



Machine Learning and the Physical World

Lecture 3 : Gaussian Processes

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Model+Data → Predict

Data + Model $\overset{\text{Compute}}{\overrightarrow{}}$ Prediction

Model+Data → Predict

$$\text{Data} + \text{Model} \xrightarrow{\text{Compute}} \text{Prediction}$$

- We do not have enough knowledge

$$\text{Model} \not\xrightarrow{\text{Compute}} \text{Prediction}$$

Model+Data → Predict



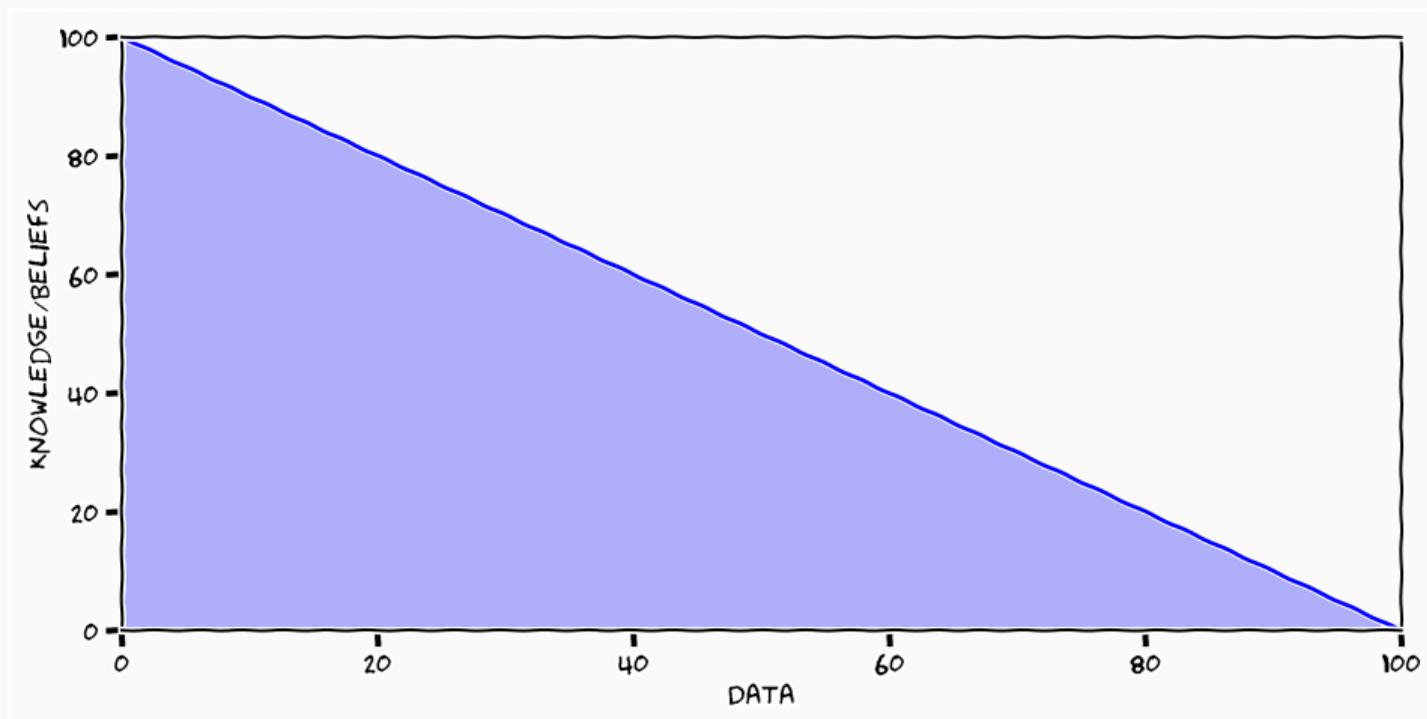
- We do not have enough knowledge



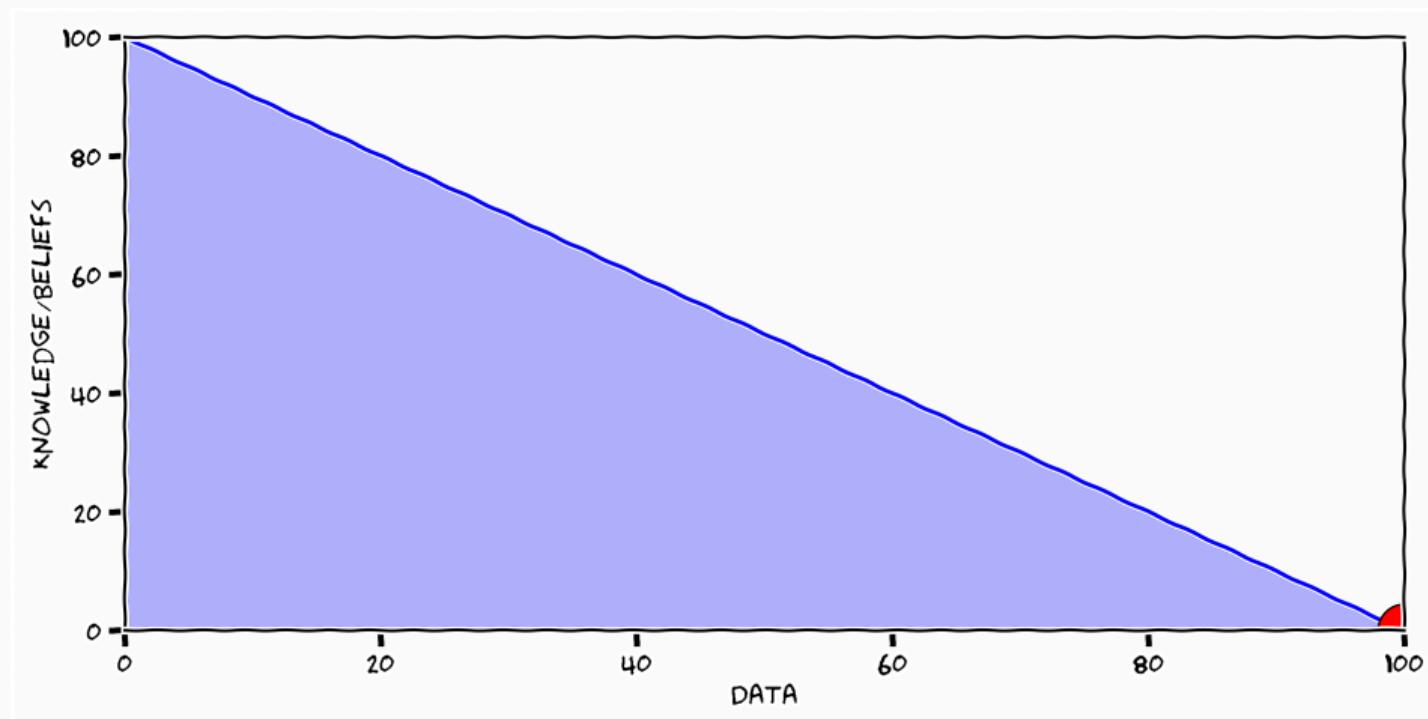
- We do not have enough data



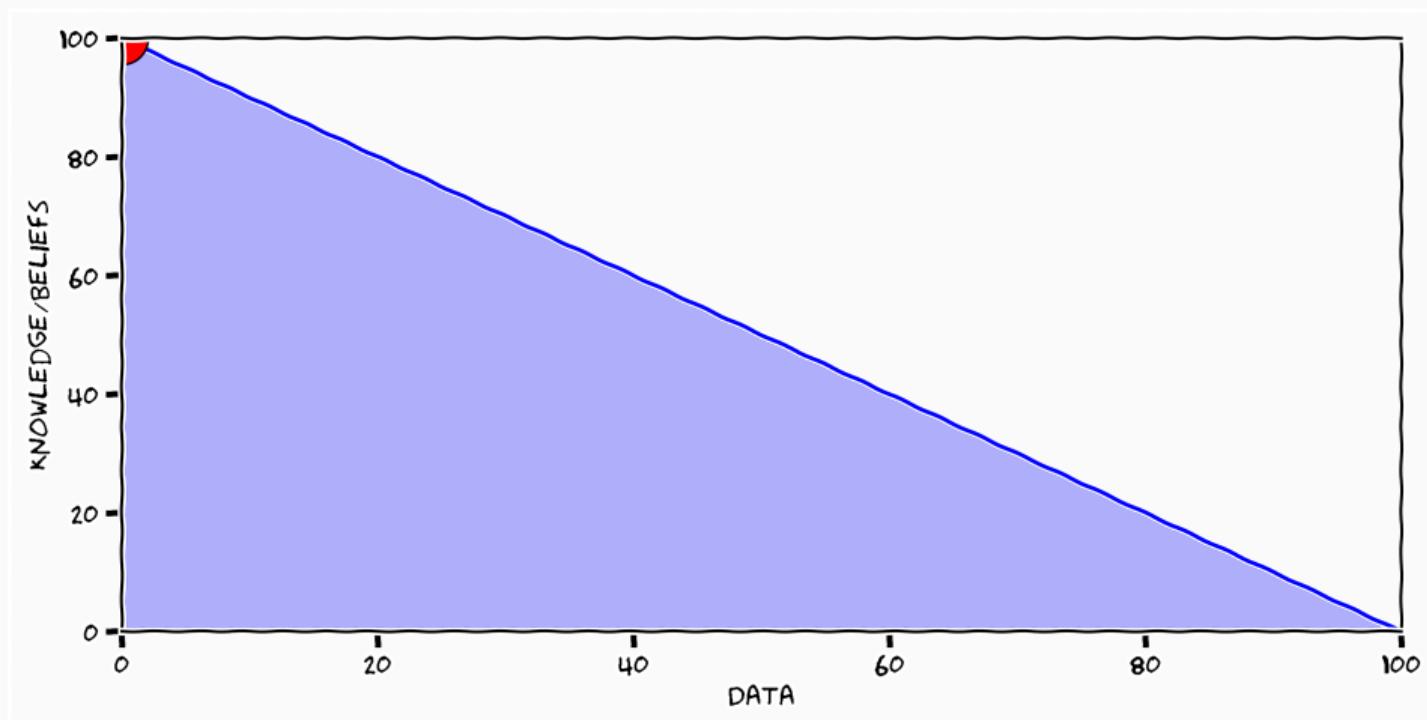
Data and Knowledge



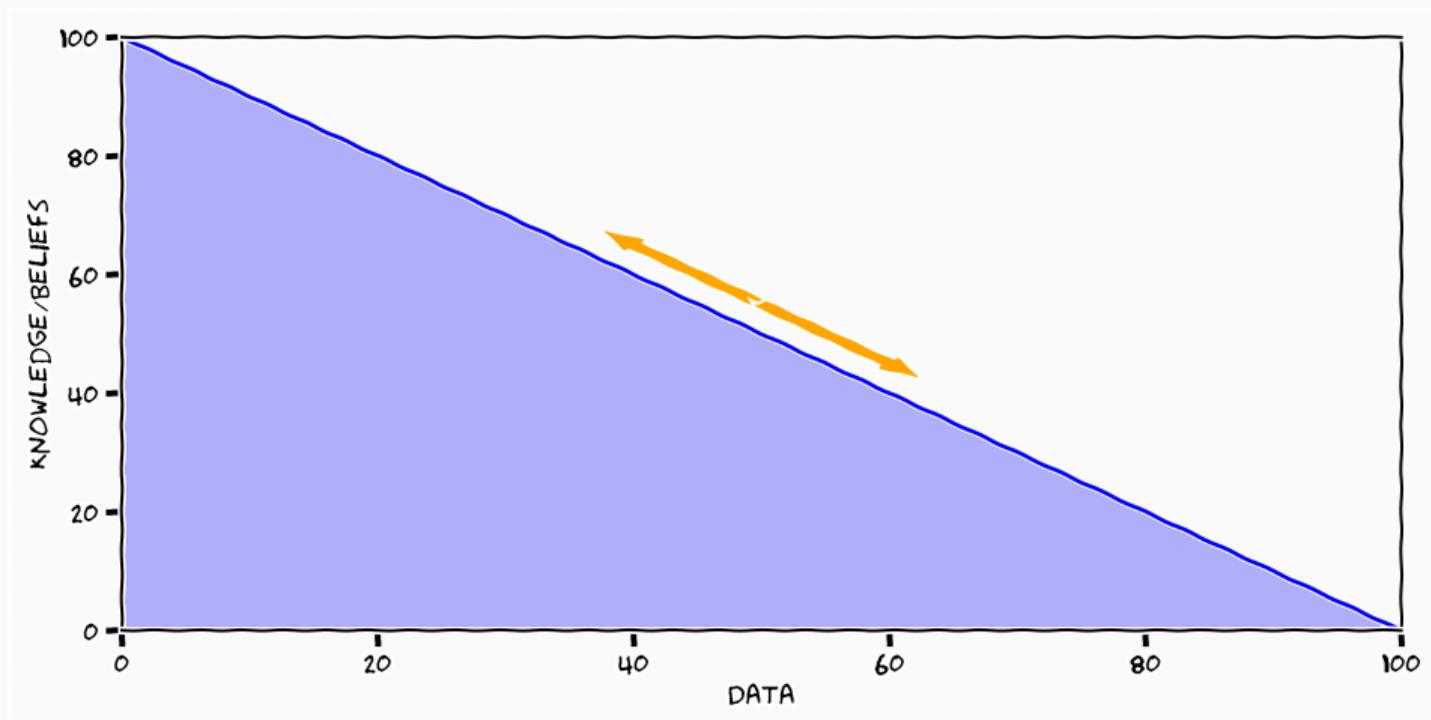
Data and Knowledge



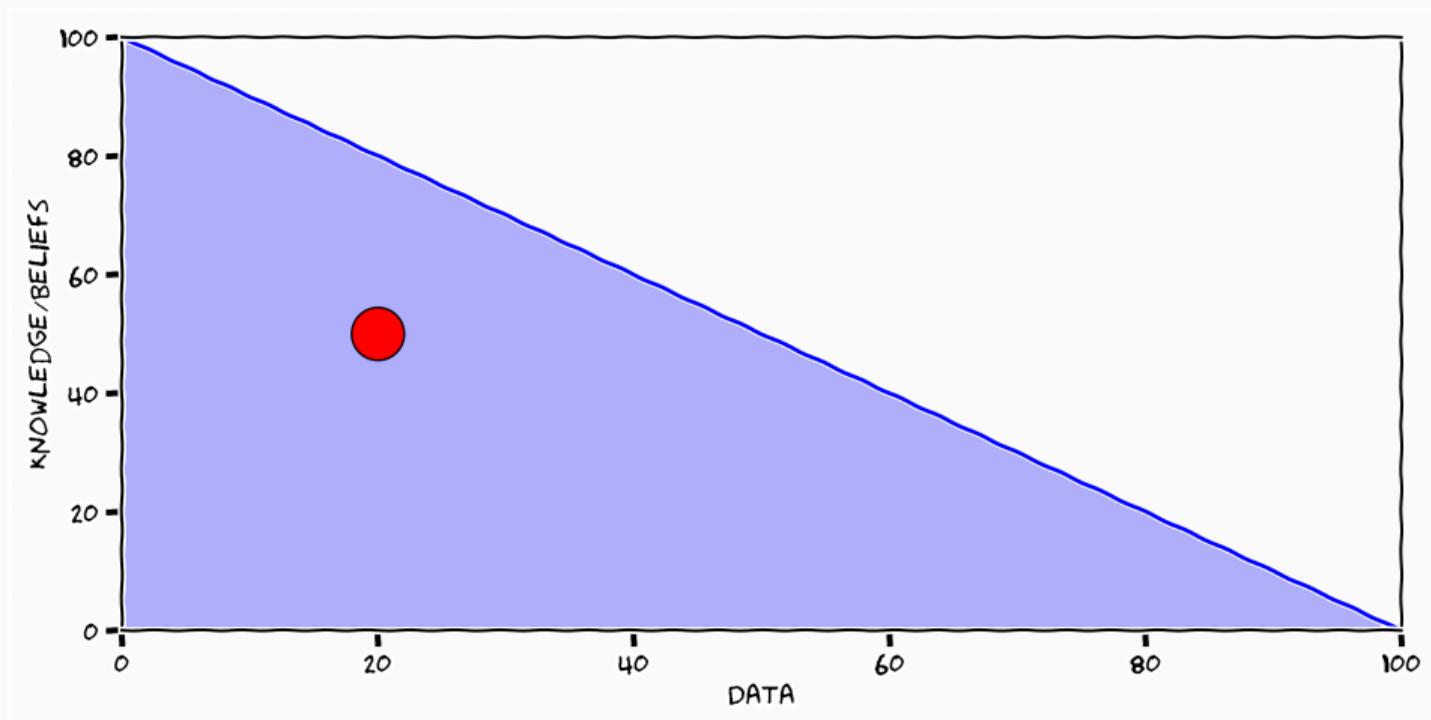
Data and Knowledge



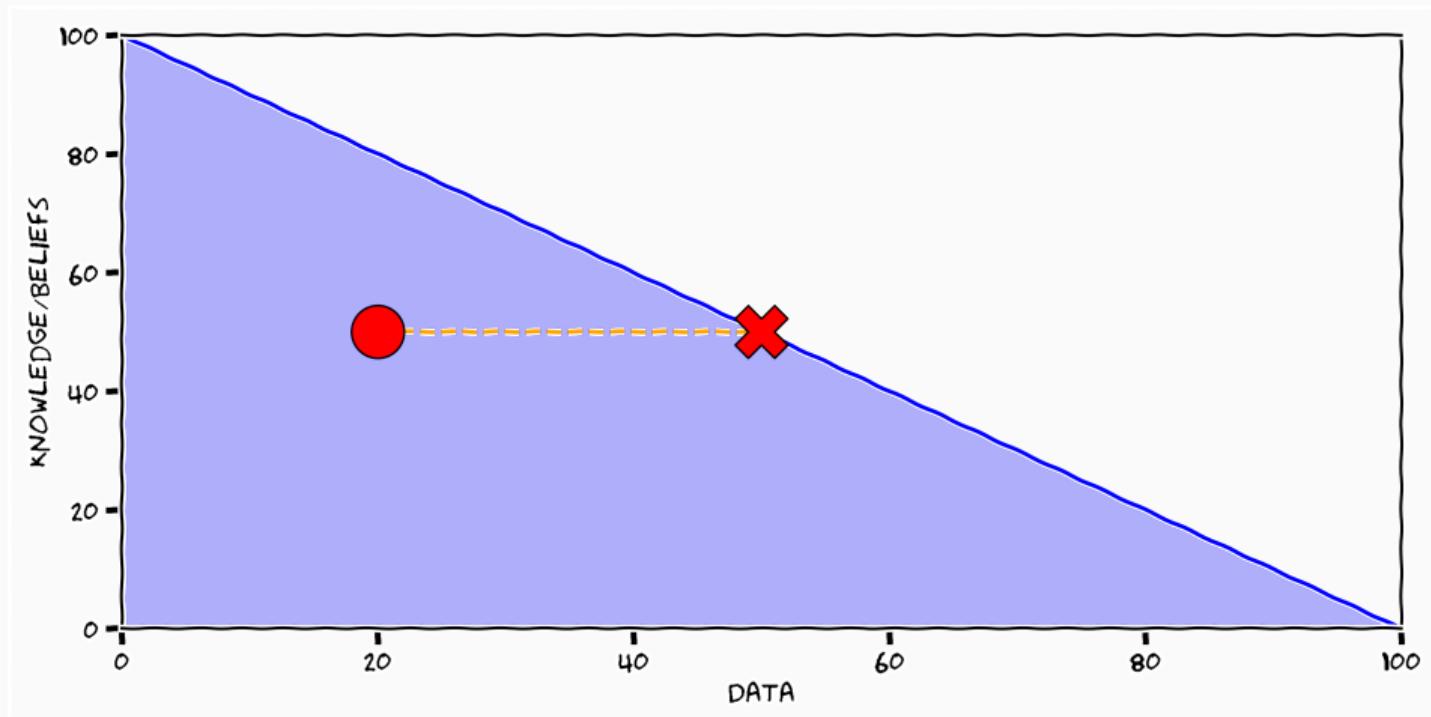
Data and Knowledge



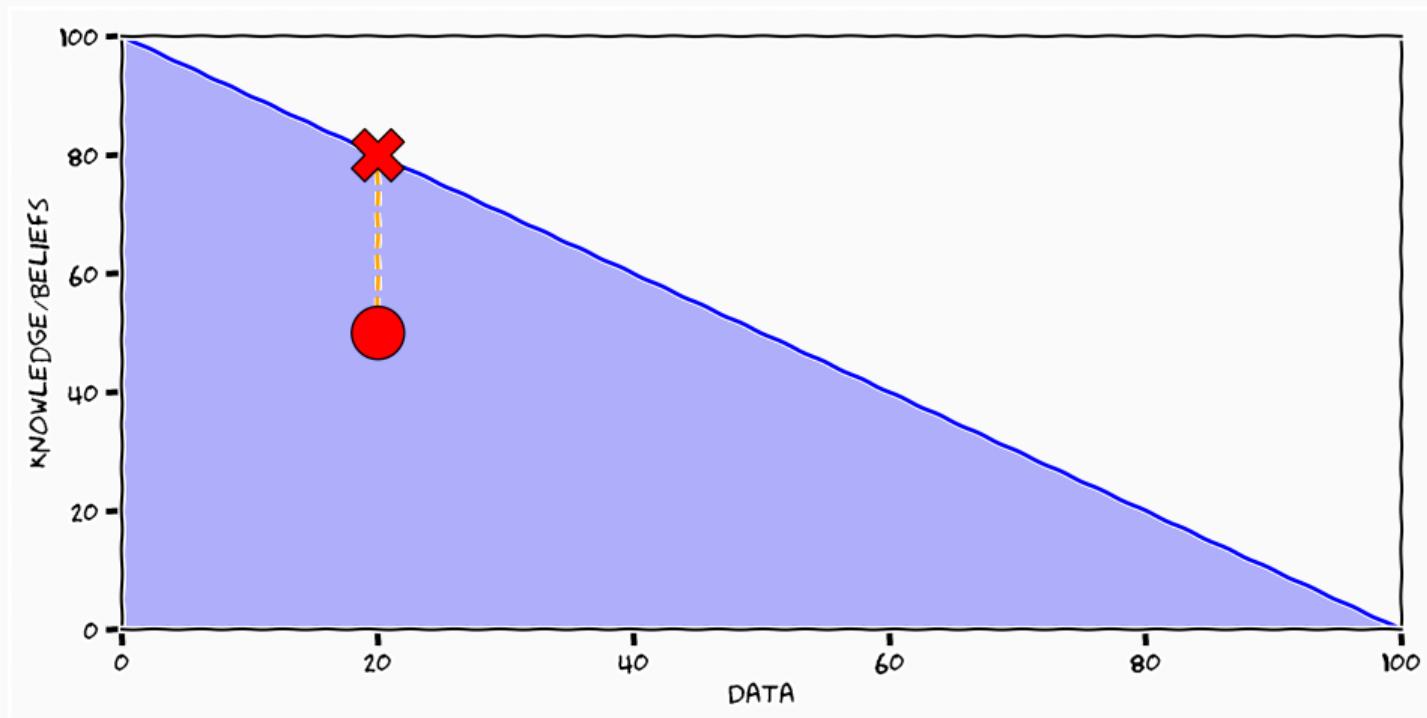
