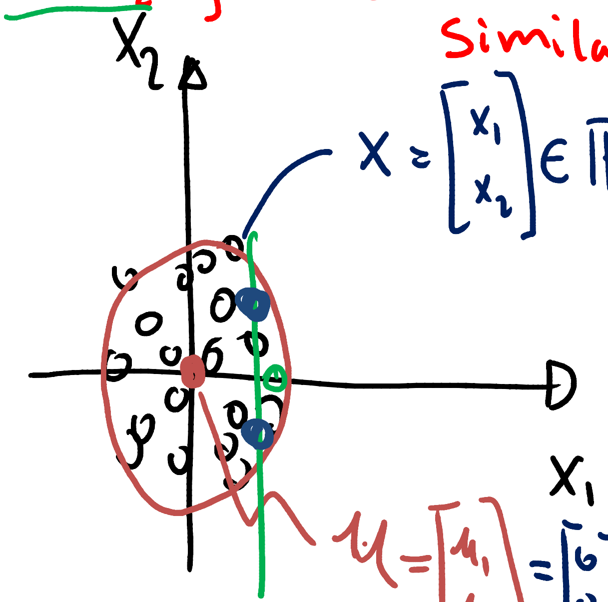
Gaussian basics

$$\left.\begin{aligned}[1\ 0]\begin{bmatrix}1\\0\end{bmatrix}&=1\\ [1\ 0]\begin{bmatrix}0\\1\end{bmatrix}&=0\end{aligned}\right\}$$

dot products measure similarity



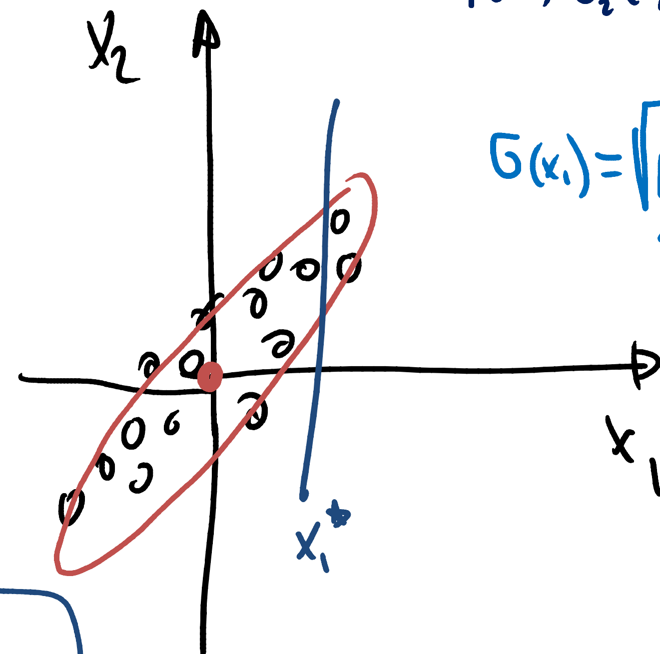
$X=\begin{bmatrix}x_1\\x_2\end{bmatrix}\in\mathbb{R}^2$

$\mu=\begin{bmatrix}\mu_1\\\mu_2\end{bmatrix}=\begin{bmatrix}0\\0\end{bmatrix}$

$\mathbb{E}(x_1x_2)$

$$\begin{bmatrix}x_1\\x_2\end{bmatrix}\sim N\left(\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}1&\boxed{0}\\0&1\end{bmatrix}\right)$$

$$\rho_{x_1x_2}=\frac{\mathrm{cov}(x_1,x_2)}{\sigma_1(x_1)\,\sigma_2(x_2)}$$



$\sigma(x_1)=\sqrt{\mathbb{E}(x_1^2)}$

$$\begin{bmatrix}x_1\\x_2\end{bmatrix}\sim N\left(\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}1&0.5\\0.5&1\end{bmatrix}\right)$$

Gaussian basics

$x^T \Sigma x$

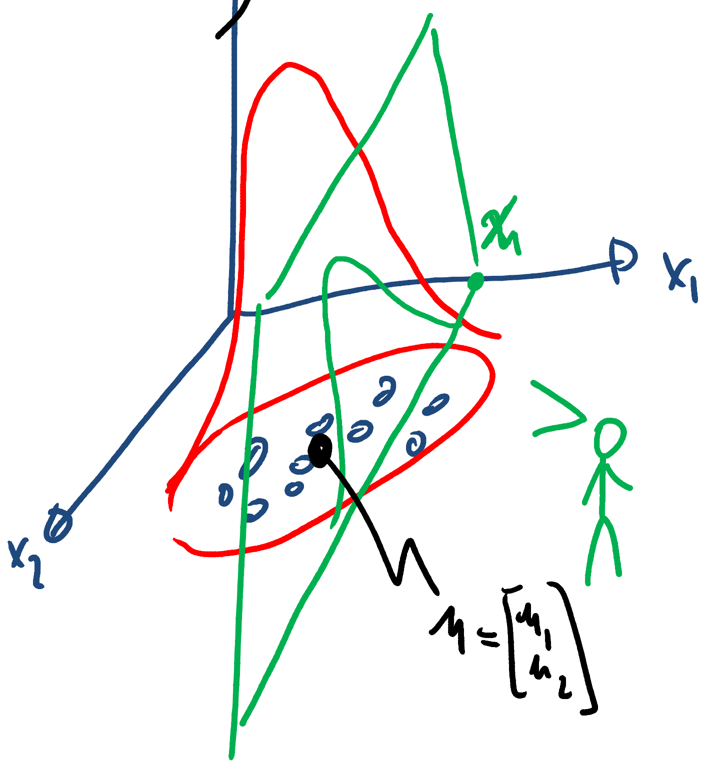
$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \sim N\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}\right)$$

