UNIVERSITY OF CAMBRIDGE

Machine Learning and the Physical World

Lecture 3 : Gaussian Processes

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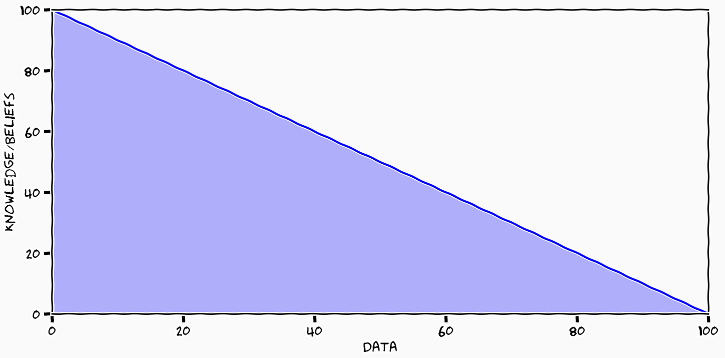
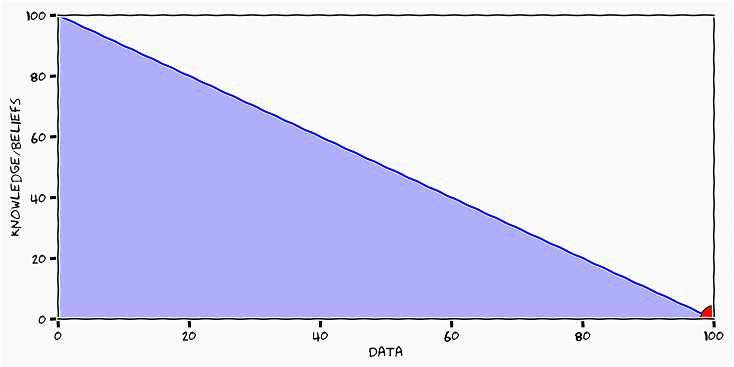
15th of October, 2020

http://carlhenrik.com

Data and Knowledge



Data and Knowledge



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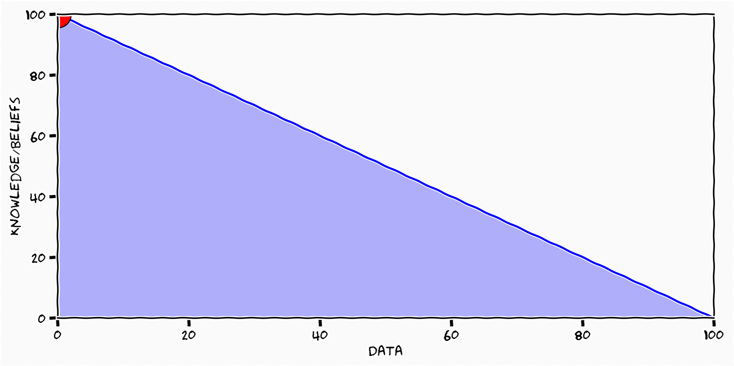

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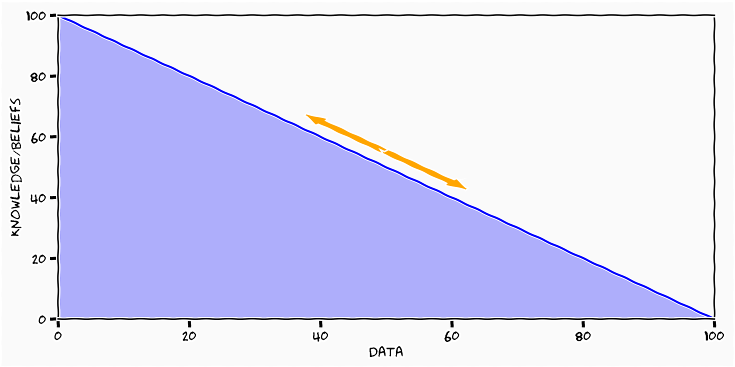

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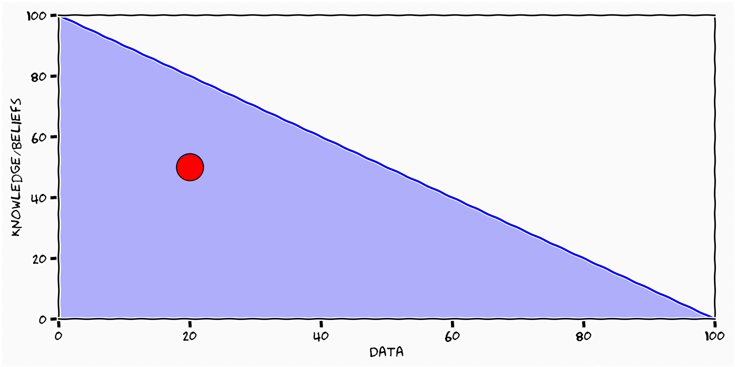

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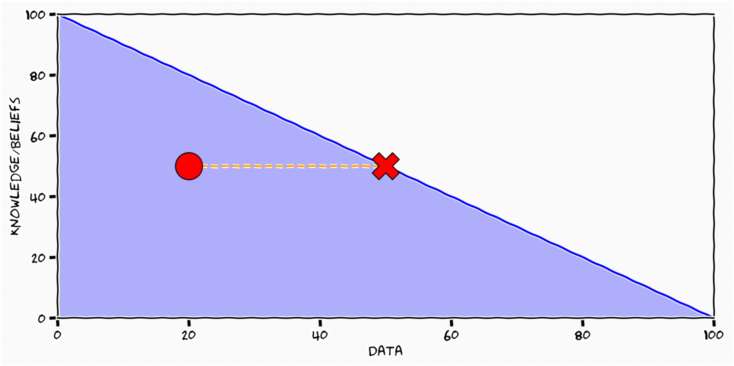

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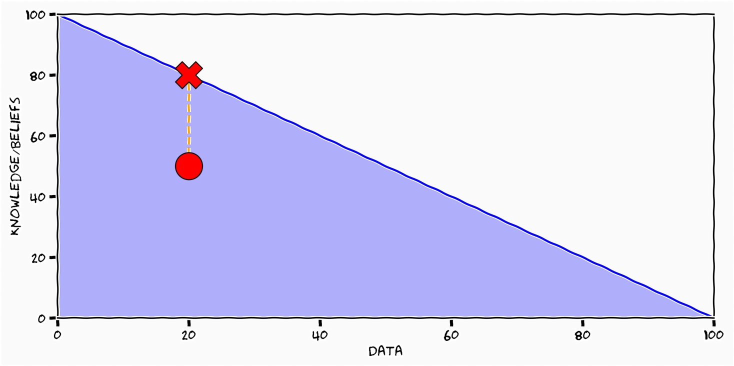

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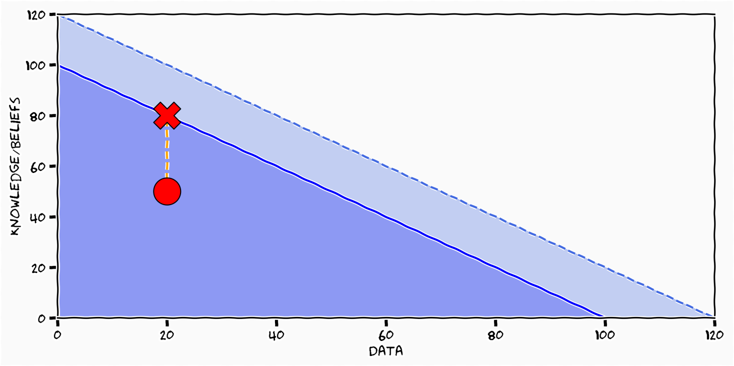

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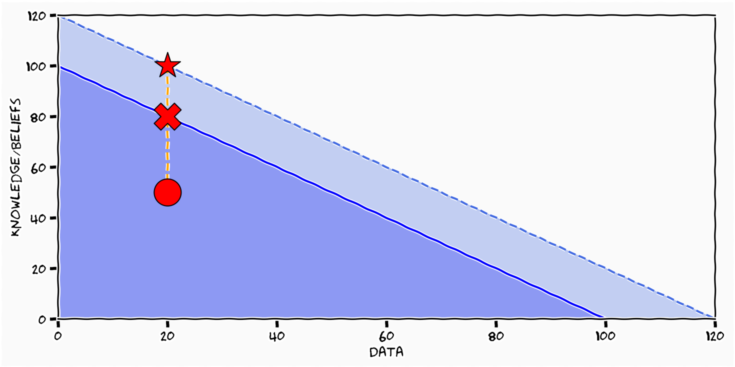
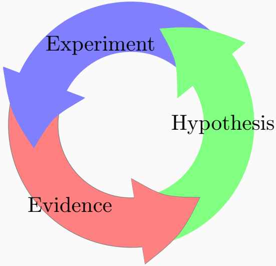
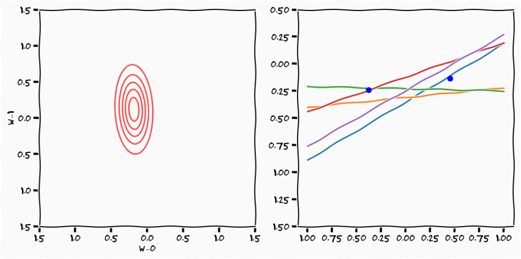


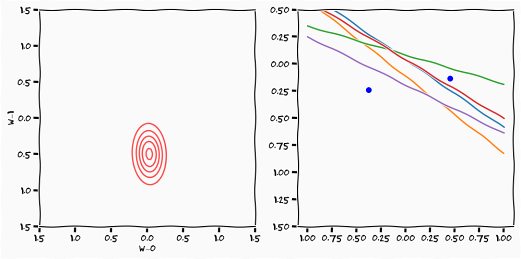
The Scientific Principle



$$p(\theta \mid y) = \frac{p(y \mid \theta)p(\theta)}{\int p(y \mid \theta)p(\theta)\mathrm{d}\theta}$$

Knowledge is Relative





We must speak our minds openly, debate our disagreements honestly, but always pursue solidarity.

The leader of the free world

Machine Learning

- Machine Learning as a Framework

$$\text{Data} + \text{Model} \overbrace{\rightarrow}^{Compute} \text{Prediction}$$

Machine Learning

- Machine Learning as a Framework

$$\text{Data} + \text{Model} \overbrace{\rightarrow}^{Compute} \text{Prediction}$$

- Machine Learning as a Science
    - how to construct "handles" to allow us to input knowledge

Today

- How to specify beliefs over larger classes of hypothesis

Today

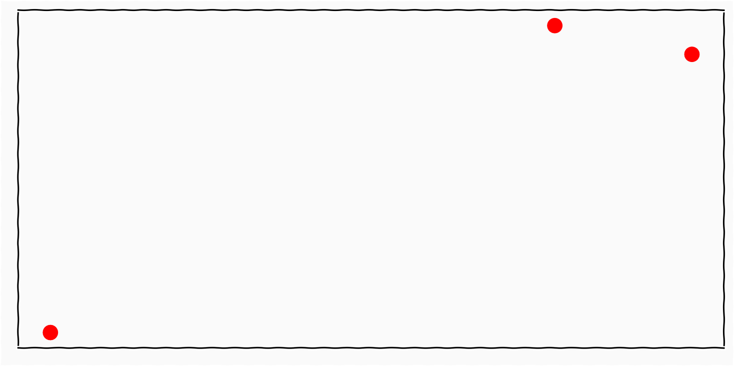
- How to specify beliefs over larger classes of hypothesis
- Non-parametrics

Today

- How to specify beliefs over larger classes of hypothesis
- Non-parametrics
- Gaussian processes

