10-301/601: Introduction to Machine Learning Lecture 27 – Gaussian Processes

Matt Gormley & Henry Chai

4/23/25

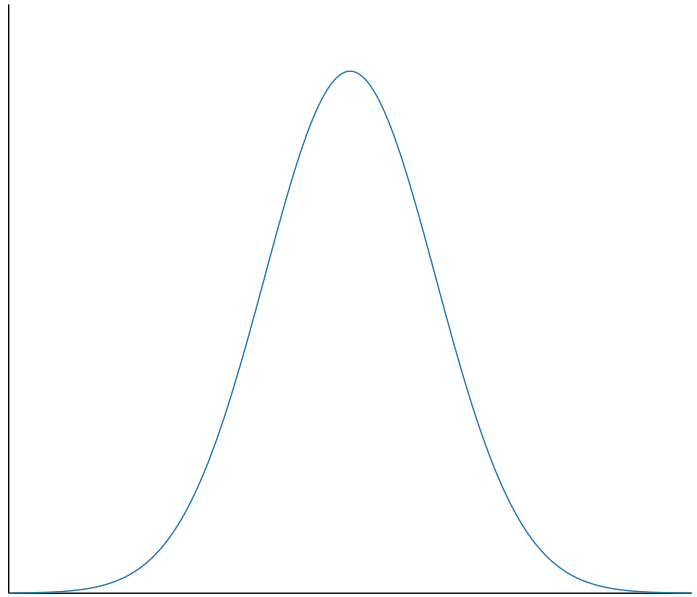
Front Matter

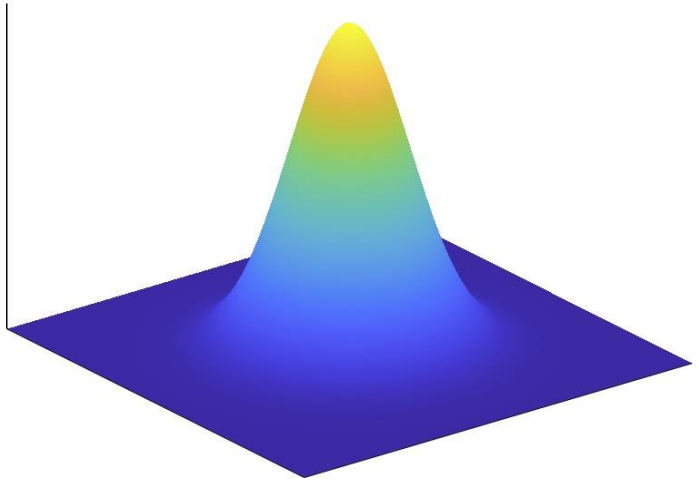
- Announcements
  - HW9 released 4/17, due 4/24 (Thursday) at 11:59 PM
    - **You may only use at most 2 late days on HW9**
  - Exam 3 on 5/1 from 1 PM to 3 PM
    - **We will not use the full 3-hour window**
    - All topics from Lectures 17 to 25 (inclusive) are in-scope, excluding the MLE/MAP portion of Lecture 17
    - Exam 1 and 2 content may be referenced but will not be the primary focus of any question
    - Please watch Piazza carefully for your room and seat assignments
    - You are allowed to bring one letter-size sheet of notes; you may put *whatever* you want on *both sides*

Gaussians

(Univariate) Gaussians:

$$x \sim \mathcal{N}(x; \mu = 0, \sigma^2 = 1)$$





- Multivariate Gaussians:

$$\boldsymbol{x} = [x_1, \ldots, x_D]^T \to \mathbb{R}^D$$

$$\sim \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu} = \mathbf{0}_D, \Sigma = I_D)$$

$\Sigma \to \mathbb{R}^{D \times D}$

covariance matrix

Some fun facts about Gaussians

- Closure under linear transformations:

If $\vec{x} \sim N(\vec{\mu}, \Sigma)$

then $A\vec{x} + \vec{b} \sim N(A\vec{\mu} + \vec{b}, A\Sigma A^T)$

- Closure under addition

If $\vec{x} \sim N(\vec{\mu}, \Sigma)$ follows $\vec{y} \sim N(\vec{m}, S)$

then $\vec{x} + \vec{y} \sim N(\vec{\mu} + \vec{m}, \Sigma + S)$

- Closure under conditioning:

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

then $x_1 \mid x_2 = c \sim N\left(\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(c - \mu_2), \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right)$

Some old friends

Gaussian process =

Bayesian linear regression + Kernels

Some old friends

Gaussian process =

Bayesian linear regression + Kernels

Recall: MAP for Linear Regression

- If we assume a linear model with additive Gaussian noise

$$\boldsymbol{y} = X\boldsymbol{w} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \rightarrow \boldsymbol{y} \sim N(X\boldsymbol{w}, \sigma^2 I_N)$$

and independent identical Gaussian priors on the weights…

why?

$$\boldsymbol{w} \sim N\left(\boldsymbol{w}_{D+1}, \frac{\sigma^2}{\lambda} I_{D+1}\right) \rightarrow p(\boldsymbol{w}) \propto \exp\left(-\frac{1}{2\sigma^2}(\lambda \boldsymbol{w}^T \boldsymbol{w})\right)$$

- … then, the MAP of $\boldsymbol{w}$ is the ridge regression solution!

$$\begin{aligned} \boldsymbol{w}_{MAP} &= \underset{\boldsymbol{w}}{\operatorname{argmin}} (X\boldsymbol{w} - \boldsymbol{y})^T (X\boldsymbol{w} - \boldsymbol{y}) + \lambda \boldsymbol{w}^T \boldsymbol{w} \\ &= (X^T X + \lambda I_{D+1})^{-1} X^T \boldsymbol{y} \end{aligned}$$

Bayesian Linear Regression

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = X\boldsymbol{w} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{w} \sim N(\mathbf{0}_{D+1}, \Sigma)$$

e.g. $\vec{w}$

identity

then,

$$\boldsymbol{y} \sim N(X\mathbf{0}_{D+1} + \mathbf{0}_N = \mathbf{0}_N, X\Sigma X^T + \sigma^2 I_N)$$

Bayesian Linear Regression

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = X\boldsymbol{w} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{w} \sim N(\mathbf{0}_{D+1}, \Sigma)$$

then,

$$\begin{bmatrix} \boldsymbol{w} \\ \boldsymbol{y} \end{bmatrix} \sim N\left(\begin{bmatrix} \mathbf{0}_{D+1} \\ \mathbf{0}_N \end{bmatrix}, \begin{bmatrix} \Sigma & ??? \\ ??? & X\Sigma X^T + \sigma^2 I_N \end{bmatrix}\right)$$

$$\text{Cov}(\vec{w}, \vec{y}) = \text{Cov}(\vec{w}, X\vec{w} + \vec{\epsilon}) = \text{Cov}(\vec{w}, X\vec{w})$$

$$= X\,\text{Cov}(\vec{w}, \vec{w})$$

$$= X\Sigma$$

Bayesian Linear Regression

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = X\boldsymbol{w} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{w} \sim N(\mathbf{0}_{D+1}, \Sigma)$$

then,

$$\begin{bmatrix} \boldsymbol{w} \\ \boldsymbol{y} \end{bmatrix} \sim N\left(\begin{bmatrix} \mathbf{0}_{D+1} \\ \mathbf{0}_N \end{bmatrix}, \begin{bmatrix} \Sigma & X\Sigma \\ X\Sigma & X\Sigma X^T + \sigma^2 I_N \end{bmatrix}\right)$$

Bayesian Linear Regression

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = X\boldsymbol{w} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{w} \sim N(\mathbf{0}_{D+1}, \Sigma)$$

then,

$$\boldsymbol{w} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{POST}, \Sigma_{POST})$$

where

$$\boldsymbol{\mu}_{POST} = \Sigma X^T (X\Sigma X^T + \sigma^2 I_N)^{-1} \boldsymbol{y},$$
$$\Sigma_{POST} = \Sigma - \Sigma X^T (X\Sigma X^T + \sigma^2 I_N)^{-1} X\Sigma$$

Bayesian Linear Regression

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = X\boldsymbol{w} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{w} \sim N(\mathbf{0}_{D+1}, \Sigma)$$

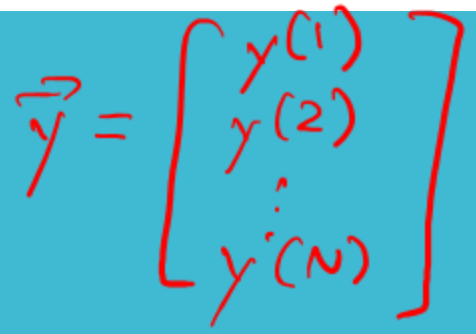
then given a new test data point $\boldsymbol{x}'$, the prediction is