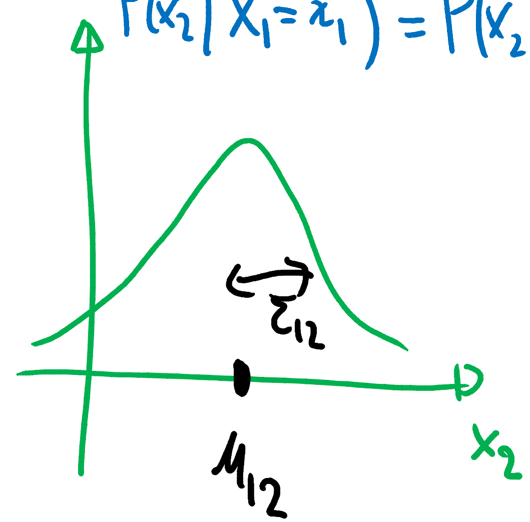
$P(x_1, x_2)$ joint

conditional

given

$$P(x_2 | X_1 = x_1) = P(x_2 | x_1)$$



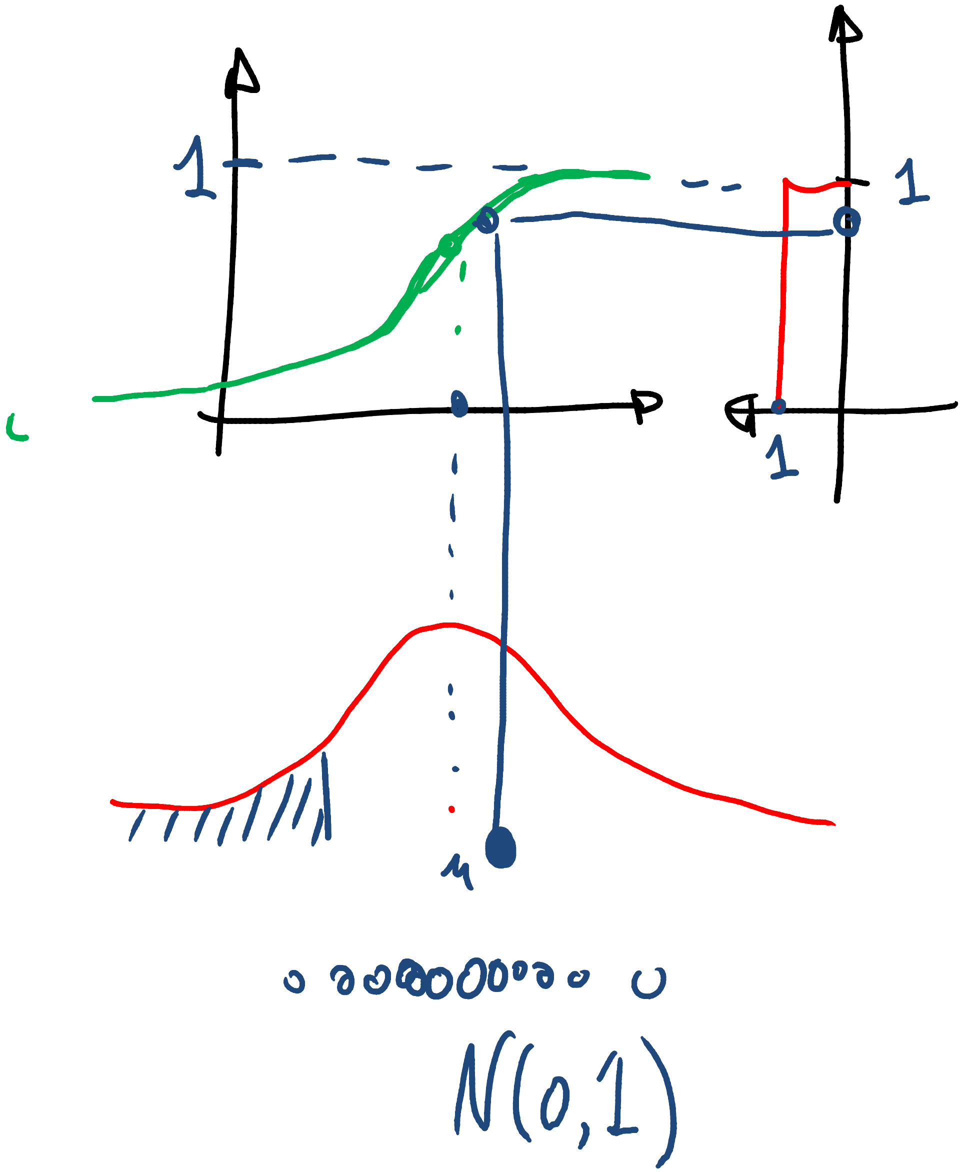


$$\mu_{12} = \mu_1 + \Sigma_{12} \Sigma_{22}^{-1} (x_2 - \mu_2)$$

$$\Sigma_{12} = \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$$

Gaussian basics

Cholesky
$\Sigma = LL^T$



$$X_i \sim N(0,1)$$

$$X_i \sim N(\mu, \sigma^2)$$

$$\sim \mu + \sigma N(0,1)$$

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}_i \sim N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

$$\underset{\uparrow \vec{x}}{\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}_i} \sim N\left(\underset{\uparrow \mu}{\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}}, \underset{\uparrow \Sigma}{\begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}} \right)$$

$X \sim N(\mu, \Sigma)$ $\quad$ $X \sim \mu + L N(0, I)$

Multivariate Gaussian Theorem (see KPM)

Theorem 4.2.1 (Marginals and conditionals of an MVN)**.** *Suppose* $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$ *is jointly Gaussian with parameters*

$$\boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix}, \quad \boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1} = \begin{pmatrix} \boldsymbol{\Lambda}_{11} & \boldsymbol{\Lambda}_{12} \\ \boldsymbol{\Lambda}_{21} & \boldsymbol{\Lambda}_{22} \end{pmatrix} \tag{4.12}$$

Then the marginals are given by

$$\begin{aligned} p(\mathbf{x}_1) &= \mathcal{N}(\mathbf{x}_1 | \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11}) \\ p(\mathbf{x}_2) &= \mathcal{N}(\mathbf{x}_2 | \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22}) \end{aligned}$$

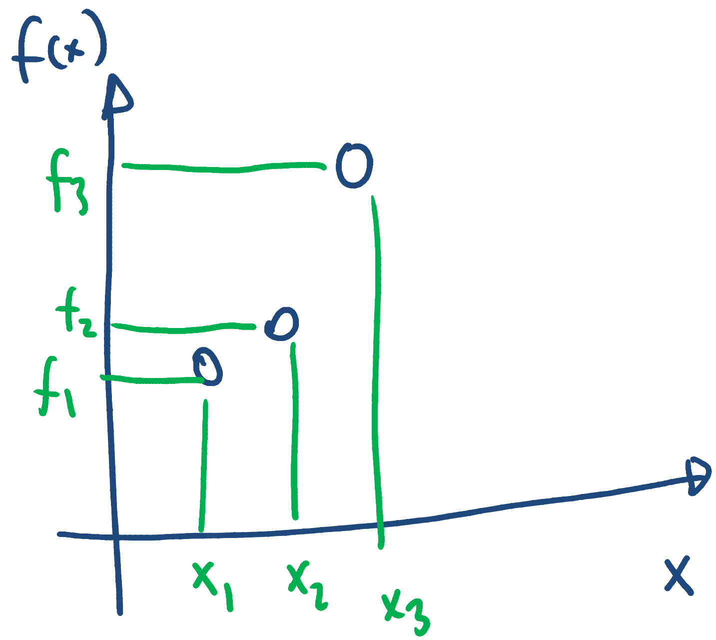
and the posterior conditional is given by