Non-parametrics

Hypothesis Classes

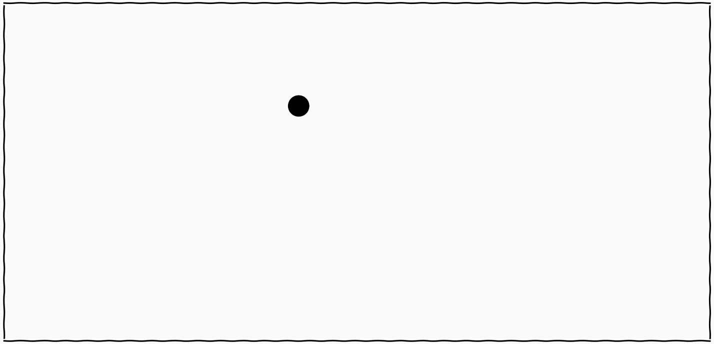


Non-parametrics

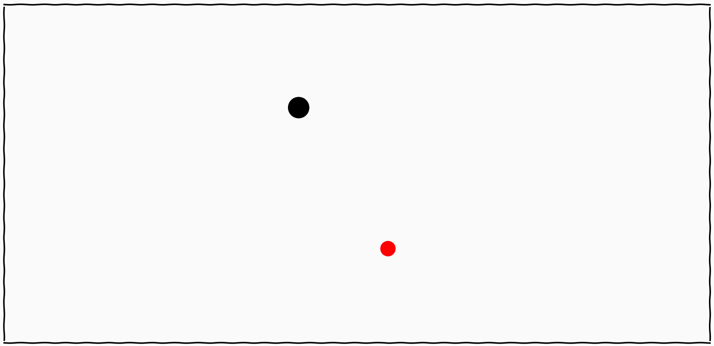
Non-parametrics

Non-parametrics

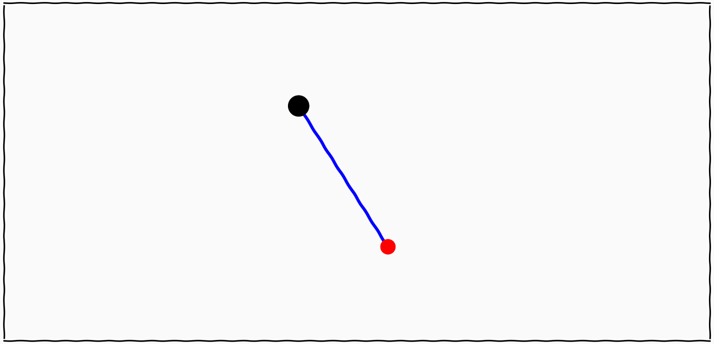
Example



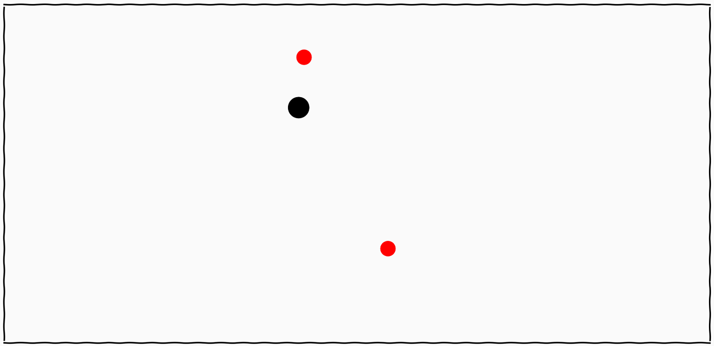
Example



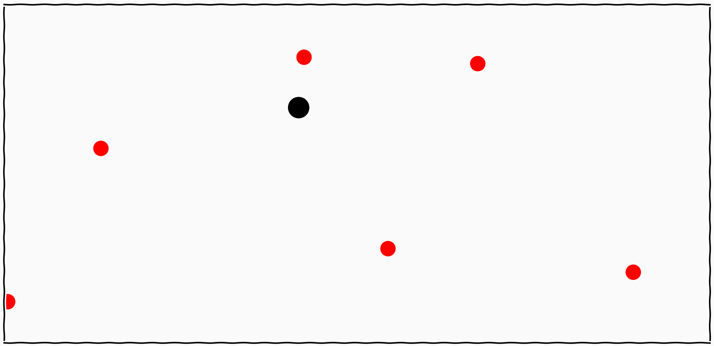
Example



Example



Example



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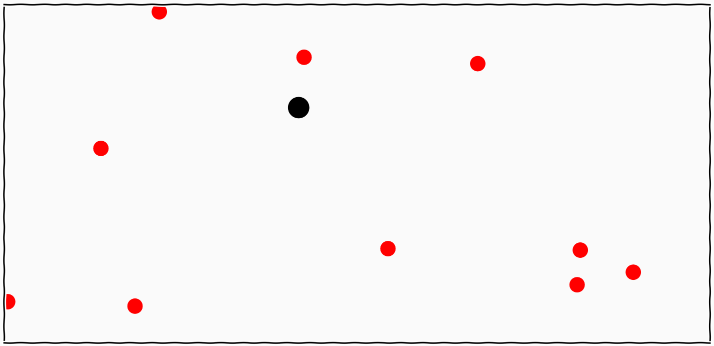
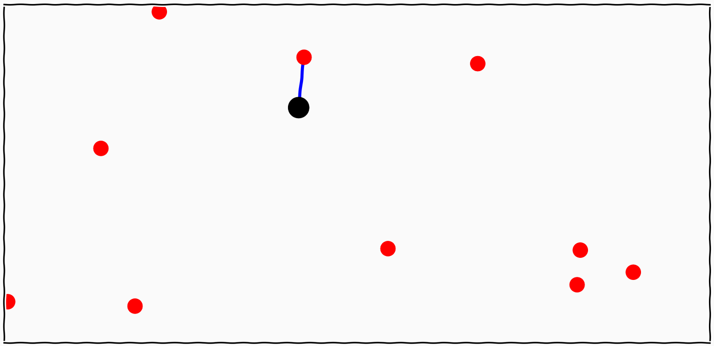
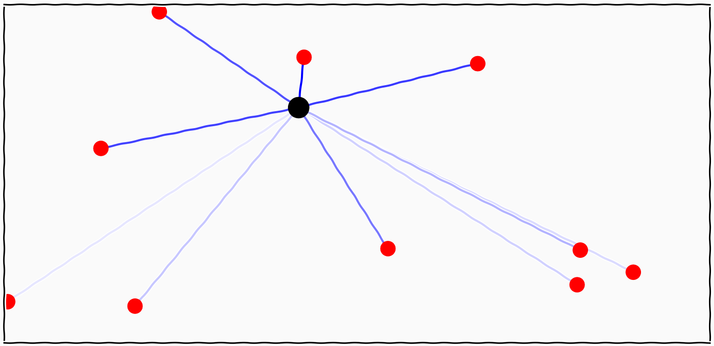


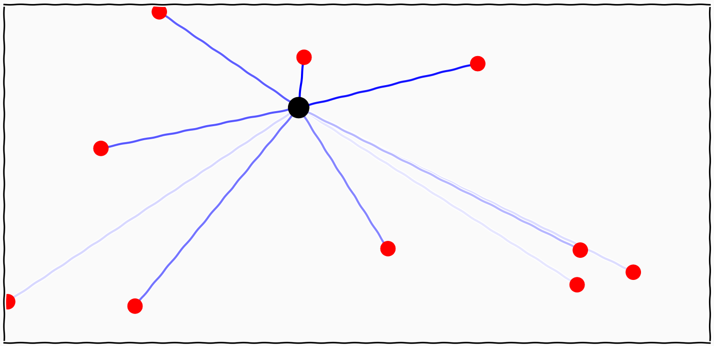
Example



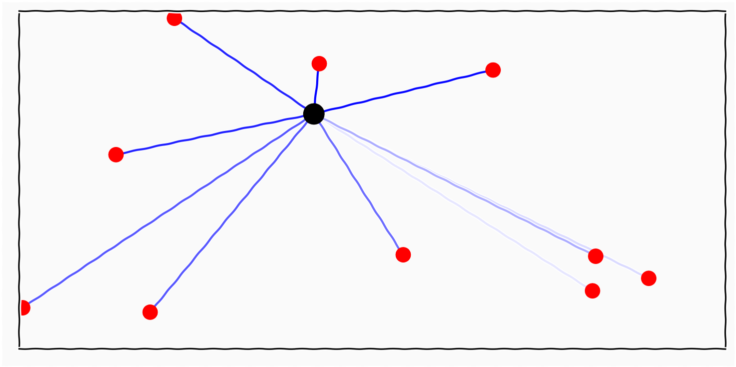
Example



Example

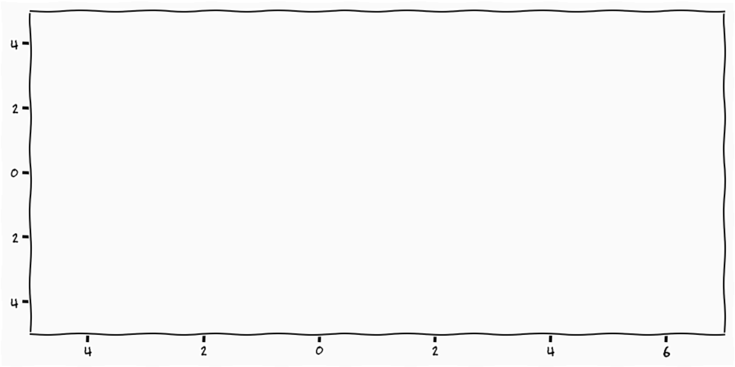


Example



Non-parametric Functions

Lets talk about functions



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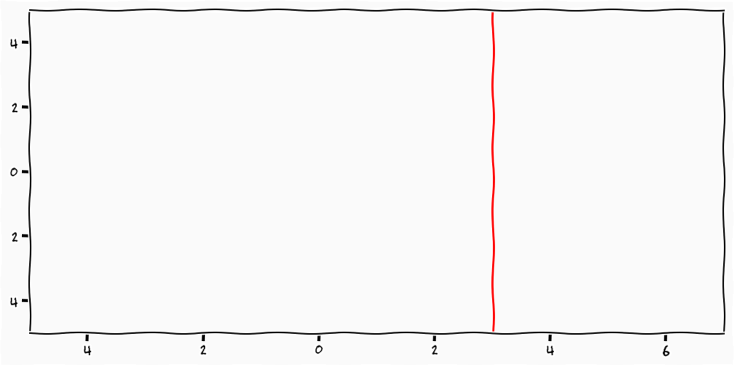
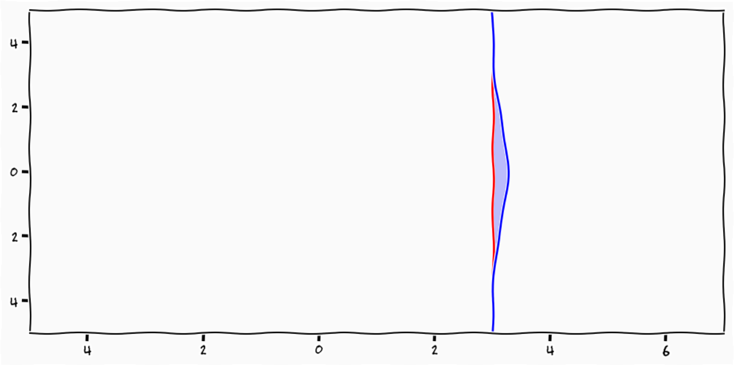
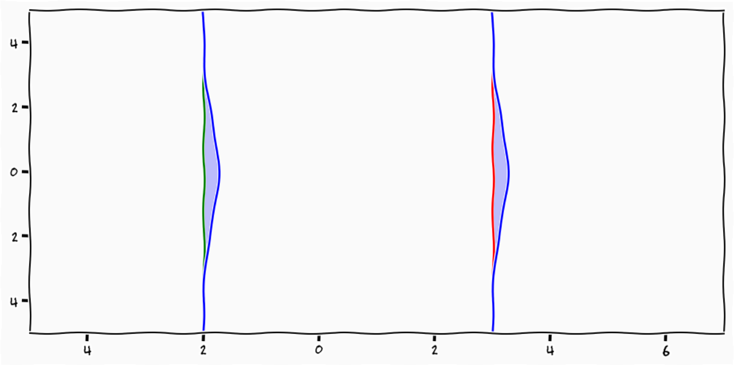


Lets talk about functions



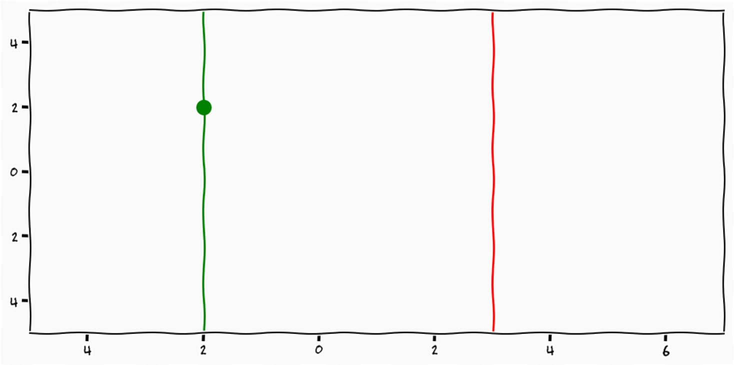
Lets talk about functions



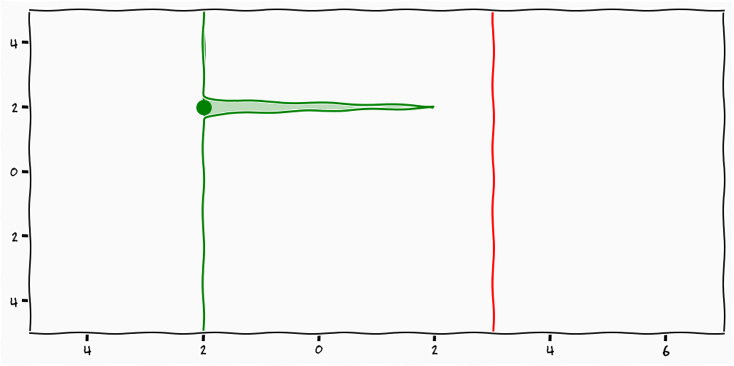
Jointly Gaussian function values

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \mathcal{N}\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix} \right)$$