Data and Knowledge



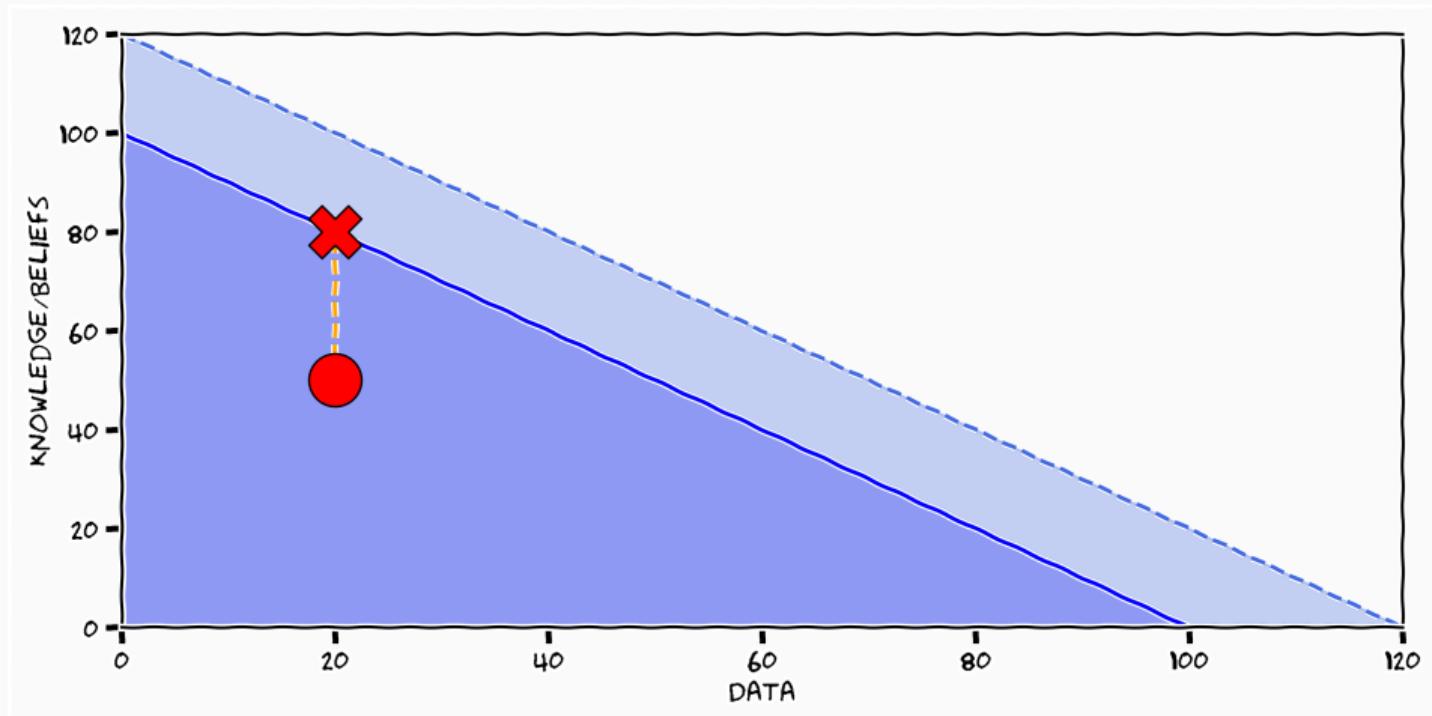
Data and Knowledge



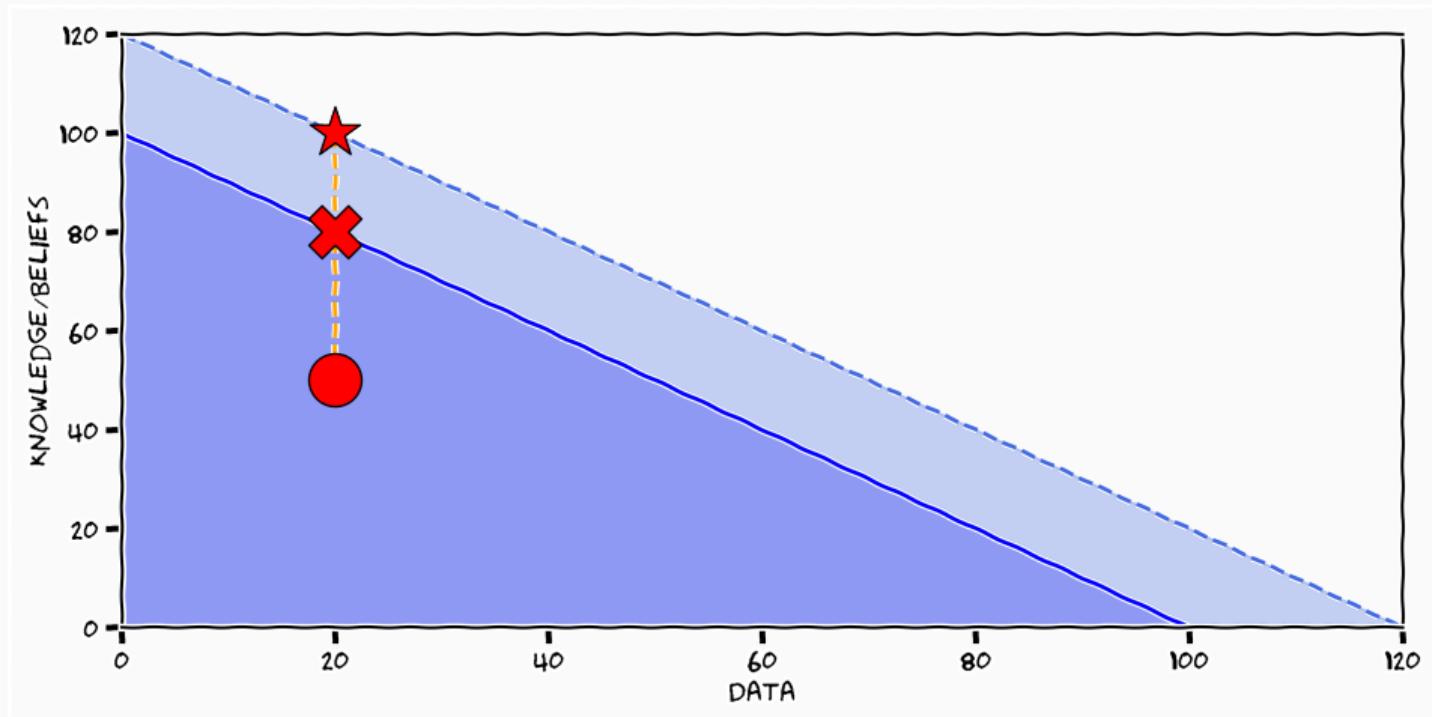
Data and Knowledge



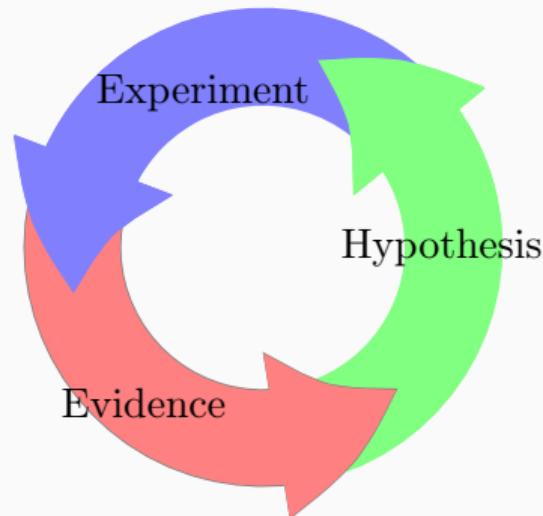
Data and Knowledge



Data and Knowledge

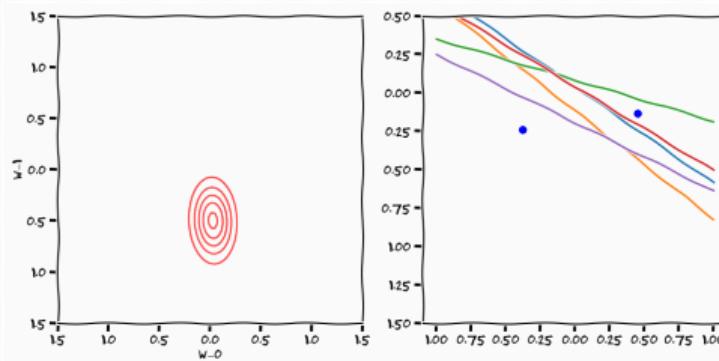
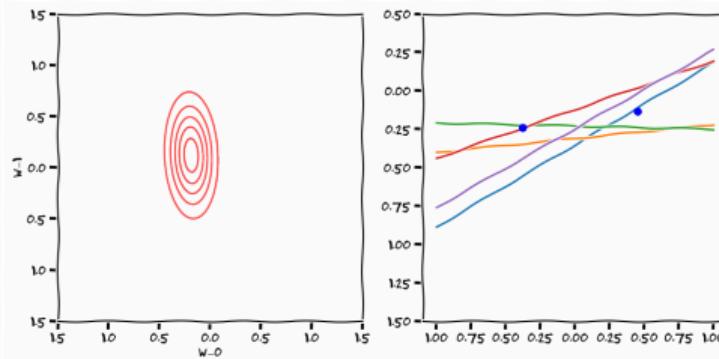


The Scientific Principle



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

Knowledge is Relative



$$\mathcal{A}_{\mathcal{H}}(\mathcal{S})$$

- \mathcal{H} - hypothesis space
- \mathcal{A} - "traverse" mechanism of the hypothesis space
- \mathcal{S} - training data

- Machine Learning as a Framework



- Machine Learning as a Framework



- Machine Learning as a Science

- how to construct "handles" to allow us to input knowledge

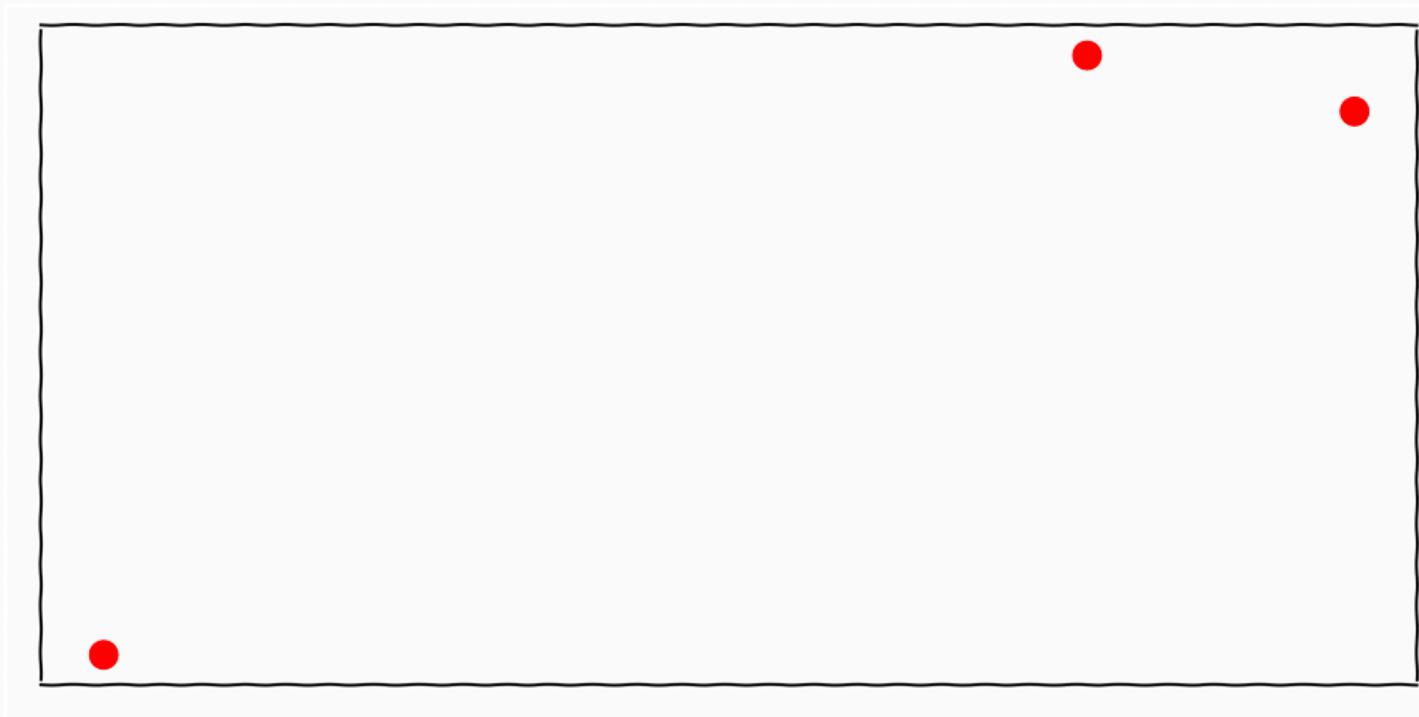
- How to specify beliefs over larger classes of hypothesis