$$\boxed{\begin{aligned} p(\mathbf{x}_1|\mathbf{x}_2) &= \mathcal{N}(\mathbf{x}_1 | \boldsymbol{\mu}_{1|2}, \boldsymbol{\Sigma}_{1|2}) \\ \boldsymbol{\mu}_{1|2} &= \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2) \\ &= \boldsymbol{\mu}_1 - \boldsymbol{\Lambda}_{11}^{-1}\boldsymbol{\Lambda}_{12}(\mathbf{x}_2 - \boldsymbol{\mu}_2) \\ &= \boldsymbol{\Sigma}_{1|2}\left(\boldsymbol{\Lambda}_{11}\boldsymbol{\mu}_1 - \boldsymbol{\Lambda}_{12}(\mathbf{x}_2 - \boldsymbol{\mu}_2)\right) \\ \boldsymbol{\Sigma}_{1|2} &= \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21} = \boldsymbol{\Lambda}_{11}^{-1} \end{aligned}}$$

Gaussian basics

x's given

want to model f's



$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} \sim \left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix} \right)$$

$$\sim \left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.7 & 0.2 \\ 0.7 & 1 & 0.6 \\ 0.2 & 0.6 & 1 \end{bmatrix} \right)$$

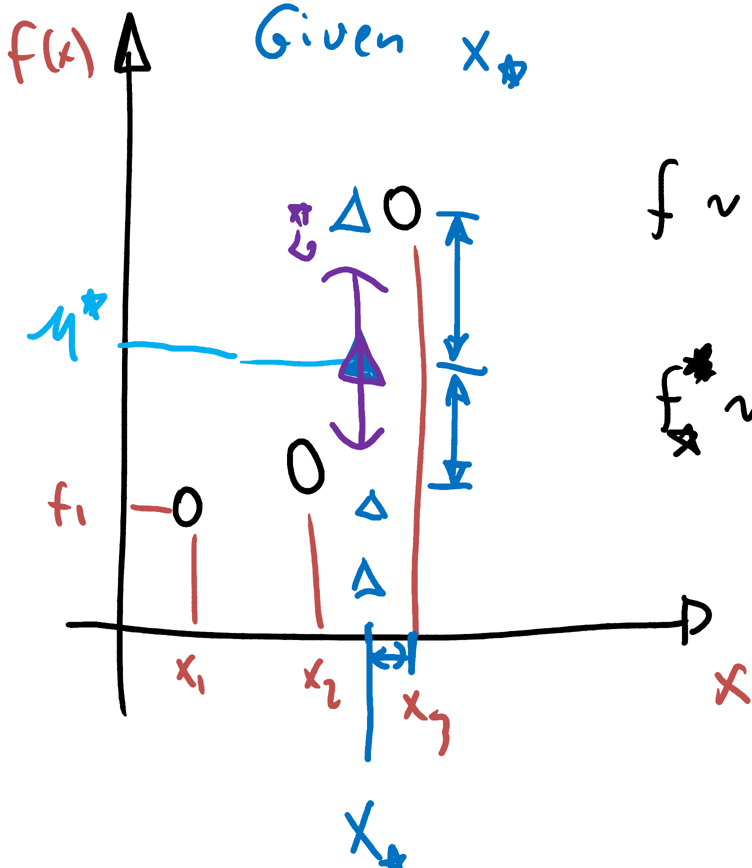
K

$$K_{ij} = e^{-\lambda \|x_i - x_j\|^2} = \begin{cases} 0 & \|x_i - x_j\| \to \infty \\ 1 & x_i = x_j \end{cases}$$

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

Gaussian basics

Given Data $D=\{(x_1,f_1),(x_2,f_2),(x_3,f_3)\}$ Given x_* $\Rightarrow f_* = ?$



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

$$K(x_*,x_*) = e^{-\|x_*-x_*\|^2} = 1$$

$$f^* \sim N(0, \underbrace{K(x_*,x_*)}_{K_{**}})$$

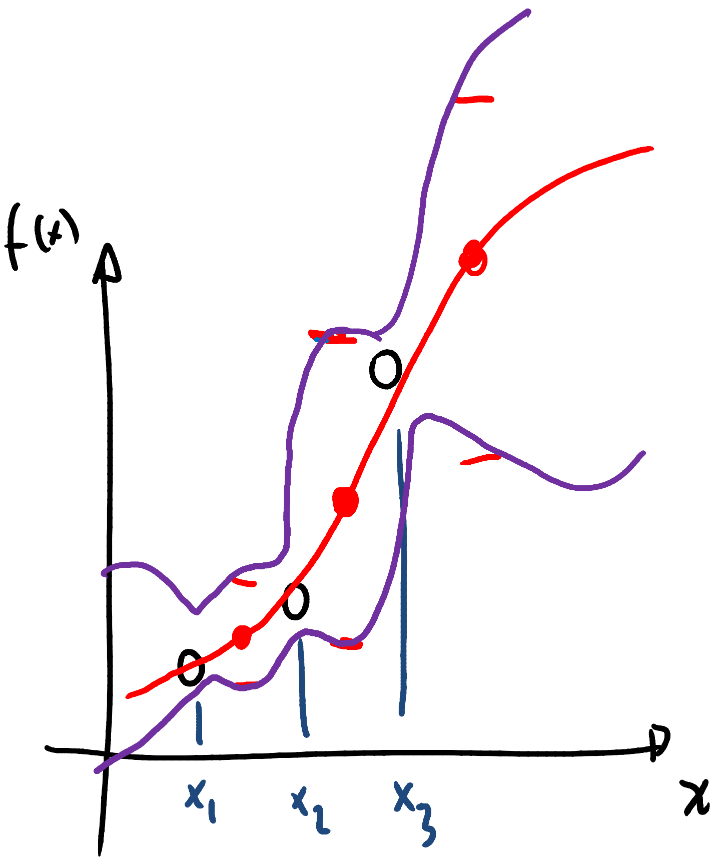
$$K_{1*} = K(x_1,x_*)$$

$$\begin{bmatrix} f\\ f_*\end{bmatrix} \sim N\left(0, \begin{bmatrix} \underbrace{\begin{bmatrix}K_{11}&K_{12}&K_{13}\\K_{21}&K_{22}&K_{23}\\K_{31}&K_{32}&K_{33}\end{bmatrix}}_{K} & \underbrace{\begin{bmatrix}K_{1*}\\K_{2*}\\K_{3*}\end{bmatrix}}_{K_*}\\ K_{*1}\;\;K_{*2}\;\;K_{*3} & \underbrace{K_{**}}_{K_{**}}\end{bmatrix}\right)$$