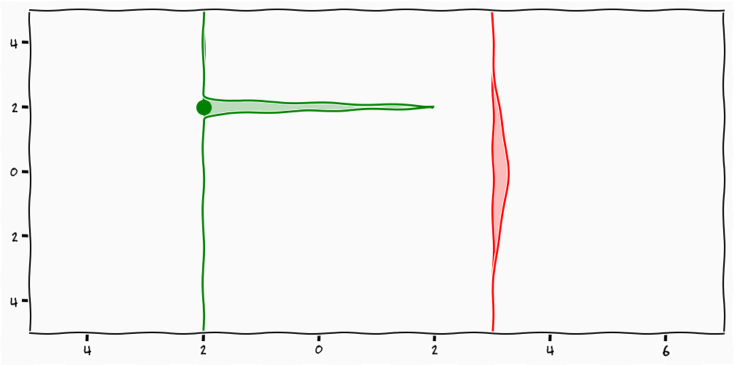
Non-parametric functions



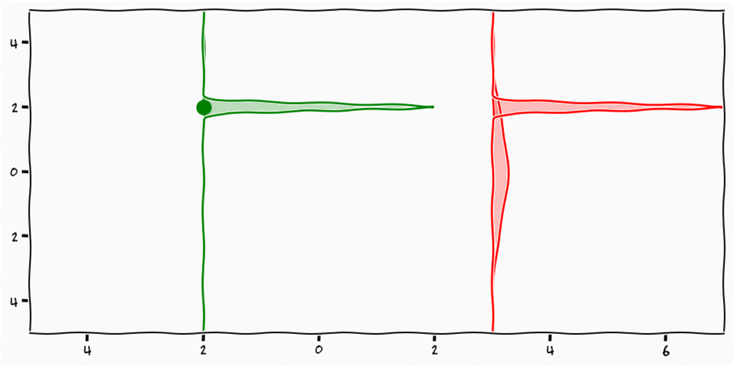
Non-parametric functions



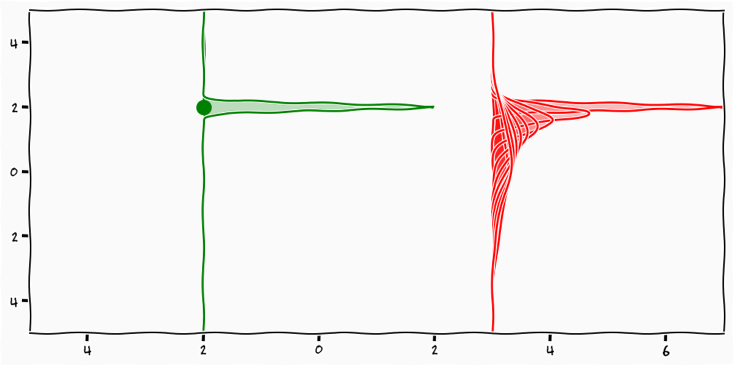
Non-parametric functions



Non-parametric functions



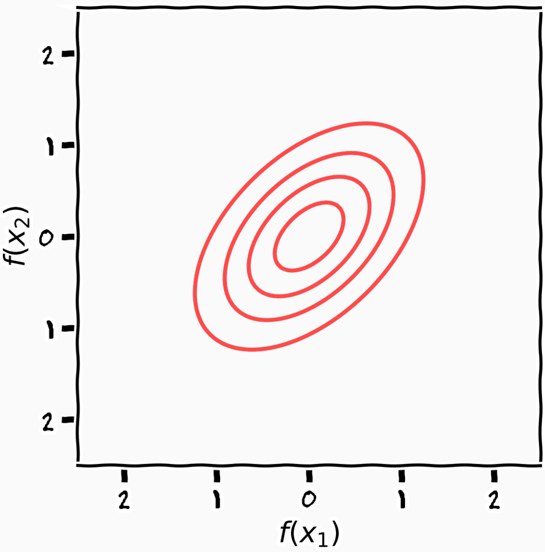
Non-parametric functions



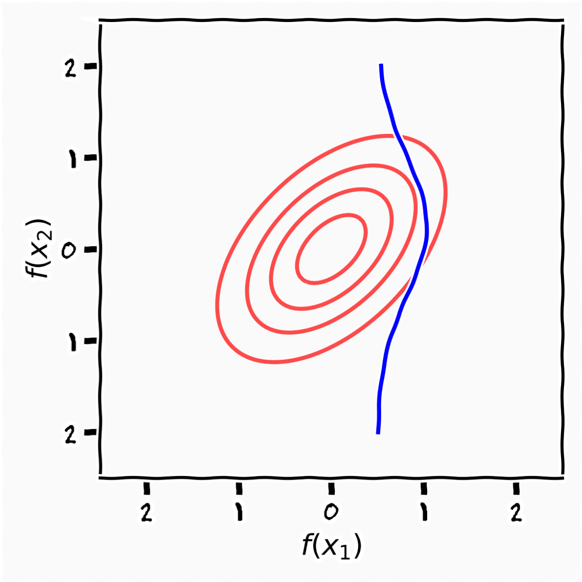
Conditional Gaussians

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

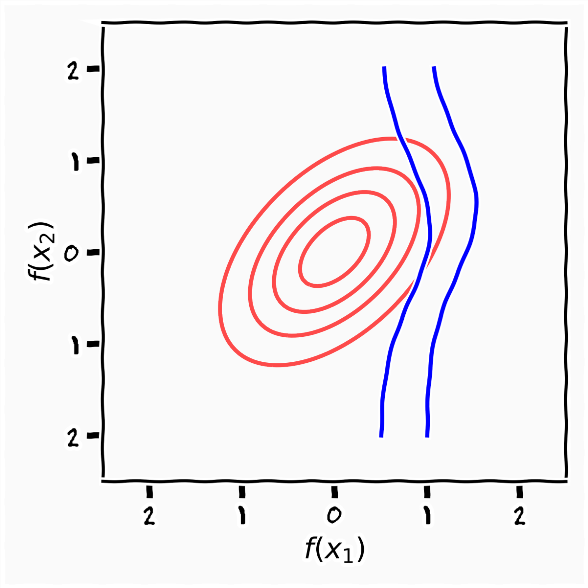
Conditional Gaussians



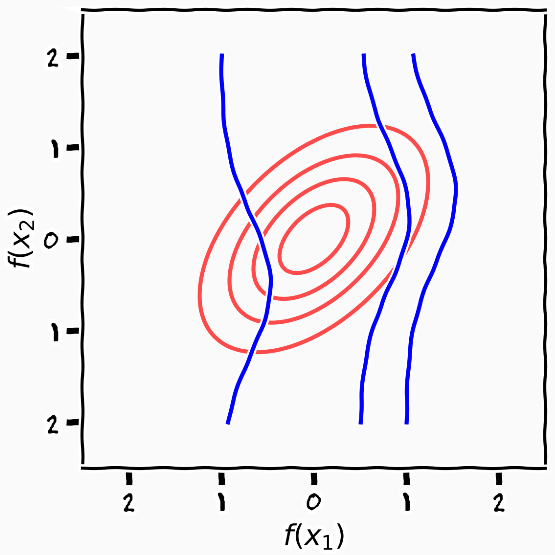
Conditional Gaussians



Conditional Gaussians



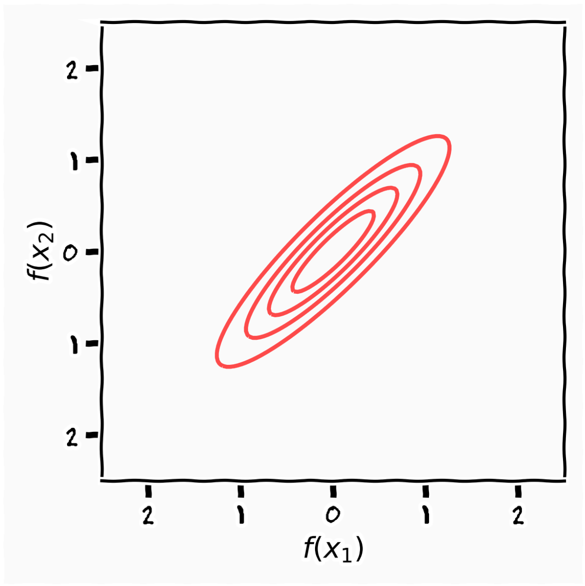
Conditional Gaussians

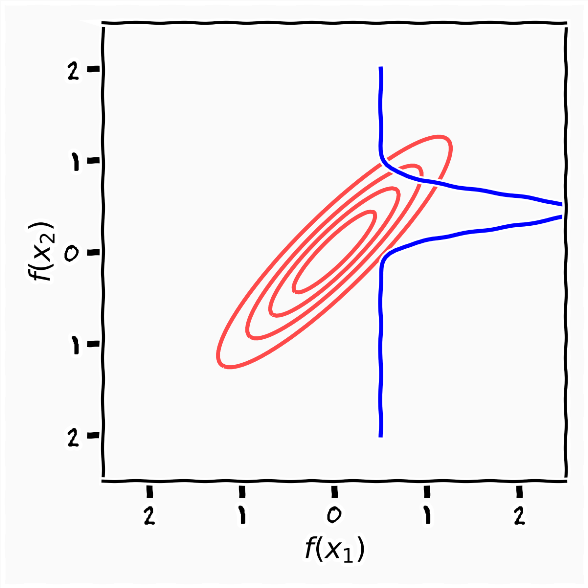


Conditional Gaussians

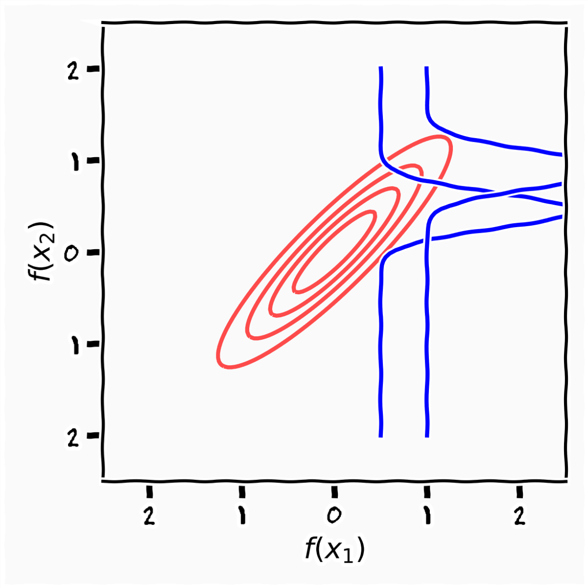
$$\mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.9 \\ 0.9 & 1 \end{bmatrix}\right)$$

Conditional Gaussians




2
1
0
1
2
$f(x_2)$
2
1
0
1
2
$f(x_1)$

Conditional Gaussians



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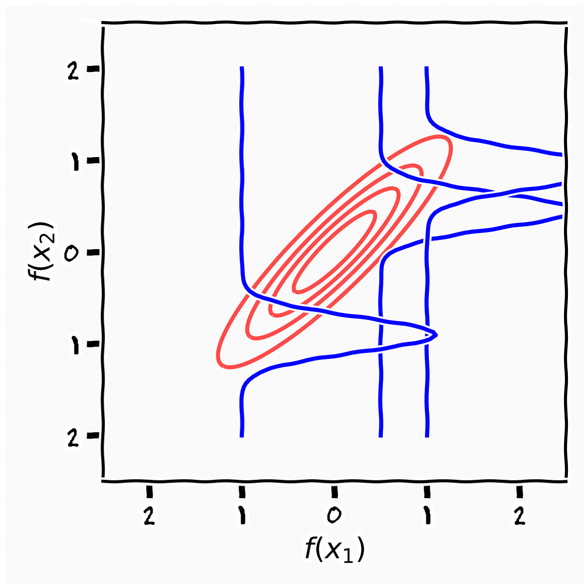
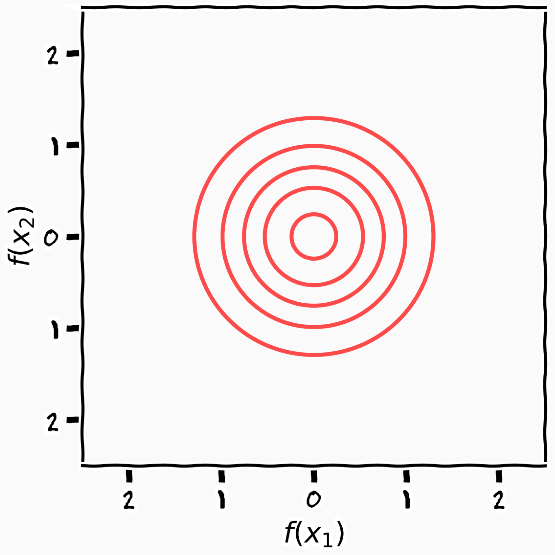


Conditional Gaussians

$$\mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right)$$

Conditional Gaussians



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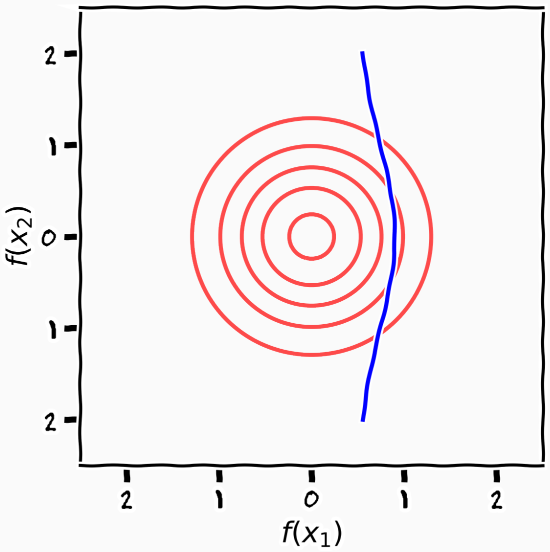

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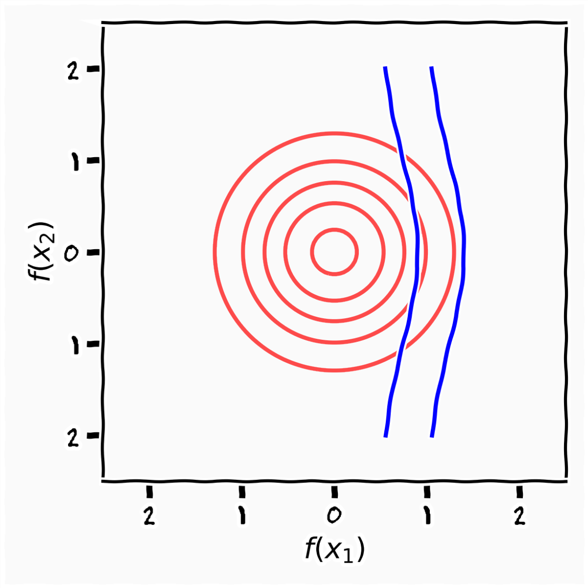

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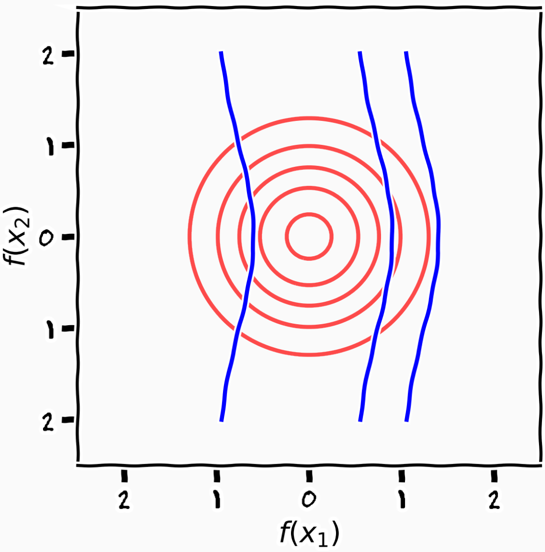
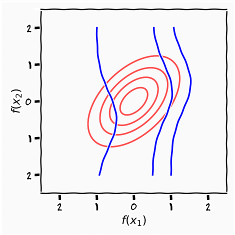
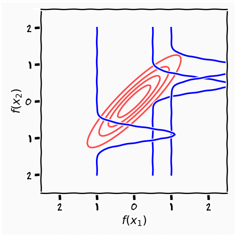


