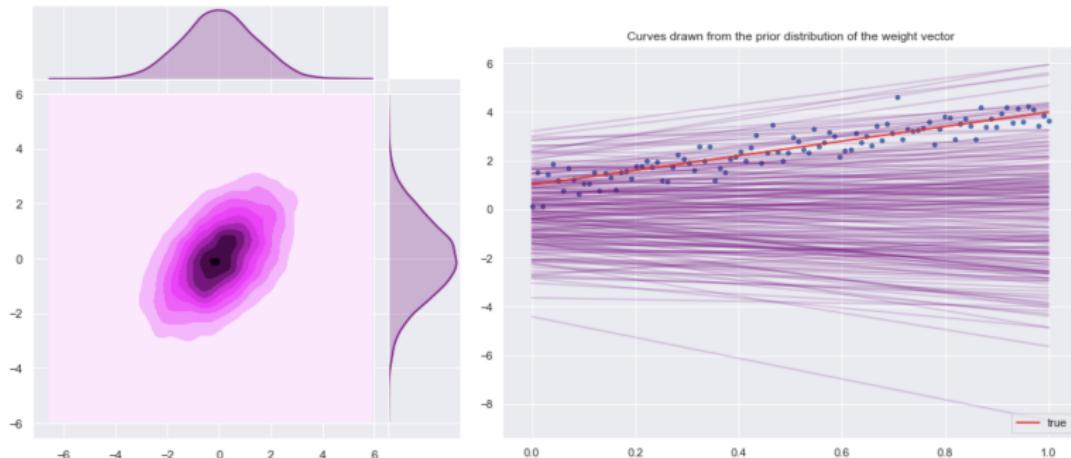


Figure: Prior Distribution, for this example $\Sigma_p = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$.

► 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]

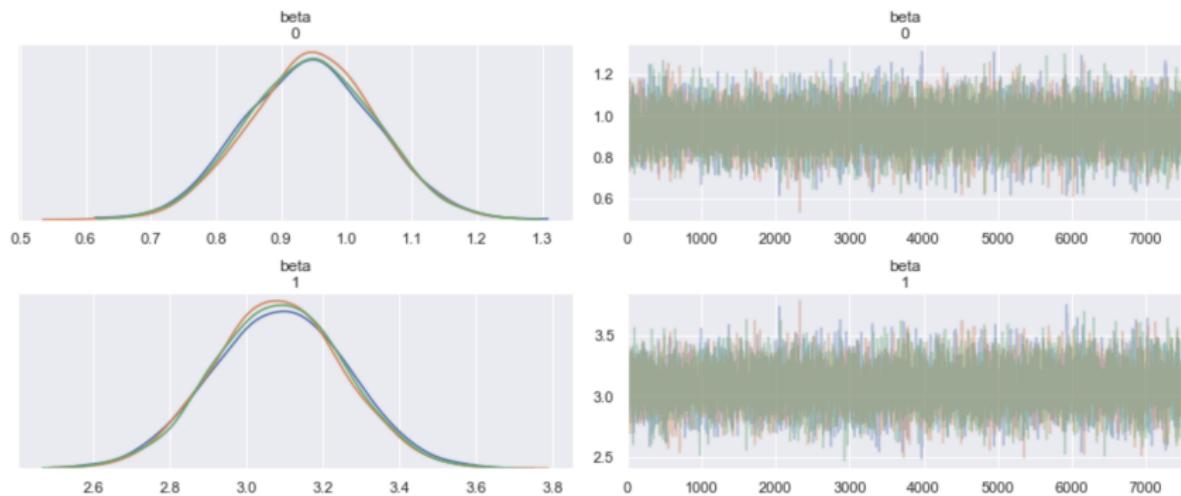


Figure: Posterior distribution of the b weight estimation using MCMC sampling (PyMC3). Here we use 3 chains.