$$\mu^* = E(f^*) = K_*^T K^{-1} f$$

$$\sigma^* = -K_*^T K^{-1} K_* + K_{**}$$

Gaussian basics



GP: a distribution over functions

A GP is a Gaussian distribution over functions:

$$f(\mathbf{x}) \sim GP(m(\mathbf{x}), \kappa(\mathbf{x}, \mathbf{x}'))$$

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})]$$

$$\kappa(\mathbf{x}, \mathbf{x}') = \mathbb{E}\left[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))^T\right]$$

$$\boxed{k(x, x') = \exp(-\tfrac{1}{2}(x - x')^2)}$$

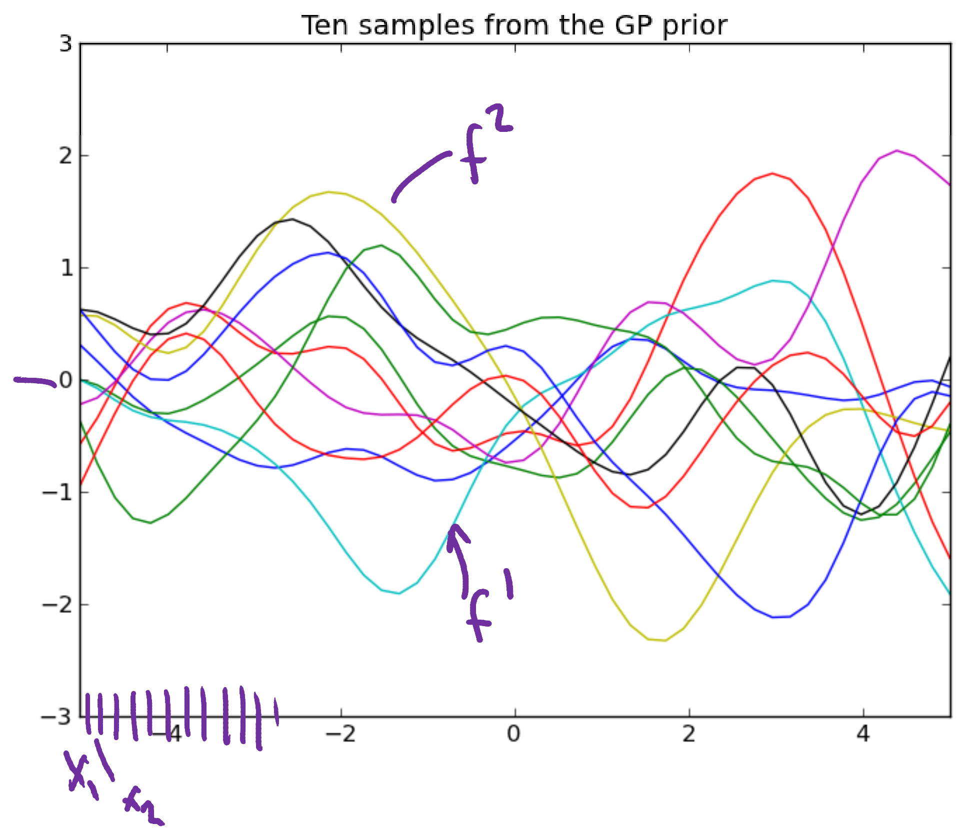
Create $x_{1:N}$

Create $\mu = 0_N$, $K_{N \times N}$

$K = L L^T$

$f^i \sim N(0_N, K)$

$\sim N(0, I) L$



Sampling from *P(f)*

```
from __future__ import division
import numpy as np
import matplotlib.pyplot as pl

def kernel(a, b):
    """ GP squared exponential kernel """
    sqdist = np.sum(a**2,1).reshape(-1,1) + np.sum(b**2,1) - 2*np.dot(a, b.T)
    return np.exp(-.5 * sqdist)

n = 50                                          # number of test points.
Xtest = np.linspace(-5, 5, n).reshape(-1,1)     # Test points.
K_ = kernel(Xtest, Xtest)                       # Kernel at test points.

# draw samples from the prior at our test points.
L = np.linalg.cholesky(K_ + 1e-6*np.eye(n))
f_prior = np.dot(L, np.random.normal(size=(n,10)))

pl.plot(Xtest, f_prior)
```