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

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

Non-parametrics

Hypothesis Classes

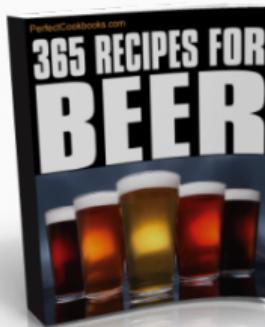


Non-parametrics

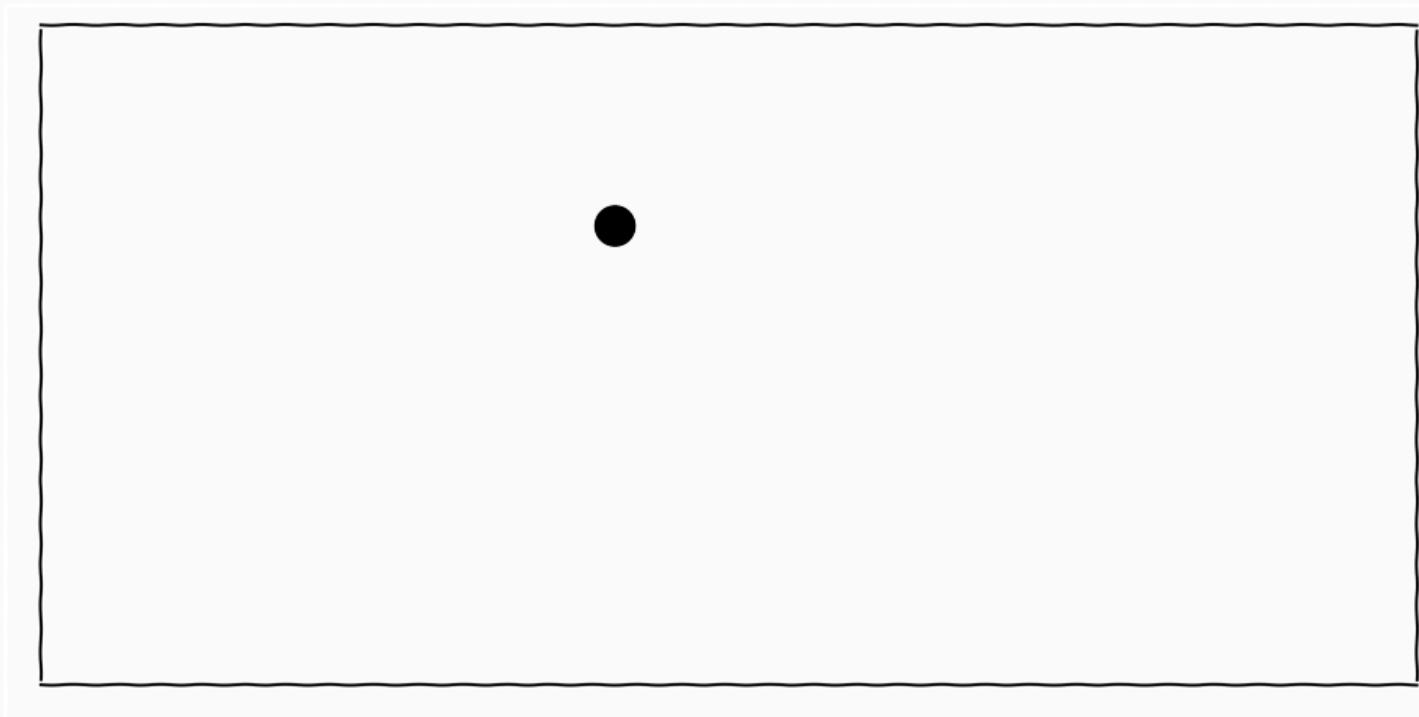




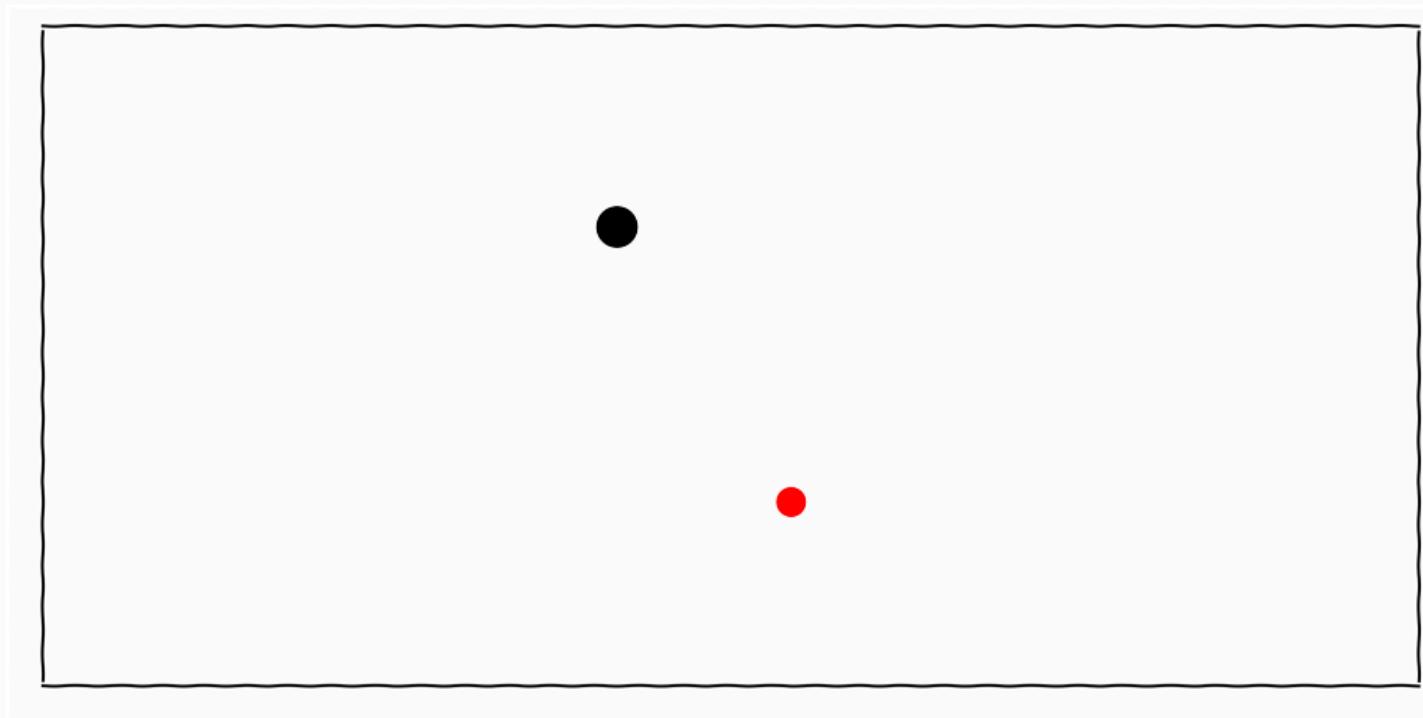
Non-parametrics



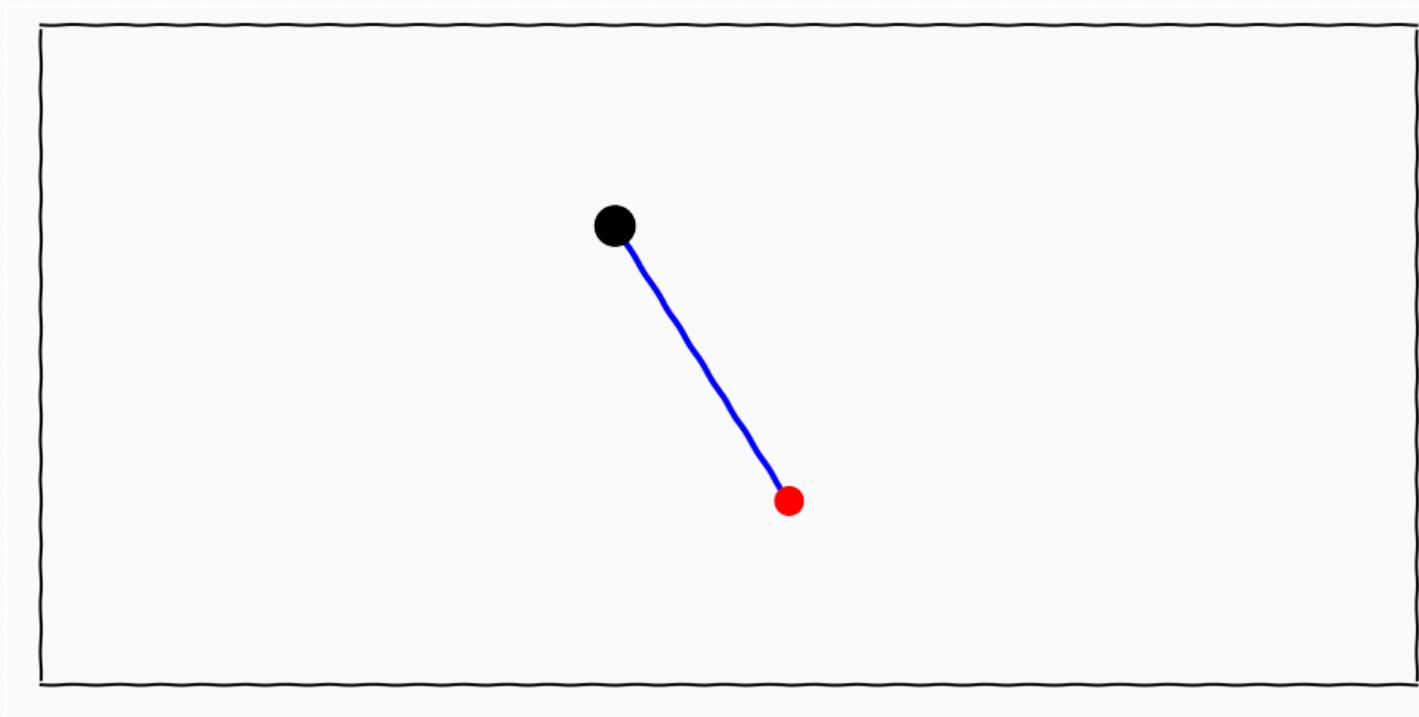
Example



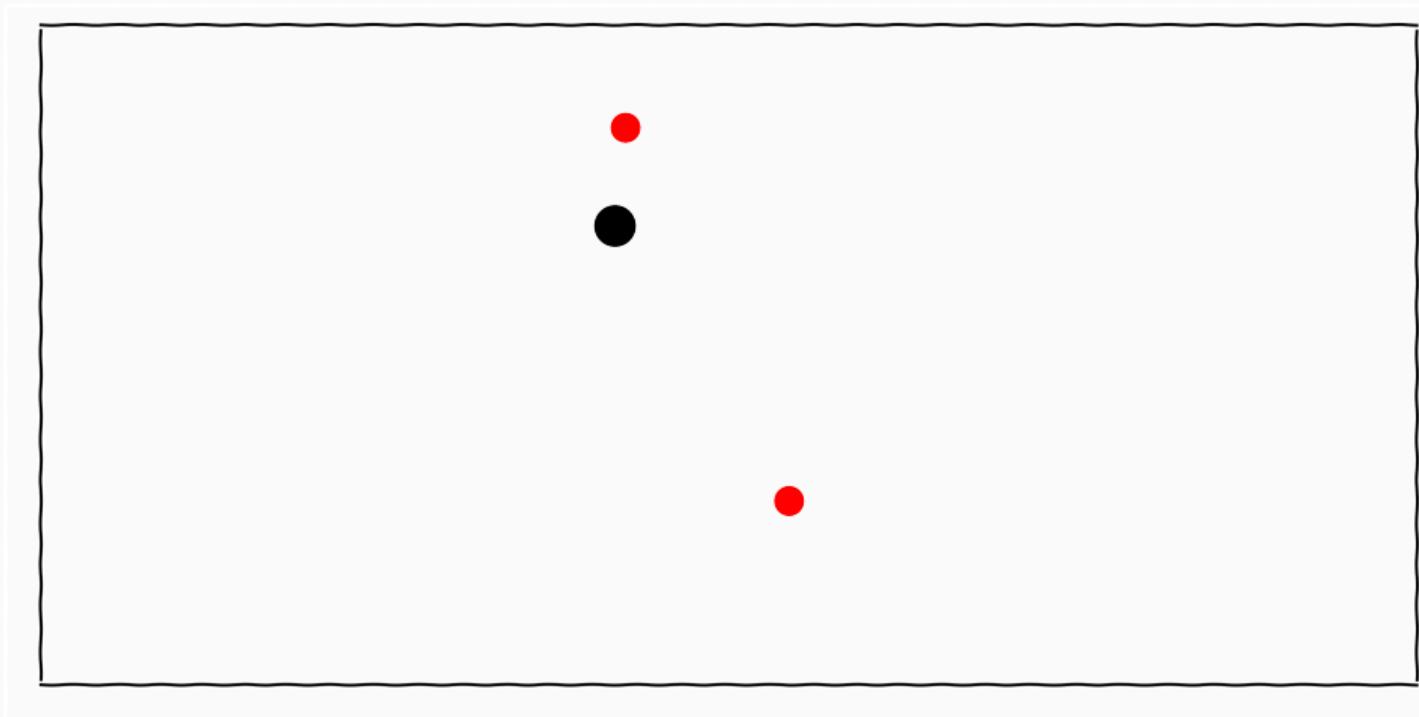
Example



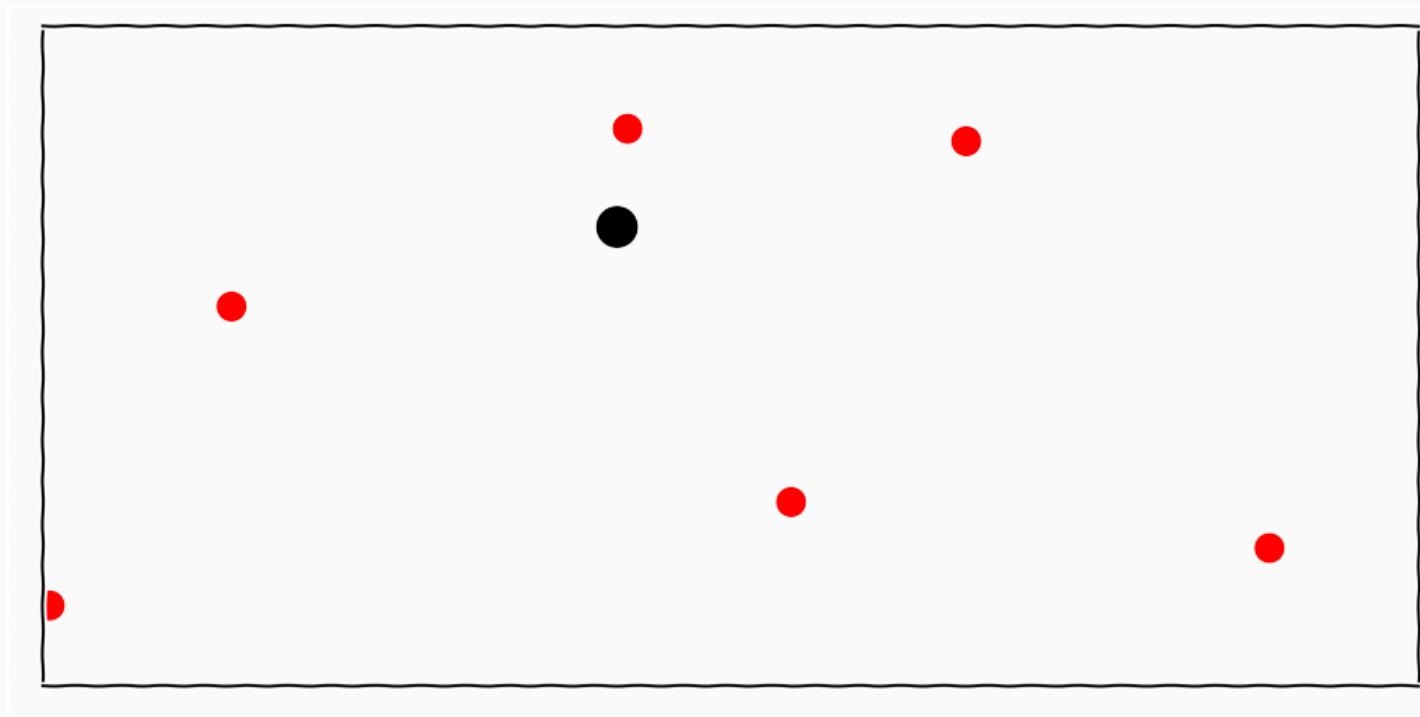
Example



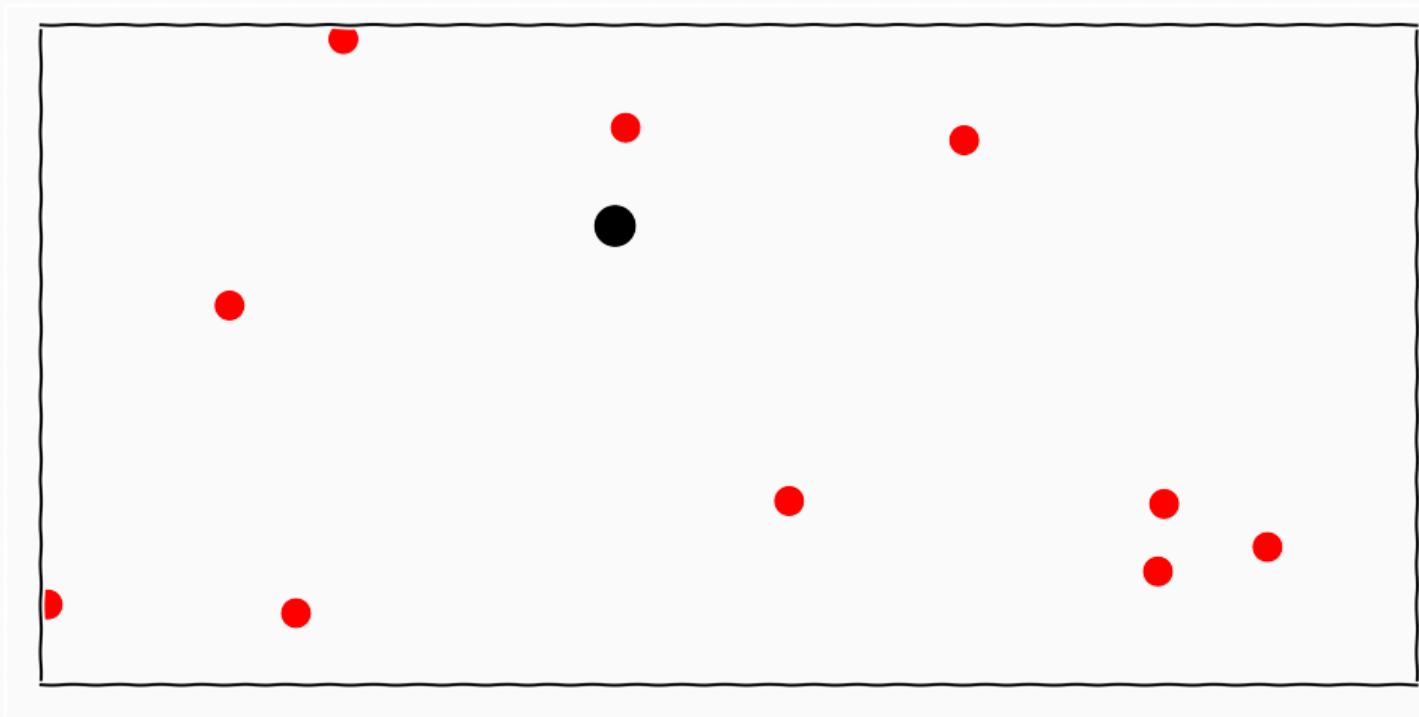
Example



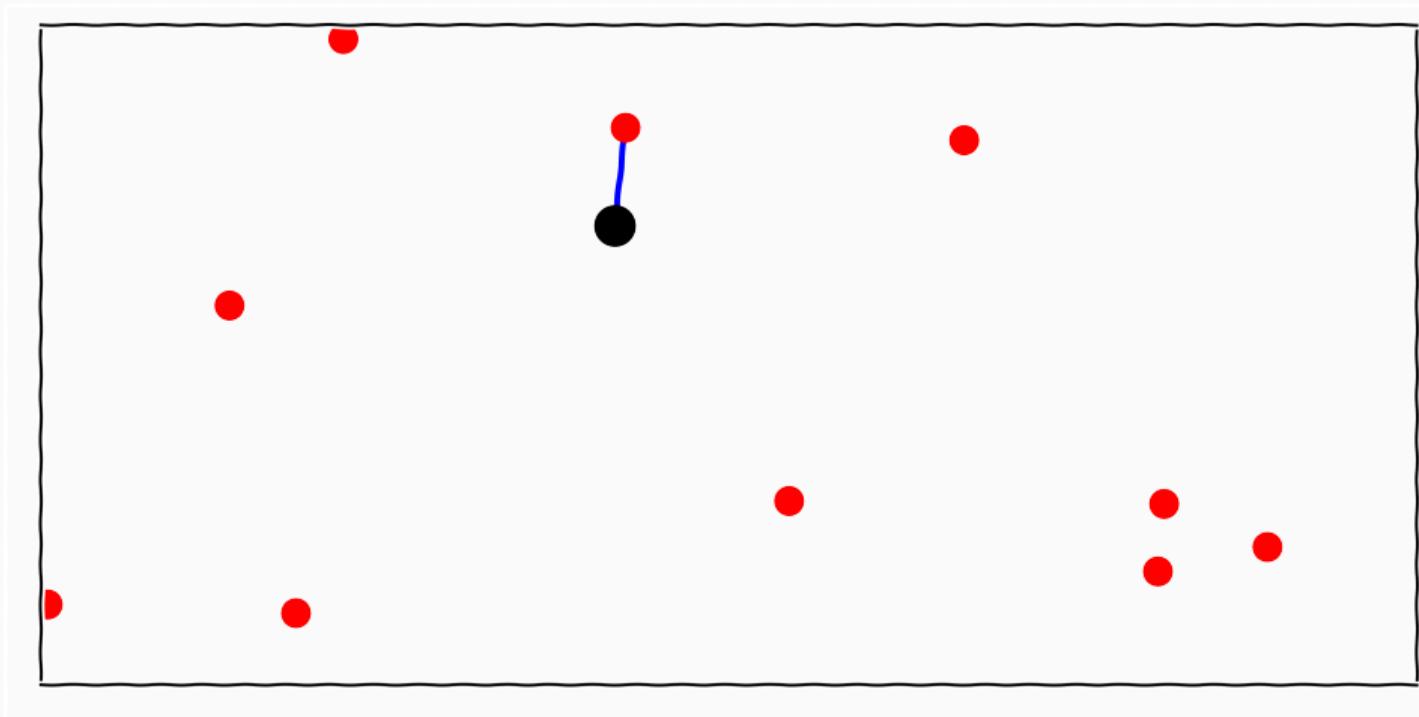
Example



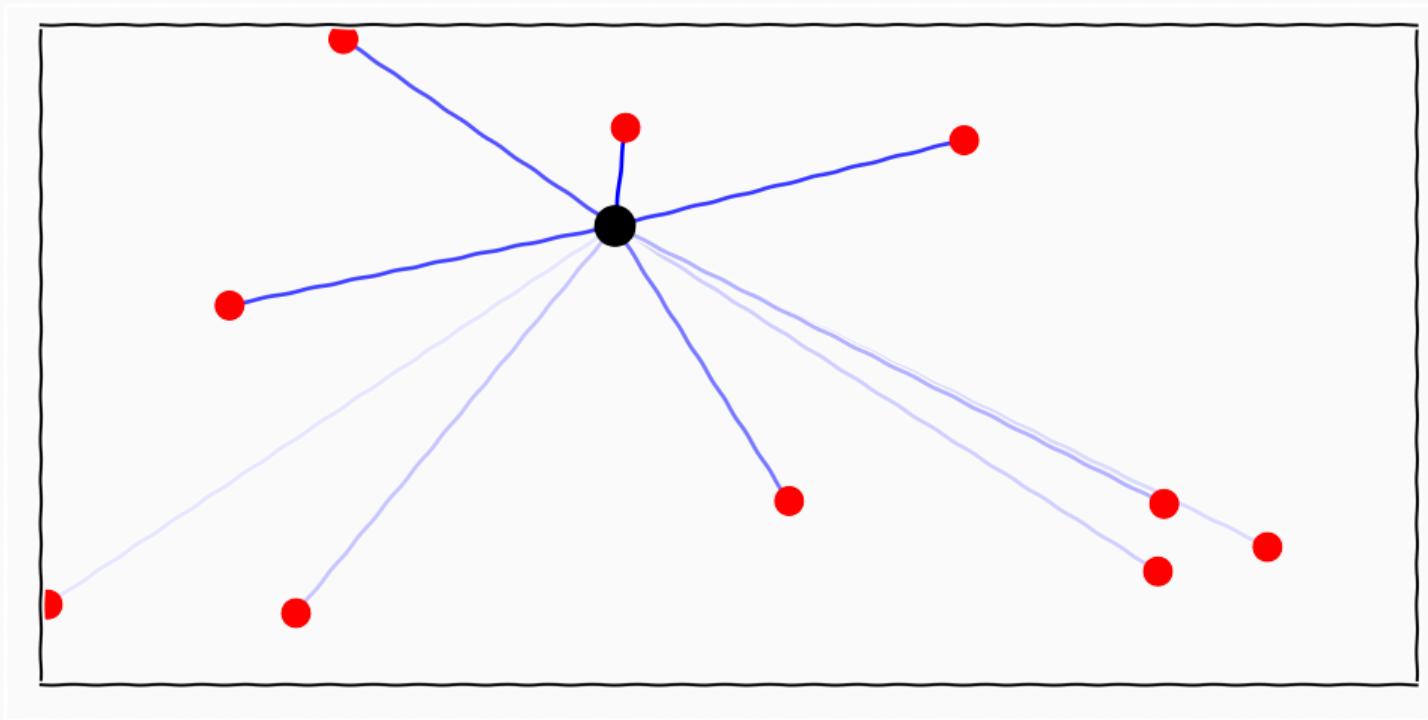
Example



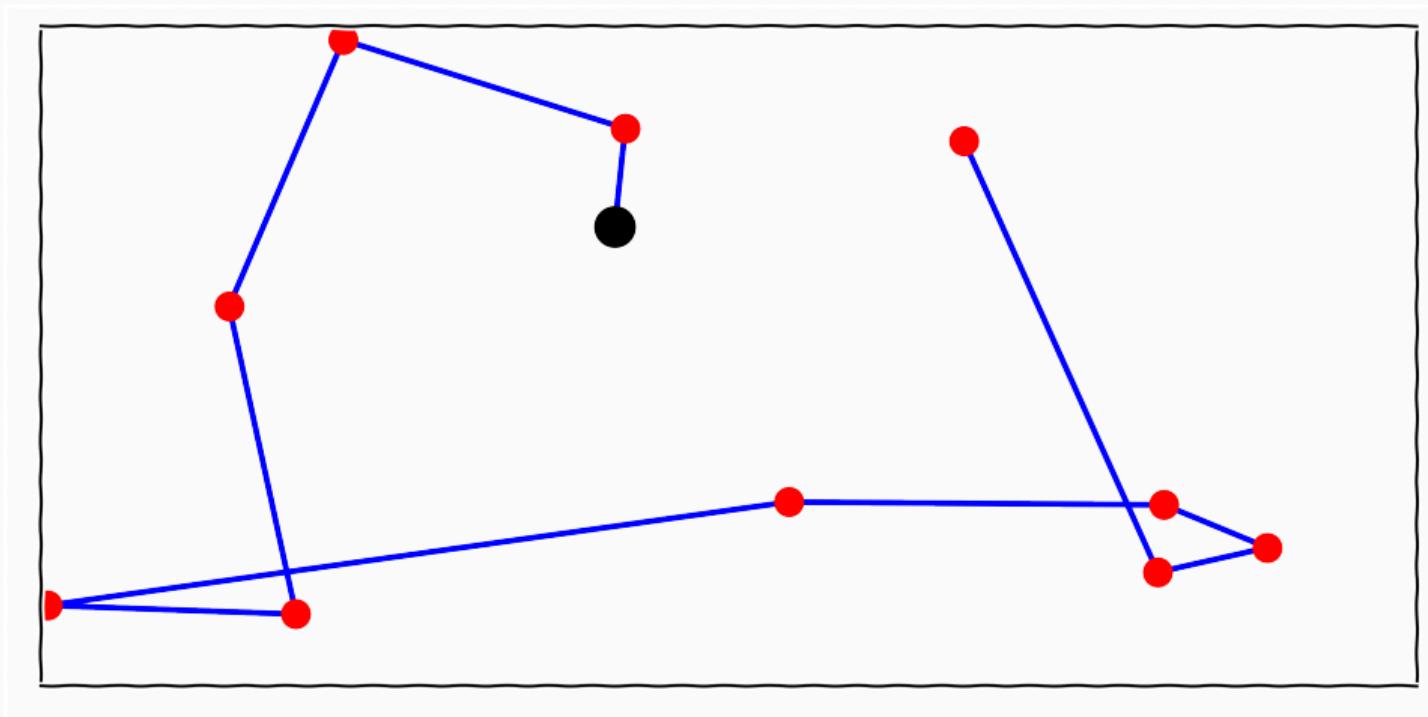
Example