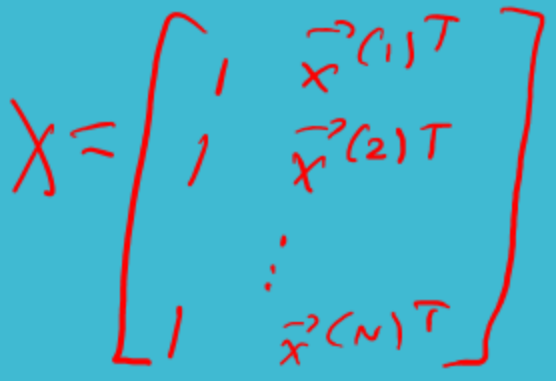
$$y' \mid \boldsymbol{y} = \boldsymbol{x}'^T \boldsymbol{w} \mid \boldsymbol{y} \sim N\left(\boldsymbol{x}'^T \boldsymbol{\mu}_{POST}, \boldsymbol{x}'^T \Sigma_{POST} \boldsymbol{x}'\right)$$

where

$$\boldsymbol{\mu}_{POST} = \Sigma X^T (X\Sigma X^T + \sigma^2 I_N)^{-1} \boldsymbol{y},$$
$$\Sigma_{POST} = \Sigma - \Sigma X^T (X\Sigma X^T + \sigma^2 I_N)^{-1} X\Sigma$$

Bayesian Linear Regression





- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\vec{\boldsymbol{y}} = X\boldsymbol{w} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{w} \sim N(\mathbf{0}_{D+1}, \Sigma)$$

then given a new test data point $\boldsymbol{x}'$, the prediction is

$$y' \mid \boldsymbol{y} = \boldsymbol{x}'^T \boldsymbol{w} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{PRED}, \Sigma_{PRED})$$

where

$$\boldsymbol{\mu}_{PRED} = \boldsymbol{x}'^T \Sigma X^T (X\Sigma X^T + \sigma^2 I_N)^{-1} \boldsymbol{y},$$

$$\Sigma_{PRED} = \boldsymbol{x}'^T \Sigma \boldsymbol{x}' - \boldsymbol{x}'^T \Sigma X^T (X\Sigma X^T + \sigma^2 I_N)^{-1} X\Sigma \boldsymbol{x}'$$

Some old friends

Gaussian process =

Bayesian linear regression + Kernels

Some new friends

Gaussian process =

Bayesian linear regression + Kernels

Bayesian Linear Regression

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = X\boldsymbol{w} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{w} \sim N(\mathbf{0}_{D+1}, \Sigma)$$

then given a new test data point $\boldsymbol{x}'$, the prediction is

$$y' \mid \boldsymbol{y} = \boldsymbol{x}'^T \boldsymbol{w} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{PRED}, \Sigma_{PRED})$$

where

$$\boldsymbol{\mu}_{PRED} = \boldsymbol{x}'^T \Sigma X^T (X\Sigma X^T + \sigma^2 I_N)^{-1} \boldsymbol{y},$$

$$\Sigma_{PRED} = \boldsymbol{x}'^T \Sigma \boldsymbol{x}' - \boldsymbol{x}'^T \Sigma X^T (X\Sigma X^T + \sigma^2 I_N)^{-1} X\Sigma \boldsymbol{x}'$$

Bayesian Non-linear Regression…

$$\Phi = \begin{bmatrix} 1 & \phi(\boldsymbol{x}^{(1)})^T \\ 1 & \phi(\boldsymbol{x}^{(2)})^T \\ \vdots & \vdots \\ 1 & \phi(\boldsymbol{x}^{(N)})^T \end{bmatrix}$$

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = \Phi\boldsymbol{\omega} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{\omega} \sim N(\mathbf{0}_{D'+1}, \Sigma)$$

then given a new test data point $\boldsymbol{x}'$, the prediction is

$$y' \mid \boldsymbol{y} = \phi(\boldsymbol{x}')^T\boldsymbol{\omega} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{PRED}, \Sigma_{PRED})$$

where

$$\boldsymbol{\mu}_{PRED} = \phi(\boldsymbol{x}')^T\Sigma\Phi^T(\Phi\Sigma\Phi^T + \sigma^2 I_N)^{-1}\boldsymbol{y},$$

$$\Sigma_{PRED} = \phi(\boldsymbol{x}')^T\Sigma\phi(\boldsymbol{x}') - \phi(\boldsymbol{x}')^T\Sigma\Phi^T(\Phi\Sigma\Phi^T + \sigma^2 I_N)^{-1}\Phi\Sigma\phi(\boldsymbol{x}')$$

Bayesian Non-linear Regression can be "kernelized"

$$\Phi = \begin{bmatrix} 1 & \phi(\boldsymbol{x}^{(1)})^T \\ 1 & \phi(\boldsymbol{x}^{(2)})^T \\ \vdots & \vdots \\ 1 & \phi(\boldsymbol{x}^{(N)})^T \end{bmatrix}$$

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = \Phi\boldsymbol{\omega} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{\omega} \sim N(\mathbf{0}_{D'+1}, \Sigma)$$

then given a new test data point $\boldsymbol{x}'$, the prediction is

$$y' \mid \boldsymbol{y} = \phi(\boldsymbol{x}')^T\boldsymbol{\omega} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{PRED}, \Sigma_{PRED})$$

where

$$\boldsymbol{\mu}_{PRED} = \phi(\boldsymbol{x}')^T\Sigma\Phi^T(\Phi\Sigma\Phi^T + \sigma^2 I_N)^{-1}\boldsymbol{y},$$

$$\Sigma_{PRED} = \phi(\boldsymbol{x}')^T\Sigma\phi(\boldsymbol{x}') - \phi(\boldsymbol{x}')^T\Sigma\Phi^T(\Phi\Sigma\Phi^T + \sigma^2 I_N)^{-1}\Phi\Sigma\phi(\boldsymbol{x}')$$

- Define a **kernel function** as

$$K(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T\Sigma\phi(\boldsymbol{x}')$$

$K(X, X) = \Phi\Sigma\Phi^T$

Bayesian Linear Regression can be kernelized!

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = \Phi\boldsymbol{\omega} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{\omega} \sim N(\mathbf{0}_{D'+1}, \Sigma)$$

then given a new test data point $\boldsymbol{x}'$, the prediction is

$$y' \mid \boldsymbol{y} = \phi(\boldsymbol{x}')^T\boldsymbol{\omega} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{PRED}, \Sigma_{PRED})$$

where

$$\boldsymbol{\mu}_{PRED} = K(\boldsymbol{x}', X)(K(X, X) + \sigma^2 I_N)^{-1}\boldsymbol{y},$$

$$\Sigma_{PRED} = K(\boldsymbol{x}', \boldsymbol{x}') - K(\boldsymbol{x}', X)(K(X, X) + \sigma^2 I_N)^{-1}K(X, \boldsymbol{x})$$

- Define the kernel function to be

$$K(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T\Sigma\phi(\boldsymbol{x}')$$

Wait, what happened to the weights?

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$\boldsymbol{y} = \Phi\boldsymbol{\omega} + \boldsymbol{\epsilon} \text{ where } \boldsymbol{\epsilon} \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \boldsymbol{\omega} \sim N(\mathbf{0}_{D'+1}, \Sigma)$$

then given a new test data point $\boldsymbol{x}'$, the prediction is

$$y' \mid \boldsymbol{y} = \phi(\boldsymbol{x}')^T\boldsymbol{\omega} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{PRED}, \Sigma_{PRED})$$

where

$$\boldsymbol{\mu}_{PRED} = K(\boldsymbol{x}', X)(K(X, X) + \sigma^2 I_N)^{-1}\boldsymbol{y},$$

$$\Sigma_{PRED} = K(\boldsymbol{x}', \boldsymbol{x}') - K(\boldsymbol{x}', X)(K(X, X) + \sigma^2 I_N)^{-1}K(X, \boldsymbol{x})$$

- Define the kernel function to be

$$K(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T\Sigma\phi(\boldsymbol{x}')$$

Some old friends

Gaussian process =

Bayesian linear regression + Kernels

A new perspective

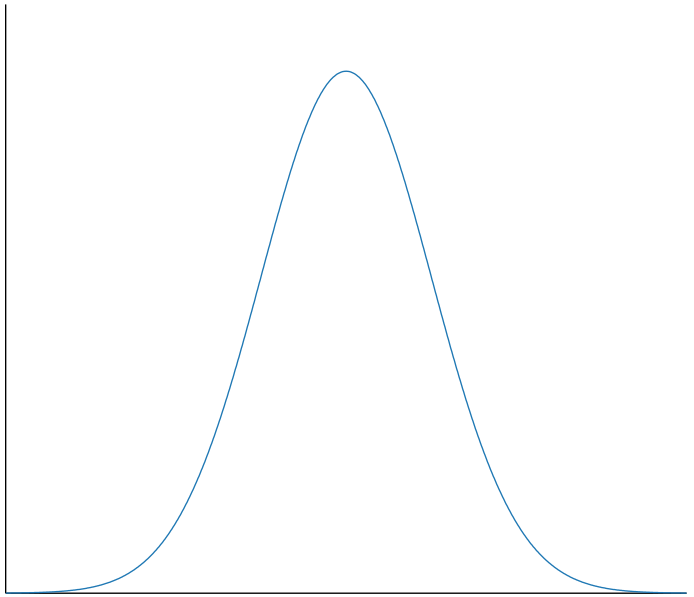
Gaussian process =

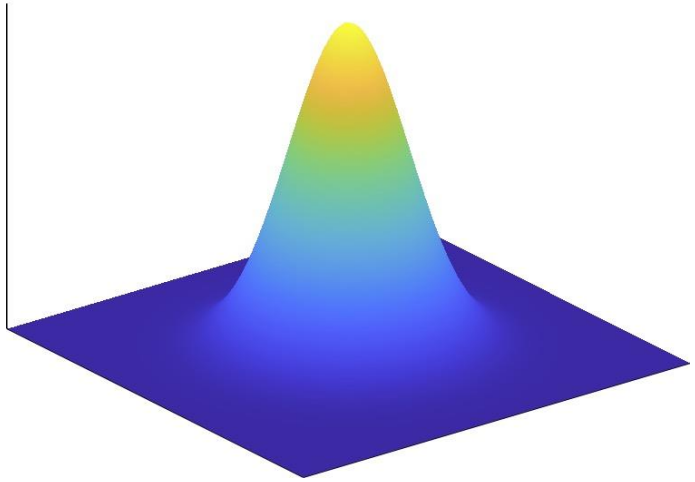
The extension of a Gaussian distribution to functions