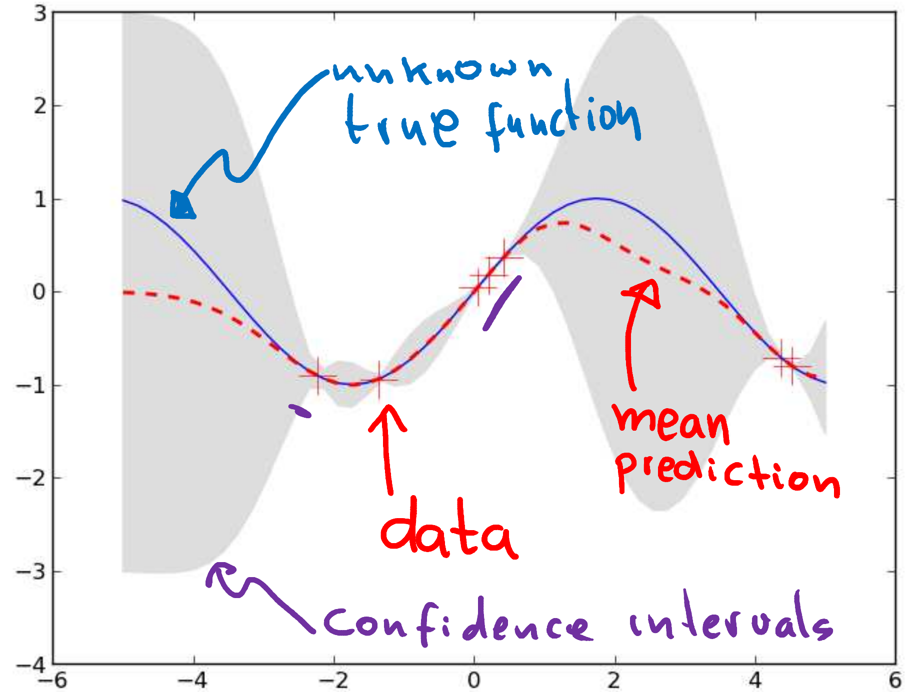
$K = LL^T$

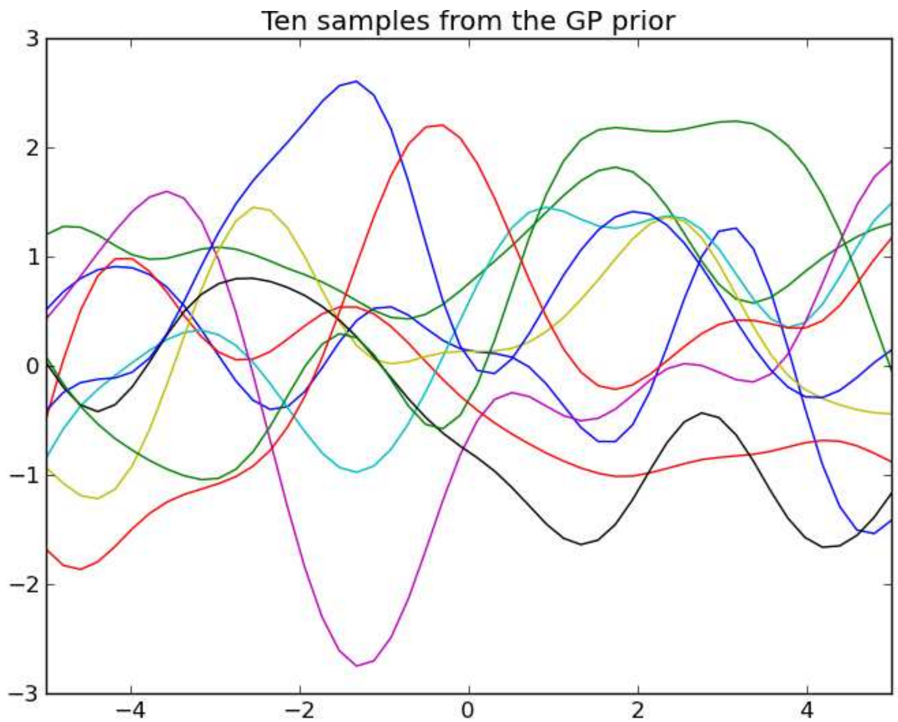
$L\mathcal{N}(0, I)$

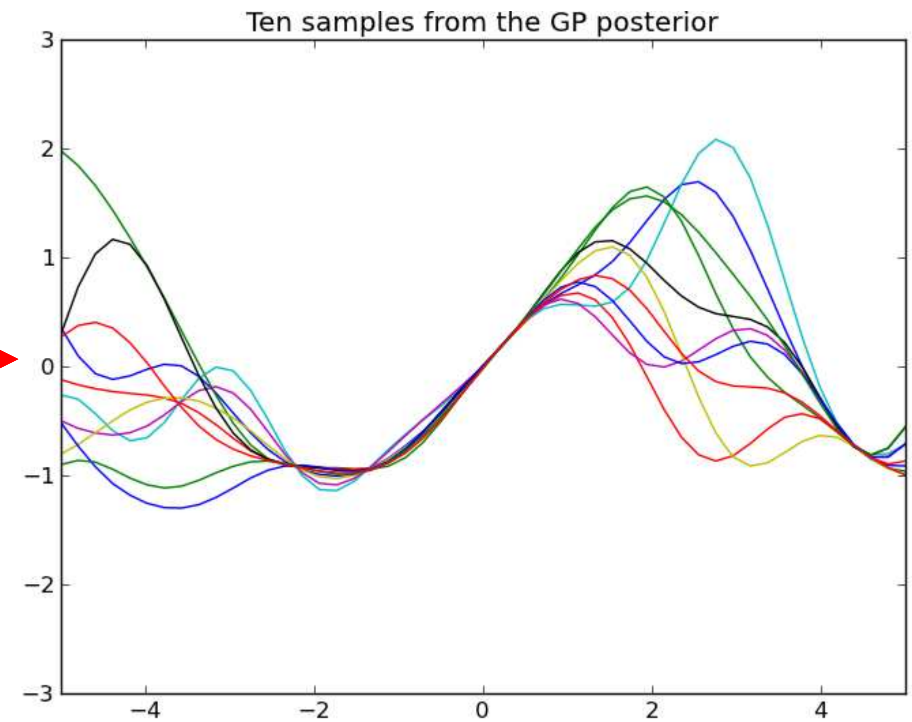
GP posterior

$$\mathcal{D} = \{(\mathbf{x}_i, f_i), i = 1 : N\}$$

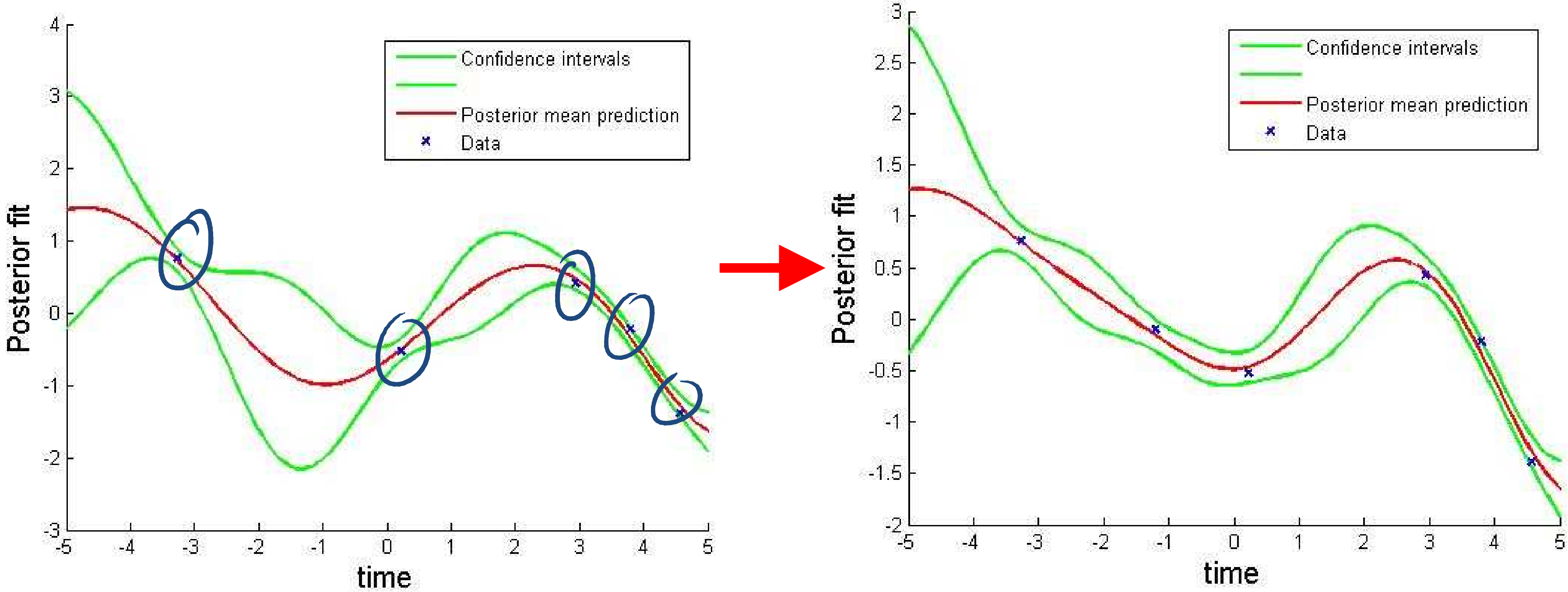
$$p(f|\mathcal{D}) = \frac{p(\mathcal{D}|f)p(f)}{p(\mathcal{D})}$$