Example

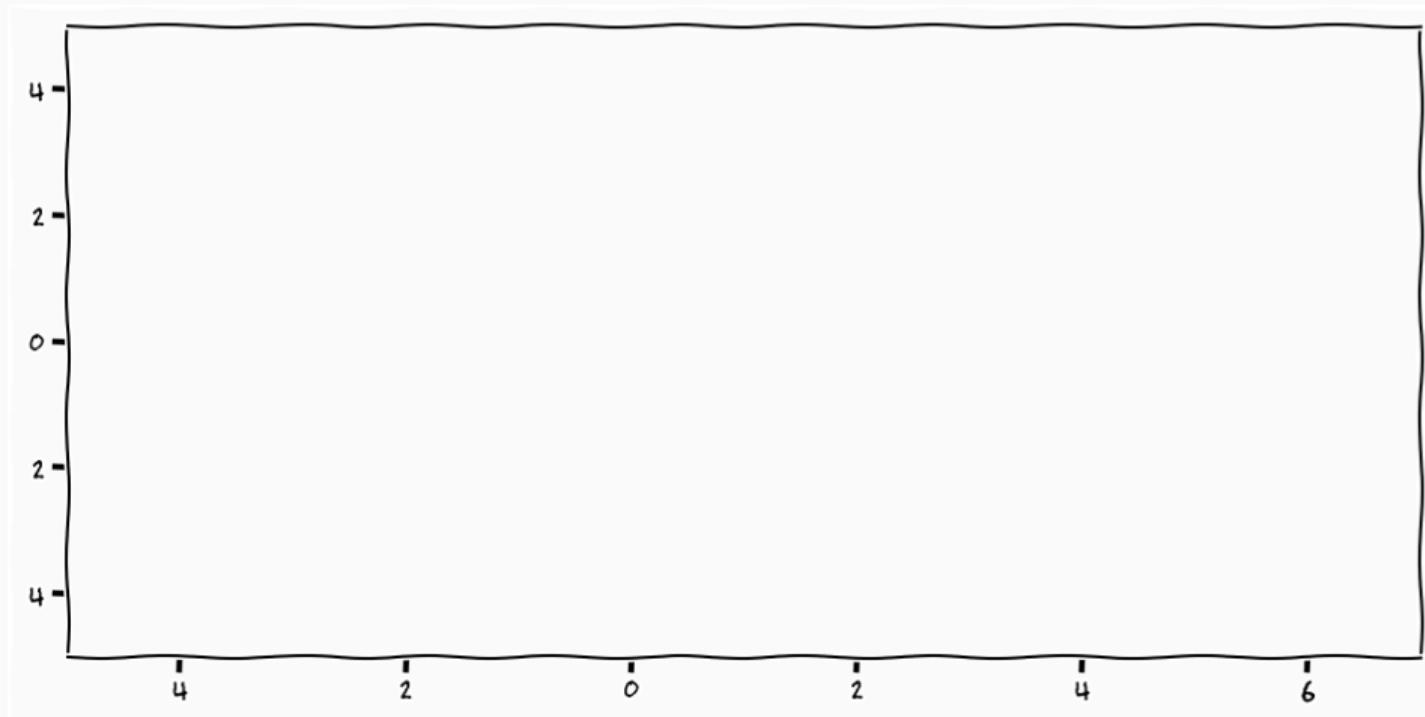


Example

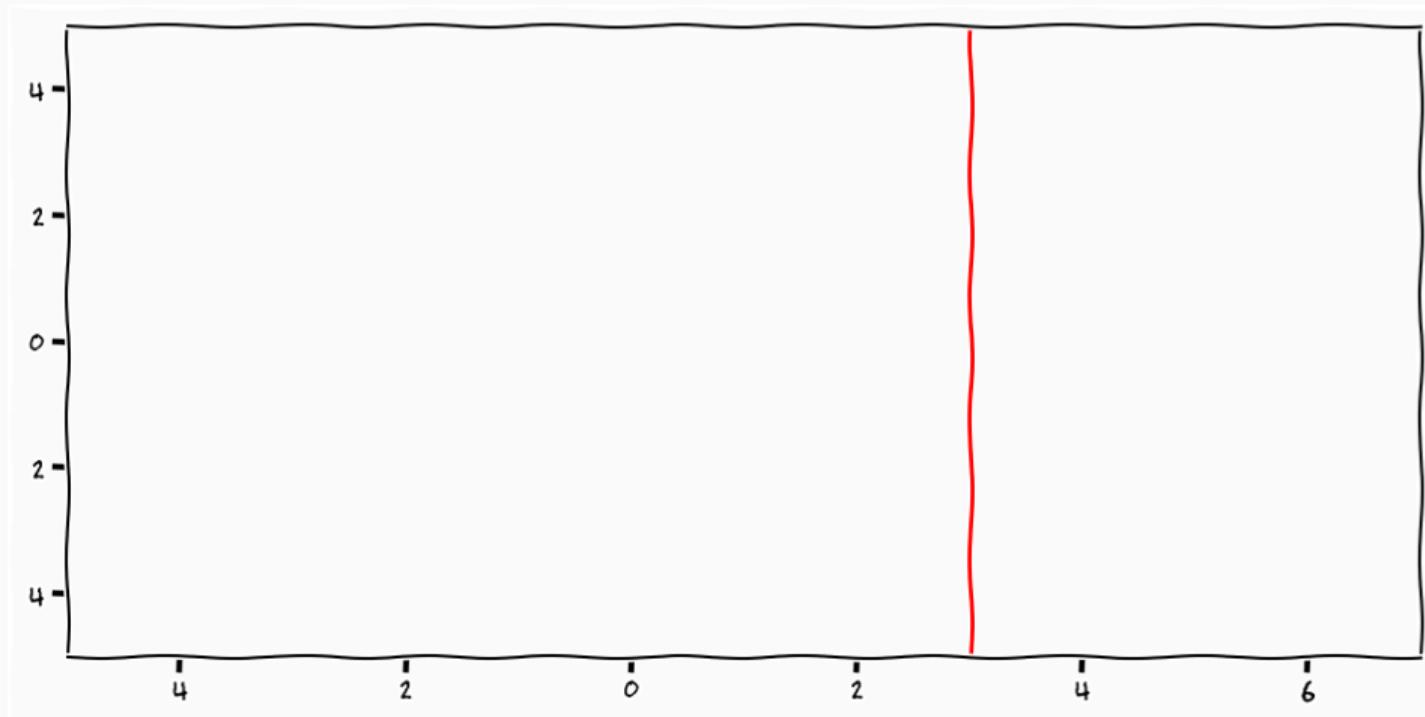


Non-parametric Functions

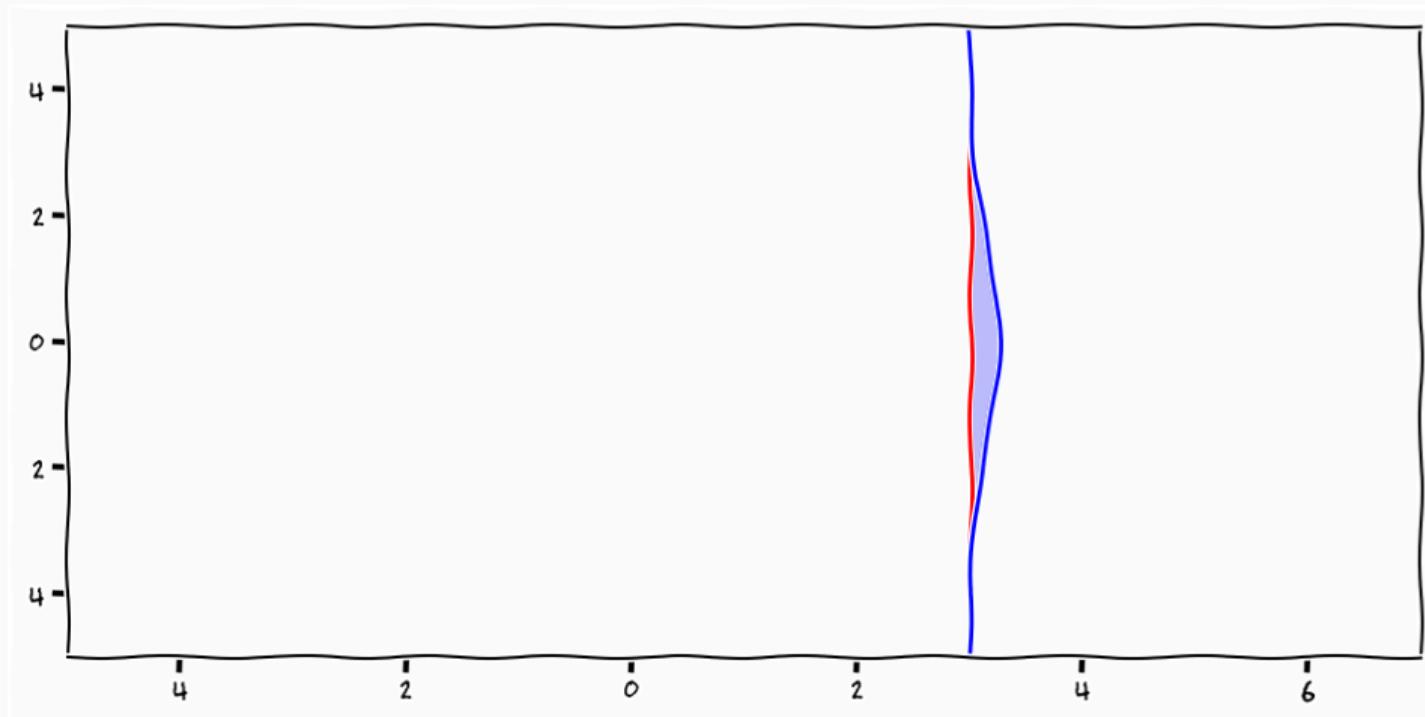
Lets talk about functions



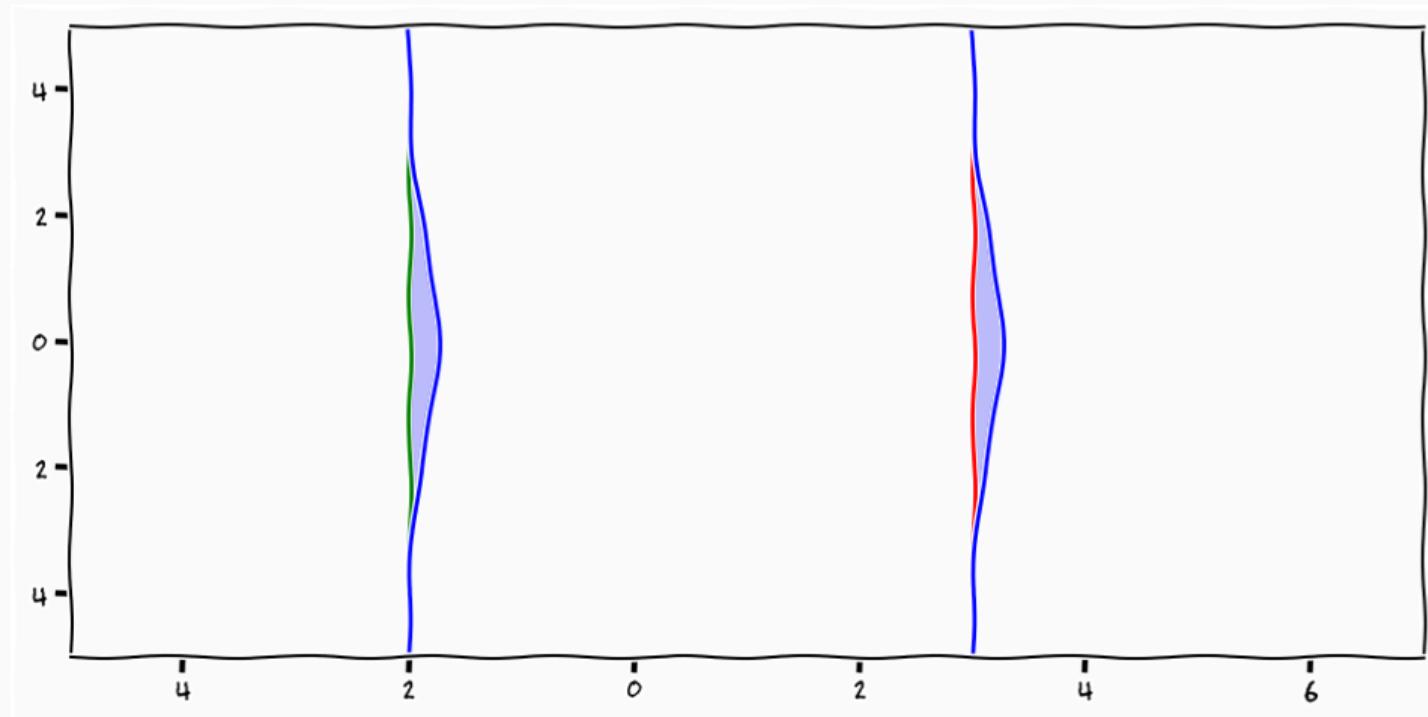
Lets talk about functions



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Lets talk about functions

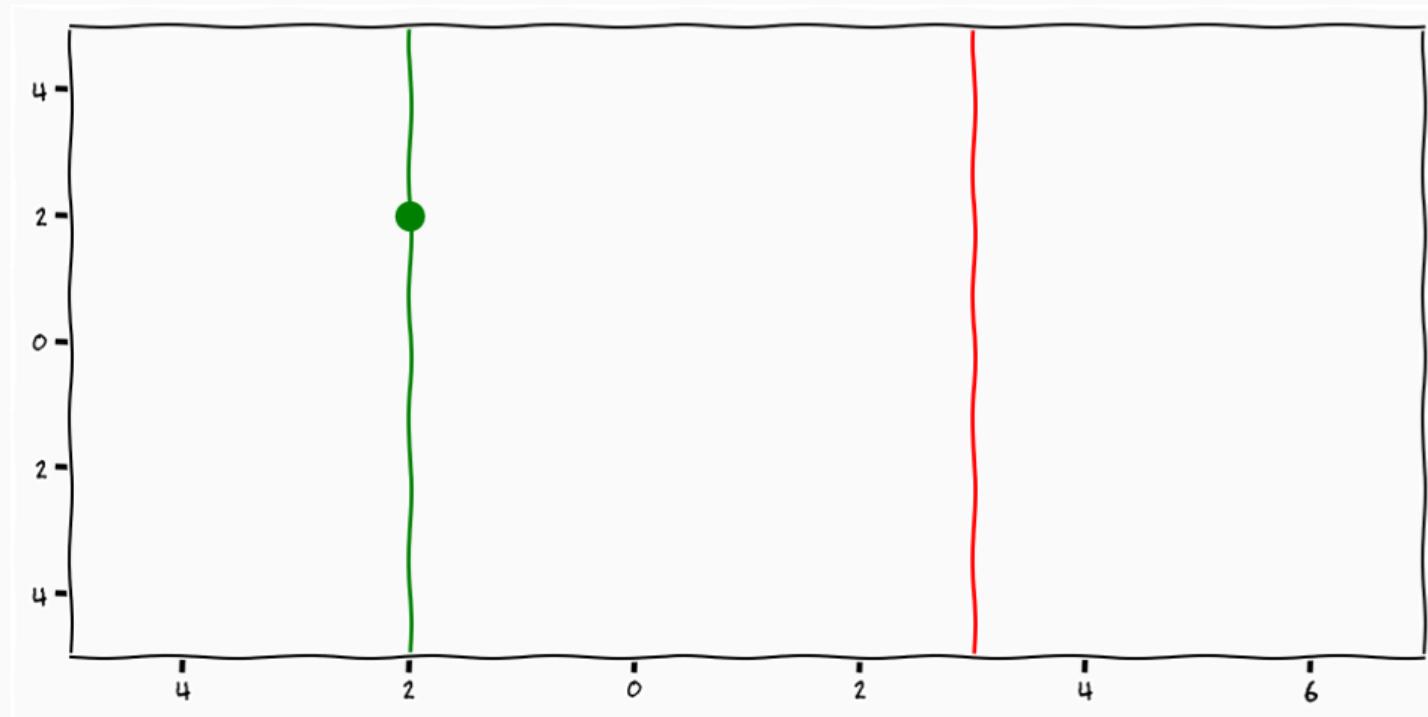


Gaussian function values

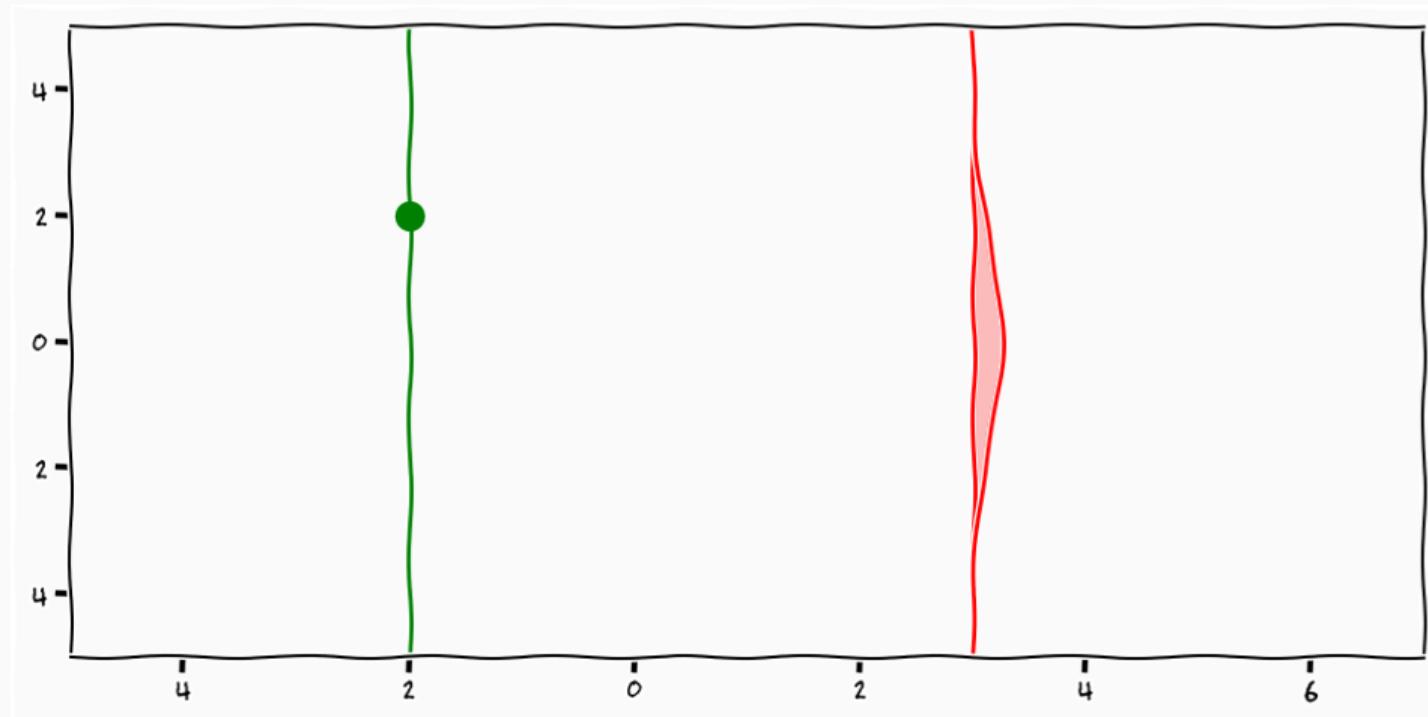
$$f_1 = \mathcal{N}(\mu_1, k_1)$$

$$f_2 = \mathcal{N}(\mu_2, k_2)$$

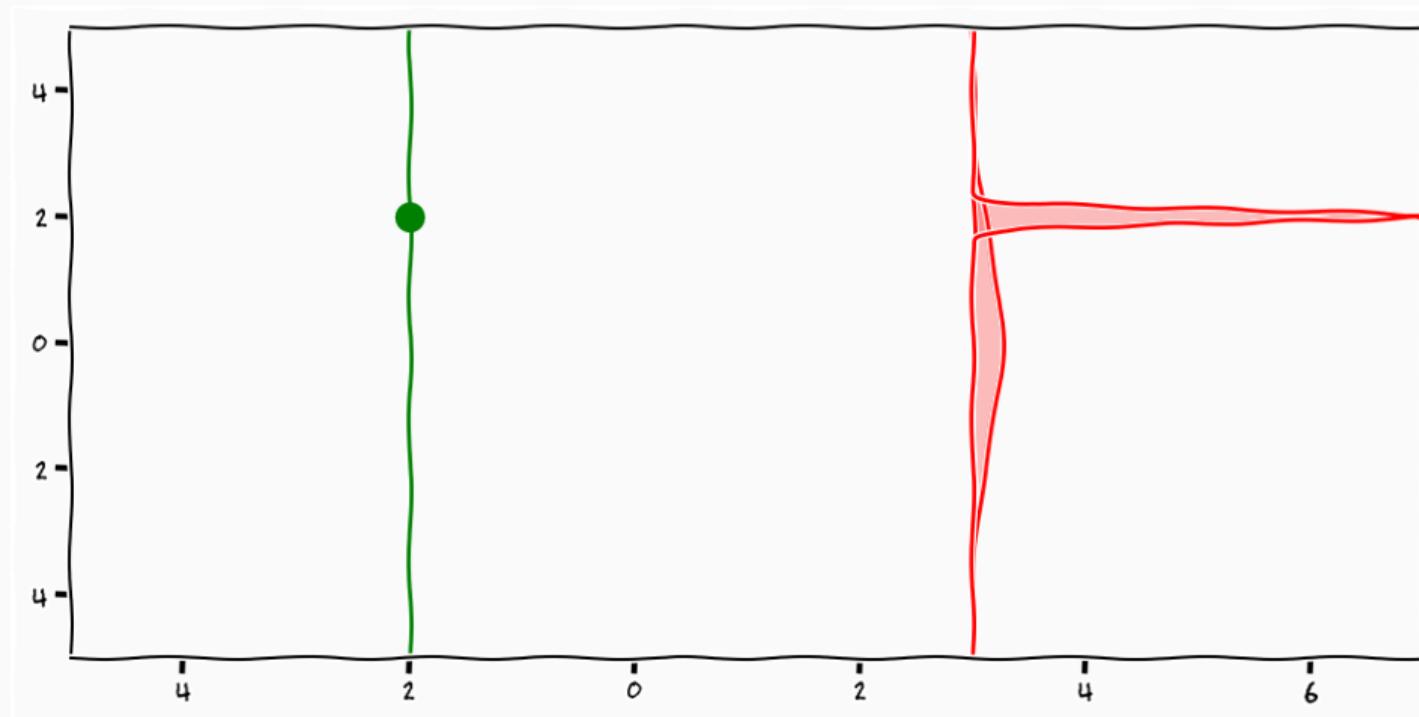
Non-parametric functions



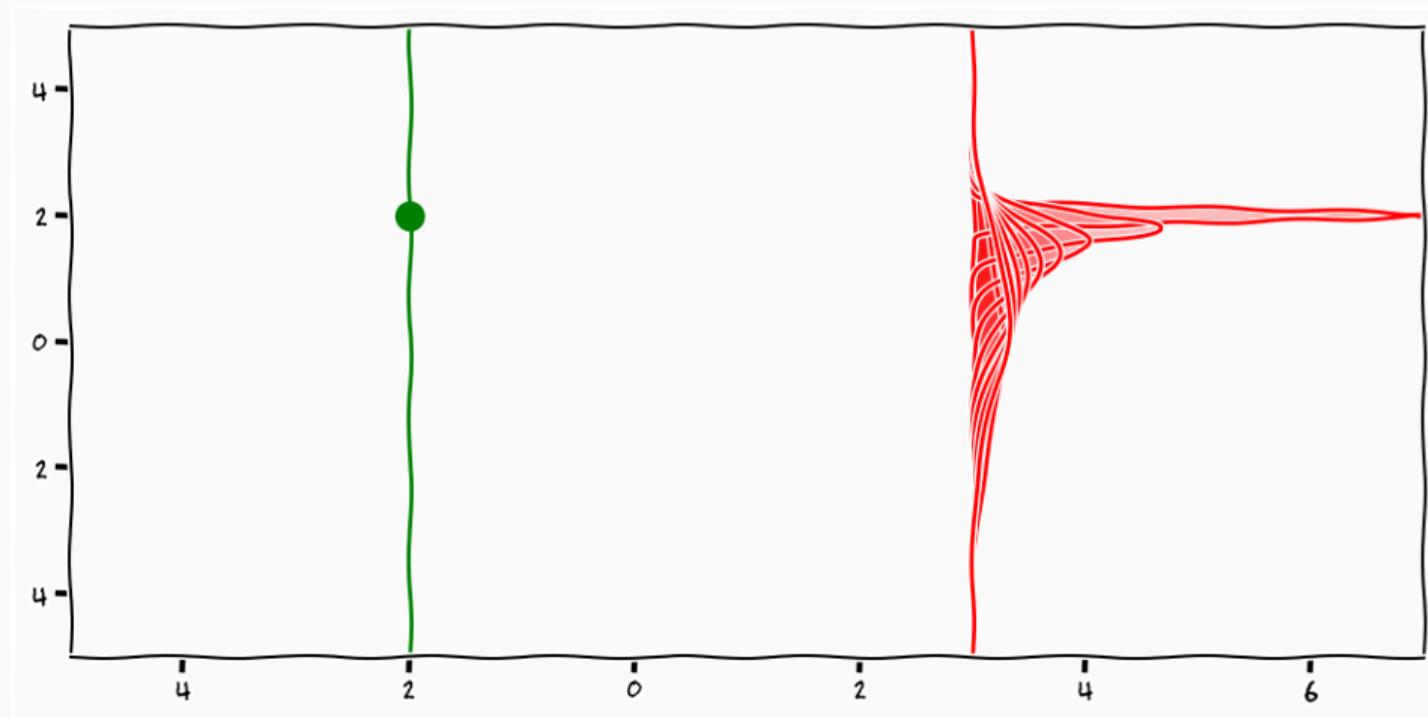
Non-parametric functions



Non-parametric functions