Posterior Distribution - Analytical Solution

[7, Chapter 2.1.1]

► Posterior

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

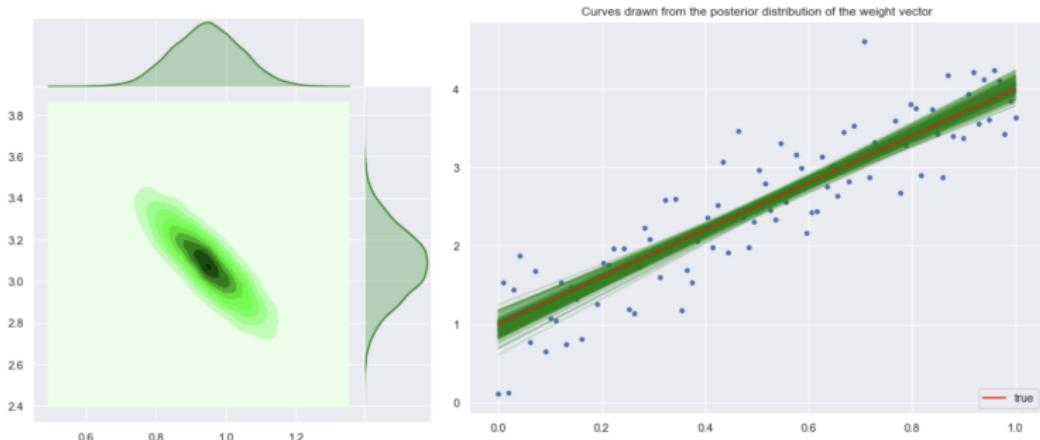


Figure: Posterior Distribution.

Predictive Distribution - Analytical Solution

[7, Chapter 2.1.1]

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

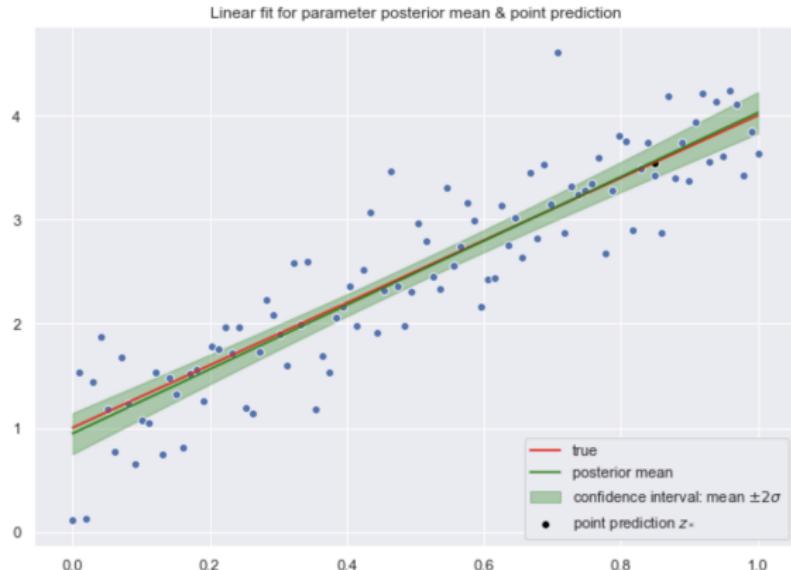


Figure: Prediction Interval.

The Kernel Trick

[7, Chapter 2.1.2]

Let us consider a map $\phi : \mathbb{R}^d \rightarrow \mathbb{R}^N$ 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 is analogous to the standard linear model replacing X with $\Phi := \phi(X)$. Set $\phi_* = \phi(x_*)$,

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

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

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

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]

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} .