Active learning with GPs



Noiseless GP regression

we observe a training set $\mathcal{D} = \{(\mathbf{x}_i, f_i), i = 1 : N\}$, where $f_i = f(\mathbf{x}_i)$

Given a test set $\mathbf{X}_*$ of size $N_* \times D$, we want to predict the function outputs $\mathbf{f}_*$.

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}_* \end{pmatrix}, \begin{pmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix}\right)$$

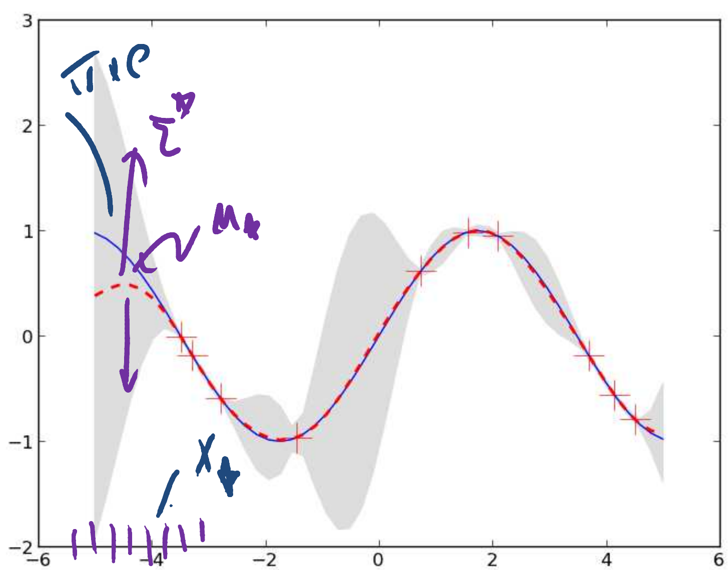
where $\mathbf{K} = \kappa(\mathbf{X}, \mathbf{X})$ is $N \times N$, $\mathbf{K}_* = \kappa(\mathbf{X}, \mathbf{X}_*)$ is $N \times N_*$, and $\mathbf{K}_{**} = \kappa(\mathbf{X}_*, \mathbf{X}_*)$ is $N_* \times N_*$.

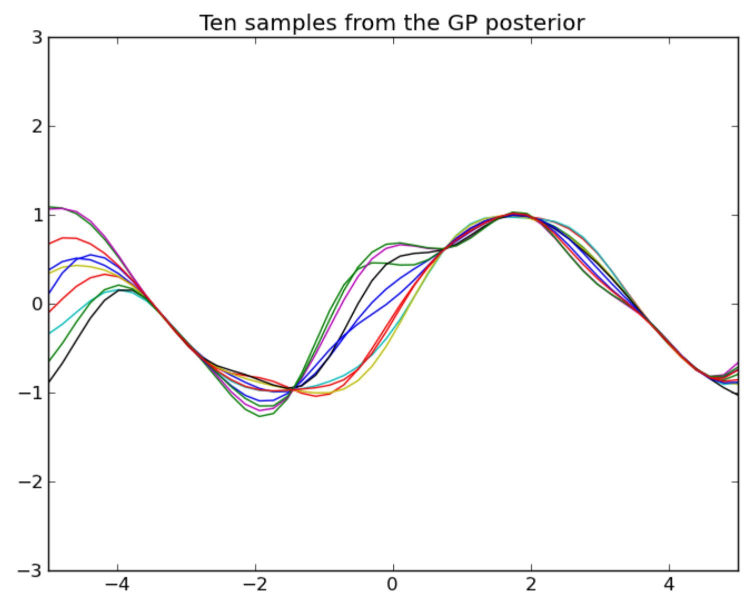
$$\kappa(x, x') = \sigma_f^2 \exp\left(-\frac{1}{2\ell^2}(x - x')^2\right)$$

Noiseless GP regression

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}_* \end{pmatrix}, \begin{pmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix} \right)$$

$$\begin{aligned} p(\mathbf{f}_* | \mathbf{X}_*, \mathbf{X}, \mathbf{f}) &= \mathcal{N}(\mathbf{f}_* | \boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*) \\ \boldsymbol{\mu}_* &= \boldsymbol{\mu}(\mathbf{X}_*) + \mathbf{K}_*^T \mathbf{K}^{-1} (\mathbf{f} - \boldsymbol{\mu}(\mathbf{X})) \\ \boldsymbol{\Sigma}_* &= \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}^{-1} \mathbf{K}_* \end{aligned}$$