Gaussians

- (Univariate) Gaussians:

$$x \sim \mathcal{N}(x; \mu = 0, \sigma^2 = 1)$$





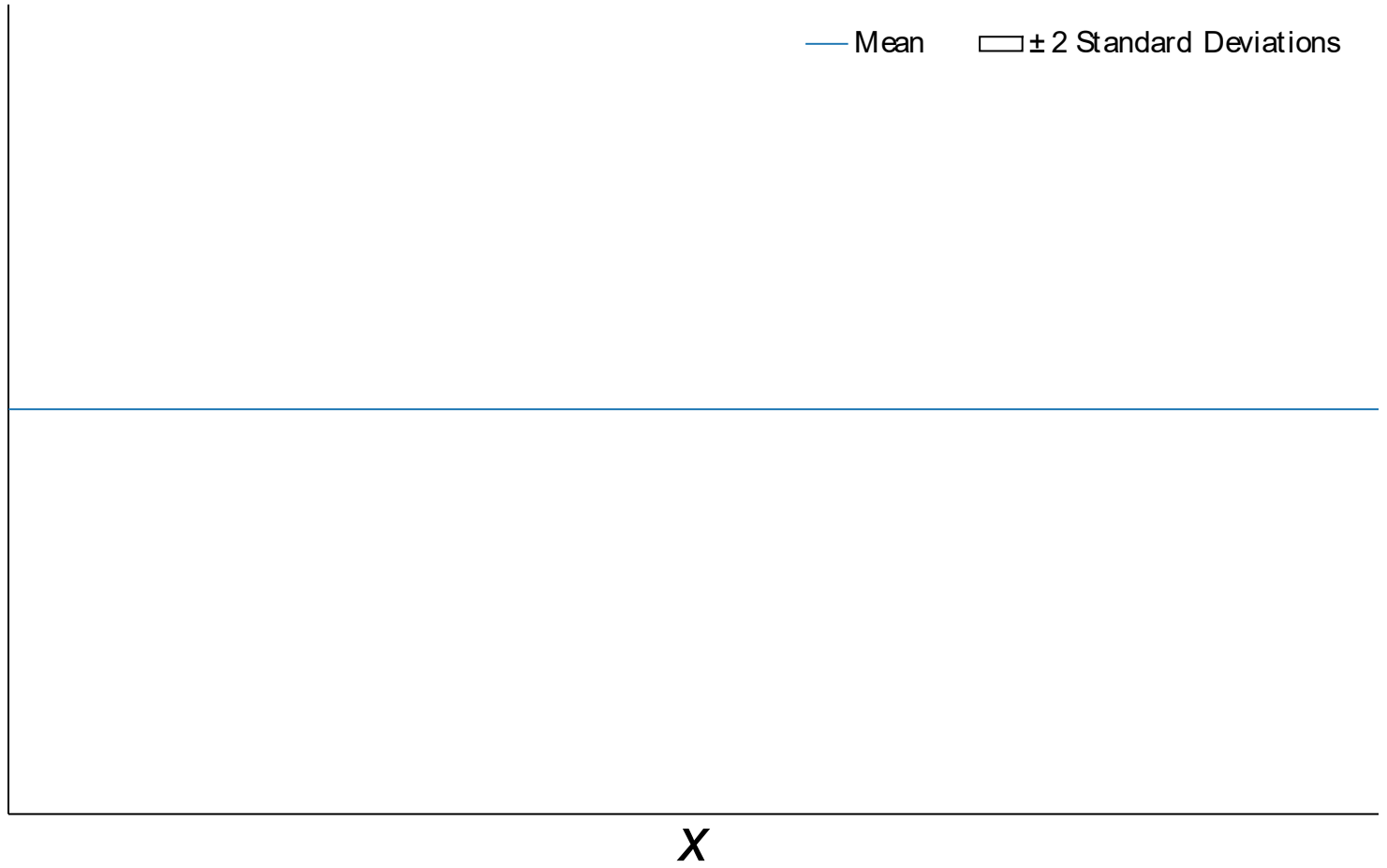
- Multivariate Gaussians:

$$\boldsymbol{x} = [x_1, \ldots, x_D]^T$$

$$\sim \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu} = \mathbf{0}_D, \Sigma = I_D)$$

Gaussian Process (GP)

$$f: \mathbb{R}^p \mapsto \mathbb{R} \sim \mathcal{GP}(f; \mu(x), \Sigma(x, x'))$$

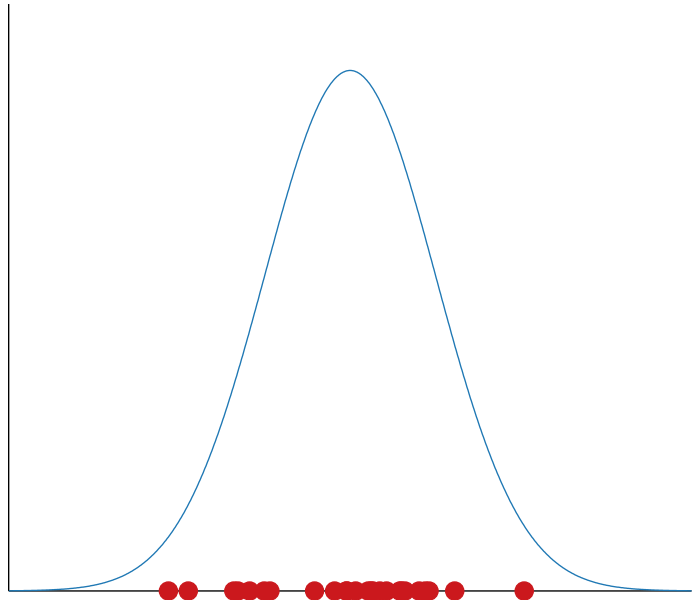


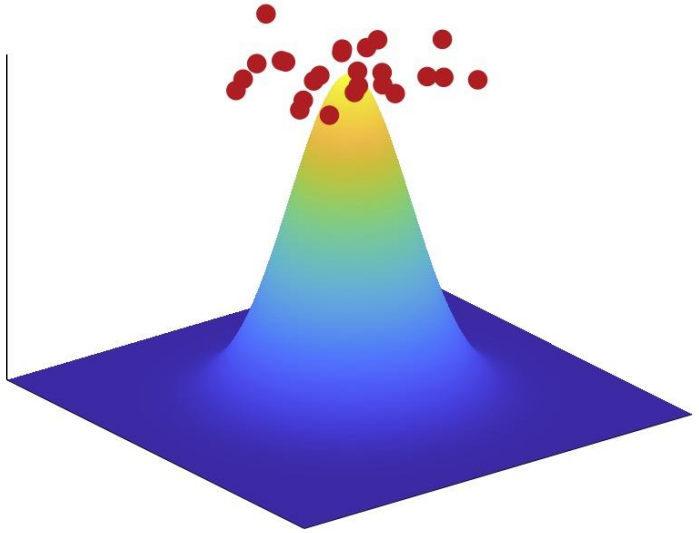
$$f \sim \mathcal{GP}(\mu, \Sigma) \rightarrow f(x) \sim \mathcal{N}\big(\mu(x), \Sigma(x, x)\big)$$

Gaussians

- (Univariate) Gaussians:

$$x \sim \mathcal{N}(x; \mu = 0, \sigma^2 = 1)$$





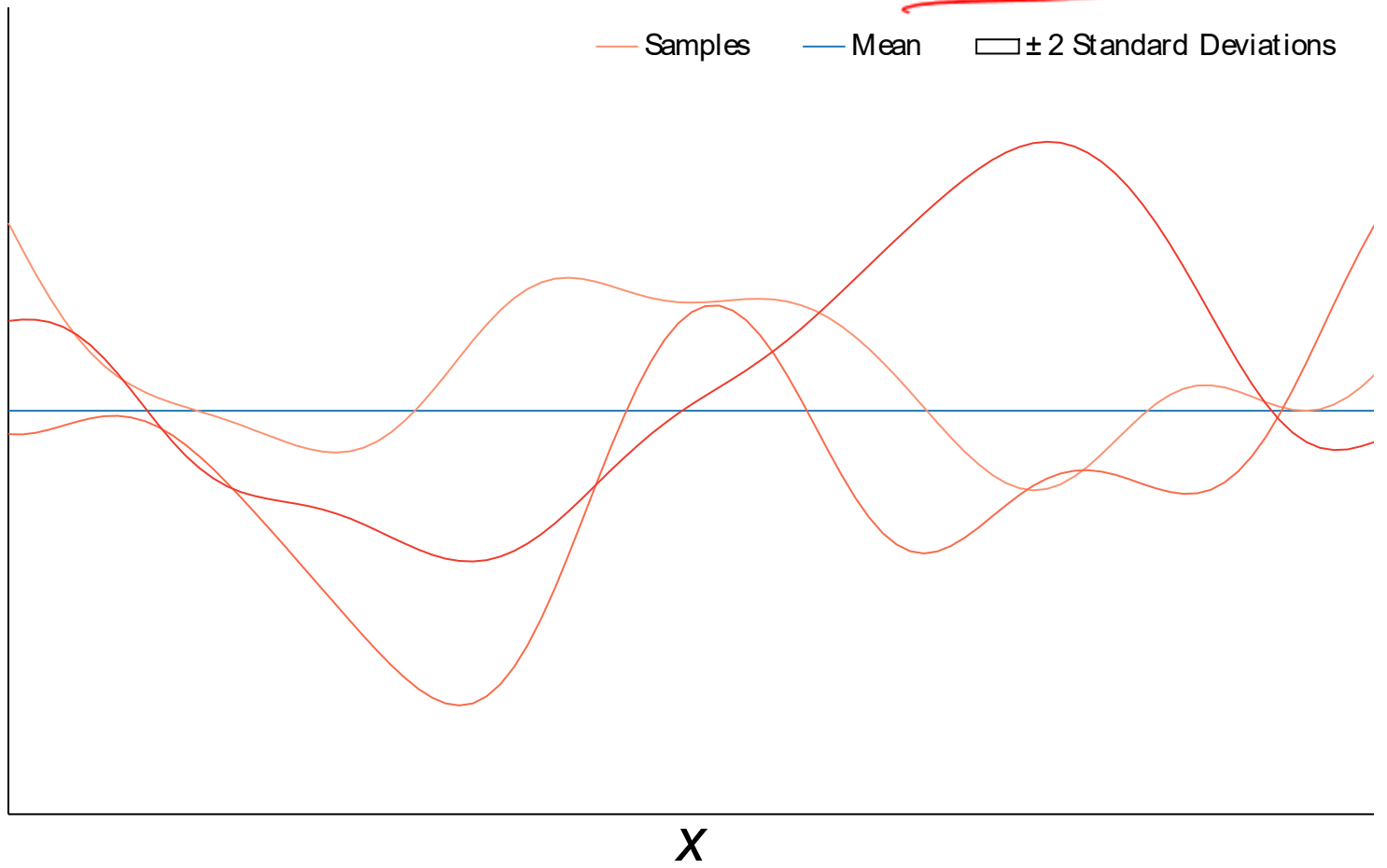
- Multivariate Gaussians:

$$\boldsymbol{x} = [x_1, \ldots, x_D]^T$$

$$\sim \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu} = \mathbf{0}_D, \Sigma = I_D)$$

Gaussian Process (GP)

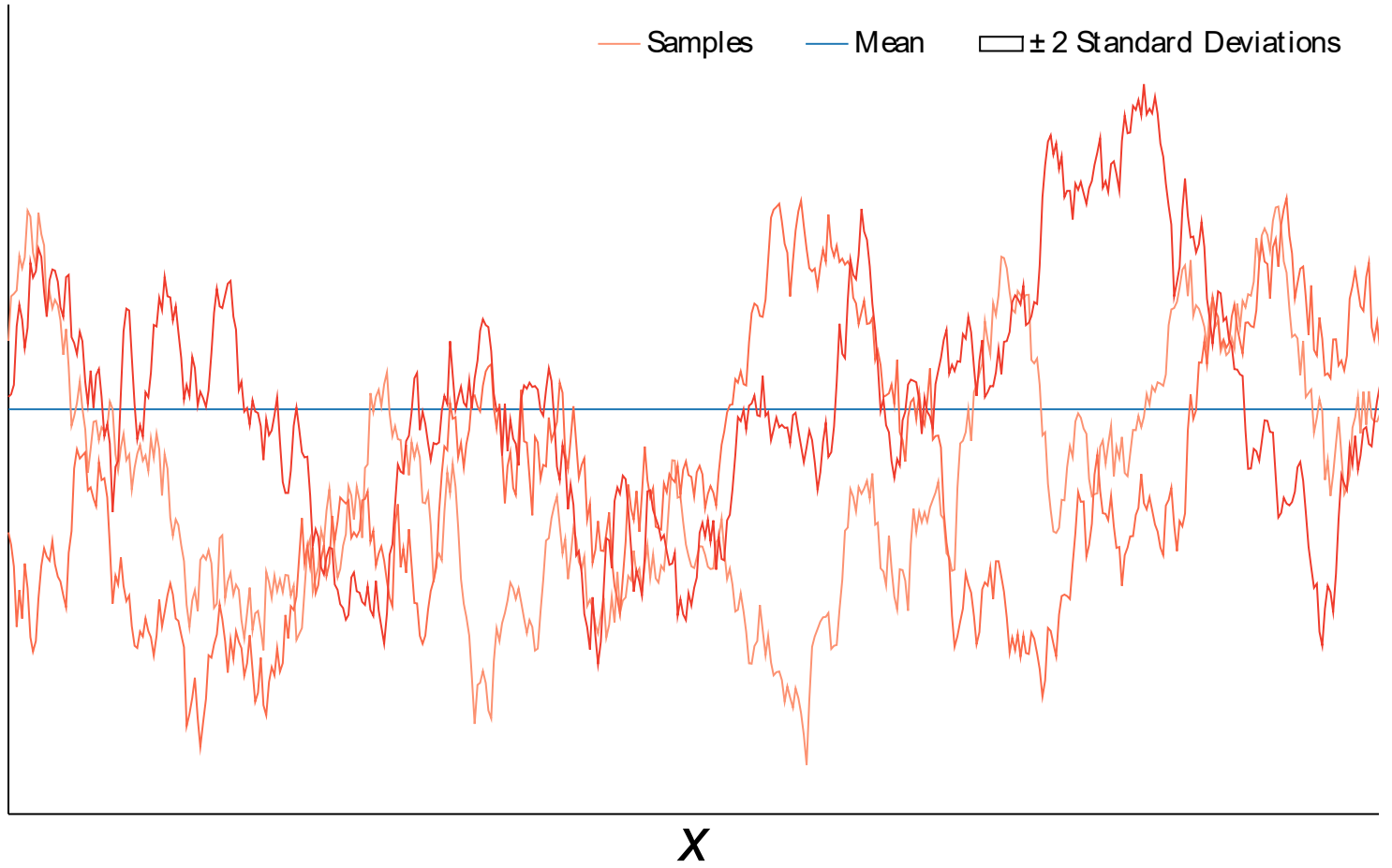
$$f: \mathbb{R}^p \mapsto \mathbb{R} \sim \mathcal{GP}(f; \mu(x) = 0, \Sigma(x, x') = \exp(-(x - x')^2))$$



$$f \sim \mathcal{GP}(\mu, \Sigma) \rightarrow f(x) \sim \mathcal{N}\big(\mu(x), \Sigma(x, x)\big)$$

Gaussian Process (GP)

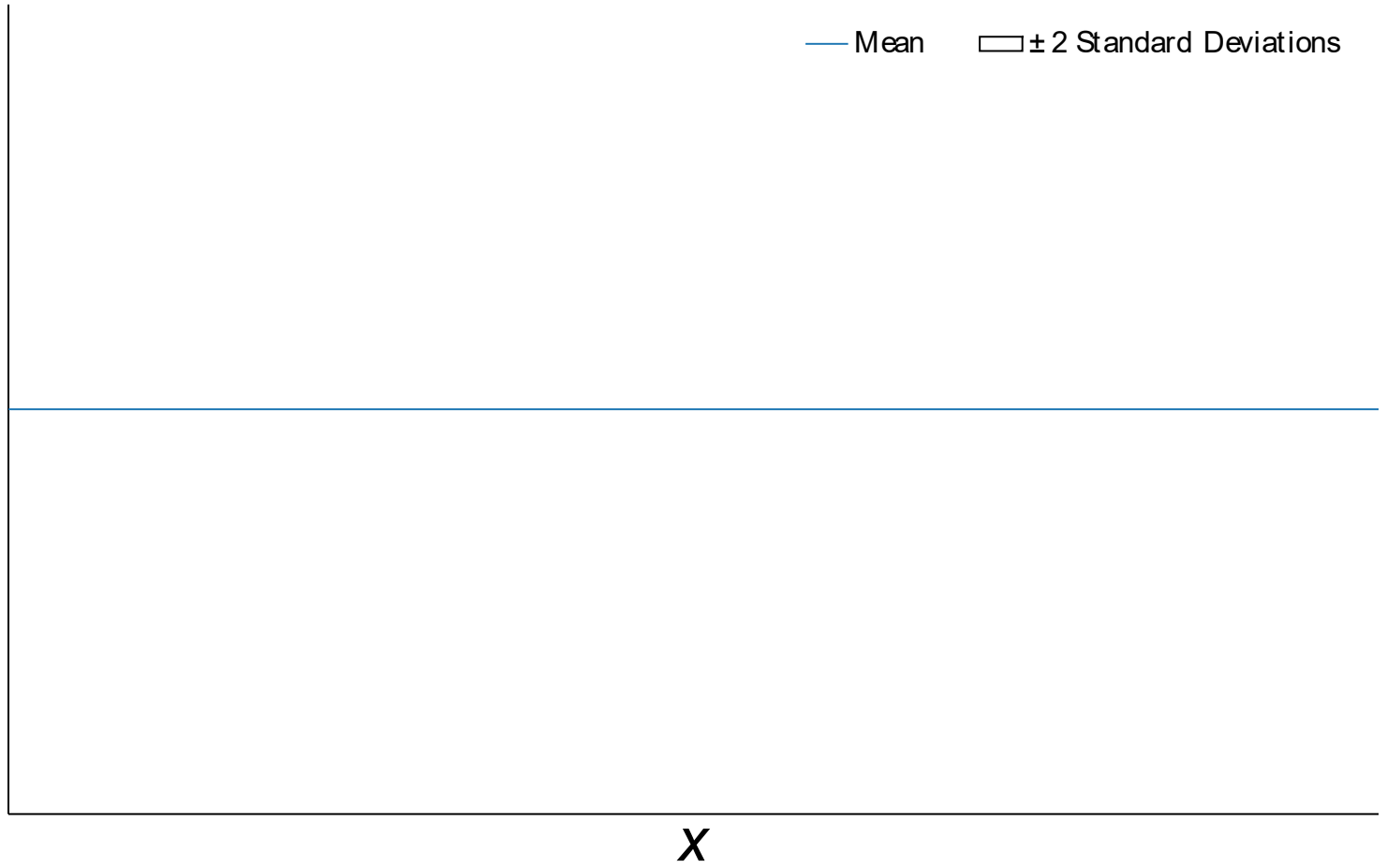
$$f: \mathbb{R}^p \mapsto \mathbb{R} \sim \mathcal{GP}(f; \mu(x) = 0, \Sigma(x, x') = \exp(-|x - x'|))$$