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

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

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

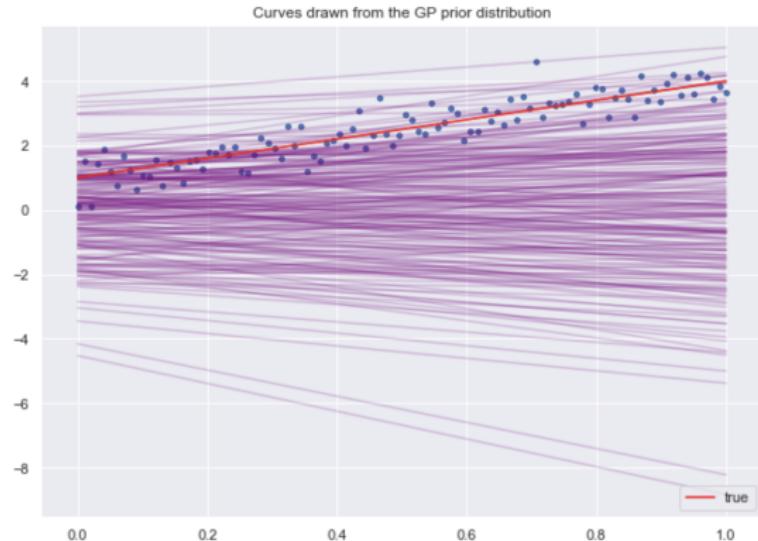


Figure: We sample from the prior space of functions by plotting their realization on $n_* = 80$ points.

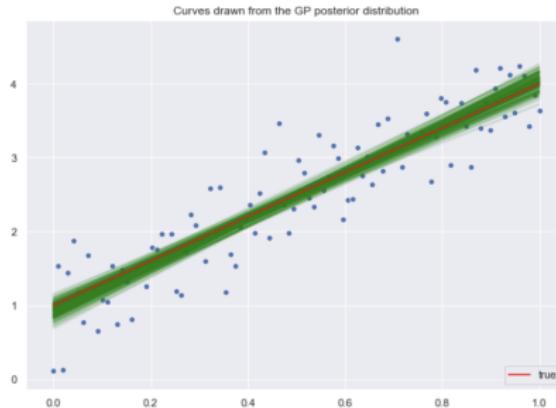
Linear Regression - Function Space View

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



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

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

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]

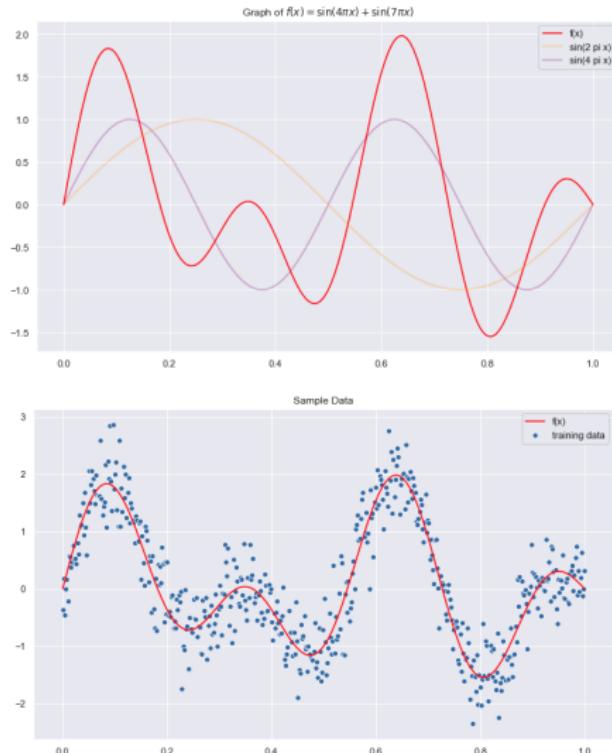


Figure: Non-Linear Example with $n = 500$ training points.

Prior Distribution

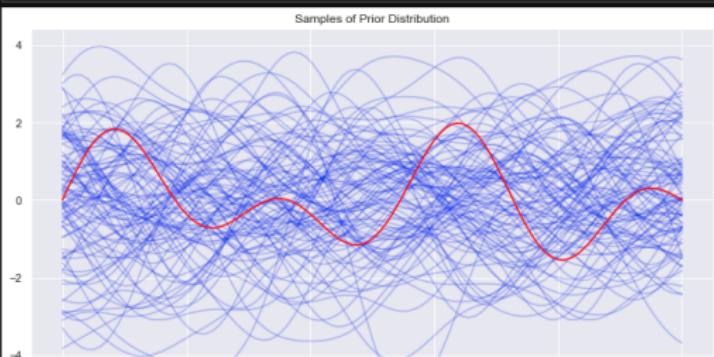
```
for i in range(0, 100):
    # Sample from prior distribution.
    z_star = np.random.multivariate_normal(mean=np.zeros(n_star),
    , cov=K_star2)
    # Plot function.
    sns.lineplot(x=x_star, y=z_star, color='blue', alpha=0.2, ax
=ax)
```