Non-parametric functions



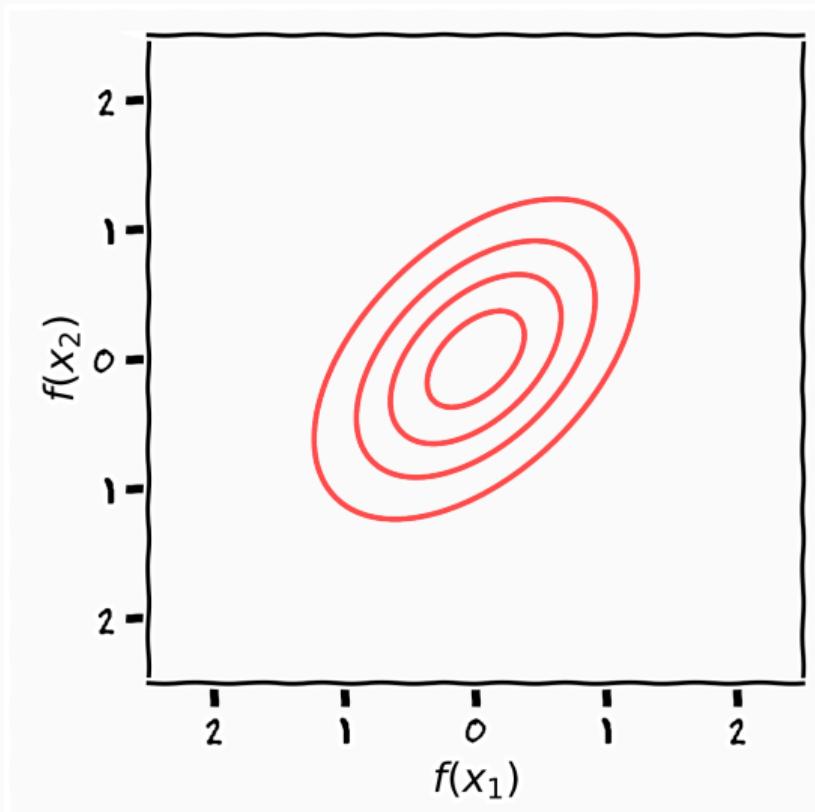
Jointly Gaussian function values

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

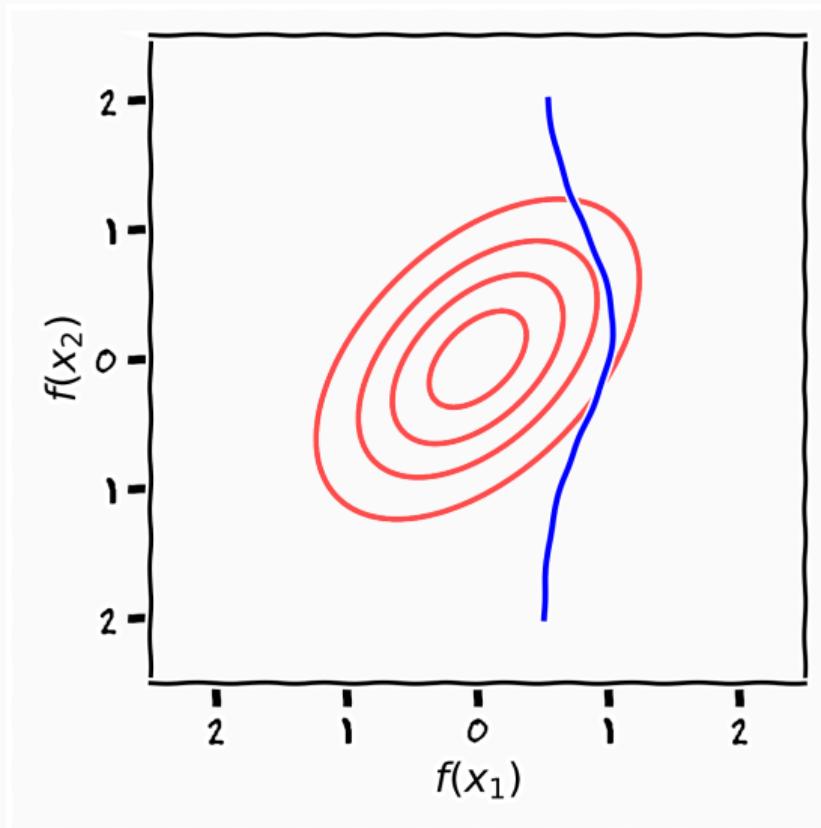
Conditional Gaussians

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix} \right)$$

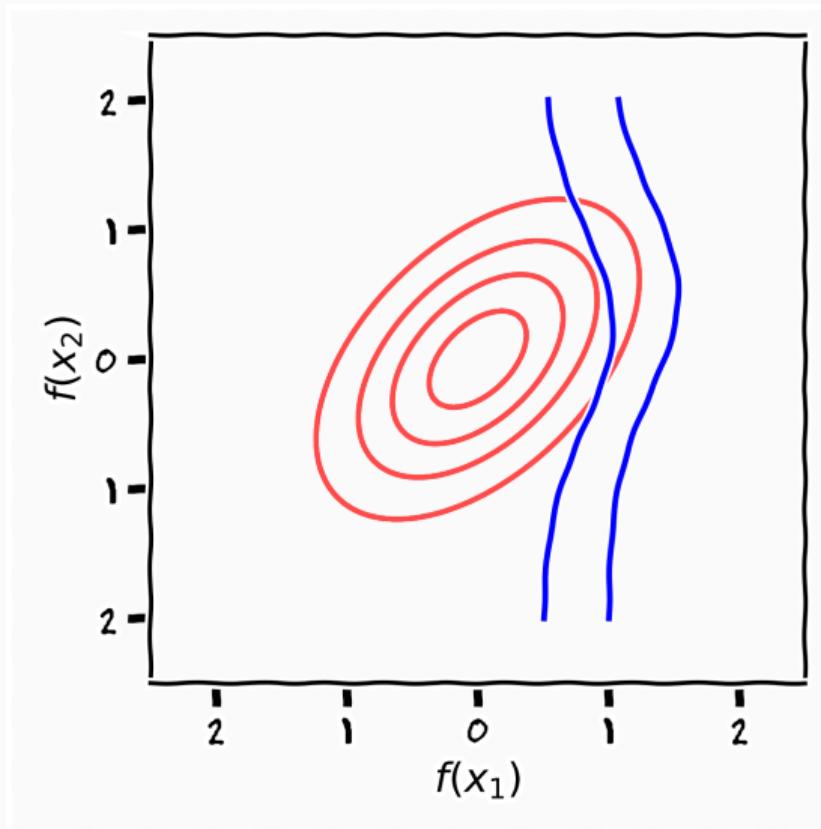
Conditional Gaussians



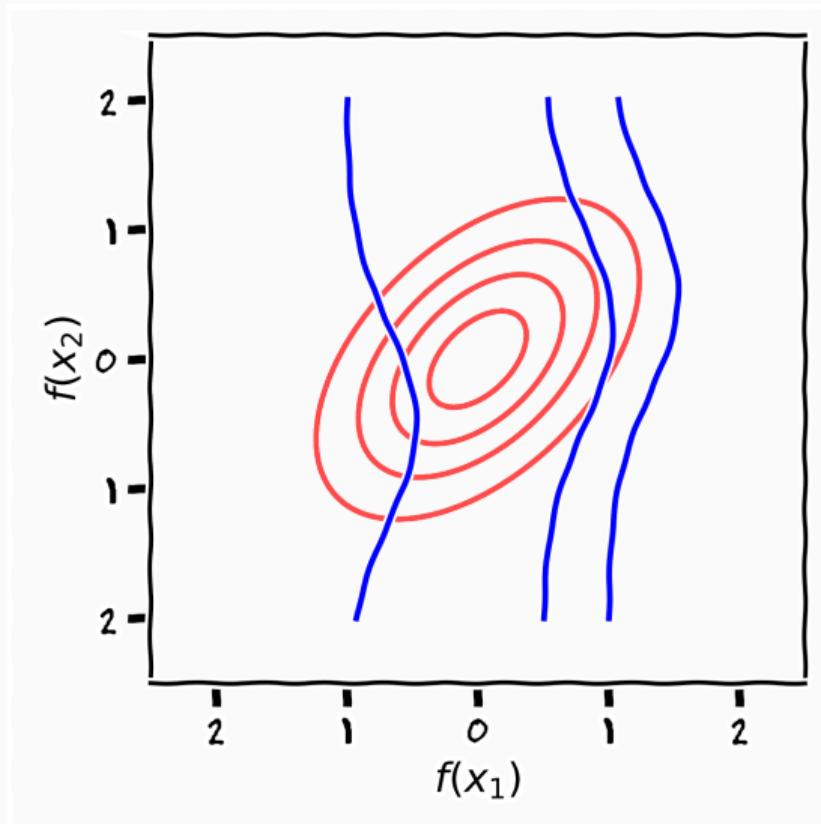
Conditional Gaussians



Conditional Gaussians



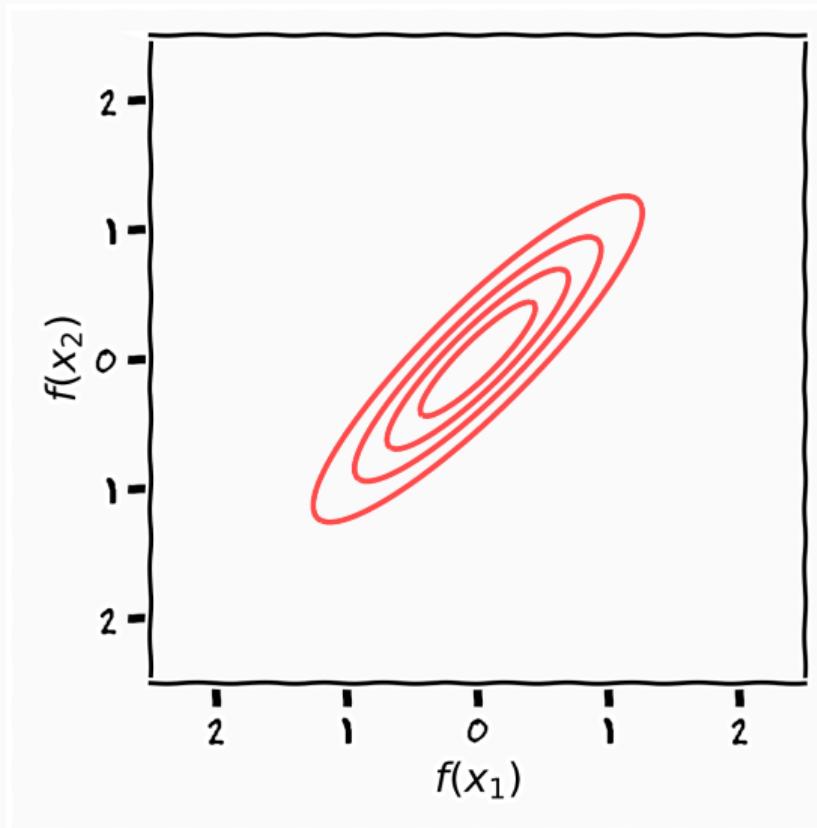
Conditional Gaussians



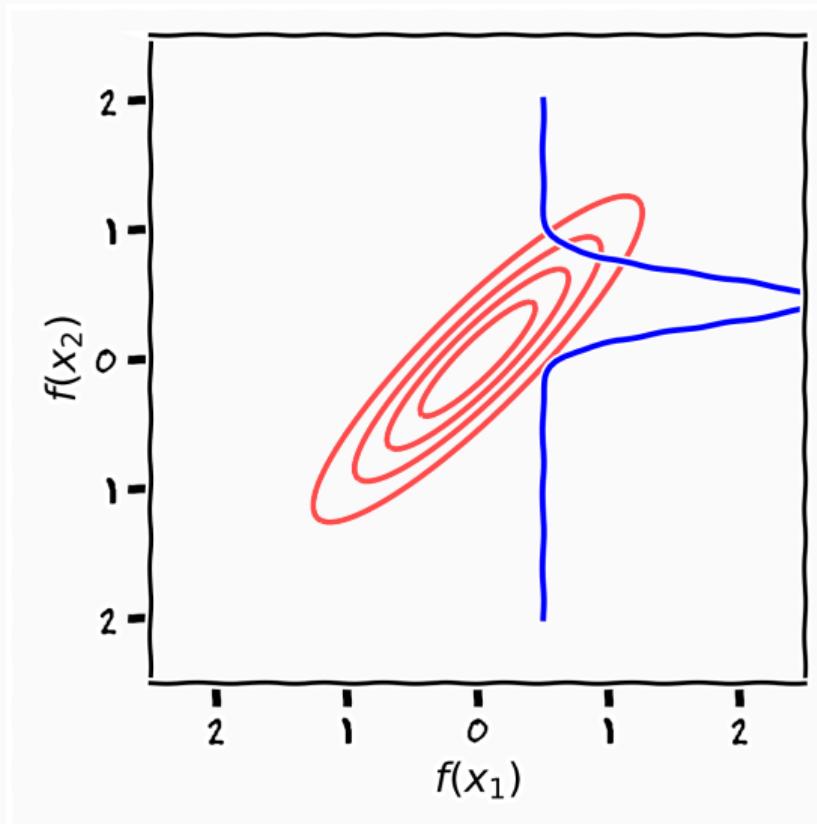
Conditional Gaussians

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.9 \\ 0.9 & 1 \end{bmatrix} \right)$$