$$f \sim \mathcal{GP}(\mu, \Sigma) \rightarrow f(x) \sim \mathcal{N}\big(\mu(x), \Sigma(x, x)\big)$$

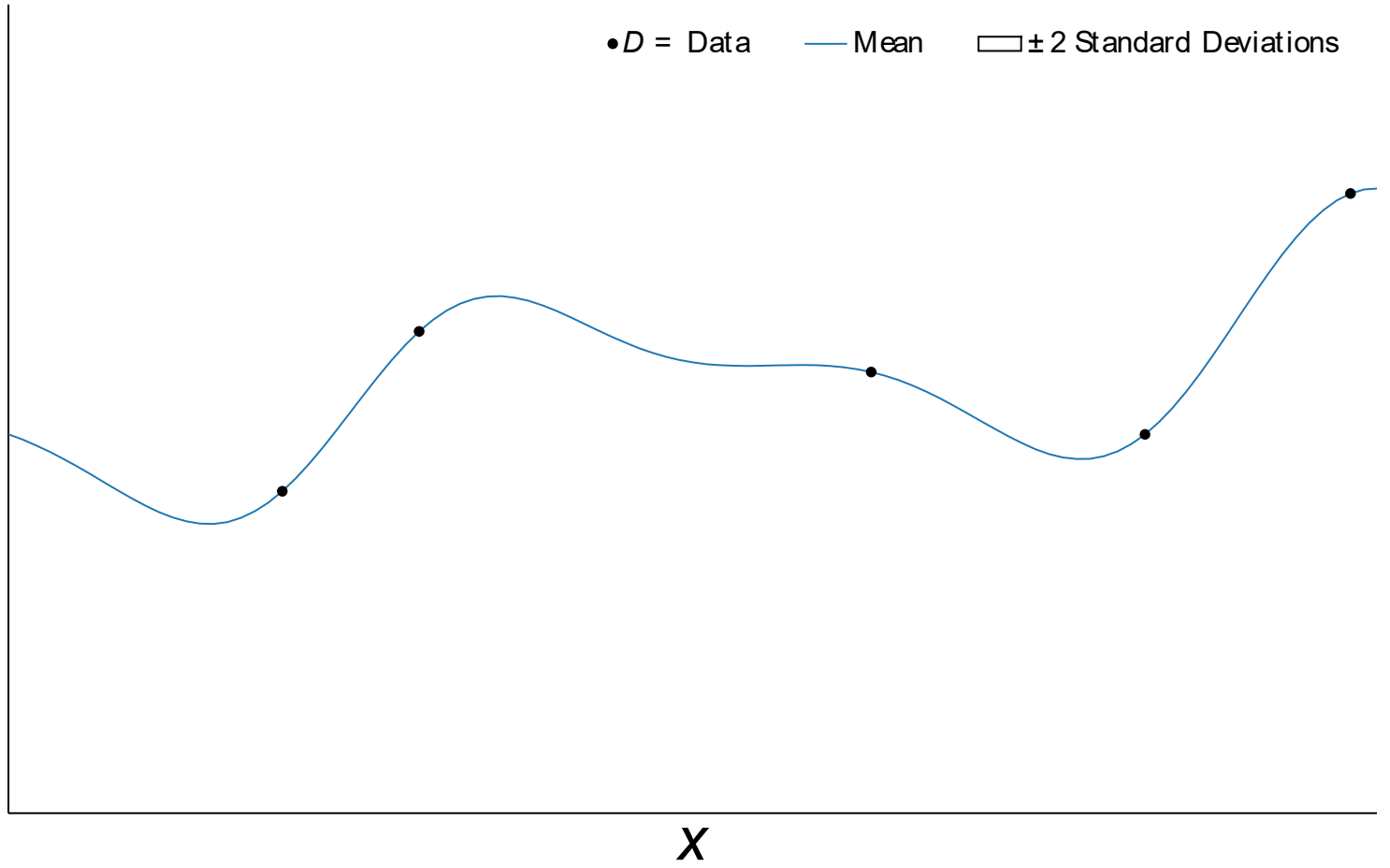
GP Prior

$$f: \mathbb{R}^p \mapsto \mathbb{R} \sim \mathcal{GP}(f; \mu(x) = 0, \Sigma(x, x') = \exp(-(x - x')^2))$$



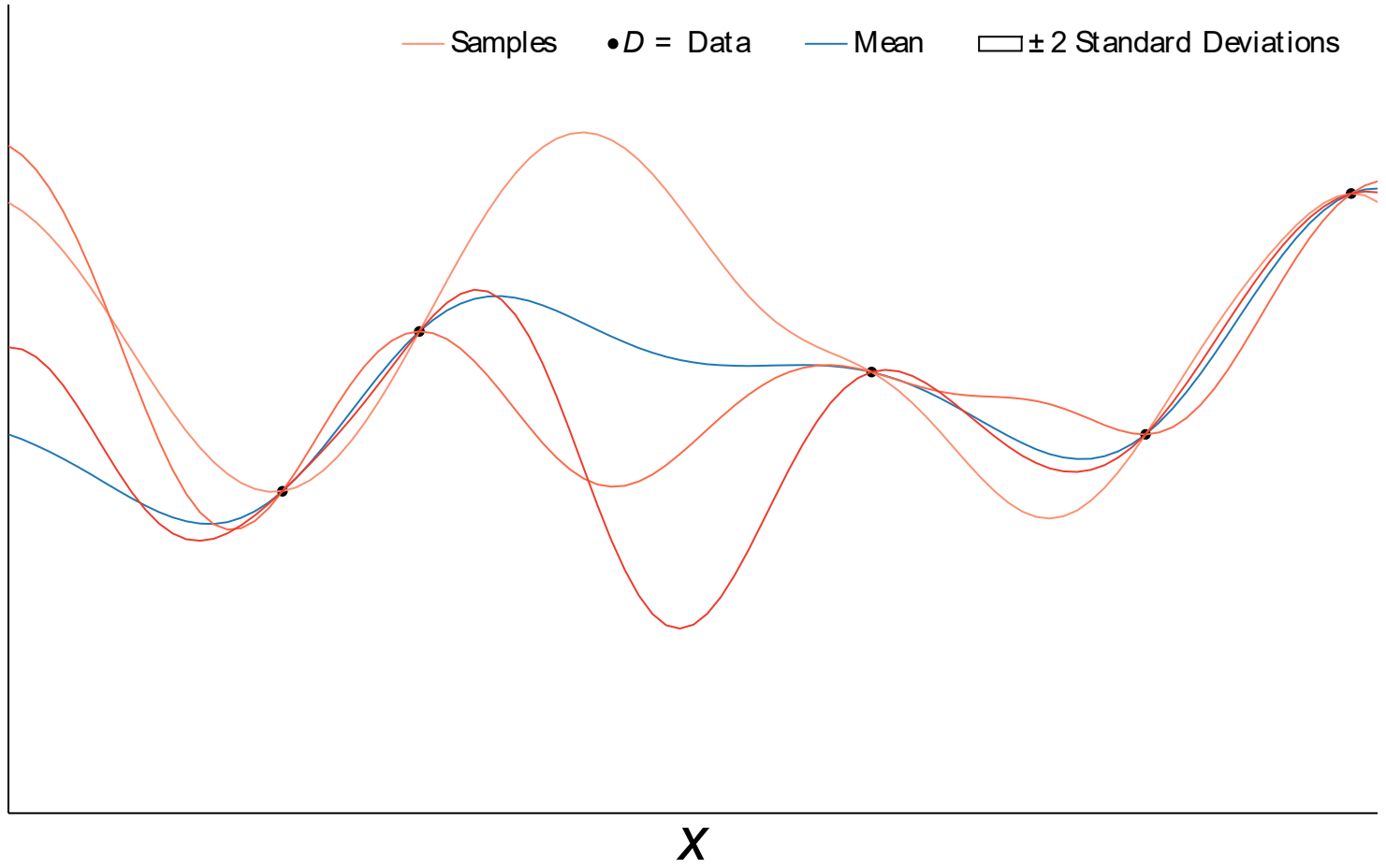
GP Posterior

$$f \mid \mathcal{D} \sim \mathcal{GP}(f; \mu_{\mathcal{D}}, \Sigma_{\mathcal{D}})$$