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

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

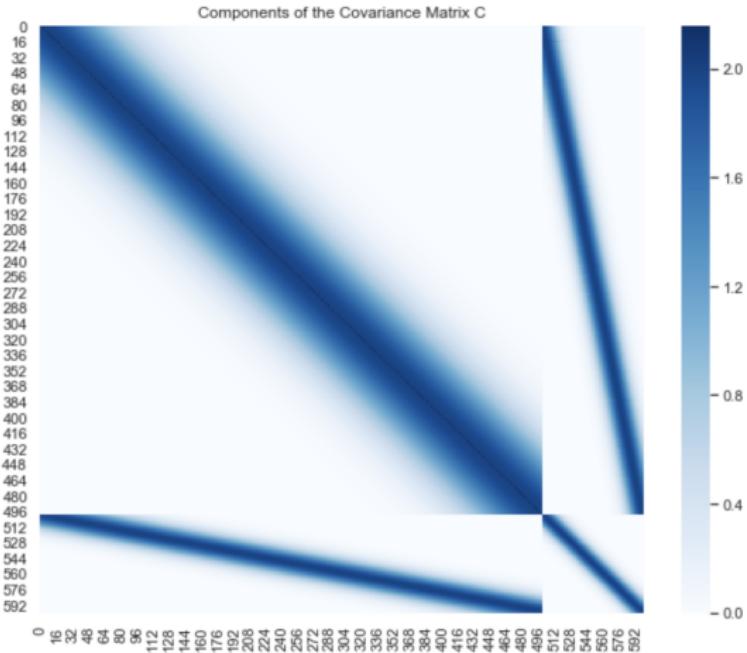
for i in range(0, 100):
    # Sample from prior distribution.
    z_star = np.random.multivariate_normal(mean=np.zeros(n_star), cov=K_star2)
    # Plot function.
    sns.lineplot(x=x_star, y=z_star, color='blue', alpha=0.2)

    # 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');
```



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

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

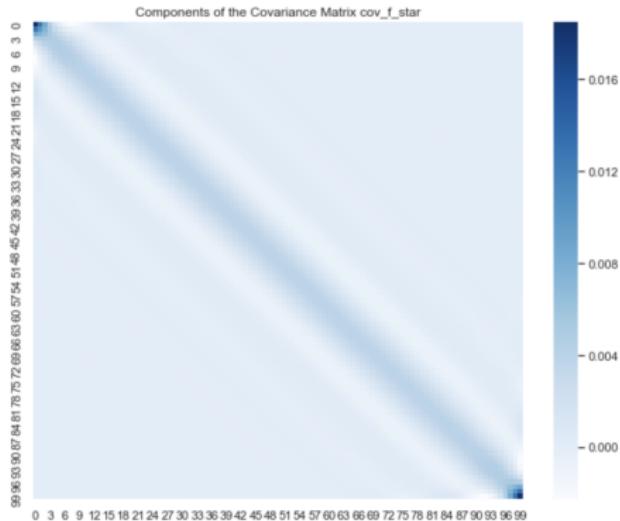


Figure: Covariance matrix of the posterior (conditional) distribution.

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

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

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');
```