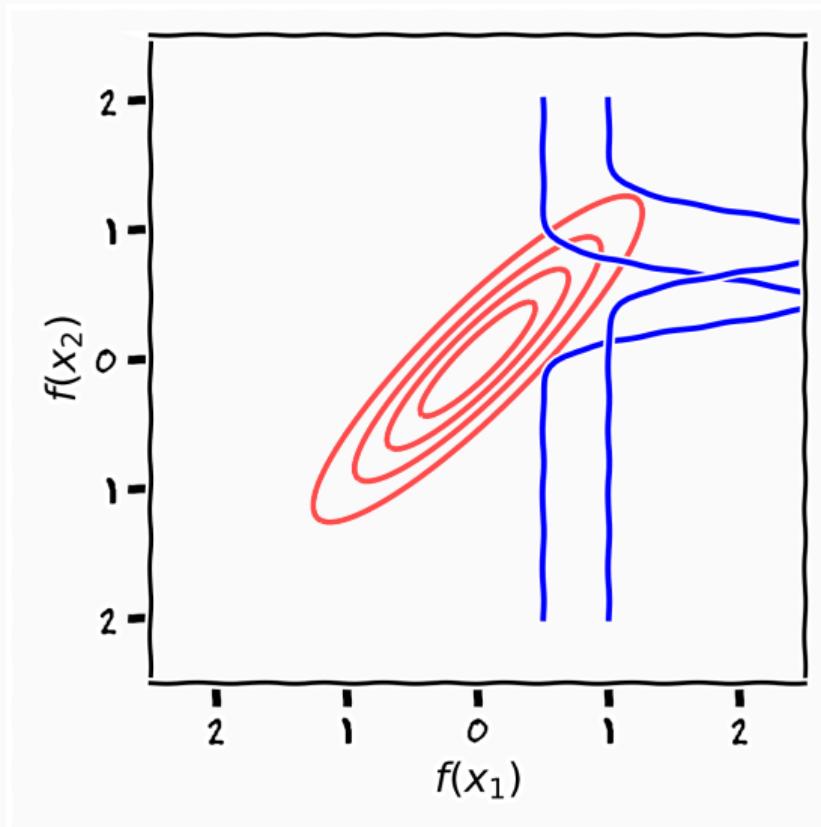
Conditional Gaussians



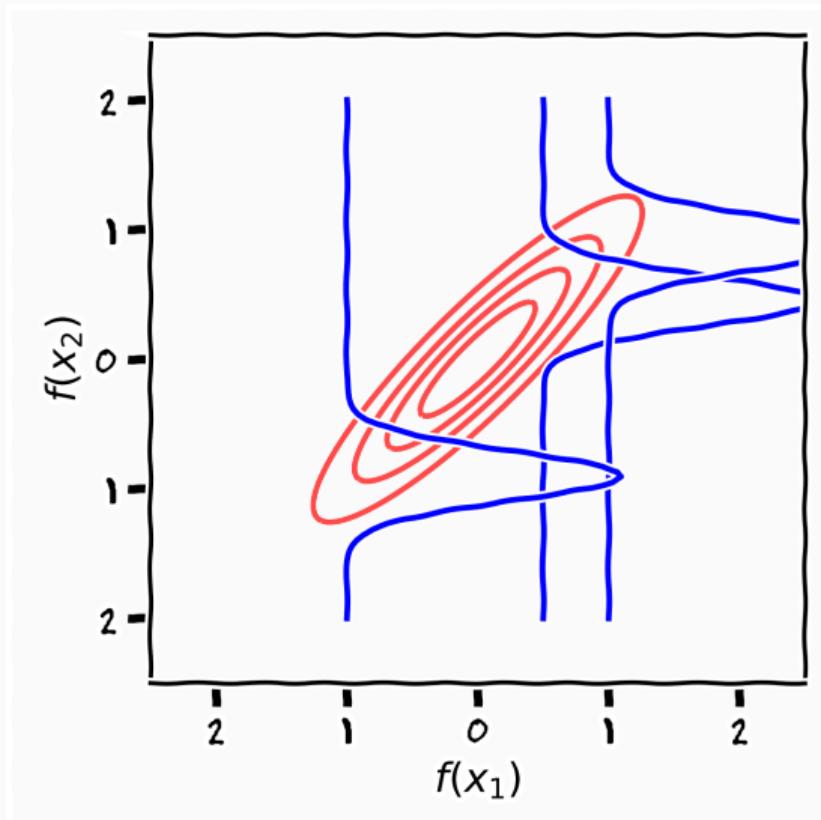
Conditional Gaussians



Conditional Gaussians



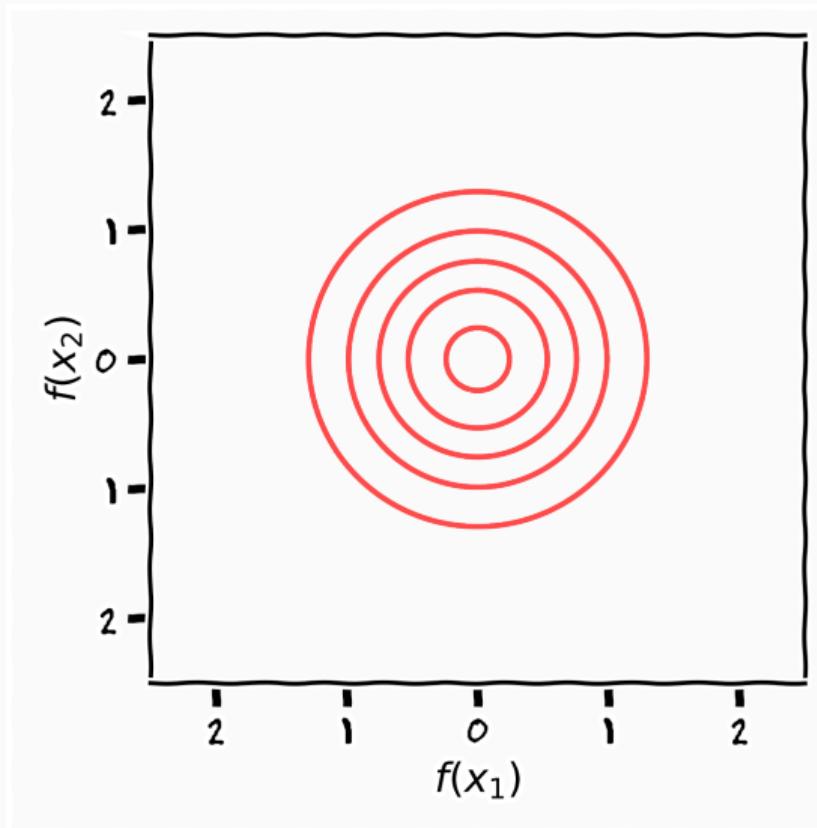
Conditional Gaussians



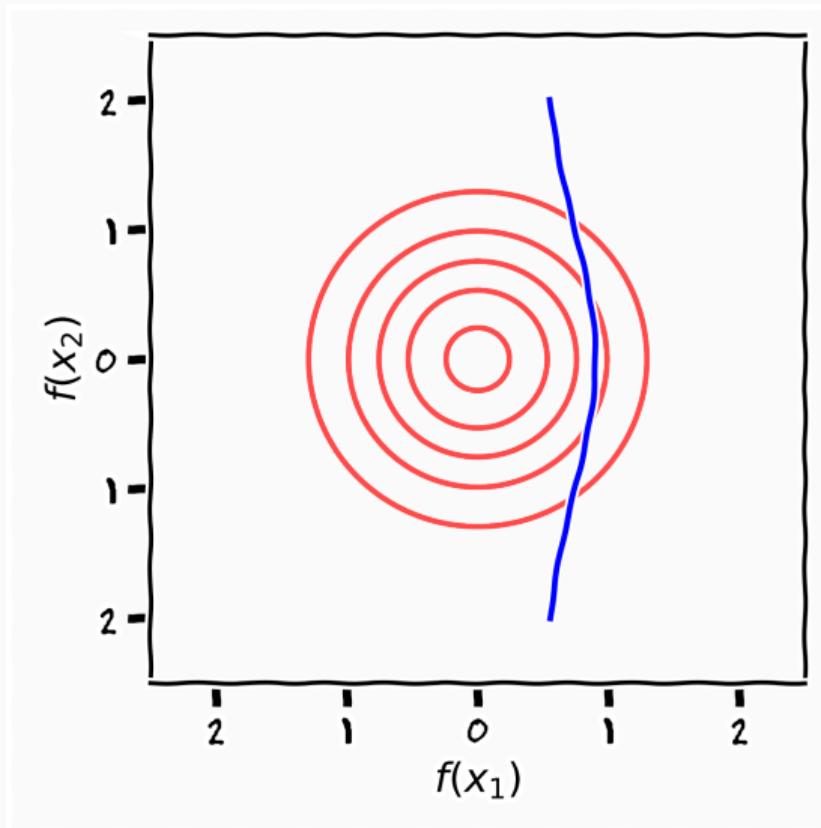
Conditional Gaussians

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

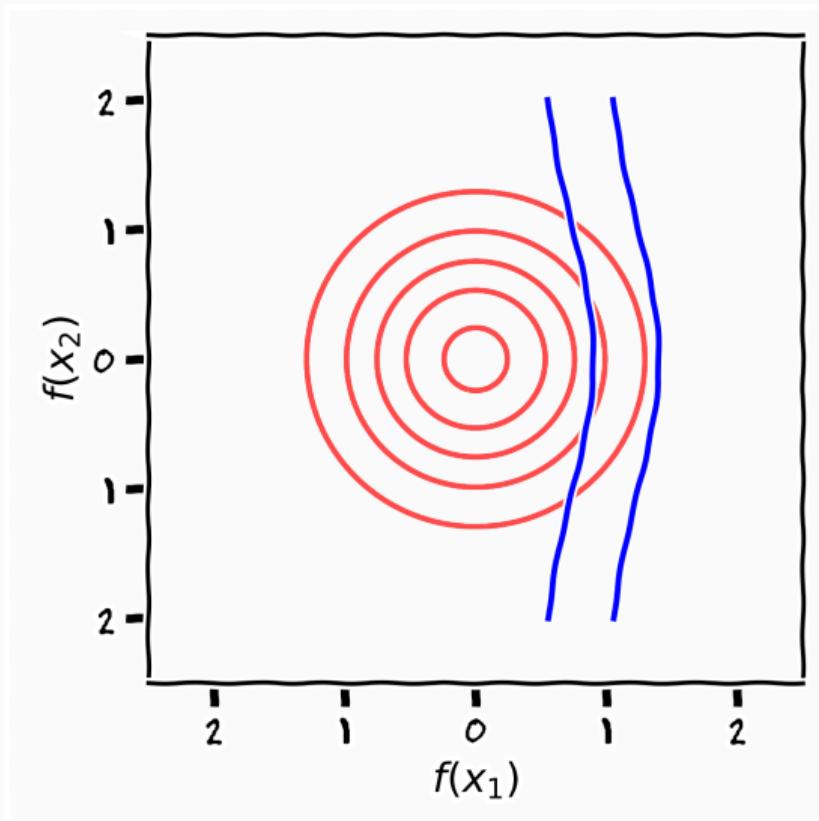
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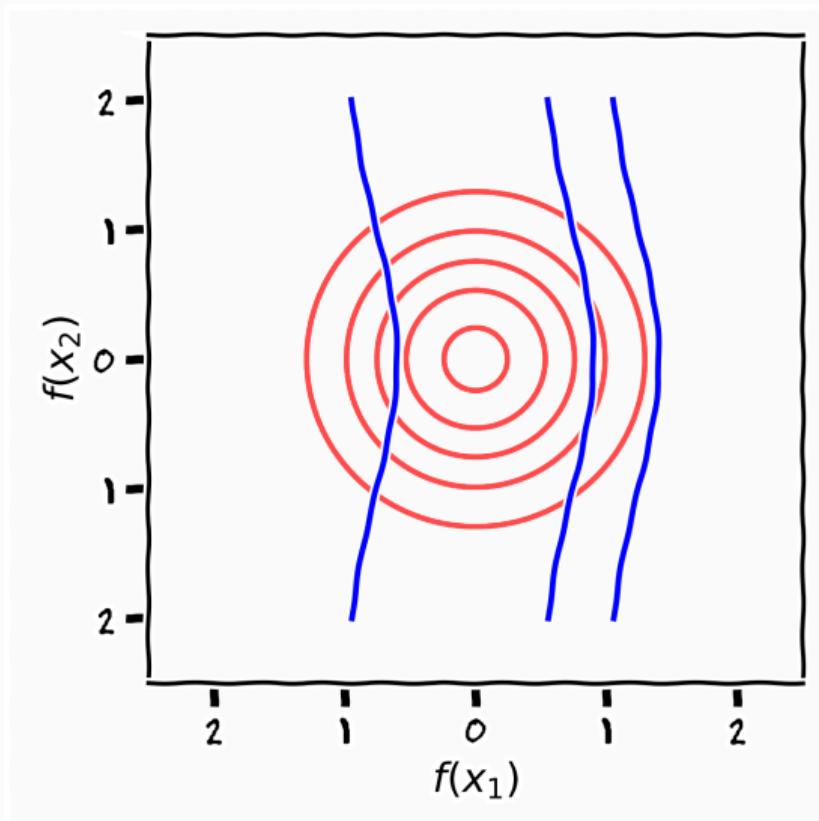
Conditional Gaussians



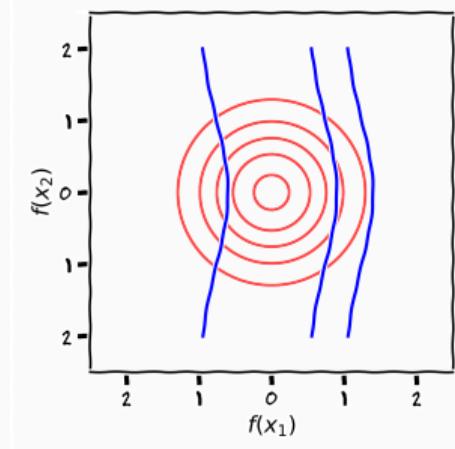
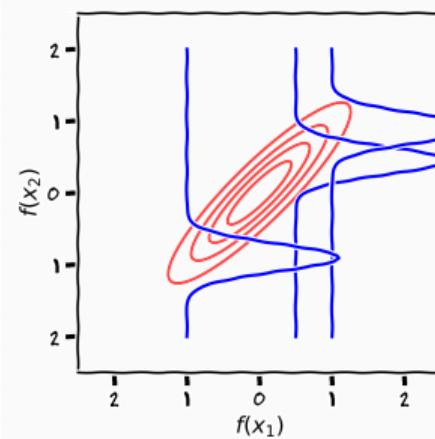
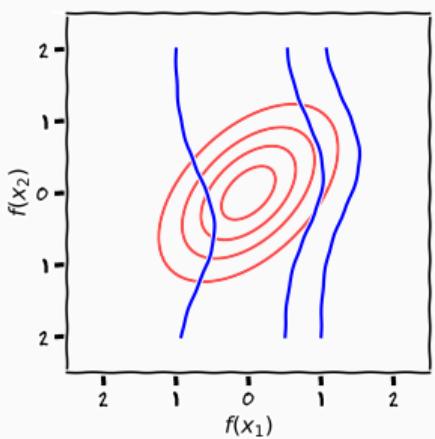
Conditional Gaussians



Conditional Gaussians



Conditional Gaussians

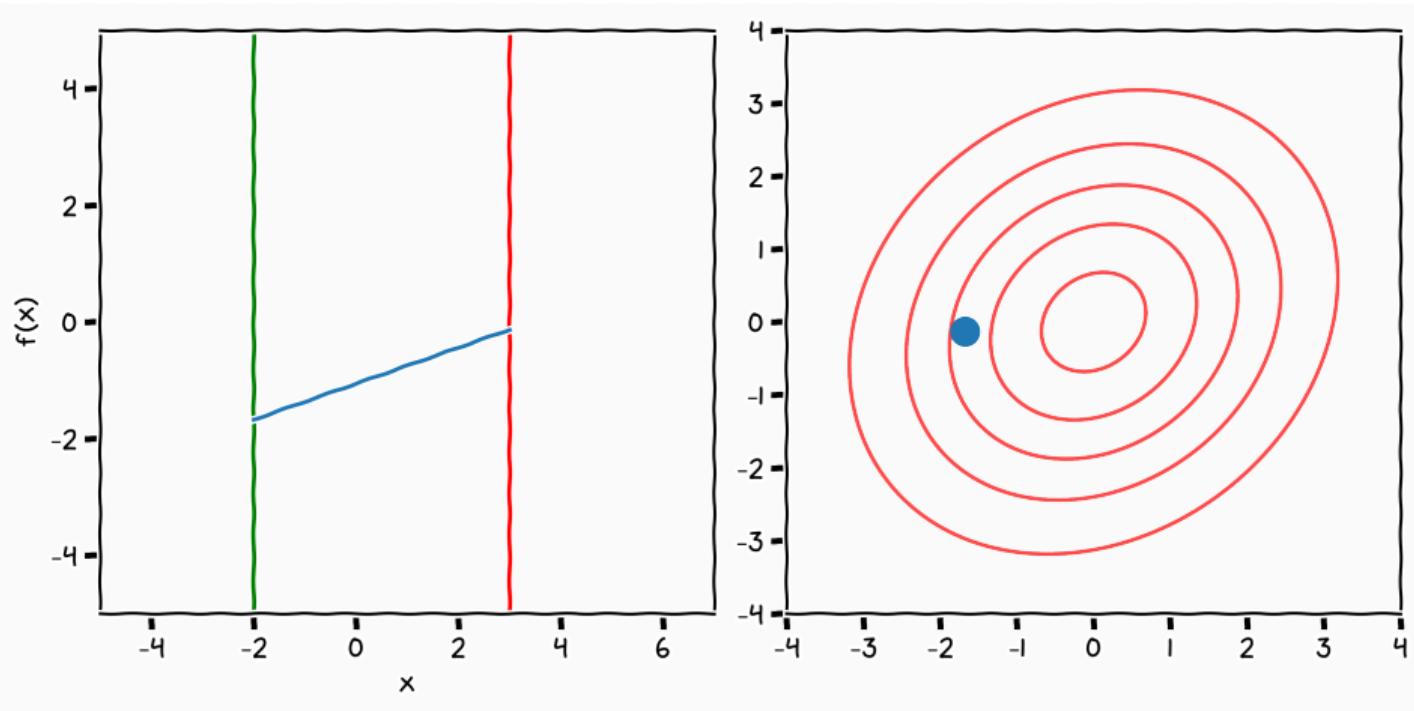


$$N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}\right)$$

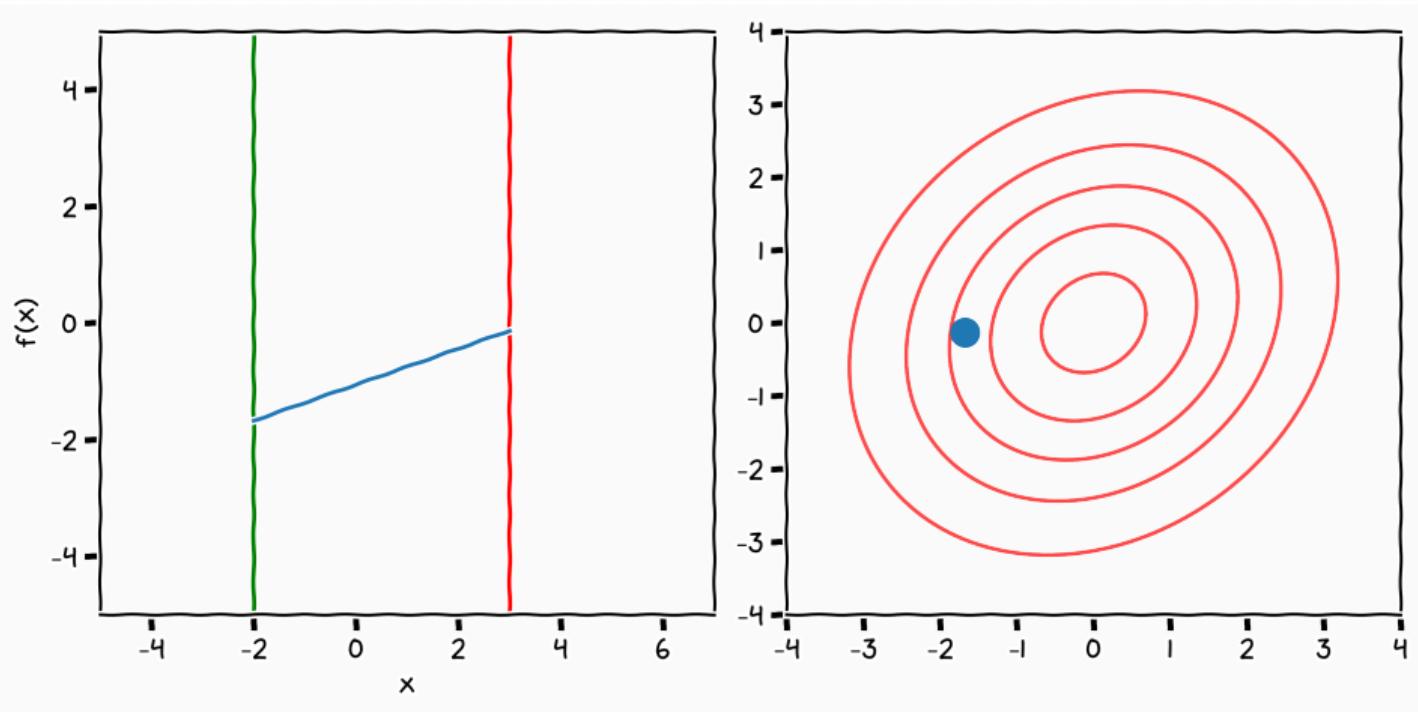
$$N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.9 \\ 0.9 & 1 \end{bmatrix}\right)$$

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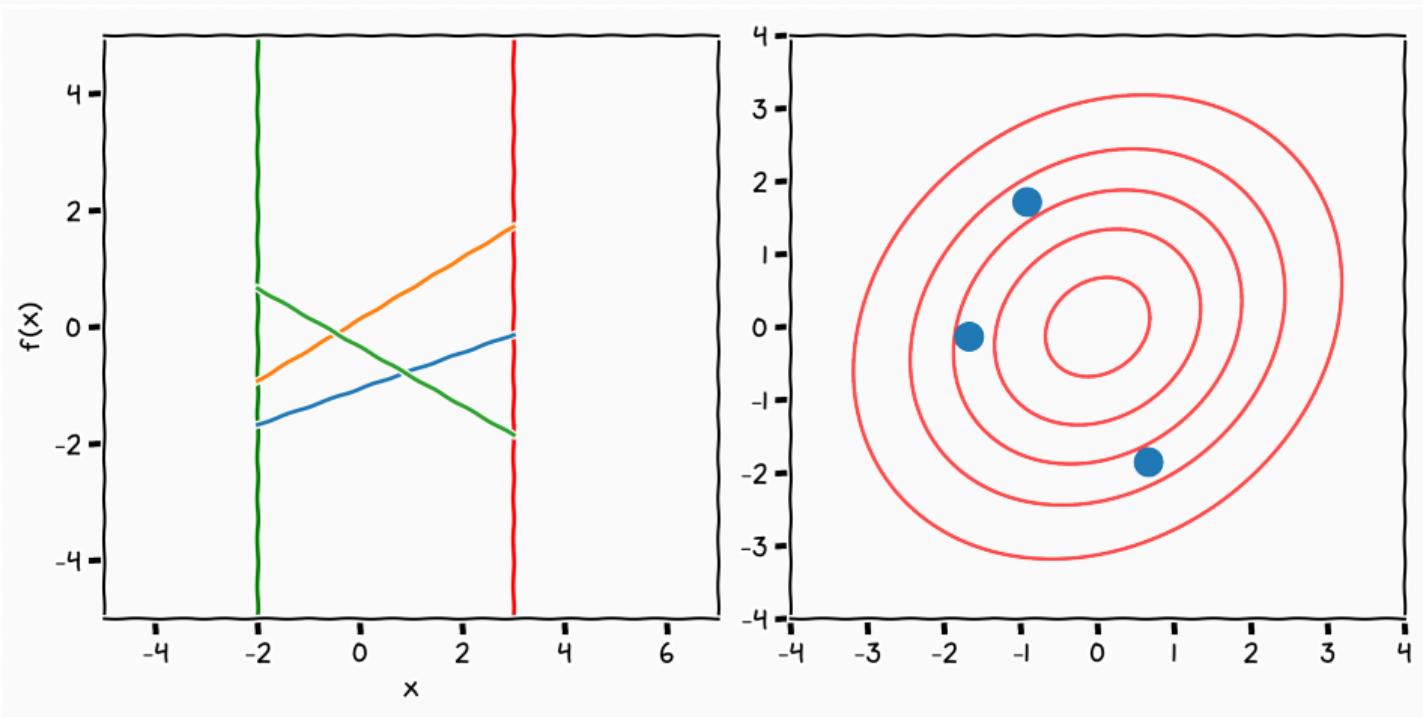
Gaussian Samples