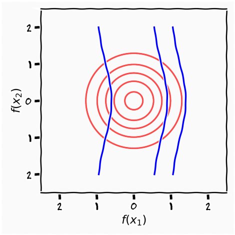
Conditional Gaussians



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

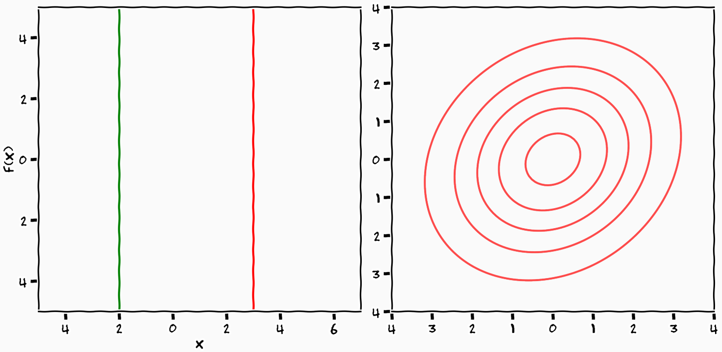


$$\mathrm{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.9 \\ 0.9 & 1 \end{bmatrix}\right)$$

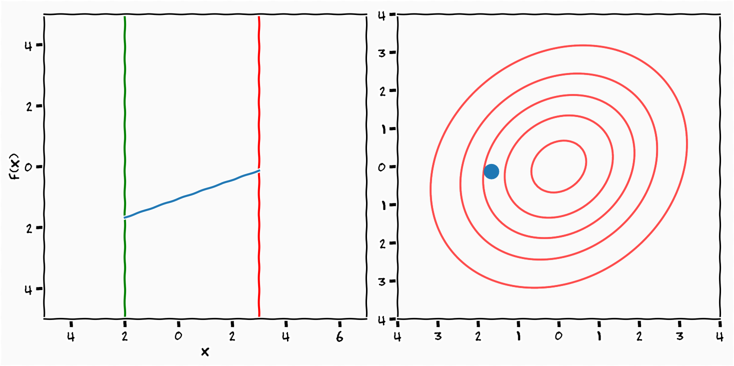


$$\mathrm{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right)$$

Gaussian Samples



Gaussian Samples



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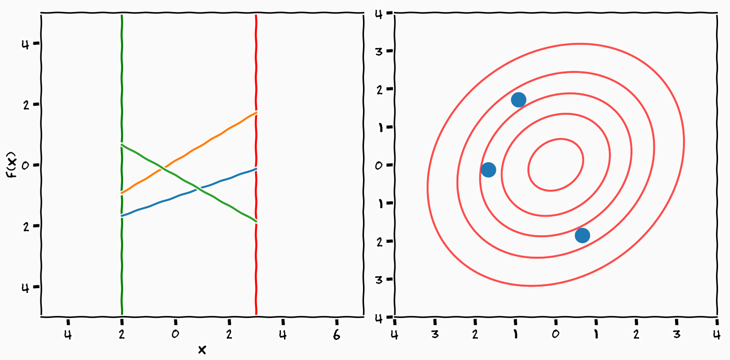

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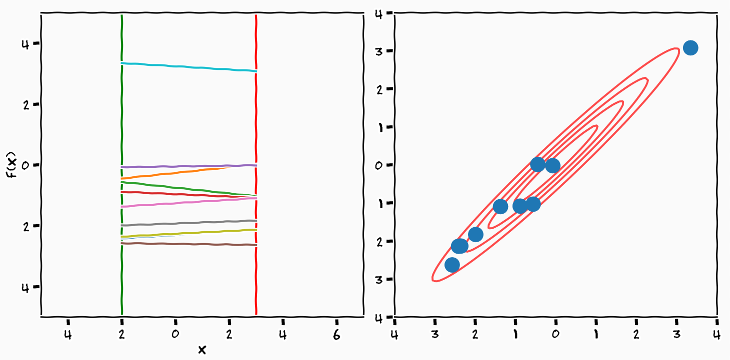
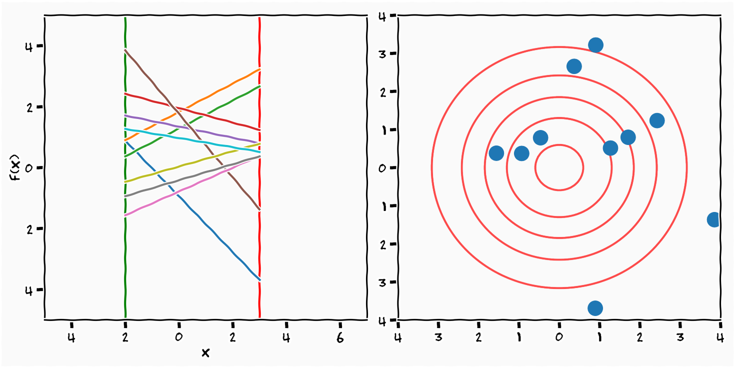
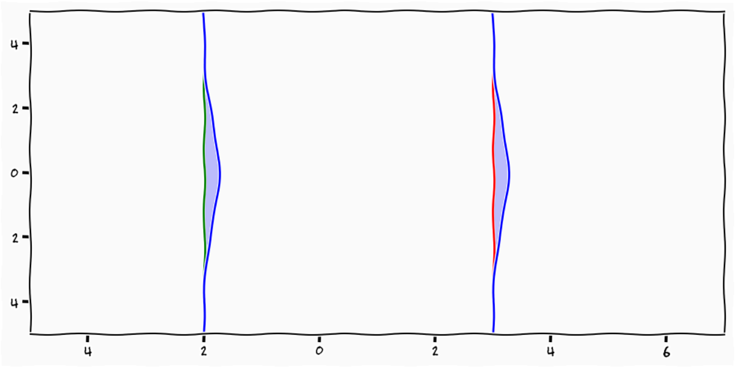


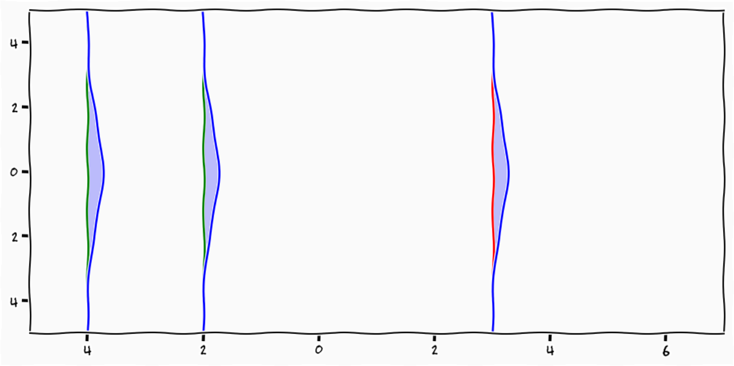
Gaussian Samples



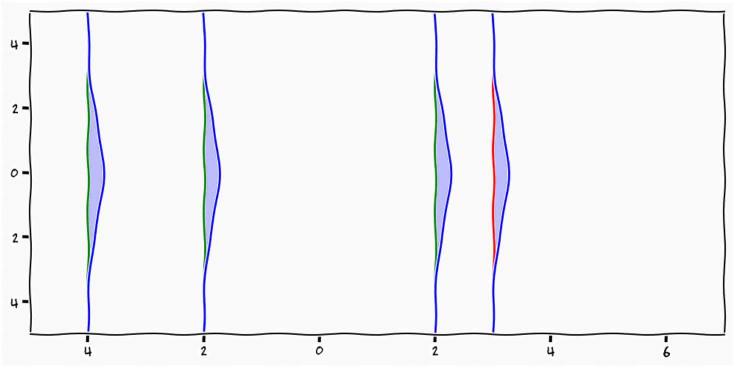
Lets talk about functions



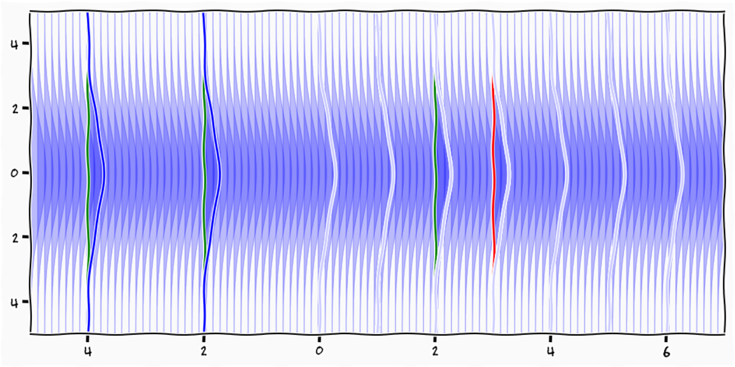
Non-parametric functions



Non-parametric functions



Non-parametric functions



Jointly Gaussian functions II

$$p(\mathbf{f}) = \mathcal{N}\left(\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{bmatrix} \middle| \begin{bmatrix} \mu(x_1) \\ \mu(x_2) \\ \vdots \\ \mu(x_N) \end{bmatrix}, \begin{bmatrix} k_{11} & k_{12} & \dots & k_{1N} \\ k_{21} & k_{22} & \dots & k_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ k_{N1} & k_{N2} & \dots & k_{NN} \end{bmatrix} \right)$$

Gaussian Distribution - Marginal

$$p(x_1, x_2) = \mathcal{N}\left(\begin{array}{c|c} x_1 & \mu_1 \\ x_2 & \mu_2 \end{array} , \begin{array}{cc} k_{11} & k_{12} \\ k_{21} & k_{22} \end{array} \right)$$

Gaussian Distribution - Marginal

$$p(x_1, x_2) = \mathcal{N}\left(\begin{array}{c} x_1 \\ x_2 \end{array} \middle| \begin{array}{c} \mu_1 \\ \mu_2 \end{array}, \begin{array}{cc} k_{11} & k_{12} \\ k_{21} & k_{22} \end{array} \right)$$

$$\Rightarrow p(x_1) = \int_{x_2} p(x_1, x_2) = \underline{\mathcal{N}\left(x_1 \mid \mu_1, k_{11}\right)}$$

Gaussian Distribution - Marginal

$$p(x_1, x_2) = \mathcal{N}\left(\begin{array}{c|c} x_1 & \mu_1 \\ x_2 & \mu_2 \end{array}, \begin{array}{cc} k_{11} & k_{12} \\ k_{21} & k_{22} \end{array}\right)$$

$$\Rightarrow p(x_1) = \int_{x_2} p(x_1, x_2) = \underline{\mathcal{N}\left(x_1 \mid \mu_1, k_{11}\right)}$$

$$p(x_1, x_2, \ldots, x_N) = \mathcal{N}\left(\begin{array}{c|c} x_1 & \mu_1 \\ x_2 & \mu_2 \\ \vdots & \vdots \\ x_N & \mu_N \end{array}, \begin{array}{cccc} k_{11} & k_{12} & \cdots & k_{1N} \\ k_{21} & k_{22} & \cdots & k_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ k_{N1} & k_{N2} & \cdots & k_{NN} \end{array}\right)$$

Gaussian Distribution - Marginal

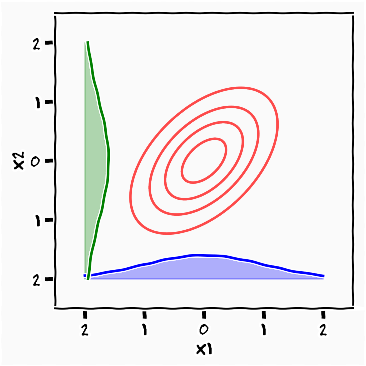
$$p(x_1, x_2) = \mathcal{N}\left(\begin{array}{c|c} x_1 & \mu_1 \\ x_2 & \mu_2 \end{array}, \begin{array}{cc} k_{11} & k_{12} \\ k_{21} & k_{22} \end{array} \right)$$

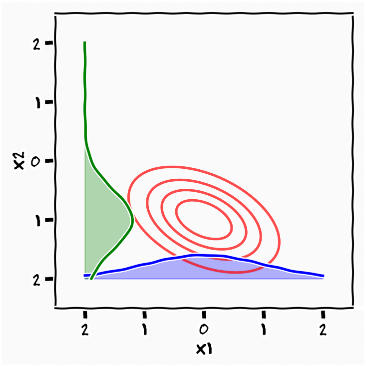
$$\Rightarrow p(x_1) = \int_{x_2} p(x_1, x_2) = \underline{\mathcal{N}\left(x_1 \mid \mu_1, k_{11}\right)}$$

$$p(x_1, x_2, \ldots, x_N) = \mathcal{N}\left(\begin{array}{c|c} x_1 & \mu_1 \\ x_2 & \mu_2 \\ \vdots & \vdots \\ x_N & \mu_N \end{array}, \begin{array}{cccc} k_{11} & k_{12} & \cdots & k_{1N} \\ k_{21} & k_{22} & \cdots & k_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ k_{N1} & k_{N2} & \cdots & k_{NN} \end{array} \right)$$

$$\Rightarrow \quad p(x_1) = \int_{x_2, \ldots, x_N} p(x_1, x_2, \ldots, x_N) = \underline{\mathcal{N}\left(x_1 \mid \mu_1, k_{11}\right)}$$

Gaussian Distribution - Marginal



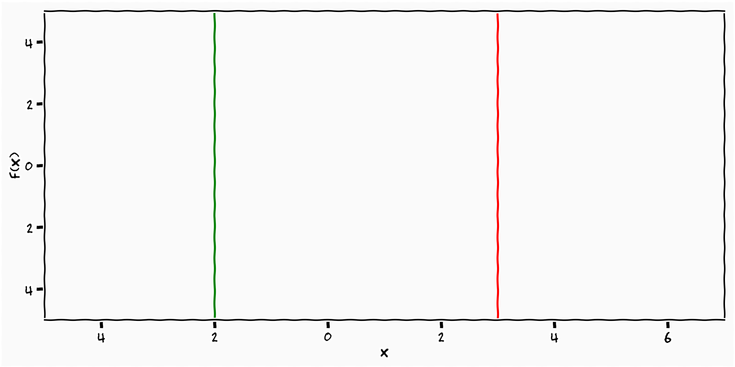


Marginal Property (Consistency)

