

## Gaussian Processes

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### 1 Motivational examples for Gaussian Processes (GP)

- State of the art nonlinear regressions done with GP Bayes filter
- Used in reverse kinematics, dynamics, modeling
- Concrete example: *Modeling of soil properties*<sup>1</sup>
  - Task: Model the distribution of soil pH throughout Honduras land
  - A limited set of datapoints of soil pH at fixed locations through the country is provided
  - Variables influencing soil pH: sunlight, rainfall amount, topography, vegetation etc
  - Used state of the art GP Bayes filter to predict the mean soil pH and the prediction variance, or confidence (1)

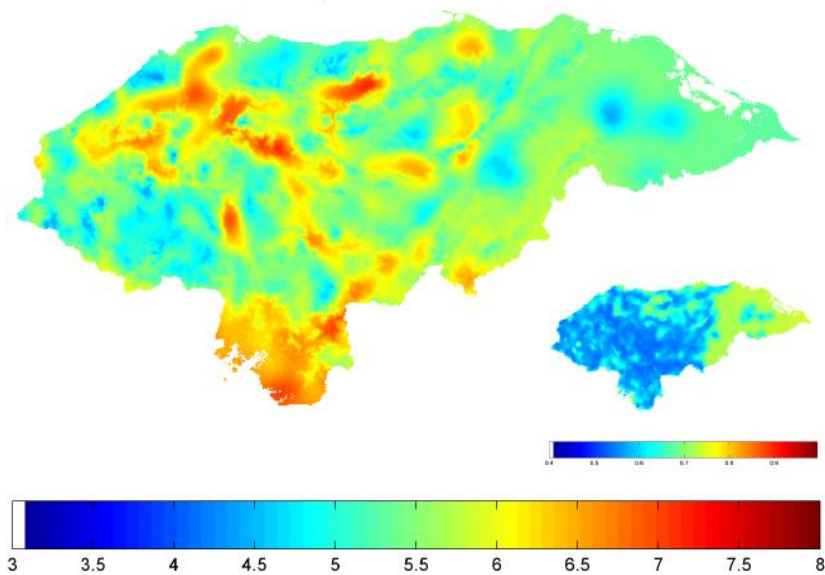


Figure 1: Predicted map of pH in topsoil and 67% confidence interval.

<sup>1</sup>J. P. Gonzalez, S. Cook, T. Oberthur, A. Jarvis, J. A. Bagnell and M. Bernardine, *Creating Low-Cost Soil Maps for Tropical Agriculture using Gaussian Processes*, JCAI 2007, Jan 2007.

## 2 High level idea behind GP's

- Consider a function as a really long list of numbers, a vector of numbers
- For discrete set of locations build a Gaussian distribution on the vector
- Generalize discrete covariance to continuous functions
- Graphically

Consider  $\vec{f}(x) = [f(x_1), f(x_2), f(x_3), \dots, f(10)]^T$  then we can form a Gaussian distribution on this vector of the form:

$$p(\vec{f}(x)) = \frac{1}{z} e^{-(\vec{f}-\mu_f)^T \Sigma^{-1} (\vec{f}-\mu_f)} \quad (1)$$

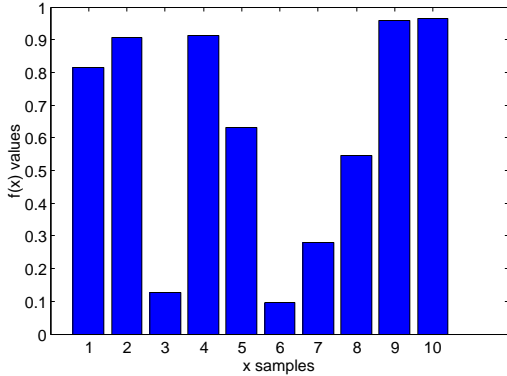


Figure 2: Sample points for GP filter

Generalizing the idea of a distribution of a vector  $\vec{f}(x)$  to continuous functions and using the expansion of the matrix exponent:

$$(\vec{f} - \mu_f)^T \Sigma^{-1} (\vec{f} - \mu_f) = \sum_i \sum_j (f_i - \mu_i) \Sigma_{ij}^{-1} (f_j - \mu_j) \quad (2)$$

we obtain a distribution of continuous functions:

$$p(f) = \frac{1}{z} e^{-\frac{1}{2} \int dx \int dx' f(x) \Delta(x, x') f(x')} \quad (3)$$