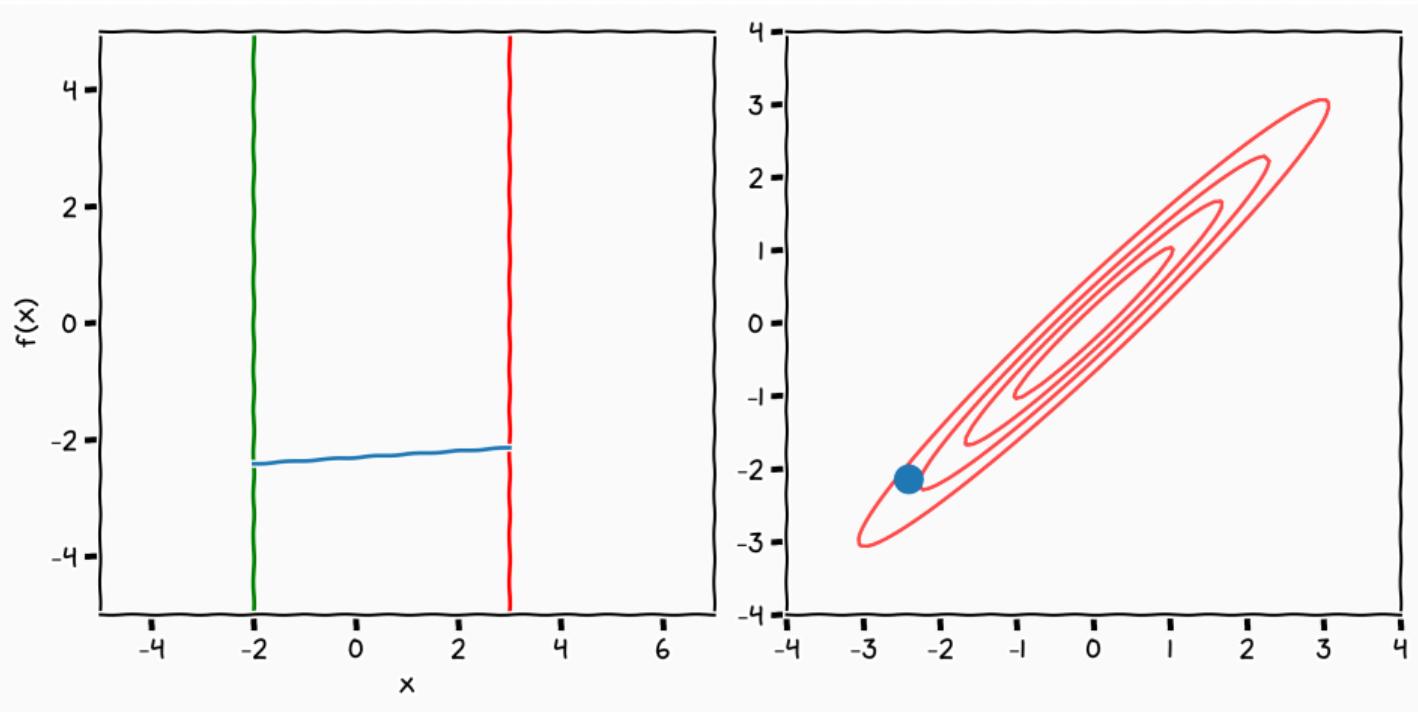
Gaussian Samples



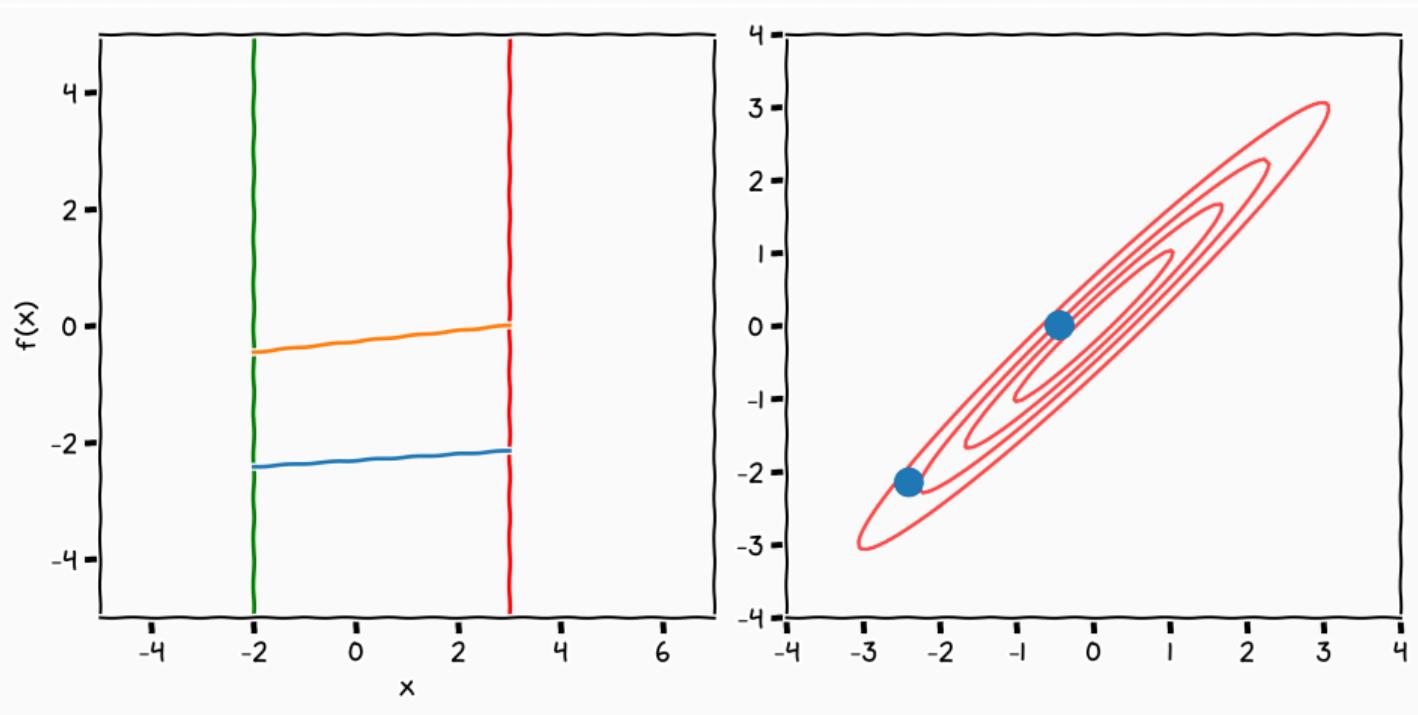
Gaussian Samples



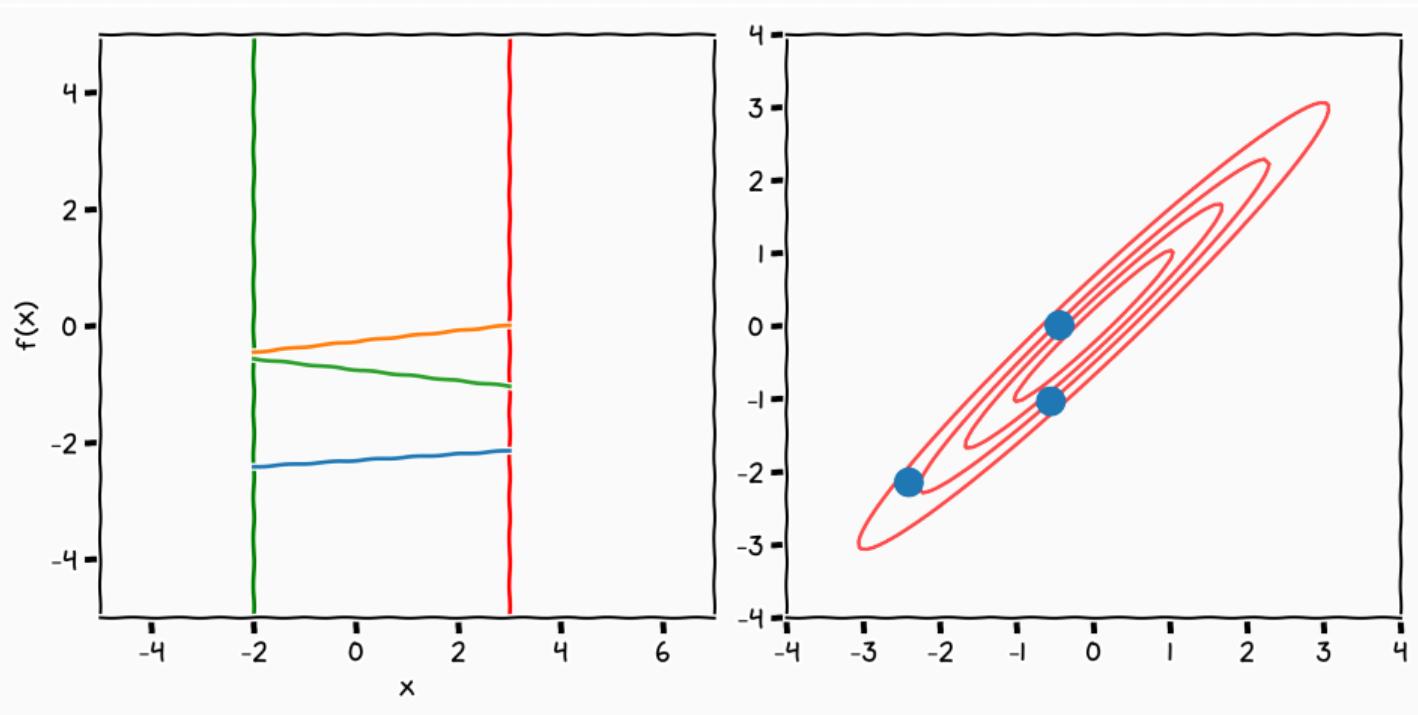
Gaussian Samples



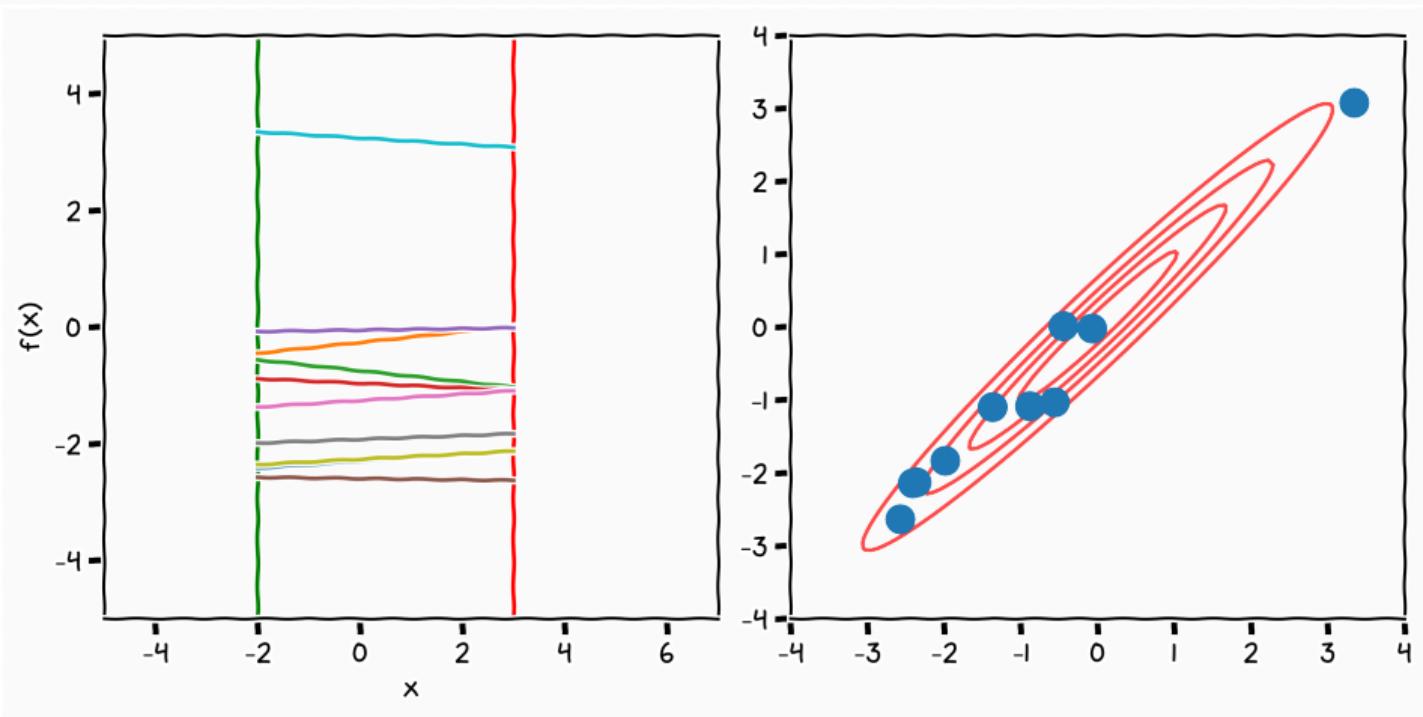
Gaussian Samples



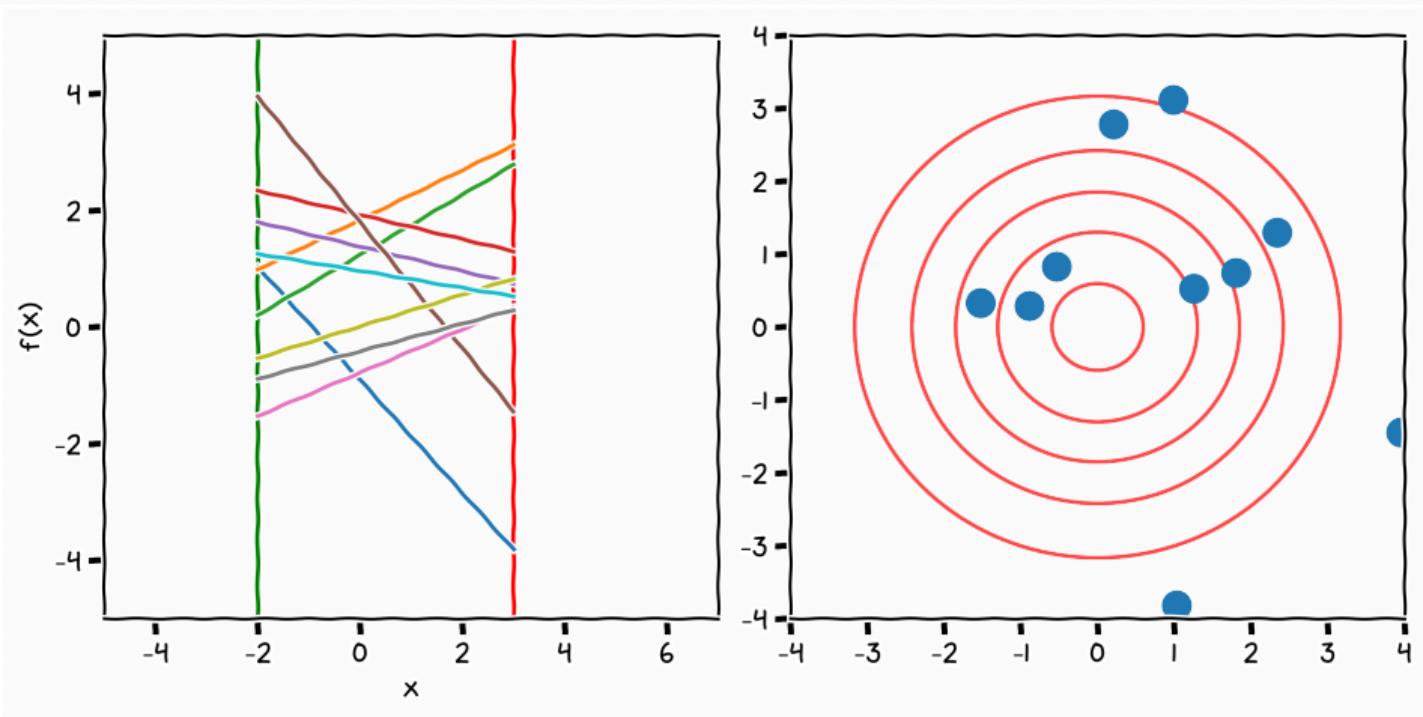
Gaussian Samples



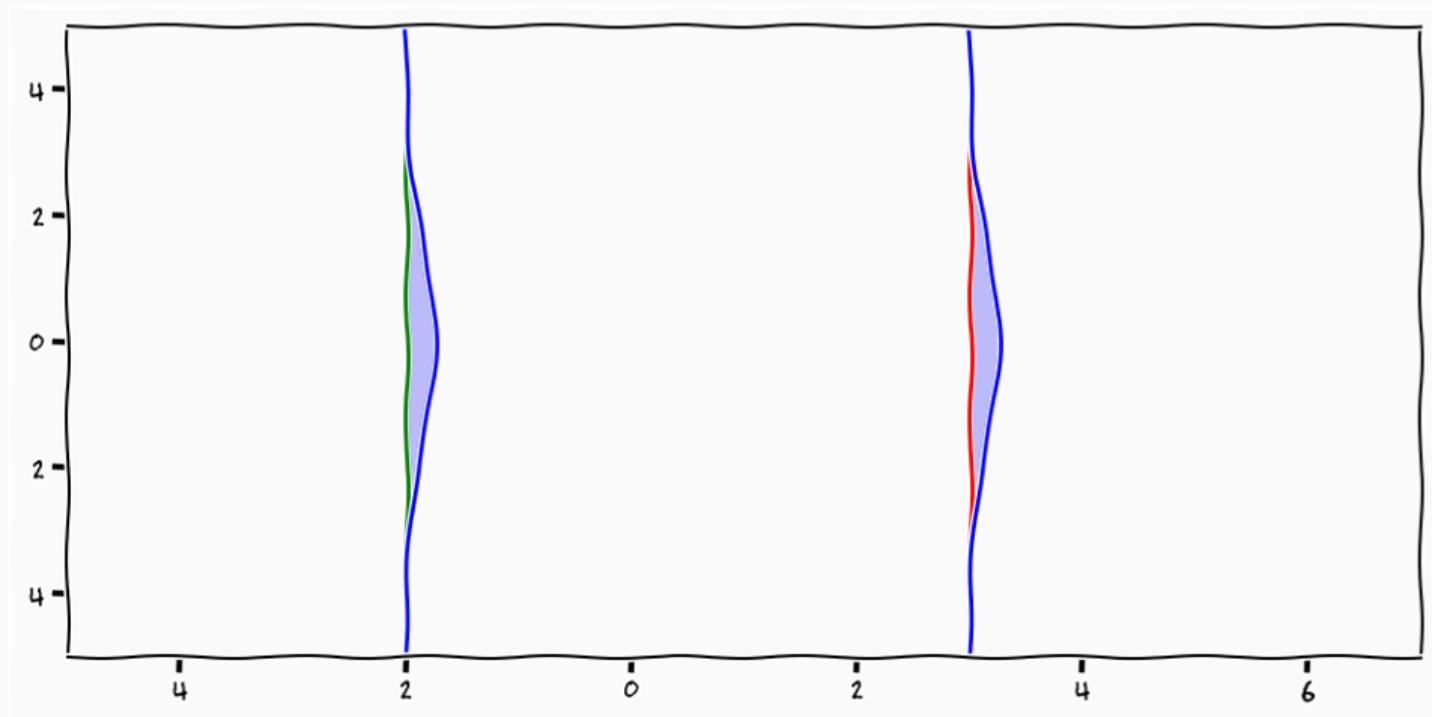
Gaussian Samples



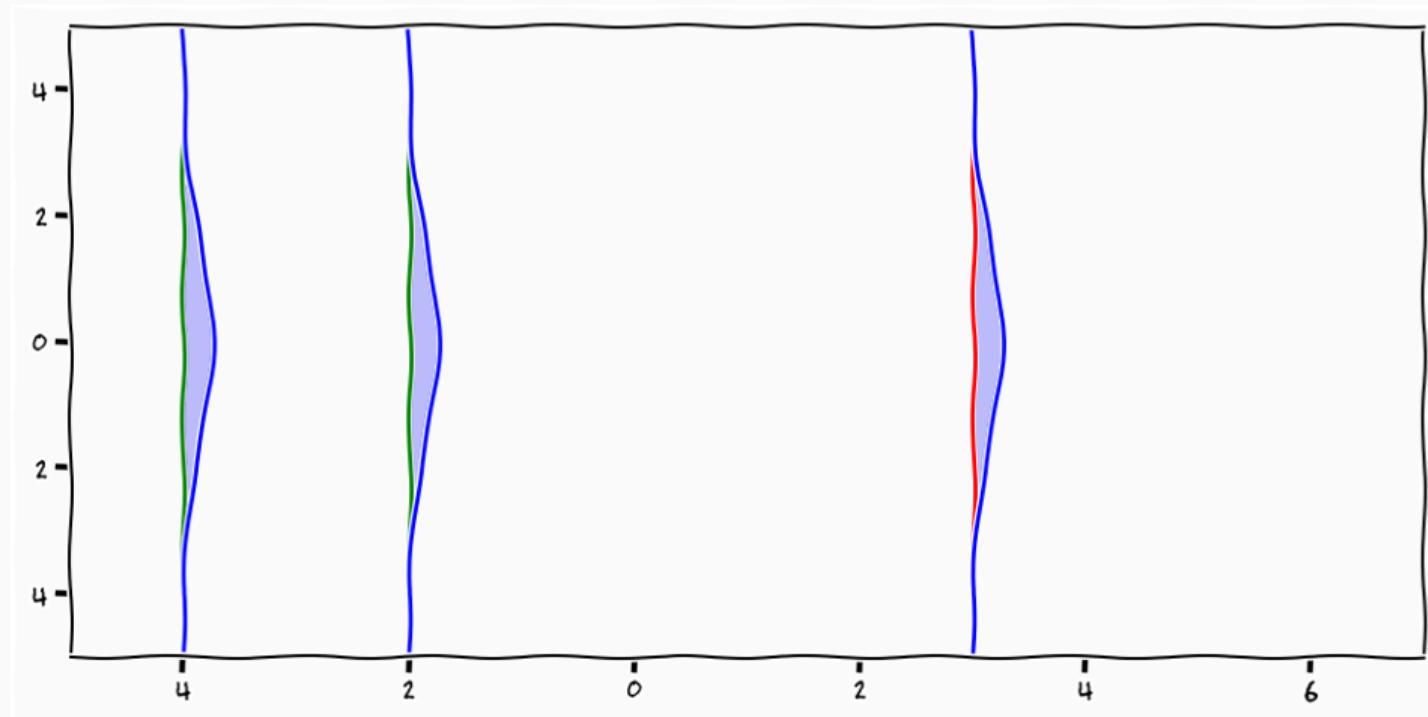
Gaussian Samples



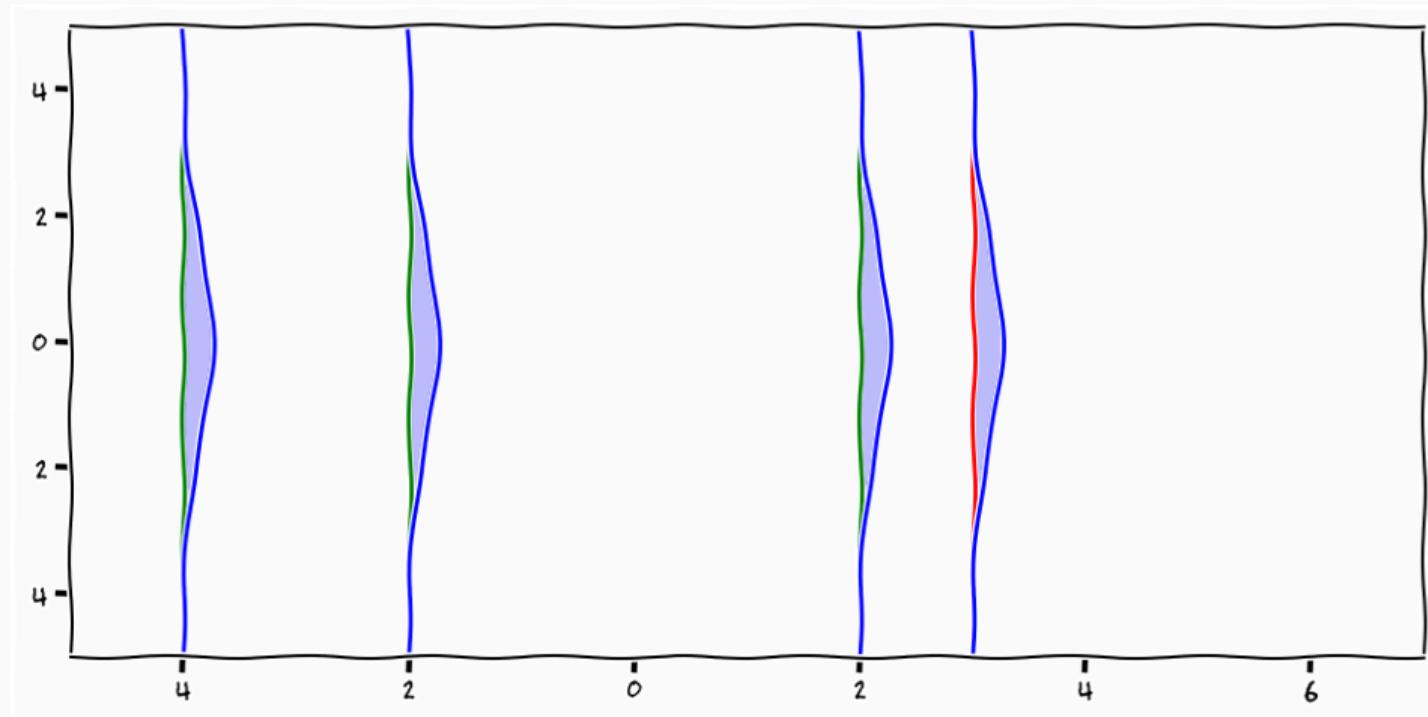
Lets talk about functions



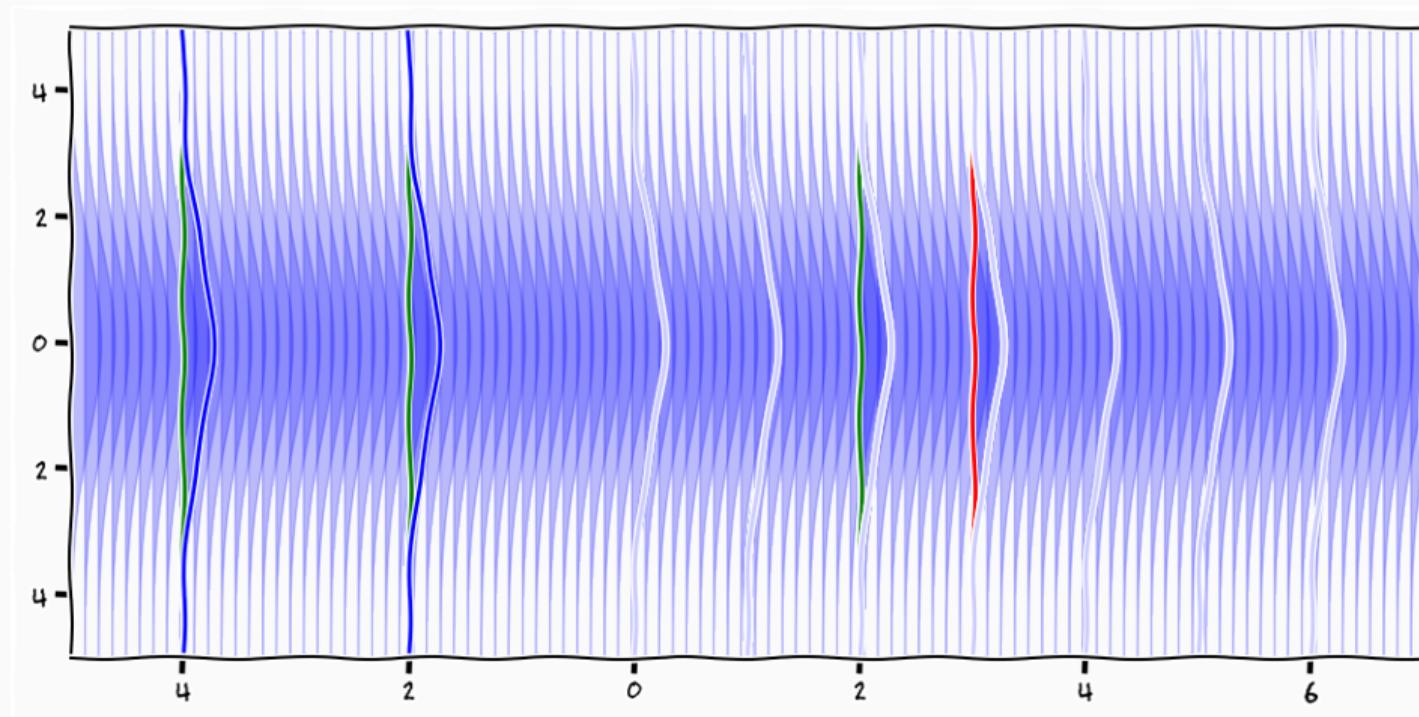
Non-parametric functions



Non-parametric functions



Non-parametric functions



Jointly Gaussian functions II

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

Gaussian Distribution - Marginal

$$p(\textcolor{red}{x}_1, x_2) = \mathcal{N} \left(\begin{array}{c|cc} \textcolor{red}{x}_1 & \mu_1 & k_{11} & k_{12} \\ x_2 & \mu_2 & k_{21} & k_{22} \end{array} \right)$$

Gaussian Distribution - Marginal

$$\begin{aligned} p(\textcolor{magenta}{x}_1, x_2) &= \mathcal{N} \left(\begin{array}{c|cc} x_1 & \mu_1 & k_{11} & k_{12} \\ x_2 & \mu_2 & k_{21} & k_{22} \end{array} \right) \\ \Rightarrow p(\textcolor{magenta}{x}_1) &= \int_{x_2} p(\textcolor{magenta}{x}_1, x_2) = \underline{\mathcal{N}(\textcolor{magenta}{x}_1 \mid \mu_1, k_{11})} \end{aligned}$$

Gaussian Distribution - Marginal

$$p(\mathbf{x}_1, x_2) = \mathcal{N} \left(\begin{array}{c|cc} \mathbf{x}_1 & \mu_1 & k_{11} & k_{12} \\ x_2 & \mu_2 & k_{21} & k_{22} \end{array} \right)$$

$$\Rightarrow p(\mathbf{x}_1) = \int_{x_2} p(\mathbf{x}_1, x_2) = \underline{\mathcal{N}(\mathbf{x}_1 | \mu_1, k_{11})}$$