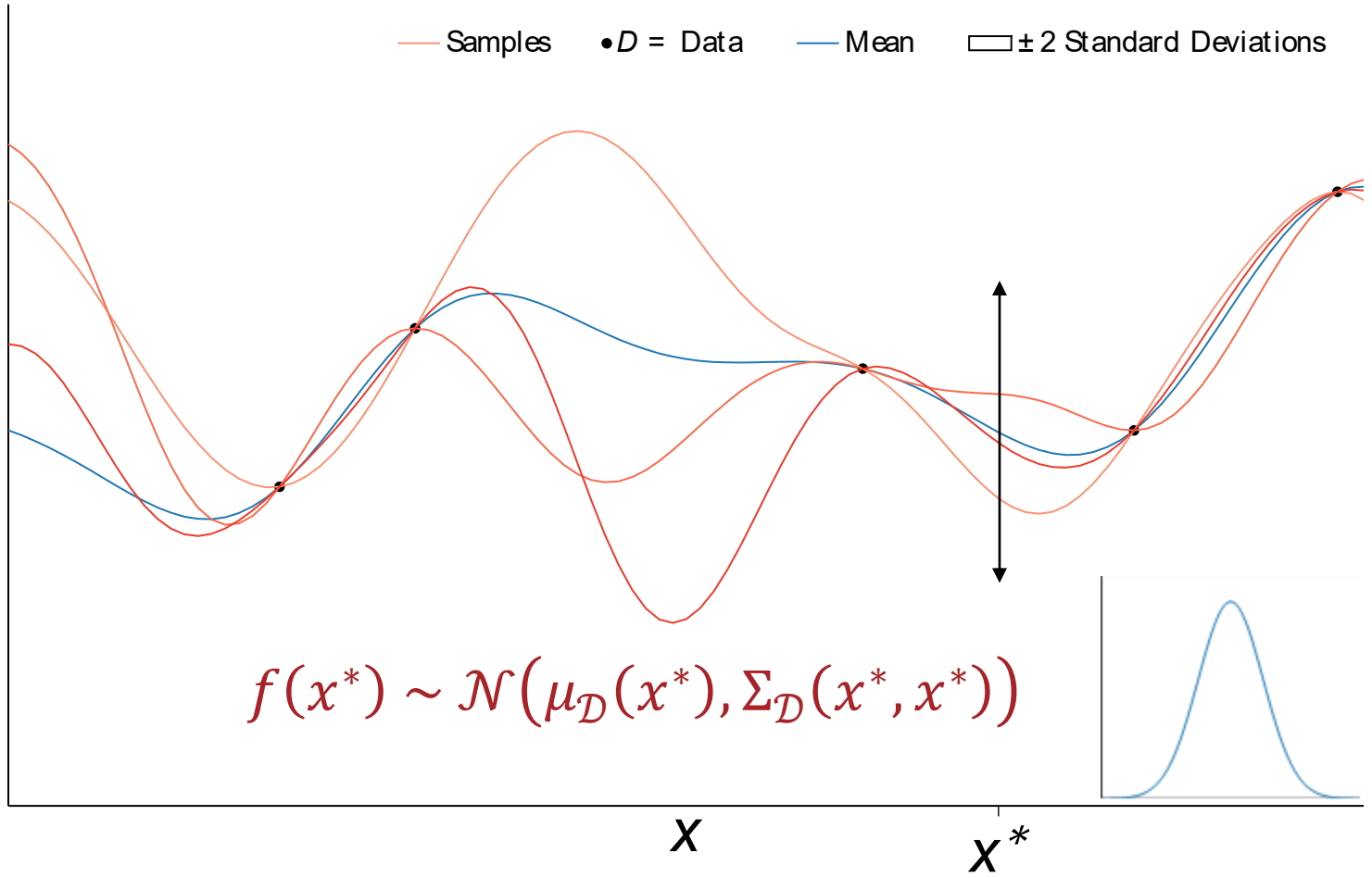
GP Posterior

$$f \mid \mathcal{D} \sim \mathcal{GP}(f; \mu_{\mathcal{D}}, \Sigma_{\mathcal{D}})$$

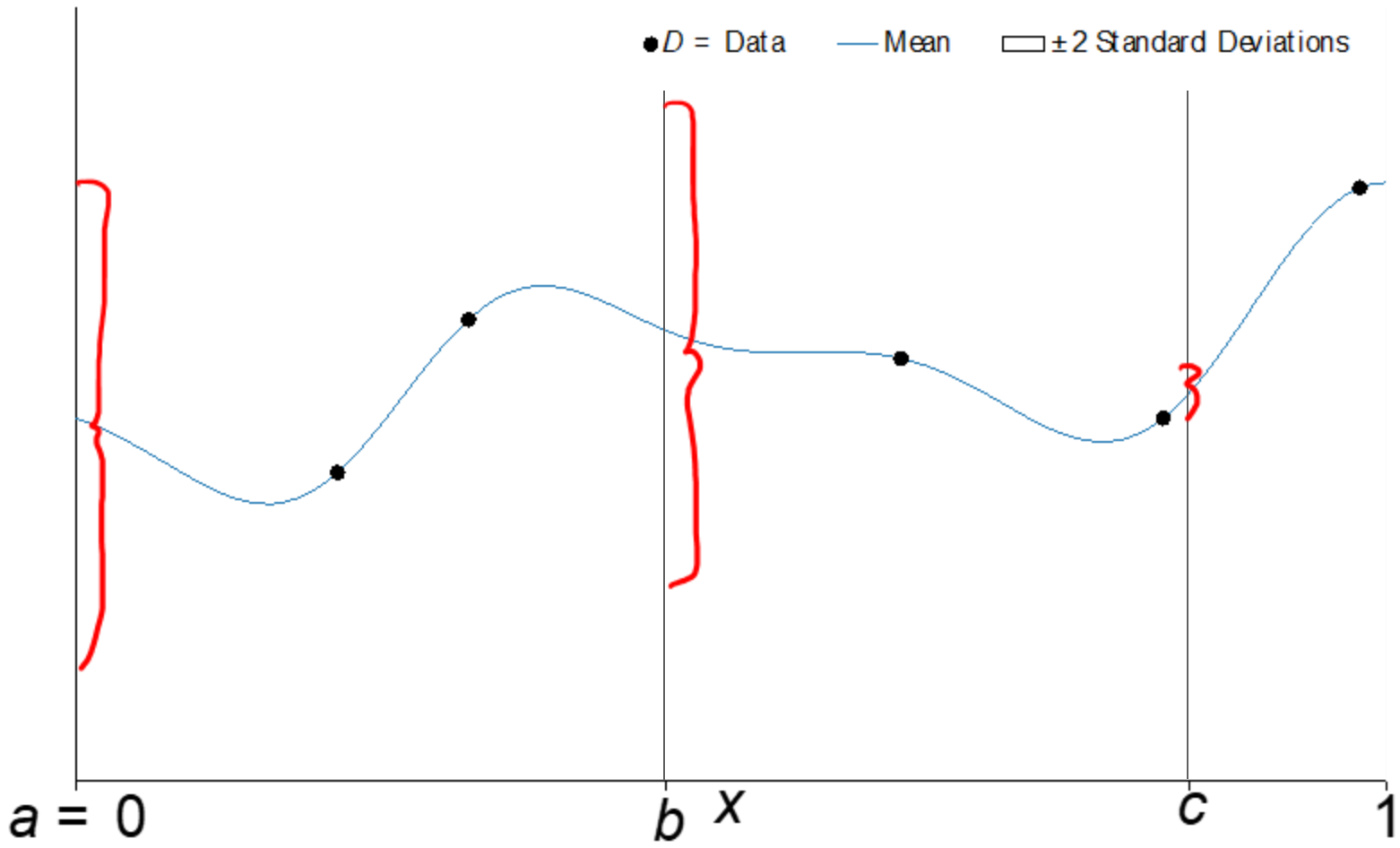


GP Posterior

$$f \mid \mathcal{D} \sim \mathcal{GP}(f; \mu_{\mathcal{D}}, \Sigma_{\mathcal{D}})$$