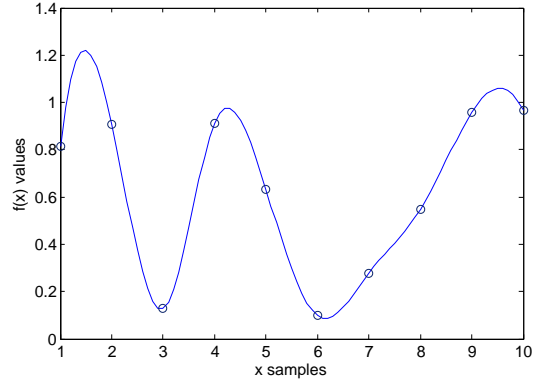


Figure 3: Sample function passing through training points for GP filter

However, in the continuous function case the normalizer  $\frac{1}{z}$  is effectively an integral over all functions, which is infinite. This is a big problem, however there exists a solution: marginalize all functions by looking at a discrete number of points. To do that we apply the marginalization rules:

$$\mu_f = 0, \quad \Sigma_{ff} = \begin{pmatrix} \kappa(x_1, x_1) & \kappa(x_1, x_2) & \dots & \kappa(x_1, x_n) \\ \kappa(x_2, x_1) & \kappa(x_2, x_2) & \dots & \kappa(x_2, x_n) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(x_n, x_1) & \kappa(x_n, x_2) & \dots & \kappa(x_n, x_n) \end{pmatrix} \quad (4)$$

where  $\kappa(x, x')$  is the kernel function and effectively portrays how each point  $x$  influences point  $x'$ . The kernel function is one of the most important concepts in Gaussian processes and is used to form the covariance  $\Sigma$ .

## 2.1 Kernel functions

Kernel functions must be positive definite and symmetric as the matrix  $\Sigma$  they for has those properties.

*Sample kernel functions:*

- $\kappa(x, x') = e^{-\frac{(x-x')^2}{L}}$   
This is one of the simplest kernel functions that works surprisingly well. The parameter  $L$  is the characteristic length and defines the distance over which the correlation of 2 points  $(x, x')$  is effective. The smaller the length scale, the less each point will influence its neighbor.
- $\kappa(x, x') = \delta(x - x')$   
Effectively says that each point has no influence on its neighbor.
- $\kappa(x, x') = \vec{x}^T \vec{x}'$   
This kernel function results in Bayes linear regression.

## 3 How to apply algorithm

Consider a few datapoints in  $\mathbb{R}^2$  as shown on right. We are interested in predicting the value of  $f(x^*)$ .

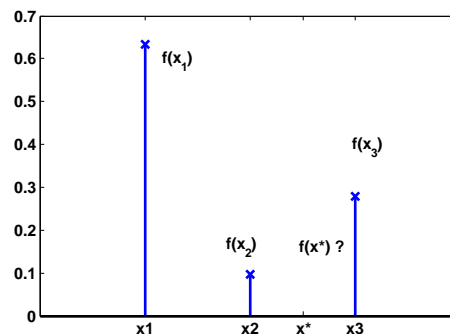


Figure 4: Training datapoints  $x_1, x_2, x_3$  and one unknown datapoint  $f(x^*)$ .

Let  $\vec{x} \equiv [x_1, x_2, x_3]^T$  and  $\vec{f} \equiv [f(x_1), f(x_2), f(x_3)]^T$  then we have the distribution of points:

$$\begin{pmatrix} \vec{f} \\ f(x^*) \end{pmatrix} \sim \mathbb{N} \left( 0, \begin{bmatrix} K_{\vec{x}\vec{x}} & K_{\vec{x}x^*} \\ K_{x^*\vec{x}} & K_{x^*x^*} \end{bmatrix} \right) \quad (5)$$

We are interested in the conditional distribution  $p = f(x^*)|f(x_1)f(x_2)f(x_3)$  therefore we can compute the mean and variance of the value  $f(x^*)$  using rules for conditionalizing the Gaussian distribution.

$$\begin{aligned} \mu_{f^*} &= K_{\vec{x}x^*}^T K_{\vec{x}\vec{x}}^{-1} \vec{f} \\ \Sigma_{f^*} &= K_{x^*x^*} - K_{\vec{x}x^*}^T K_{\vec{x}\vec{x}}^{-1} K_{\vec{x}x^*} \end{aligned}$$