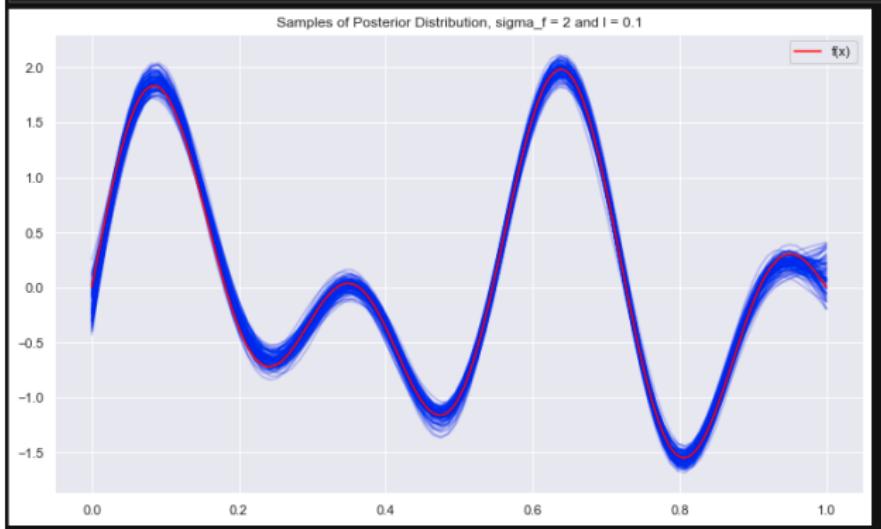


Figure: We sample from the posterior space of functions by plotting their realization on $n_* = 100$ points.

Hyperparameter Estimation

[7, Chapter 2.3, 5]

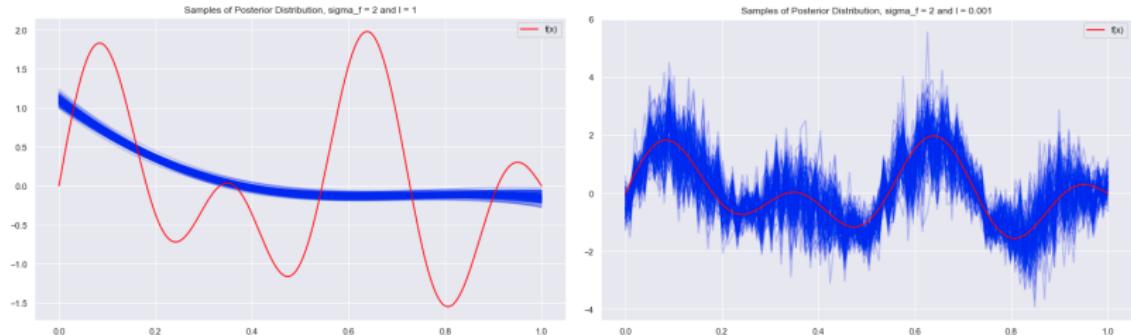


Figure: Samples from two gaussian processes with different scale parameters (left: $\ell = 1$ and right: $\ell = 0.001$).

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

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

If $k : \mathcal{X}_1 \times \mathcal{X}_1 \rightarrow \mathbb{R}$ and $h : \mathcal{X}_2 \times \mathcal{X}_2 \rightarrow \mathbb{R}$ 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 $T_k : L^2(\mathcal{X}, \mu) \rightarrow L^2(\mathcal{X}, \mu)$ (where (\mathcal{X}, μ) is a finite measure space and $k \in L^\infty(\mathcal{X} \times \mathcal{X}, \mu \times \mu)$).

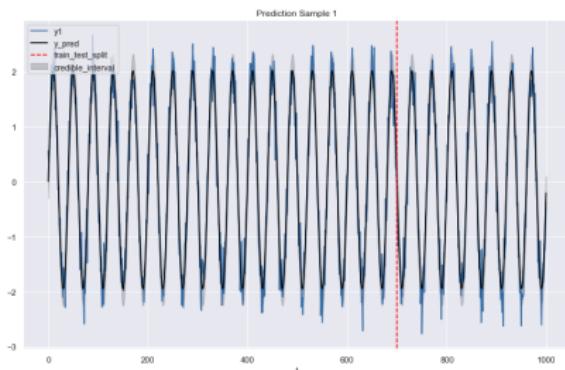
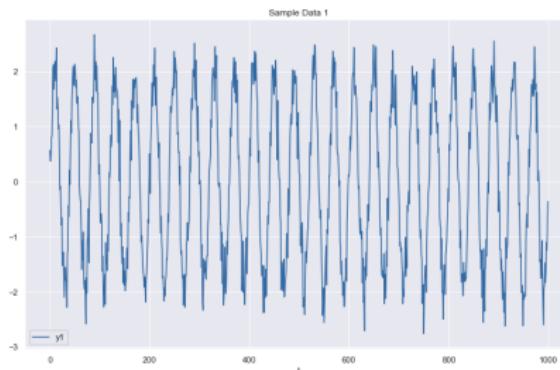
$$(T_k\phi)(x) = \int_{\mathcal{X}} k(x, x')\phi(x')d\mu(x')$$