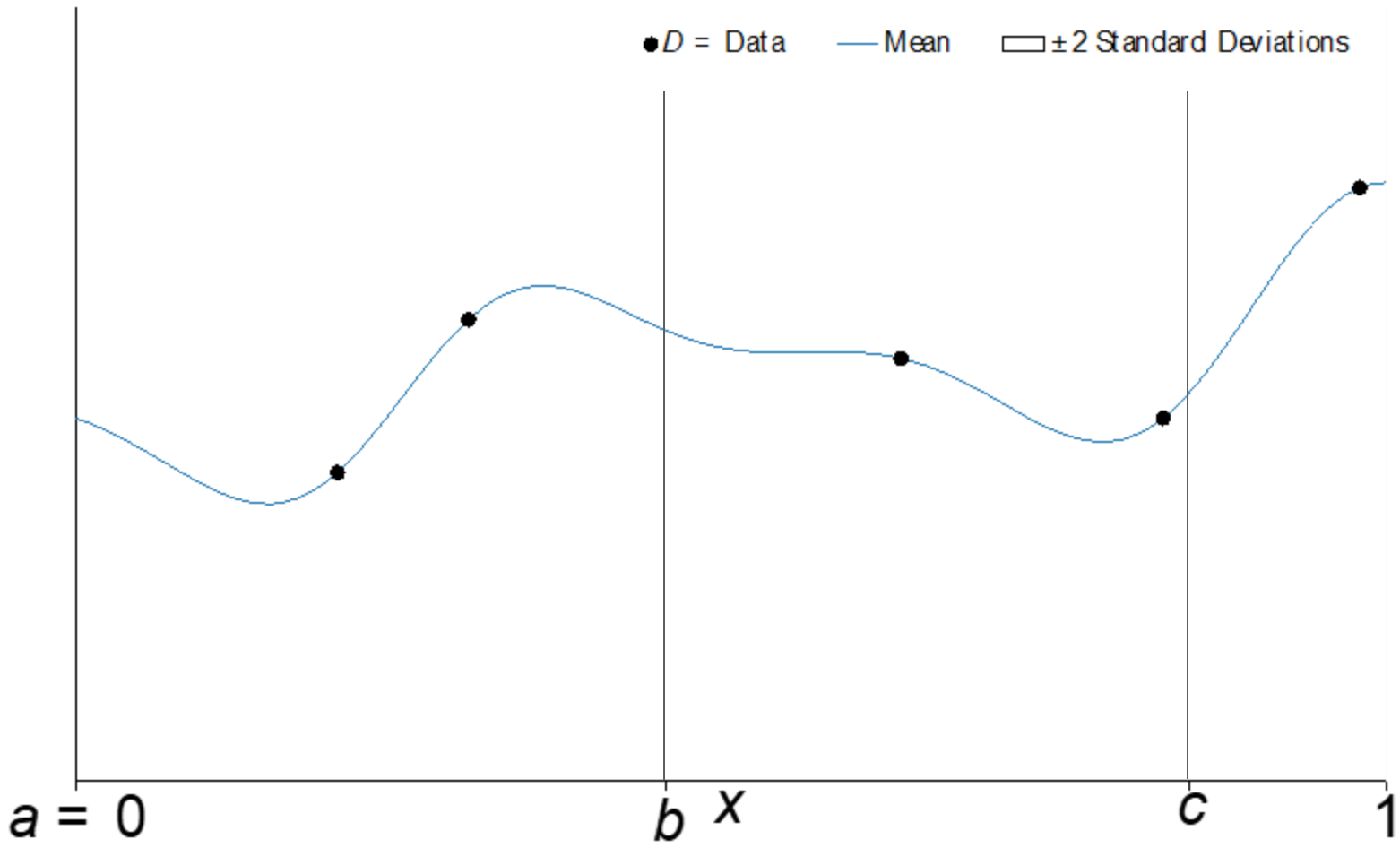


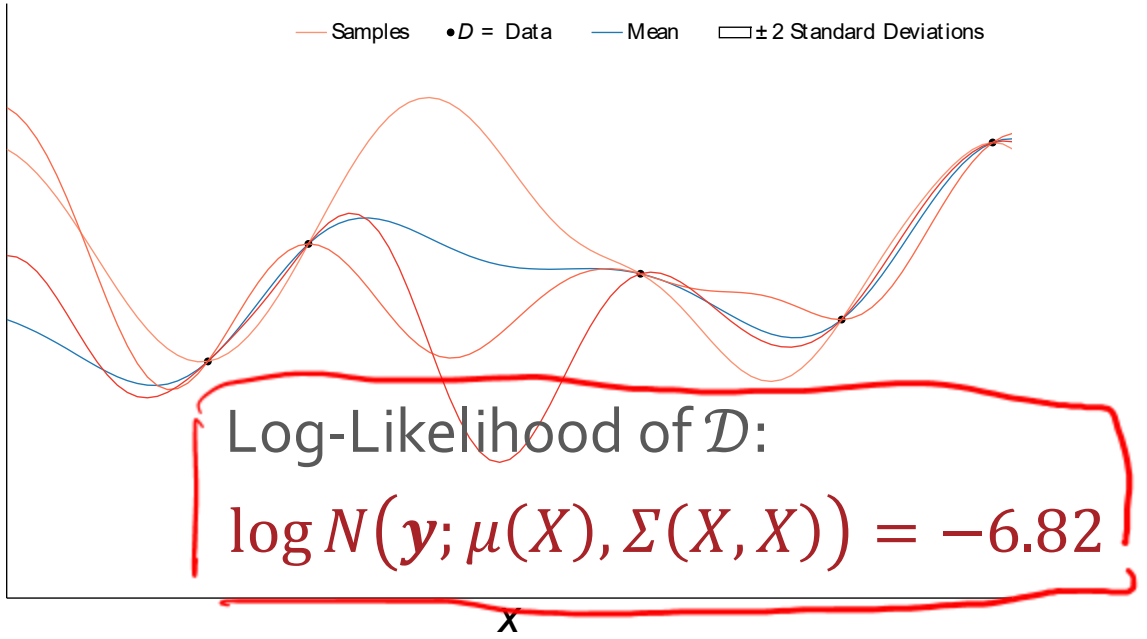
Active Learning

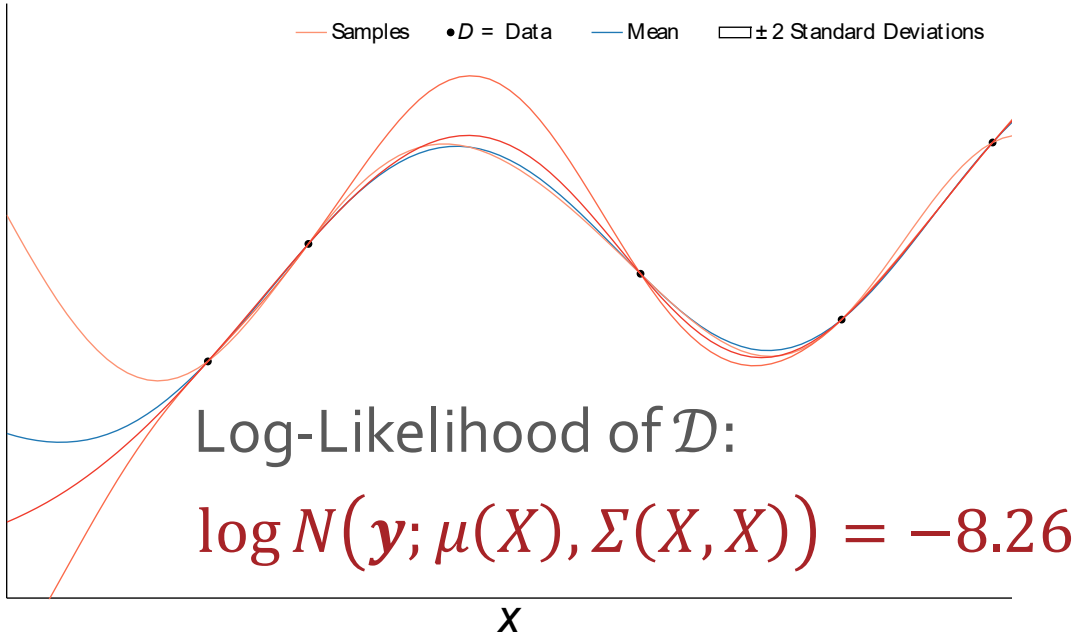


Suppose you can add one data point to your training dataset.

Which value of x would you add and why?





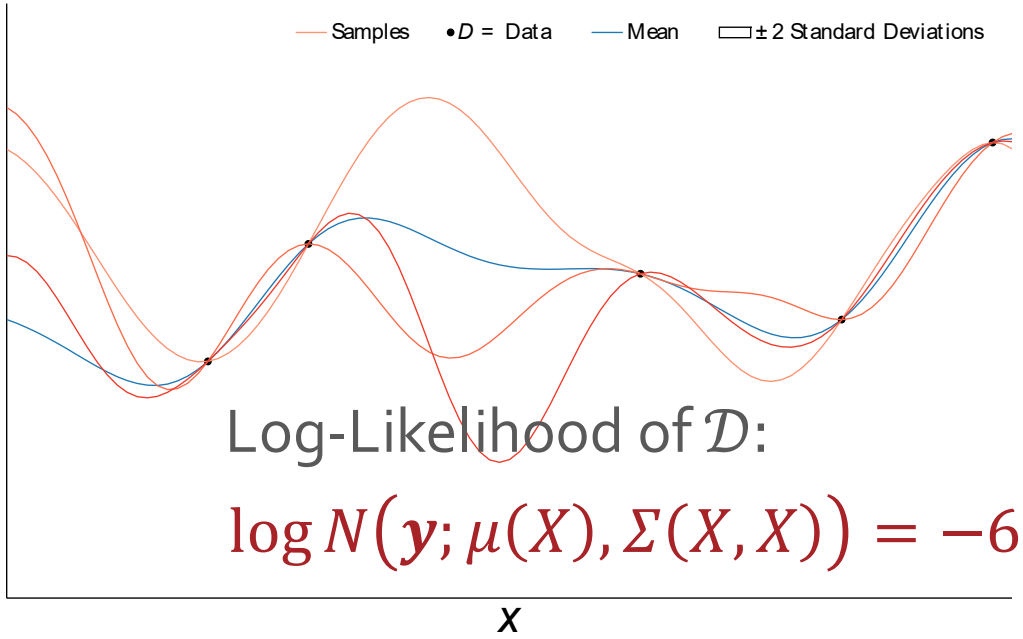


$$f \sim \mathcal{GP}\left(f;\ 0, (1^2)\exp\left(-\frac{(x-x')^2}{1^2}\right)\right)$$

$$f \sim \mathcal{GP}\left(f;\ 0, (2^2)\exp\left(-\frac{(x-x')^2}{2^2}\right)\right)$$