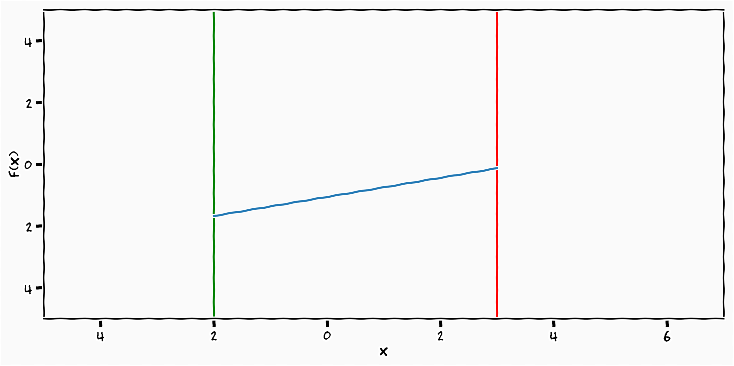
For all measurable sets $F_i \subseteq \mathbb{R}^n$ and probability measure $\mathcal{N}$

$$\mathcal{N}_{t_1 \cdot t_k}\left(F_1 \times \cdot \times F_k\right) = \mathcal{N}_{t_1 \cdots t_k, t_{k+1} \cdot t_{k+m}}\left(F_1 \times \cdot \times F_k \times \mathbb{R}^n \times \cdot \times \mathbb{R}^n\right)$$

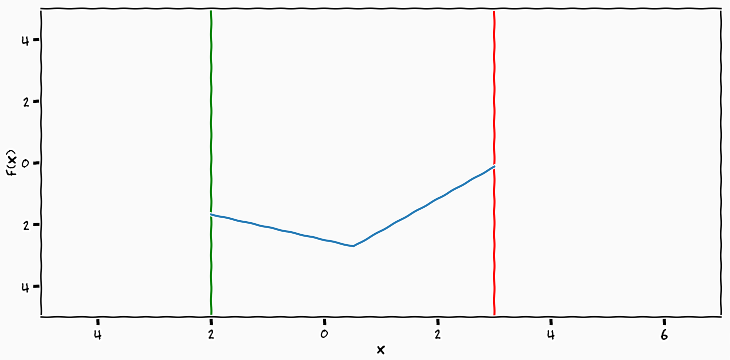
Gaussian Samples



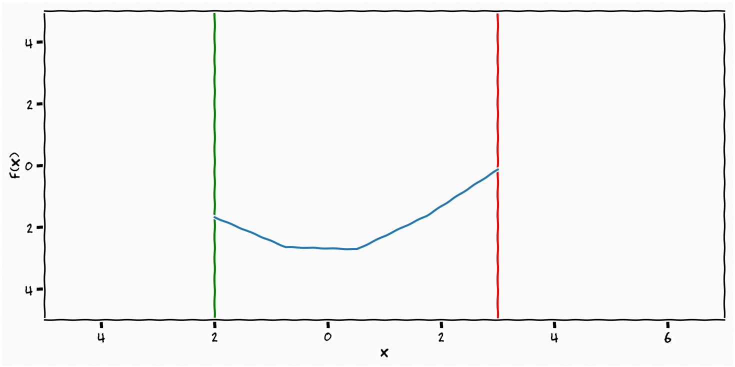
Gaussian Samples



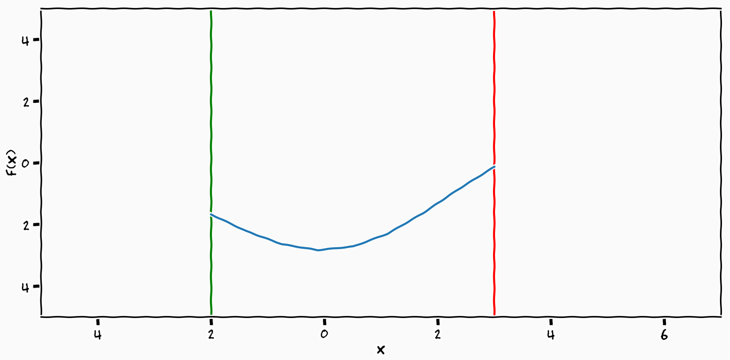
Gaussian Samples



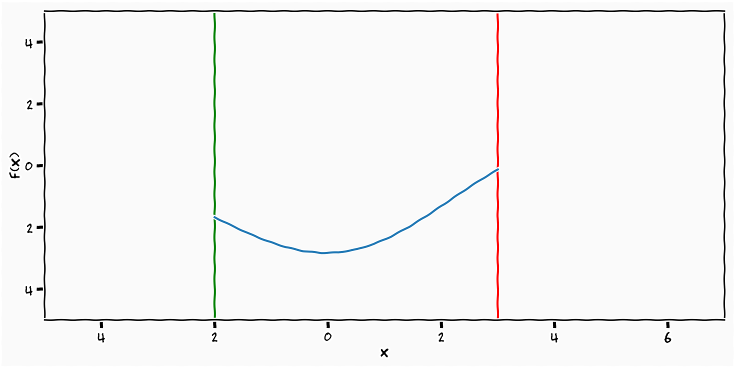
Gaussian Samples



Gaussian Samples



Gaussian Samples



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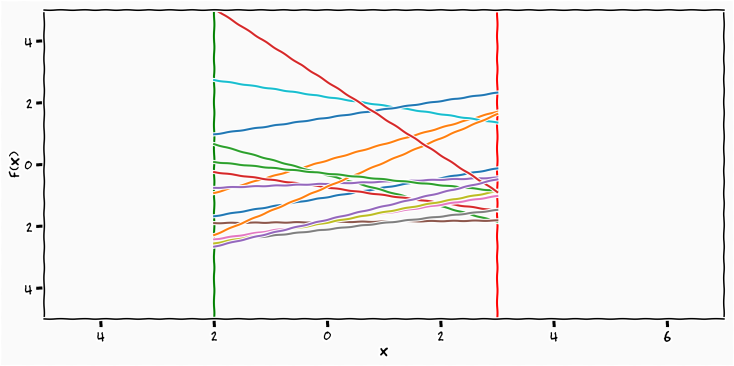
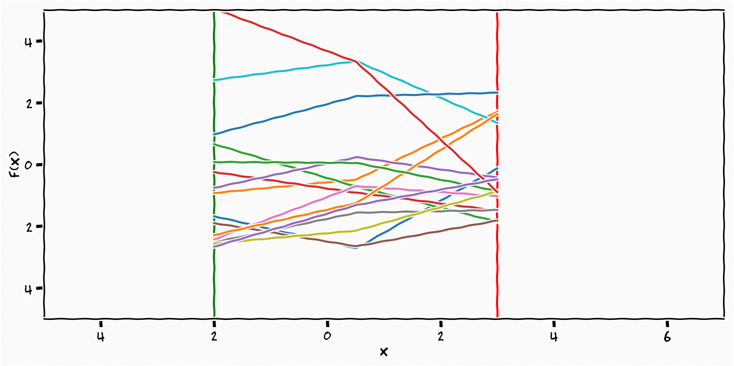
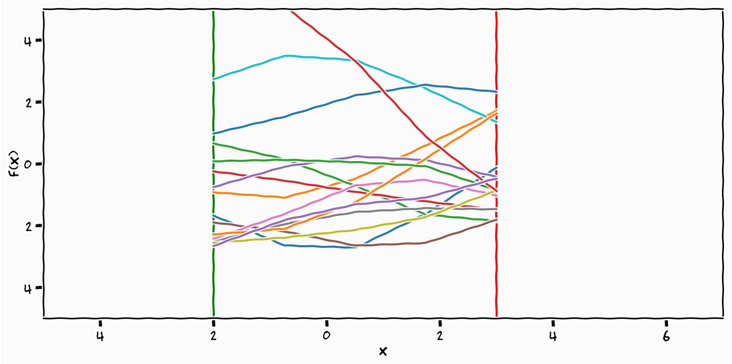


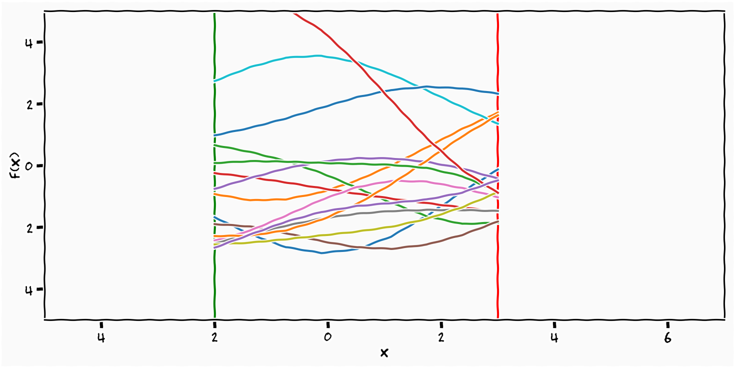
Gaussian Samples



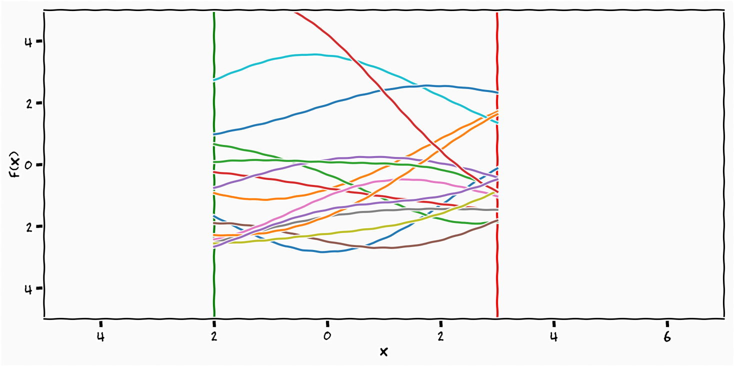
Gaussian Samples

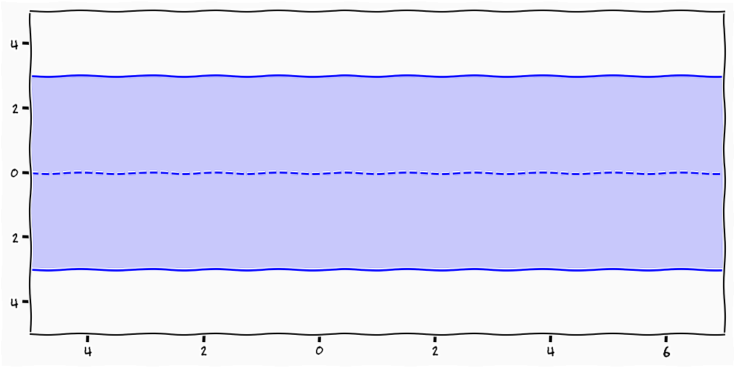


Gaussian Samples



Gaussian Samples

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Gaussian Processes: Formalism

$$p(\mathbf{f}) = \mathcal{N}\left(\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \\ \vdots \end{bmatrix} \middle| \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_N \\ \vdots \end{bmatrix}, \begin{bmatrix} k_{11} & k_{12} & \dots & k_{1N} & \dots \\ k_{21} & k_{22} & \dots & k_{2N} & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ k_{N1} & k_{N2} & \dots & k_{NN} & \dots \\ \vdots & \vdots & \dots & \vdots & \ddots \end{bmatrix} \right)$$

$$\mathcal{GP}(\cdot,\cdot) \qquad M \in \mathbb{R}^{\infty \times N} \qquad \mathcal{N}(\cdot,\cdot)$$

$$\infty \qquad \rightarrow \qquad N$$

The Gaussian distribution is the projection of the infinite Gaussian process

Gaussian Process

Definition (Gaussian Process)
A Gaussian process is a collection of random variables who are jointly Gaussian distributed index by a infinite index set

Gaussian Processes: Formalism II

$$p(\mathbf{f}) = \mathcal{N}\left(\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \\ \vdots \end{bmatrix} \middle| \begin{bmatrix} \mu(x_1) \\ \mu(x_2) \\ \vdots \\ \mu(x_N) \\ \vdots \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \dots & k(x_1, x_N) & \dots \\ k(x_2, x_1) & k(x_2, x_2) & \dots & k(x_2, x_N) & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ k(x_N, x_1) & k(x_N, x_2) & \dots & k(x_N, x_N) & \dots \\ \vdots & \vdots & \dots & \vdots & \ddots \end{bmatrix}\right)$$

"Parametrisation"

$$k_{ij} = k(x_i, x_j)$$

- We parameterise the covariance as a function of the input

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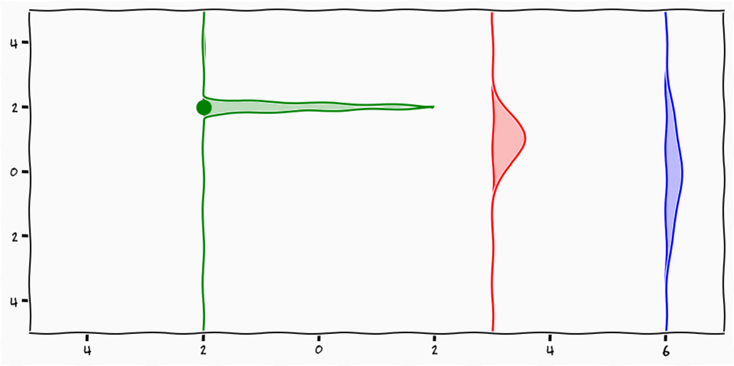
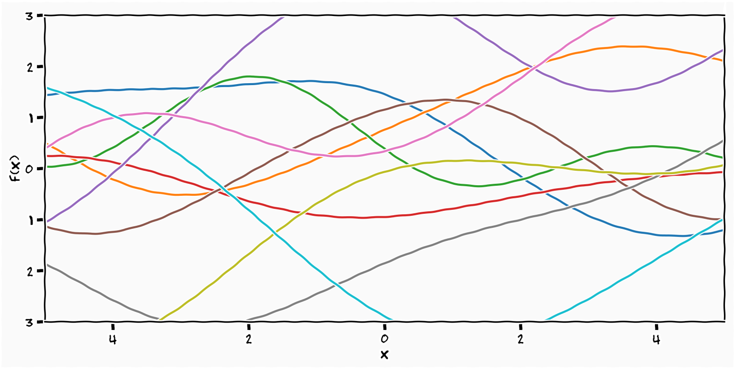
- Your "handle" to input your knowledge into a GP is the covariance function
  - *you specify the degree of covariance between data-points*
- If this "parametrisation" aligns well with your knowledge a GP is the way forward!