Example: Periodic Component I ([3])

[6, Section 1.7. Gaussian Processes]

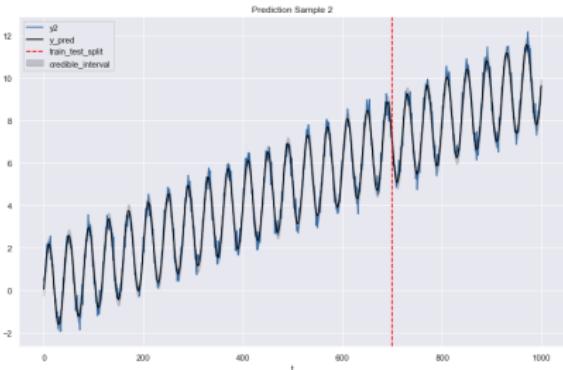
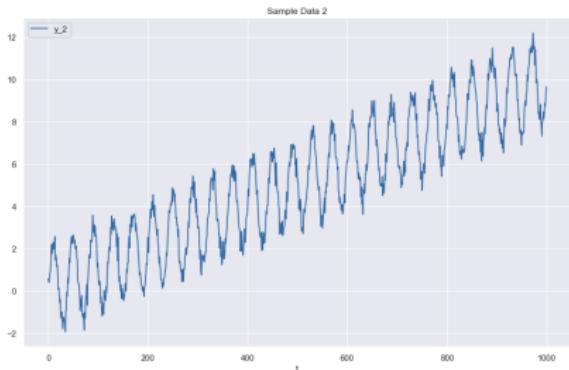
```
from sklearn.gaussian_process.kernels import WhiteKernel, ExpSineSquared, ConstantKernel  
  
k0 = WhiteKernel(noise_level=0.3**2, noise_level_bounds=(0.1**2, 0.5**2))  
  
k1 = ConstantKernel(constant_value=2) * ExpSineSquared(length_scale=1.0, periodicity=40, periodicity_bounds=(35, 45))  
  
kernel_1 = k0 + k1
```

```
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

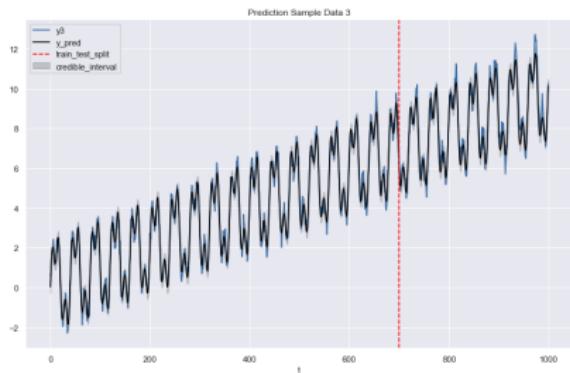
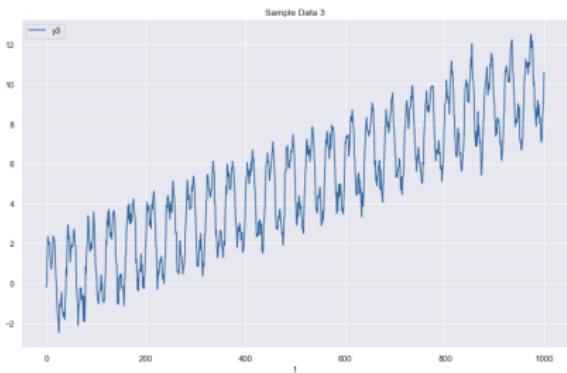
```
k0 = WhiteKernel(noise_level=0.3**2, noise_level_bounds=(0.1**2, 0.5**2))

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.

Thank You!

Contact

- ▶ [🚀 https://juanitorduz.github.io](https://juanitorduz.github.io)
- ▶ [⌚ github.com/juanitorduz](https://github.com/juanitorduz)
- ▶ [🐦 juanitorduz](https://twitter.com/juanitorduz)
- ▶ [✉️ juanitorduz@gmail.com](mailto:juanitorduz@gmail.com)