Kernel Hyperparameters

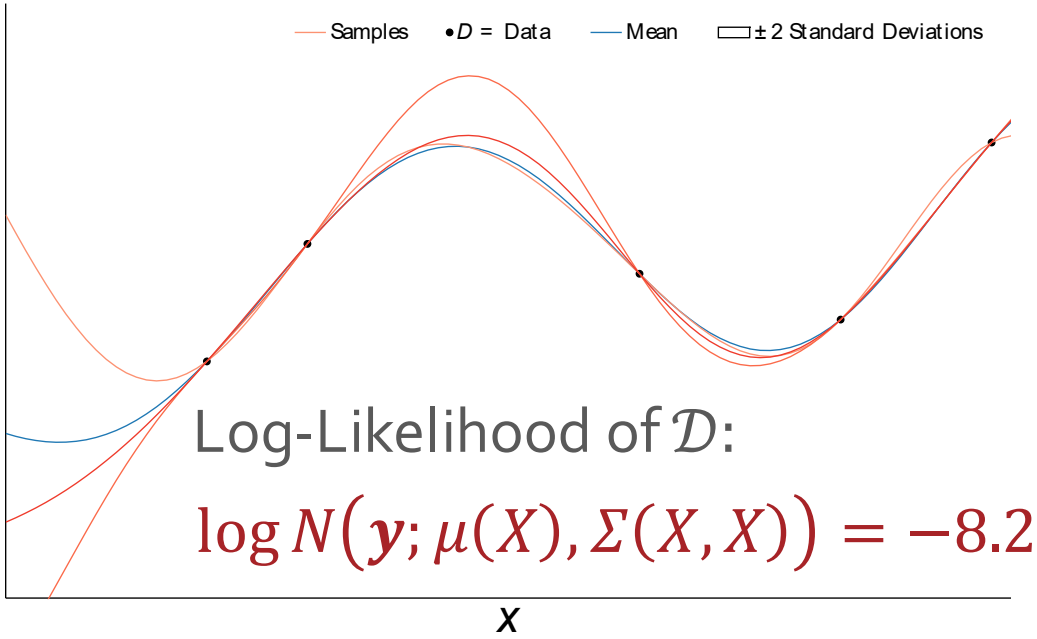
- Can be set via MLE
- As long as μ and Σ are differentiable, the log-likelihood is differentiable with respect to the kernel hyperparameters



Log-Likelihood of $\mathcal{D}$:

$$\log N\left(\boldsymbol{y}; \mu(X), \Sigma(X,X)\right) = -6.82$$

$$f \sim \mathcal{GP}\left(f;\ 0, (1^2)\exp\left(-\frac{(x-x')^2}{1^2}\right)\right)$$



Log-Likelihood of $\mathcal{D}$:

$$\log N\left(\boldsymbol{y}; \mu(X), \Sigma(X,X)\right) = -8.26$$

$$f \sim \mathcal{GP}\left(f;\ 0, (2^2)\exp\left(-\frac{(x-x')^2}{2^2}\right)\right)$$

Wait doesn't this always get zero training error???

Noise

- Assume a linear model with additive Gaussian noise and a zero-mean Gaussian prior on the weights:

$$y = \Phi\omega + \epsilon \text{ where } \epsilon \sim N(\mathbf{0}_N, \sigma^2 I_N) \text{ and } \omega \sim N(\mathbf{0}_{D'+1}, \Sigma)$$

then given a new test data point x', the prediction is

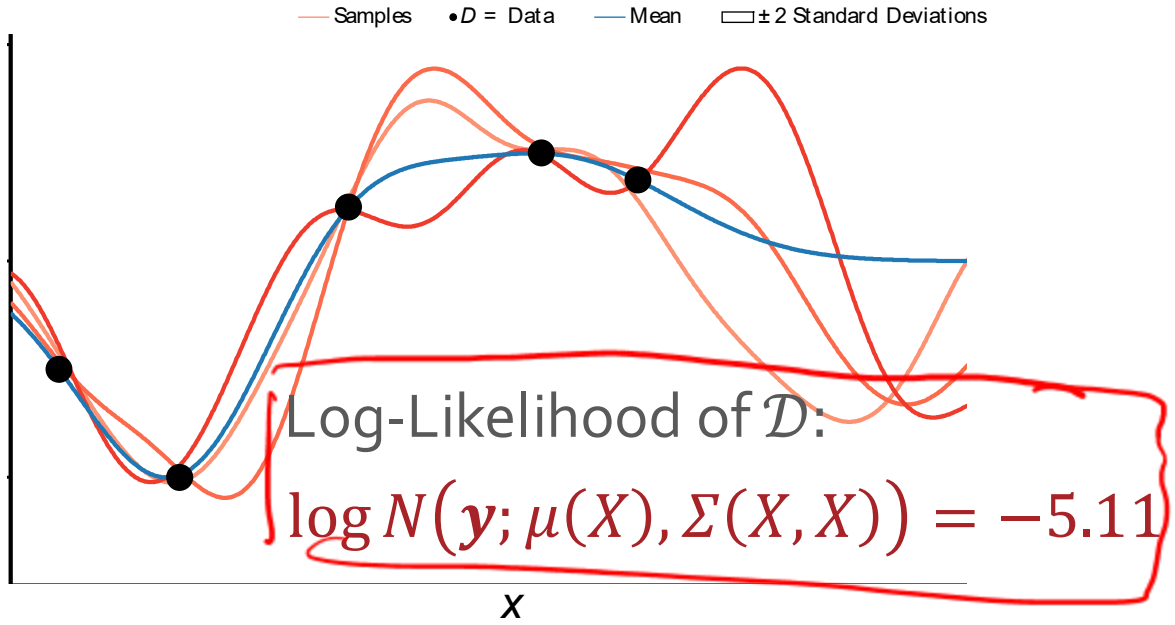
$$y' \mid y = \phi(x')^T \omega \mid y \sim N(\mu_{PRED}, \Sigma_{PRED})$$

where

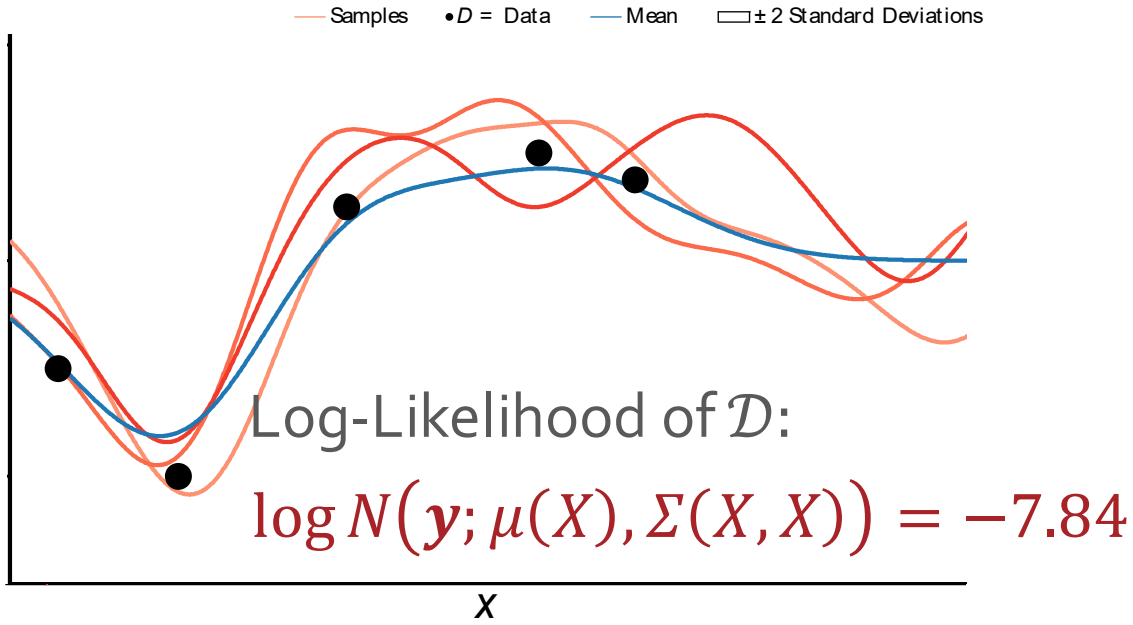
$$\mu_{PRED} = K(x', X)(K(X, X) + \sigma^2 I_N)^{-1} y,$$

$$\Sigma_{PRED} = K(x', x') - K(x', X)(K(X, X) + \sigma^2 I_N)^{-1} K(X, x)$$

- σ^2 is another hyperparameter we can tune
  - $\sigma^2 = 0$ is a noiseless fit: the mean will always pass through the observations exactly; $\sigma^2 > 0$ allows for deviations



$\sigma^2 = 0.1$



$\sigma^2 = 0.5$

Noise