Gaussian Processes

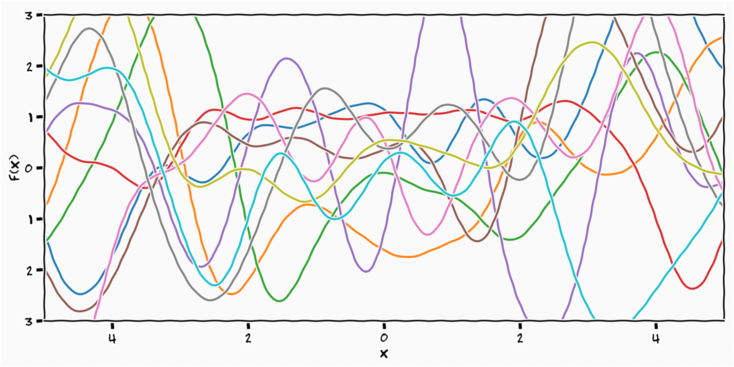


Gaussian Processes Samples



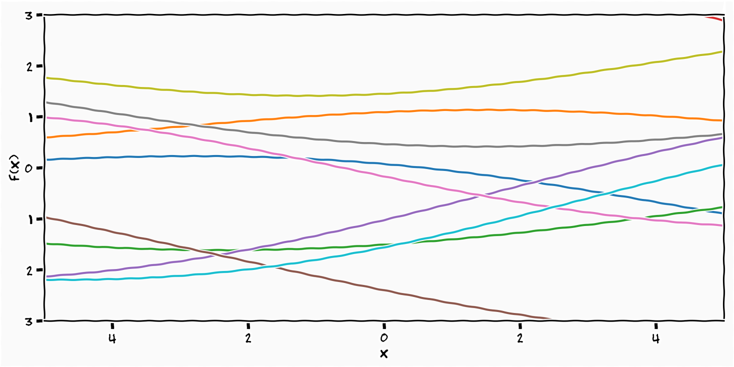
$$k(x_i, x_j) = 3 \cdot e^{-\frac{(x_i - x_j)^2}{15}}$$

Gaussian Processes Samples

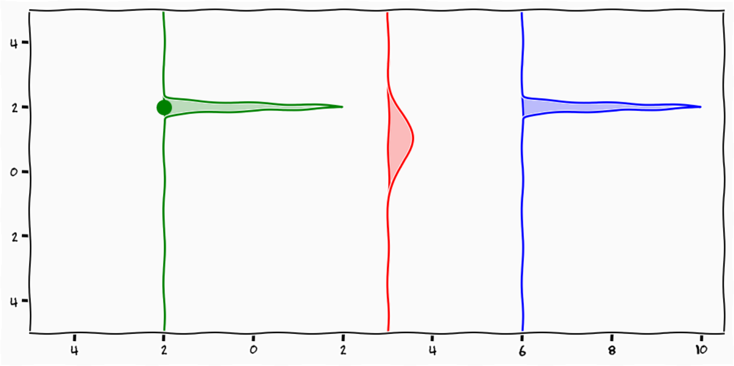


$$k(x_i, x_j) = 3 \cdot e^{-\frac{(x_i - x_j)^2}{1}}$$

Gaussian Processes Samples



$$k(x_i, x_j) = 3 \cdot e^{-\frac{(x_i - x_j)^2}{150}}$$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Bayesian Inference

Bayes' Rule

$$p(\mathbf{f}_* \mid \mathbf{f}) = \frac{p(\mathbf{f}, \mathbf{f}_*)}{p(\mathbf{f})} = \frac{p(\mathbf{f}, \mathbf{f}_*)}{\int p(\mathbf{f}, \mathbf{f}_*) \mathrm{d}\mathbf{f}_*}$$

Marginal Likelihood

$$\int p(\mathbf{f}, \mathbf{f}_*) \mathrm{d}\mathbf{f}_* = \int p(\mathbf{f} \mid \mathbf{f}_*) p(\mathbf{f}_*) \mathrm{d}\mathbf{f}_*$$

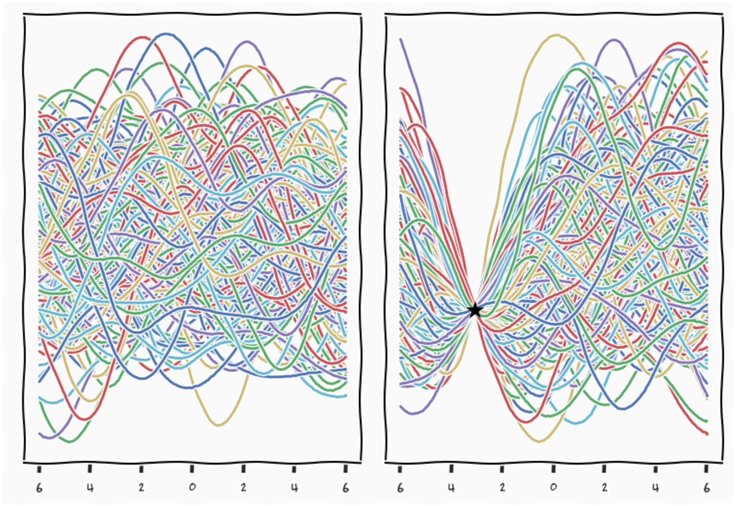
- Take every possible function value/marginal $\mathbf{f}_*$ at location $\mathbf{x}_*$ according to their probability

Marginal Likelihood

$$\int p(\mathbf{f}, \mathbf{f}_*) \mathrm{d}\mathbf{f}_* = \int p(\mathbf{f} \mid \mathbf{f}_*) p(\mathbf{f}_*) \mathrm{d}\mathbf{f}_*$$

- Take every possible function value/marginal $\mathbf{f}_*$ at location $\mathbf{x}_*$ according to their probability
- Check if these marginals are consistent with the marginals we observe $\mathbf{f}$ at location $\mathbf{x}$

Gaussian Processes: Posterior Samples



Gaussian Process: "Predictive Posterior"

$$p(\mathbf{f}, \mathbf{f}_*) = p(\mathbf{f}_* \mid \mathbf{f})p(\mathbf{f})$$

- We have defined $p(\mathbf{f}, \mathbf{f}_*)$

Gaussian Process: "Predictive Posterior"

$$p(\mathbf{f}, \mathbf{f}_*) = p(\mathbf{f}_* \mid \mathbf{f})p(\mathbf{f})$$

- We have defined $p(\mathbf{f}, \mathbf{f}_*)$
- We know through the marginal property of the Gaussian that $p(\mathbf{f})$ is consistent

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- We have defined $p(\mathbf{f}, \mathbf{f}_*)$
- We know through the marginal property of the Gaussian that $p(\mathbf{f})$ is consistent
- We know that $p(\mathbf{f}_* \mid \mathbf{f})$ is Gaussian
- $\Rightarrow$ *We can just solve for* $p(\mathbf{f}_* \mid \mathbf{f})$

Gaussian Process: "Predictive Posterior"

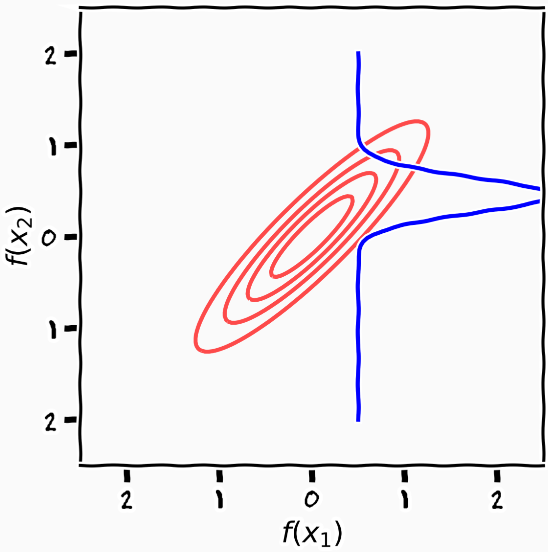
- All instantiations are jointly Gaussian

$$\left[\begin{array}{c}\mathbf{f}\\ \mathbf{f}_*\end{array}\right] \sim \mathcal{N}\left(\left[\begin{array}{c}\mathbf{0}\\ \mathbf{0}\end{array}\right], \left[\begin{array}{cc}k(\mathbf{x},\mathbf{x}) & k(\mathbf{x},\mathbf{x}_*)\\ k(\mathbf{x}_*,\mathbf{x}) & k(\mathbf{x}_*,\mathbf{x}_*)\end{array}\right]\right)$$

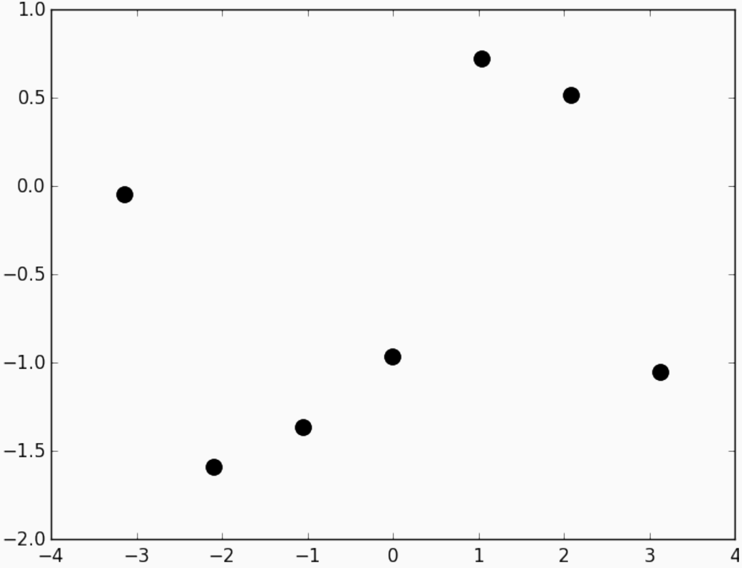
- Conditional Gaussian

$$\begin{aligned} p(f_*|\mathbf{x}_*,\mathbf{x},\mathbf{f}) = \mathcal{N}(&k(\mathbf{x}_*,\mathbf{x})^{\mathrm{T}}k(\mathbf{x},\mathbf{x})^{-1}\mathbf{f},\\ &k(\mathbf{x}_*,\mathbf{x}_*) - k(\mathbf{x}_*,\mathbf{x})^{\mathrm{T}}k(\mathbf{x},\mathbf{x})^{-1}k(\mathbf{x},\mathbf{x}_*)) \end{aligned}$$

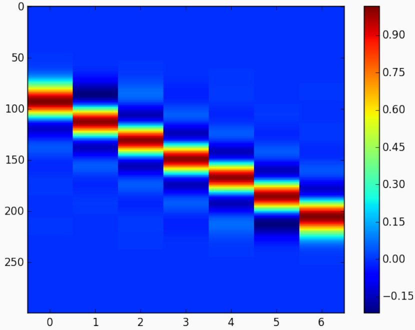
Conditional Gaussians



Gaussian Process: "Predictive Posterior"

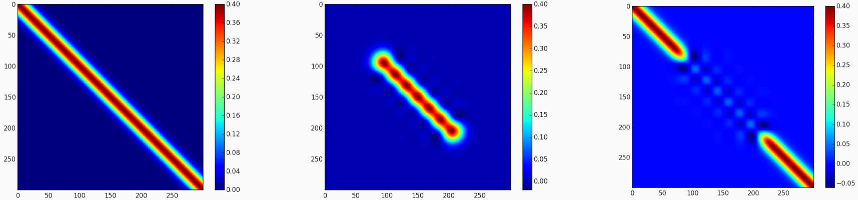


Does it make sense: Mean



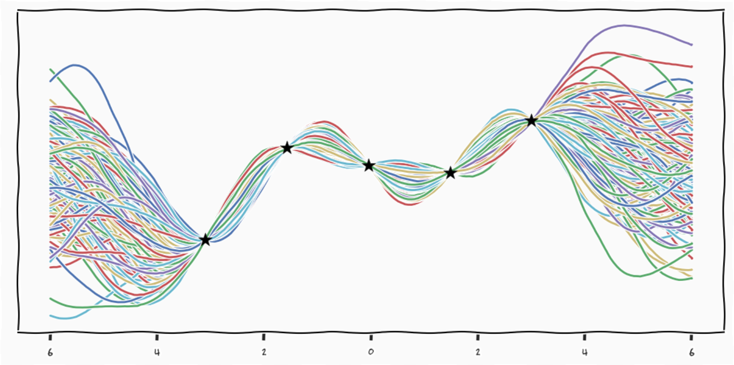
$$k(\mathbf{x}_*, \mathbf{X})^{\mathrm{T}} k(\mathbf{X}, \mathbf{X})^{-1} \mathbf{f}$$

Does it make sense: Covariance

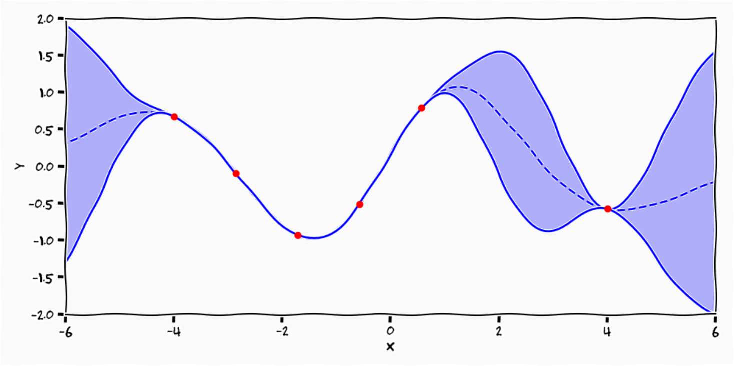


$$k(\mathbf{x}_*, \mathbf{x}_*) - k(\mathbf{x}_*, \mathbf{x})^{\mathrm{T}} k(\mathbf{x}, \mathbf{x})^{-1} k(\mathbf{x}, \mathbf{x}_*)$$