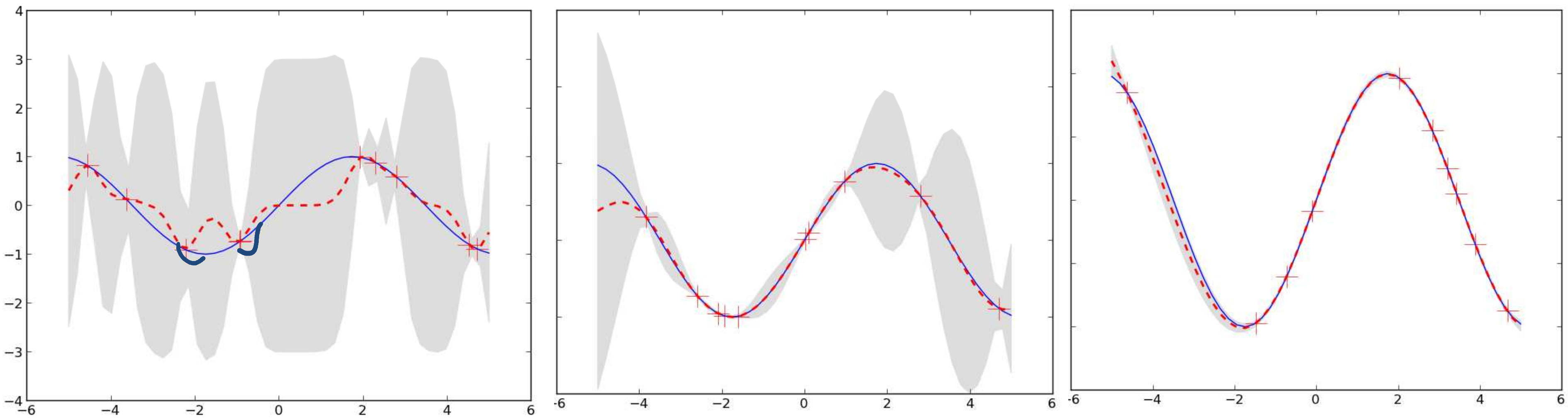


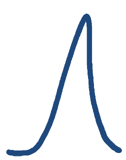
Effect of kernel width parameter

$$\kappa(x, x') = \sigma_f^2 \exp\left(-\frac{1}{2\ell^2}(x - x')^2\right)$$

Let $\sigma_f = 1$

$\ell^2 = 0.1$ $\ell^2 = 1$ $\ell^2 = 10$





Noisy GP regression

noisy

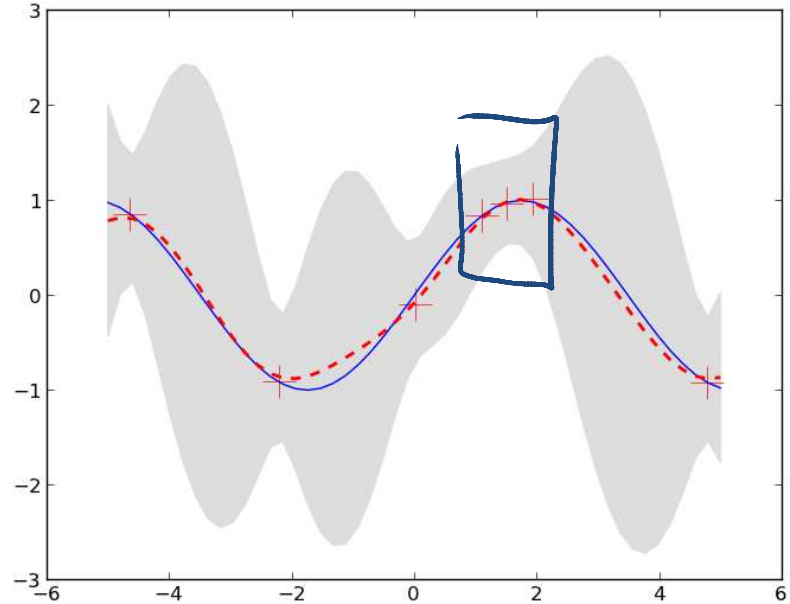
$$y = f(\mathbf{x}) + \epsilon, \text{ where } \epsilon \sim \mathcal{N}(0, \sigma_y^2)$$

$$p(\mathbf{y}|\mathbf{X}) = \int p(\mathbf{y}|\mathbf{f}, \mathbf{X}) p(\mathbf{f}|\mathbf{X}) d\mathbf{f}$$

$$p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{f}|\mathbf{0}, \mathbf{K})$$

$$p(\mathbf{y}|\mathbf{f}) = \prod_i \mathcal{N}(y_i|f_i, \sigma_y^2)$$

$$\text{cov}\,[\mathbf{y}|\mathbf{X}] = \mathbf{K} + \boxed{\sigma_y^2 \mathbf{I}_N} \triangleq \mathbf{K}_y$$



$$\begin{pmatrix} \mathbf{y} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{pmatrix} \mathbf{K}_y & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix}\right) \xrightarrow{\text{thm}} \begin{aligned} p(\mathbf{f}_*|\mathbf{X}_*, \mathbf{X}, \mathbf{y}) &= \mathcal{N}(\mathbf{f}_*|\boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*) \\ \boldsymbol{\mu}_* &= \mathbf{K}_*^T \mathbf{K}_y^{-1} \mathbf{y} \\ \boldsymbol{\Sigma}_* &= \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}_y^{-1} \mathbf{K}_* \end{aligned}$$

Noisy GP regression

In the case of a single test input, x_* this simplifies as follows

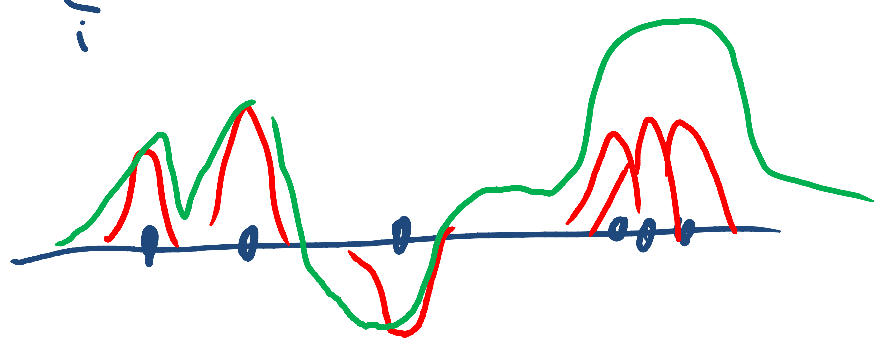
$$p(f_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) \quad = \quad \boxed{\mathcal{N}(f_*|\mathbf{k}_*^T \mathbf{K}_y^{-1} \mathbf{y}, k_{**} - \mathbf{k}_*^T \mathbf{K}_y^{-1} \mathbf{k}_*)}$$

where $\mathbf{k}_* = [\kappa(\mathbf{x}_*, \mathbf{x}_1), \ldots, \kappa(\mathbf{x}_*, \mathbf{x}_N)]$ and $k_{**} = \kappa(\mathbf{x}_*, \mathbf{x}_*)$. $=1$