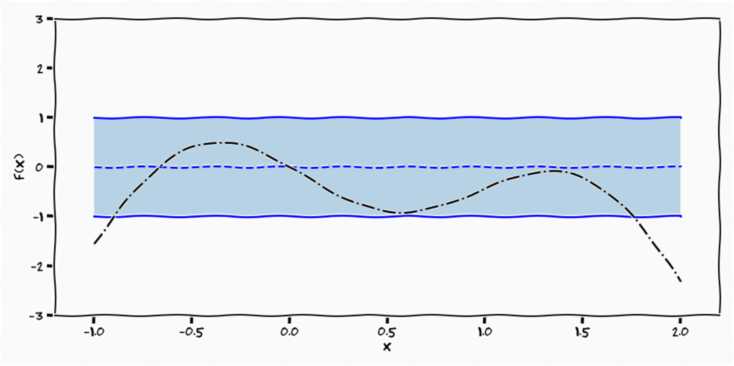
Gaussian Processes: "Predictive Posterior Samples"



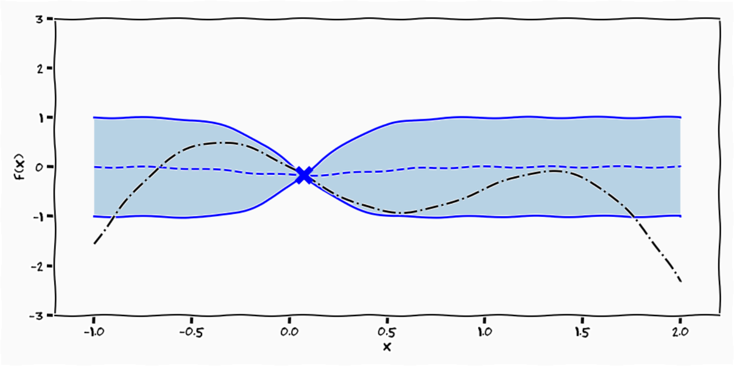
Gaussian Processes: "Predictive Posterior Process"



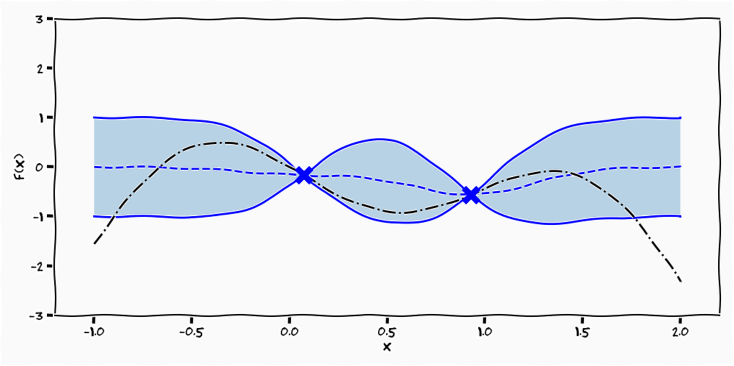
Posterior Processes



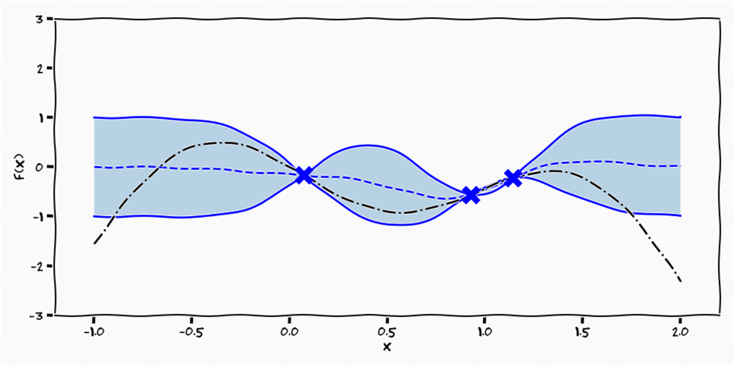
Posterior Processes



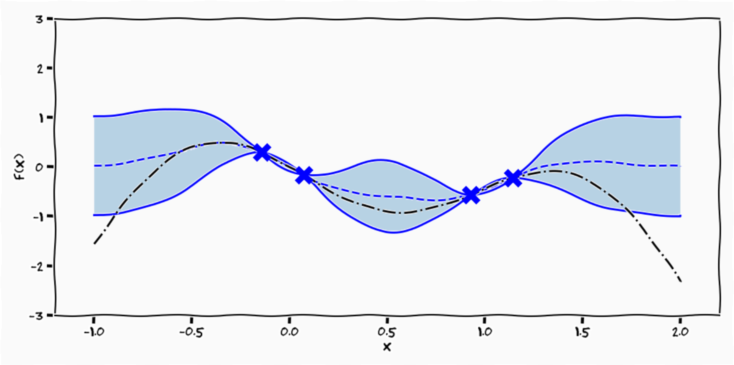
Posterior Processes



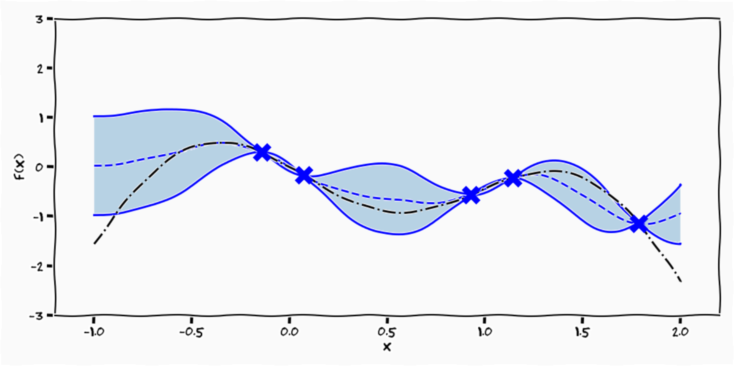
Posterior Processes



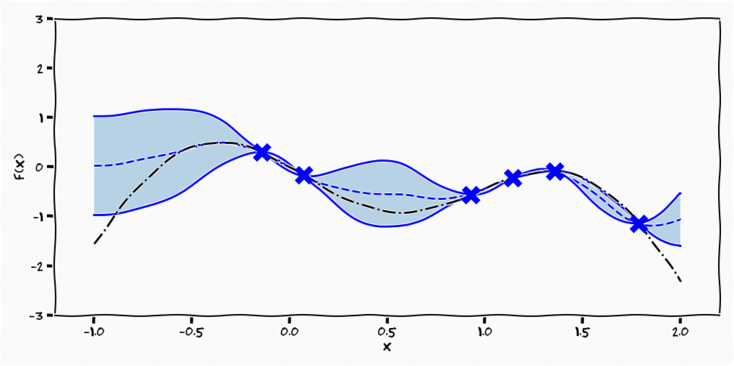
Posterior Processes



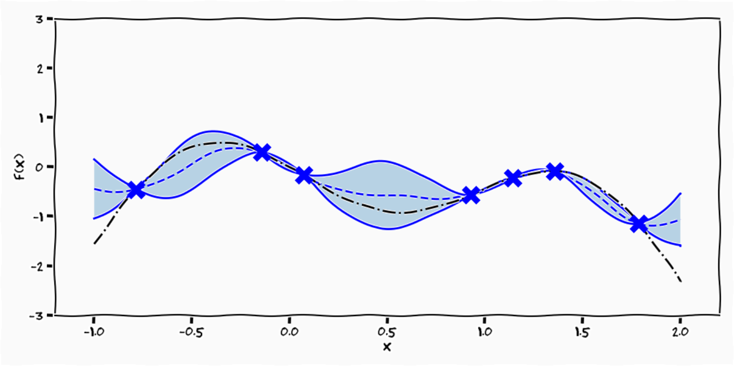
Posterior Processes



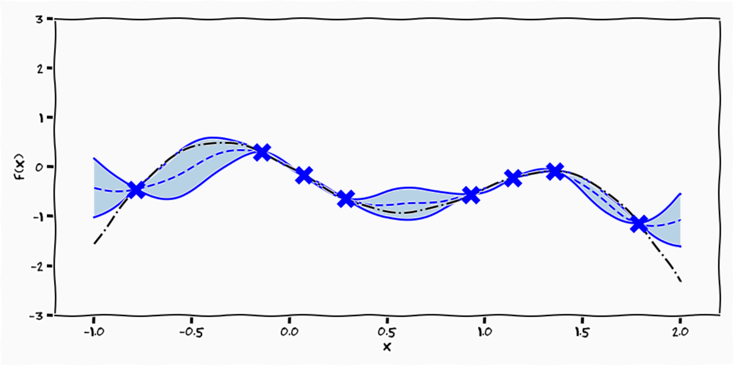
Posterior Processes



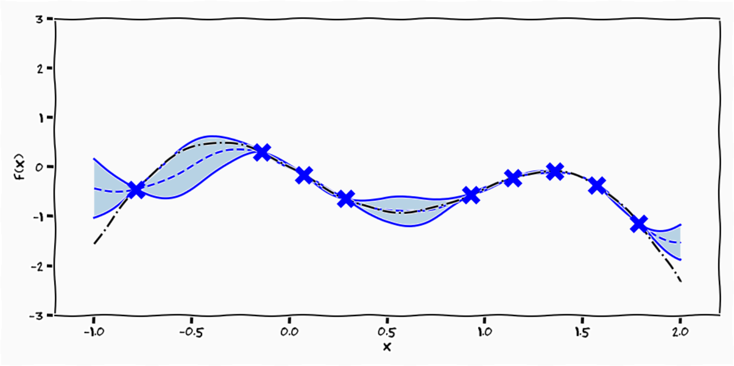
Posterior Processes



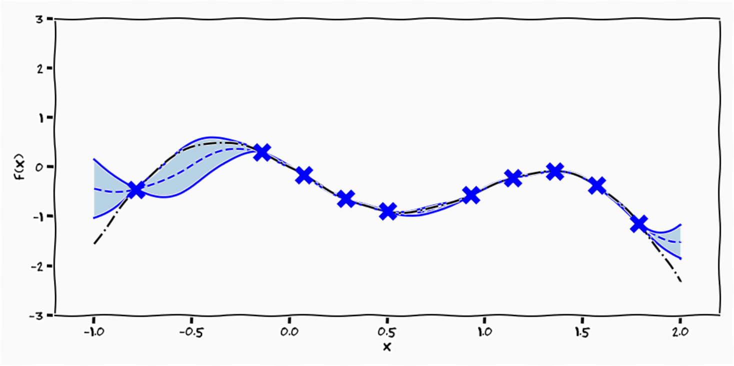
Posterior Processes



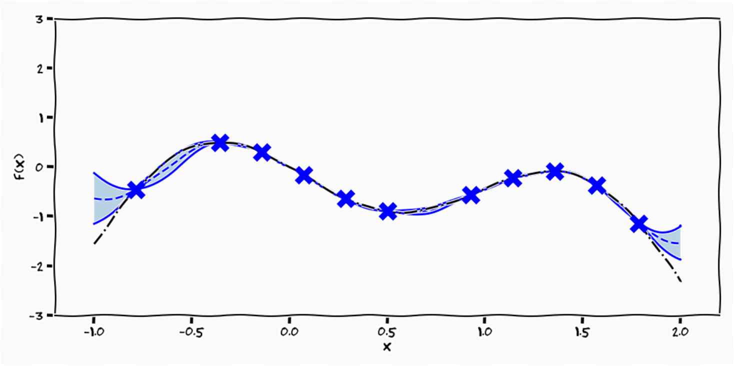
Posterior Processes



Posterior Processes



Posterior Processes



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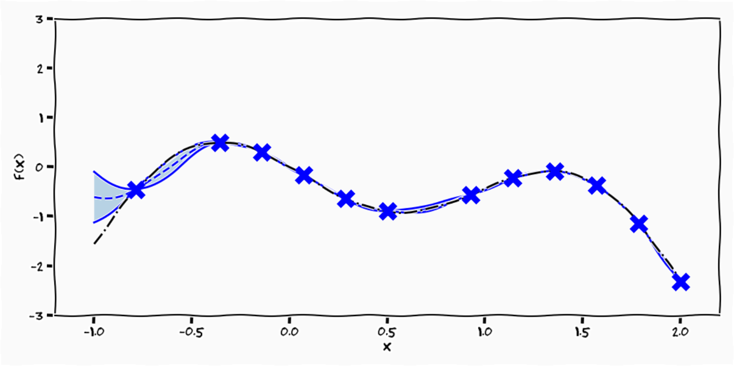
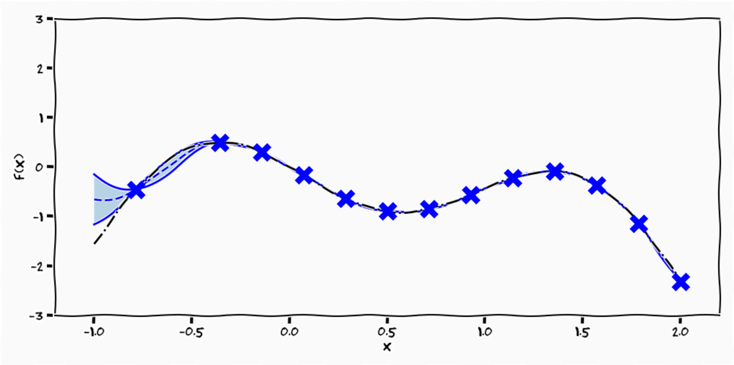
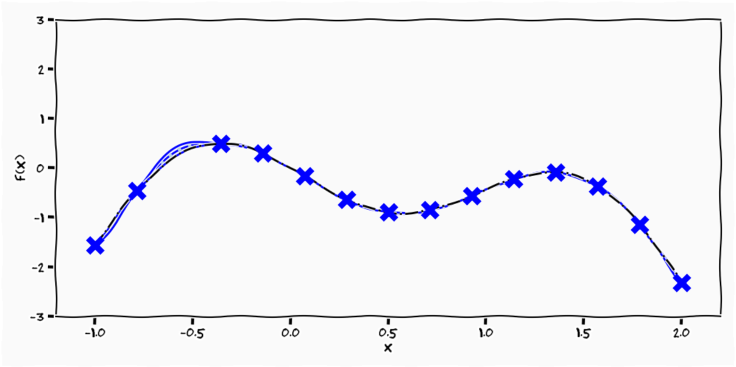


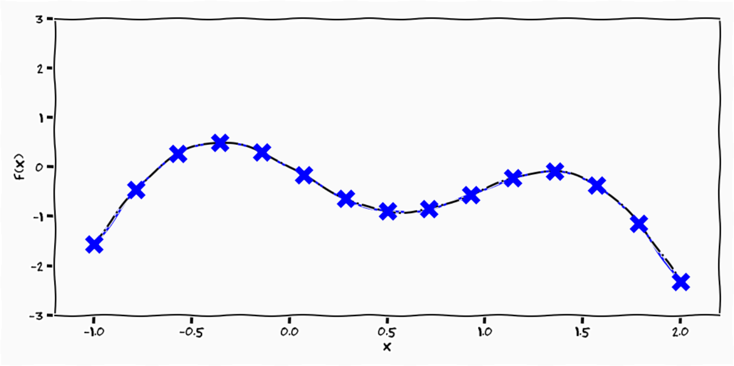
Posterior Processes



Posterior Processes



Posterior Processes



Model

- So far we have only looked at the prior
  - the same as when we sampled from $p(\mathbf{w})$ in the previous lecture
  - the "predictive posterior" has really been the "conditional prior"
- Now lets introduce a likelihood

Model

$$p(\mathbf{y},\mathbf{f}) = p(\mathbf{y} \mid \mathbf{f})p(\mathbf{f}) = p(\mathbf{f}) \prod_{i=1} \mathcal{N}(p(y_i \mid f_i))$$

$$p(\mathbf{y} \mid \mathbf{f}) = \mathcal{N}(\mathbf{y} \mid \mathbf{f}, \sigma^2 \mathbf{I})$$

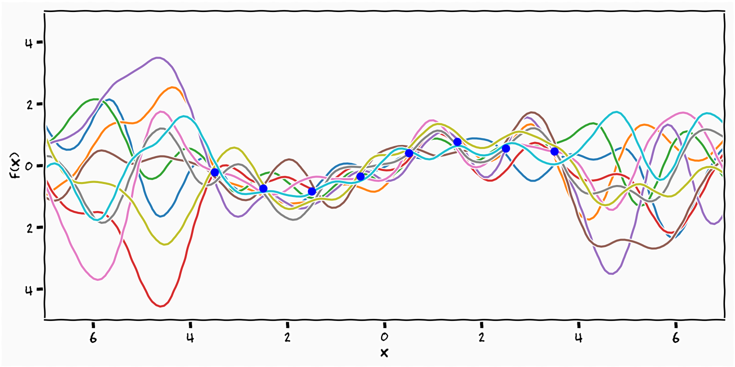
- Same motivation as with linear regression
- we want to explain away our ignorance from the data using σ

Predictive Posterior Process

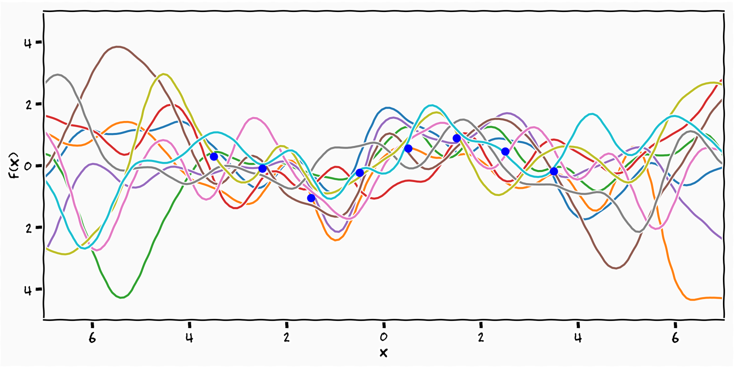
$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}, \mathbf{x}) + \sigma^2 \mathbf{I} & k(\mathbf{x}, \mathbf{x}_*) \\ k(\mathbf{x}_*, \mathbf{x}) & k(\mathbf{x}_*, \mathbf{x}_*) \end{bmatrix} \right)$$

$$\begin{aligned} p(f_* | \mathbf{x}_*, \mathbf{x}, \mathbf{y}, \boldsymbol{\theta}) = \mathcal{N}(& k(\mathbf{x}_*, \mathbf{x})^{\mathrm{T}} (K(\mathbf{x}, \mathbf{x}) + \sigma^2 \mathbf{I}))^{-1} \mathbf{y}, \\ & k(\mathbf{x}_*, \mathbf{x}_*) - k(\mathbf{x}_*, \mathbf{x})^{\mathrm{T}} (K(\mathbf{x}, \mathbf{x}) + \sigma^2 \mathbf{I})^{-1} K(\mathbf{x}, \mathbf{x}_*)) \end{aligned}$$

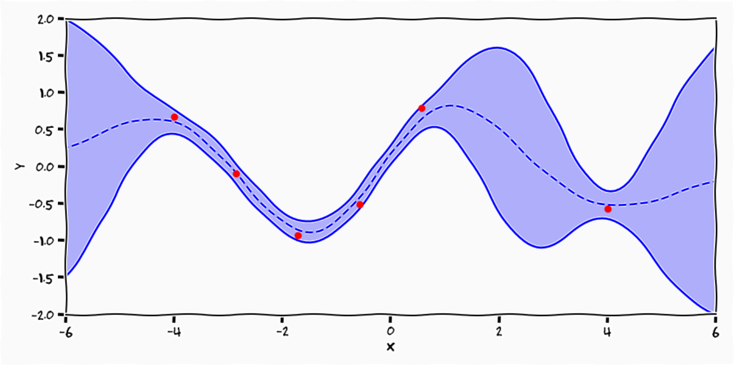
Posterior Samples



Posterior Samples



Gaussian Processes: Predictive Posterior Process



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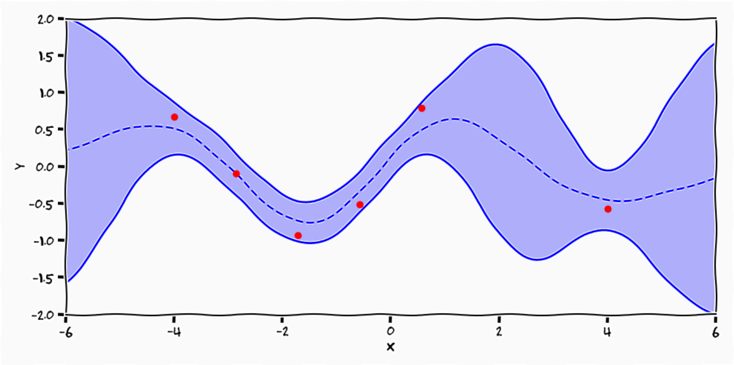
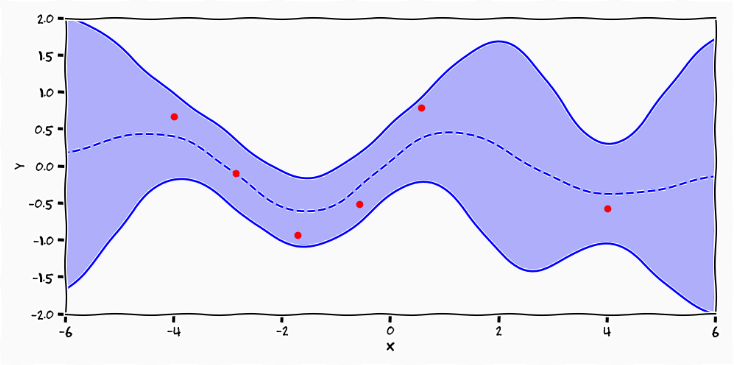
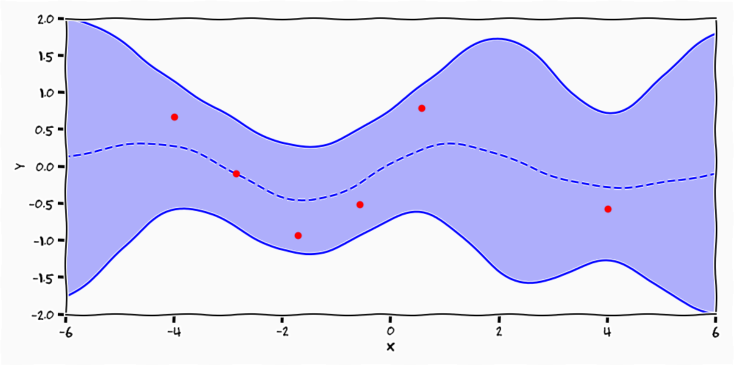


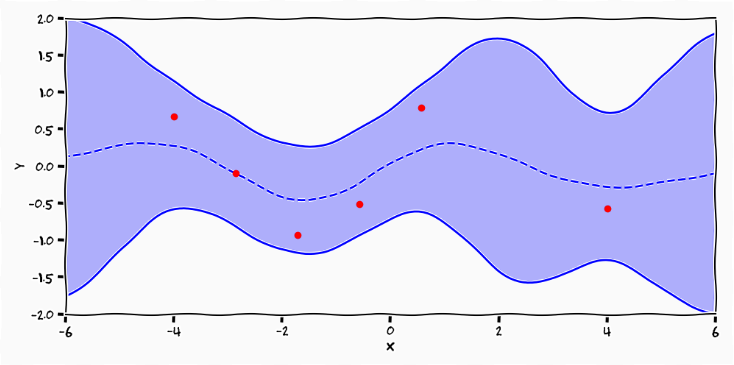
Gaussian Processes: Predictive Posterior Process



Gaussian Processes: Predictive Posterior Process



Gaussian Processes: Predictive Posterior Process



Predictive Posteriors

- Gaussian Process - *Non-parametric formulation*

$$
\begin{aligned}
p(y_* \mid \mathbf{y}, \mathbf{x}_*, \mathbf{X}, \theta) = \mathcal{N}(y_* \mid \mu_*, K_*) \\
\mu_* &= k(x_*, x)k(x, x)^{-1}\mathbf{y} \\
K_* &= k(x_*, x_*) - k(x_*, x)k(x, x)^{-1}k(x, x_*)
\end{aligned}
$$

Predictive Posteriors

- Gaussian Process - *Non-parametric formulation*

$$
\begin{aligned}
p(y_* \mid \mathbf{y}, \mathbf{x}_*, \mathbf{X}, \theta) &= \mathcal{N}(y_* \mid \mu_*, K_*) \\
\mu_* &= k(x_*, x)k(x, x)^{-1}\mathbf{y} \\
K_* &= k(x_*, x_*) - k(x_*, x)k(x, x)^{-1}k(x, x_*)
\end{aligned}
$$

- Linear Regression - *Parametric formulation*

$$
\begin{aligned}
p(y_*|\mathbf{y}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) &= \int p(y_*|\mathbf{x}_*, \mathbf{w}, \beta)p(\mathbf{w}|\mathbf{y}, \mathbf{X}, \alpha, \beta)\mathrm{d}\mathbf{w} \\
&= \mathcal{N}\left((y_* \mid \mu_*(x_*), \Sigma_*(x_*)\right) \\
\mu_* &= \left(\beta(\alpha\mathbf{I} + \beta\mathbf{x}^{\mathrm{T}}\mathbf{x})^{-1}\mathbf{x}\mathbf{y}\right)^{\mathrm{T}}\mathbf{x}_* \\
&= \mathbf{x}_*^{\mathrm{T}}\mathbf{x}\left(\beta(\alpha\mathbf{I} + \beta\mathbf{x}^{\mathrm{T}}\mathbf{x})\right)^{-1}\mathbf{y} \\
\Sigma_* &= \frac{1}{\beta} + \mathbf{x}_*^{\mathrm{T}}(\alpha\mathbf{I} + \beta\mathbf{x}^{\mathrm{T}}\mathbf{x})^{-1}\mathbf{x}
\end{aligned}
$$

Regression Models: Mean

$$k(x_*, x)k(x, x)^{-1}\mathbf{y} \qquad \mathbf{x}_*^{\mathrm{T}}\mathbf{x}\left(\beta(\alpha\mathbf{I} + \beta\mathbf{x}^{\mathrm{T}}\mathbf{x})\right)^{-1}\mathbf{y}$$

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- this leads to the interpretation of GPs as infinite basis functions

Summary

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- Non-parametrics
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- Non-parametrics
  - parametrise relationship between data
- Gaussian processes
  - Implementation: "just a big big Gaussian"
  - Theory: projection of an infinite stochastic process

Kolmogrovs Extension Theorem

For all permutations π, measurable sets $F_i \subseteq \mathbb{R}^n$ and probability measure ν

1. Exchangeable

$$\nu_{t_{\pi(1)}\cdots t_{\pi(k)}}\left(F_{\pi(1)} \times \cdot \times F_{\pi(k)}\right) = \nu_{t_1 \cdots t_k}\left(F_1 \times \cdots \times F_k\right)$$

2. Marginal

$$\nu_{t_1 \cdot t_k}\left(F_1 \times \cdot \times F_k\right) = \nu_{t_1 \cdots t_k, t_{k+1} \cdot t_{k+m}}\left(F_1 \times \cdot \times F_k \times \mathbb{R}^n \times \cdot \times \mathbb{R}^n\right)$$

In this case the finite dimensional probability measure is a realisation of an underlying stochastic process eof