$$\overline{f}_* = \underbrace{\overset{1\times N}{\mathbf{k}_*^T} \overbrace{\overset{N\times N}{\mathbf{K}_y^{-1}} \overset{N\times 1}{\mathbf{y}}}^{\alpha\ (N\times 1)}}_{\substack{\text{mean} \\ 1\times 1}} = \sum_{i=1}^{N} \alpha_i \kappa(\mathbf{x}_i, \mathbf{x}_*) \qquad \boldsymbol{\alpha} = \underbrace{\mathbf{K}_y^{-1} \mathbf{y}}_{\text{training}}$$

$$= k_*^T \alpha$$

$$= \sum_i \alpha_i e^{-\frac{1}{\lambda} \|x_i - x_*\|^2}$$



Noisy GP regression and Ridge

$$\mathbf{X} \in \mathbb{R}^{n \times d}$$

$$\mathbf{y} \in \mathbb{R}^{n}$$

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^d} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \delta^2 \|\boldsymbol{\theta}\|_2^2$$

$$X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

$$x_i \in \mathbb{R}^{1 \times d}$$

$$(\mathbf{X}^T\mathbf{X} + \delta^2 \mathbf{I}_d)\boldsymbol{\theta} = \mathbf{X}^T\mathbf{y}$$

solution can be written as $\boldsymbol{\theta} = \mathbf{X}^T\boldsymbol{\alpha}$, where $\boldsymbol{\alpha} = \delta^{-2}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$

$$X^T X \theta + \delta^2 \theta = X^T y$$

$$\delta^2 \theta = X^T (y - X\theta)$$

$$\theta = X^T \delta^{-2} (y - X\theta) = X^T \alpha$$

Noisy GP regression and Ridge

$$(\overbrace{\mathbf{X}^T\mathbf{X}}^{d\times d} + \delta^2\mathbf{I}_d)\overset{d\times 1}{\boldsymbol{\theta}} = \mathbf{X}^T\mathbf{y}$$

solution can be written as $\boldsymbol{\theta} = \mathbf{X}^T\overset{n\times 1}{\boldsymbol{\alpha}}$, where $\underline{\boldsymbol{\alpha} = \delta^{-2}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})}$

$\boldsymbol{\alpha}$ can also be written as follows: $\underline{\boldsymbol{\alpha} = (\underbrace{\mathbf{X}\mathbf{X}^T}_{n\times n} + \delta^2\mathbf{I}_n)^{-1}\mathbf{y}}$

$$\delta^2\alpha = y - X\theta$$

$$\delta^2\alpha = y - XX^T\alpha$$

$$XX^T\alpha + \delta^2 I_n\alpha = y$$

$$\alpha = \boxed{(XX^T + \delta^2 I_n)^{-1} y}$$

$$y^* = x^*\theta = x^*X^T\alpha$$

Noisy GP regression and Ridge

$$\bar{f}_* = \mathbf{k}_*^T \mathbf{K}_y^{-1} \mathbf{y}$$

$$\underset{1\times 1}{Y^*} = \underset{1\times d}{x^*} \underset{d\times 1}{\Theta}$$

$$= x^* X^T \alpha$$

$$= \underbrace{x^* X^T}_{K_*^T} \underbrace{[XX^T + \sigma^2 I_n]^{-1}}_{K_y^{-1}} Y$$

σ_y

$$= K_*^T K_y^{-1} Y$$

$$X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$1\times d$

$$K_*^T = \underbrace{\begin{bmatrix} x^* x_1^T & x^* x_2^T & \cdots & x^* x_n^T \end{bmatrix}}_{1\times n}$$

$$K_y = \underbrace{\underset{n\times d}{X} \underset{d\times n}{X^T}}_{n\times n} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \begin{bmatrix} x_1^T & \cdots & x_n^T \end{bmatrix} = \begin{bmatrix} x_1 x_1^T & \cdots \\ & \ddots \\ x_n x_1^T & \cdots \end{bmatrix}$$

d

d

Learning the kernel parameters

marginal likelihood

$$p(\mathbf{y}|\mathbf{X},\ell^2) = \int p(\mathbf{y}|\mathbf{f},\mathbf{X})p(\mathbf{f}|\mathbf{X})d\mathbf{f}$$

$$p(\mathbf{f}|\mathbf{X},\ell^2) = \mathcal{N}(\mathbf{f}|\mathbf{0},\mathbf{K})$$

$\theta = \ell$

$$p(\mathbf{y}|\mathbf{f},\ell^2) = \prod_i \mathcal{N}(y_i|f_i,\sigma_y^2)$$

$$\log p(\mathbf{y}|\mathbf{X}) = \log \mathcal{N}(\mathbf{y}|\mathbf{0},\mathbf{K}_y) = -\frac{1}{2}\mathbf{y}\mathbf{K}_y^{-1}\mathbf{y} - \frac{1}{2}\log|\mathbf{K}_y| - \frac{N}{2}\log(2\pi)$$

$$\frac{\partial}{\partial\theta_j}\log p(\mathbf{y}|\mathbf{X}) = \frac{1}{2}\mathbf{y}^T\mathbf{K}_y^{-1}\frac{\partial \mathbf{K}_y}{\partial\theta_j}\mathbf{K}_y^{-1}\mathbf{y} - \frac{1}{2}\mathrm{tr}(\mathbf{K}_y^{-1}\frac{\partial \mathbf{K}_y}{\partial\theta_j})$$

Numerical computation considerations

$$\mu_* = \overline{f_*} = \underbrace{\mathbf{k}_*^T \mathbf{K}_y^{-1} \mathbf{y}}_{\alpha}$$

$$\mathbf{K}_y = \mathbf{L}\mathbf{L}^T$$

$$\boldsymbol{\alpha} = \mathbf{K}_y^{-1}\mathbf{y} = \mathbf{L}^{-T}\underbrace{\mathbf{L}^{-1}\mathbf{y}}_{m}$$

$m = L^{-1}y$

$Lm = y$

$\underbrace{L^{-T}m}_{\alpha}$

Algorithm 15.1: GP regression

1 $\mathbf{L} = \text{cholesky}(\mathbf{K} + \sigma_y^2 \mathbf{I})$;

2 $\boldsymbol{\alpha} = \underbrace{\mathbf{L}^T}\setminus(\underbrace{\mathbf{L}\setminus\mathbf{y}}_{m})$;

3 $\mathbb{E}[f_*] = \mathbf{k}_*^T \boldsymbol{\alpha}$;

4 $\mathbf{v} = \mathbf{L} \setminus \mathbf{k}_*$;

5 $\text{var}[f_*] = \kappa(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^T\mathbf{v}$;

6 $\log p(\mathbf{y}|\mathbf{X}) = -\frac{1}{2}\mathbf{y}^T\boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{N}{2}\log(2\pi)$

$L^T \alpha = m$