$$p(\mathbf{x}_1, x_2, \dots, x_N) = \mathcal{N} \left(\begin{array}{c|ccccccc} \mathbf{x}_1 & \mu_1 & k_{11} & k_{12} & \cdots & k_{1N} \\ x_2 & \mu_2 & k_{21} & k_{22} & \cdots & k_{2N} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ x_N & \mu_N & k_{N1} & k_{N2} & \cdots & k_{NN} \end{array} \right)$$

Gaussian Distribution - Marginal

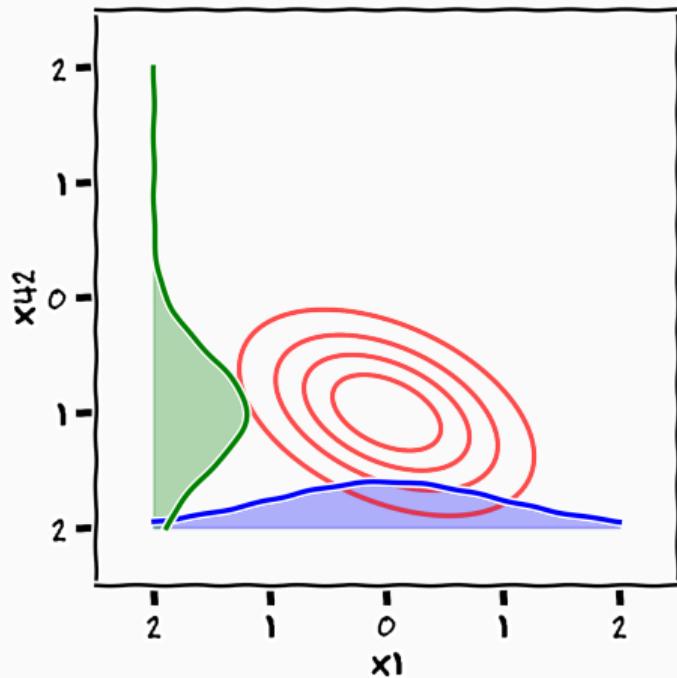
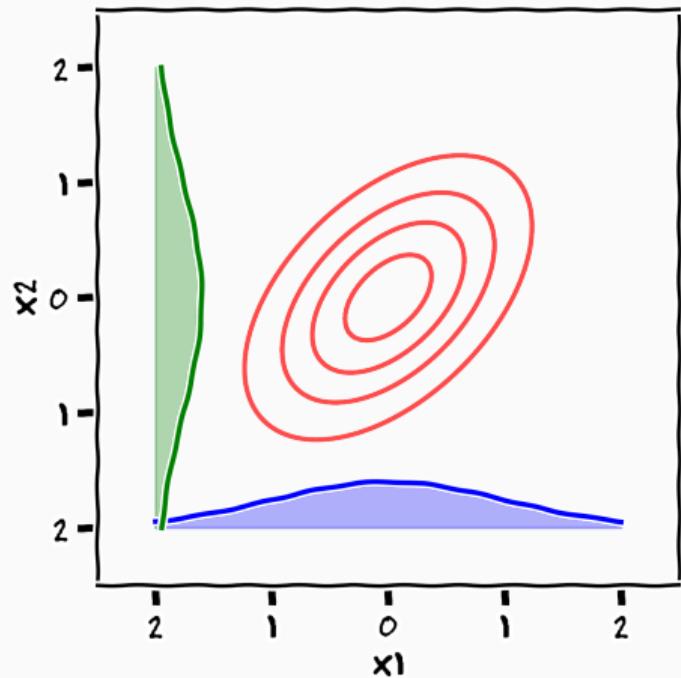
$$p(\mathbf{x}_1, x_2) = \mathcal{N} \left(\begin{array}{c|cc} \mathbf{x}_1 & \mu_1 & k_{11} & k_{12} \\ x_2 & \mu_2 & k_{21} & k_{22} \end{array} \right)$$

$$\Rightarrow p(\mathbf{x}_1) = \int_{x_2} p(\mathbf{x}_1, x_2) = \underline{\mathcal{N}(\mathbf{x}_1 \mid \mu_1, k_{11})}$$

$$p(\mathbf{x}_1, x_2, \dots, x_N) = \mathcal{N} \left(\begin{array}{c|cccccc} \mathbf{x}_1 & \mu_1 & k_{11} & k_{12} & \cdots & k_{1N} \\ x_2 & \mu_2 & k_{21} & k_{22} & \cdots & k_{2N} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ x_N & \mu_N & k_{N1} & k_{N2} & \cdots & k_{NN} \end{array} \right)$$

$$\Rightarrow p(\mathbf{x}_1) = \int_{x_2, \dots, x_N} p(\mathbf{x}_1, x_2, \dots, x_N) = \underline{\mathcal{N}(\mathbf{x}_1 \mid \mu_1, k_{11})}$$

Gaussian Distribution - Marginal

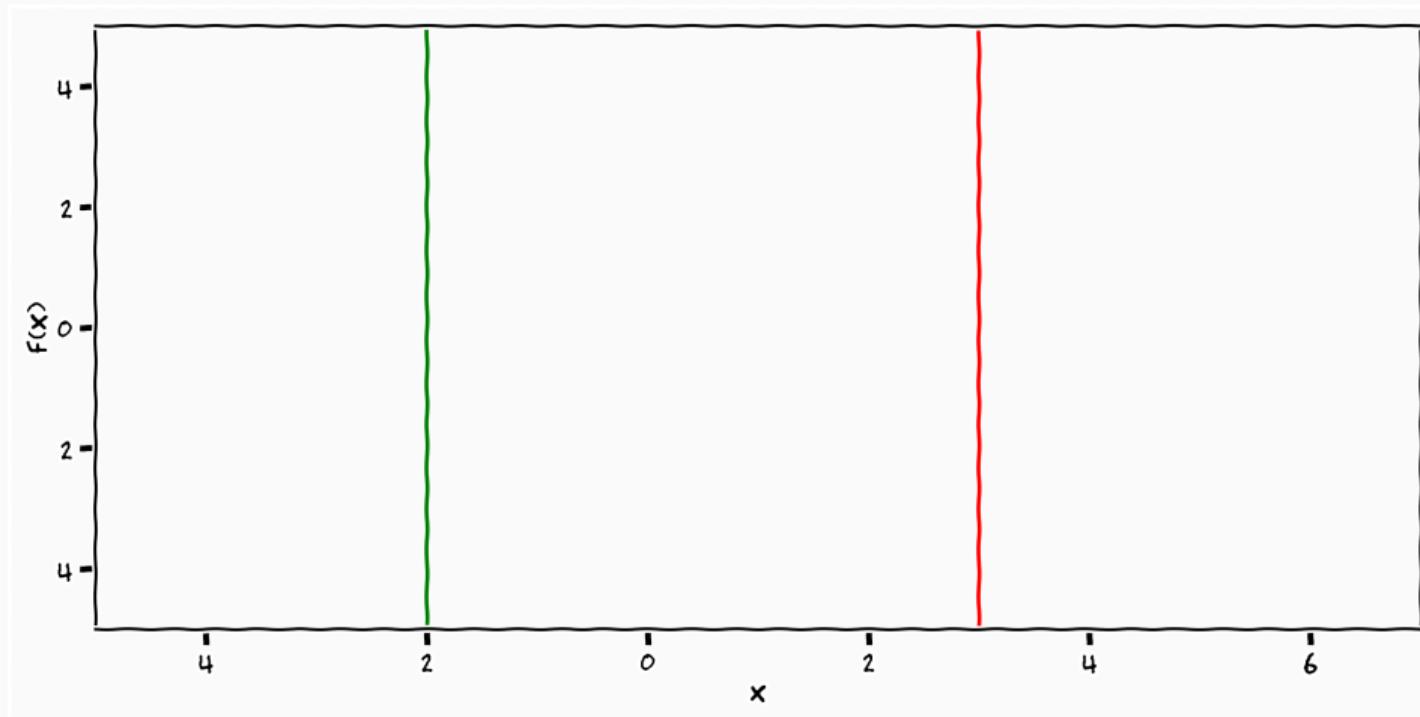


Marginal Property (Consistency)

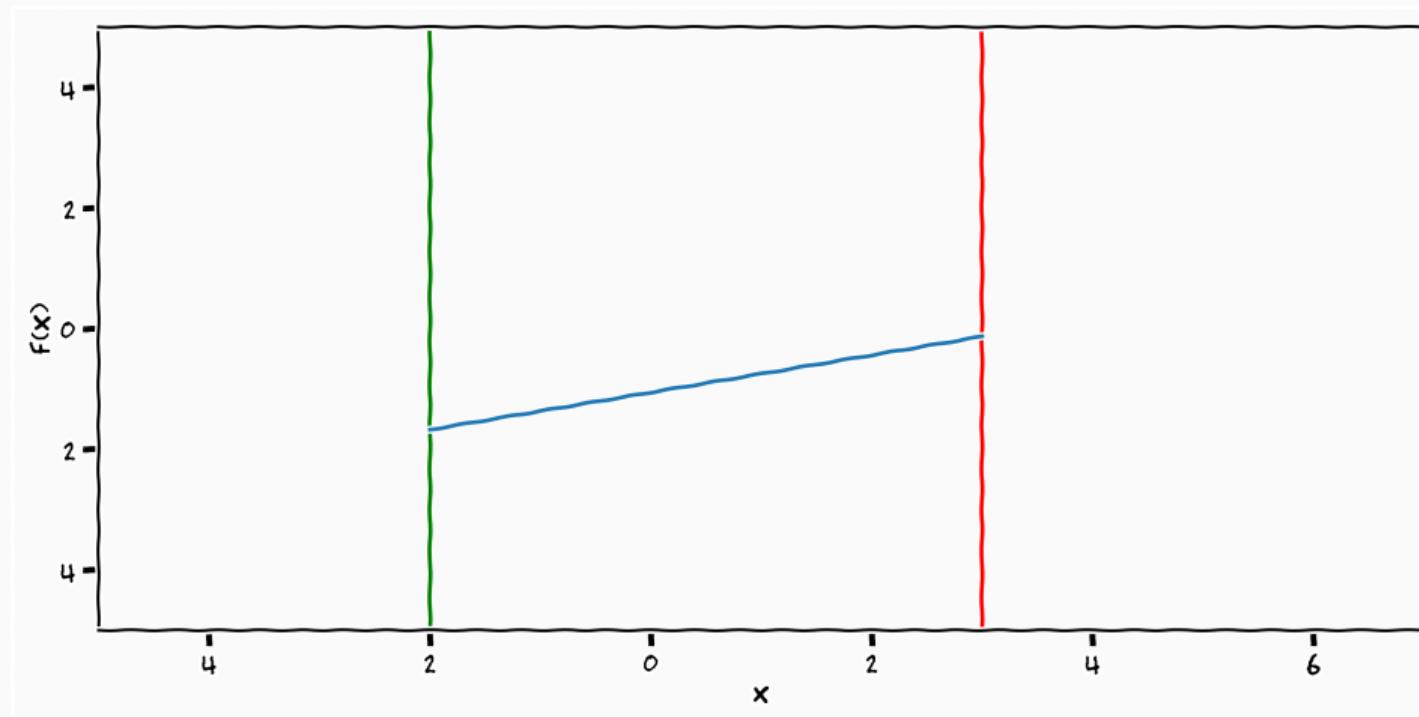
For all measurable sets $F_i \subseteq \mathbb{R}^n$ and probability measure \mathcal{N}

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

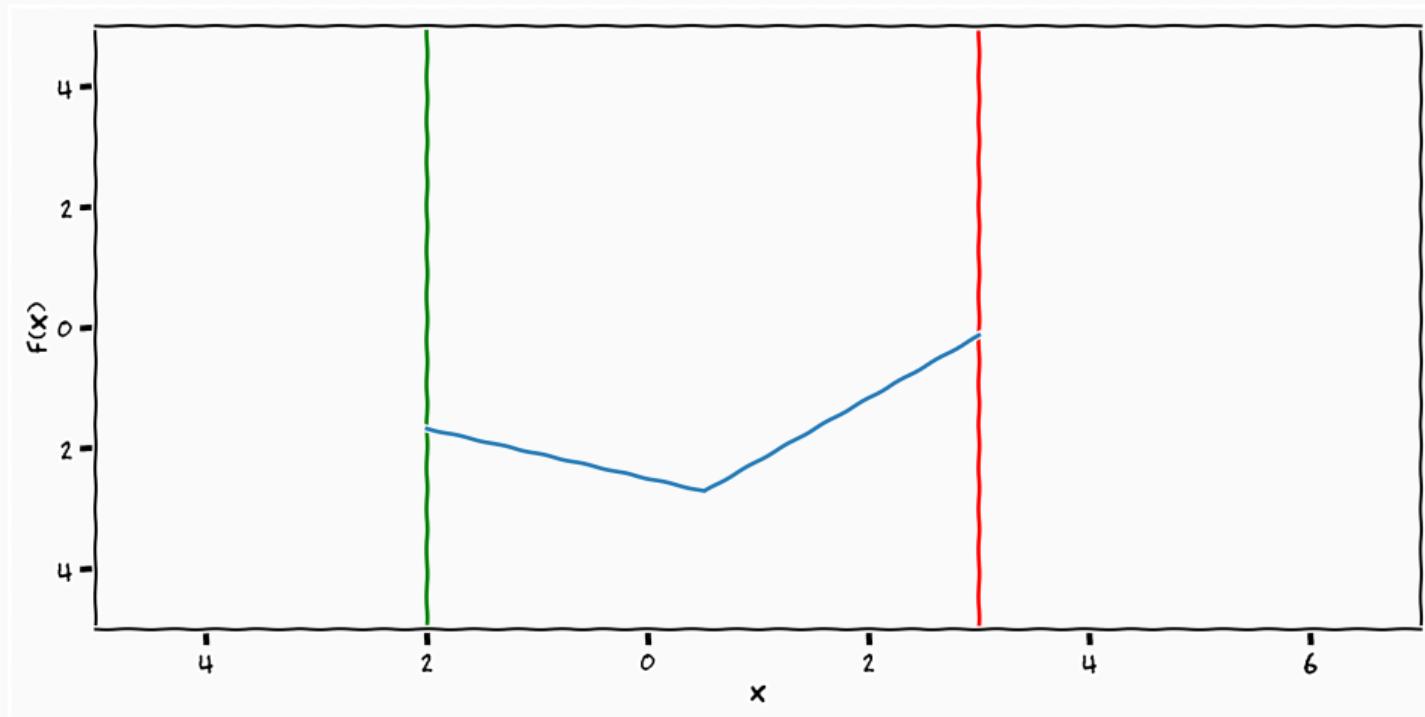
Gaussian Samples



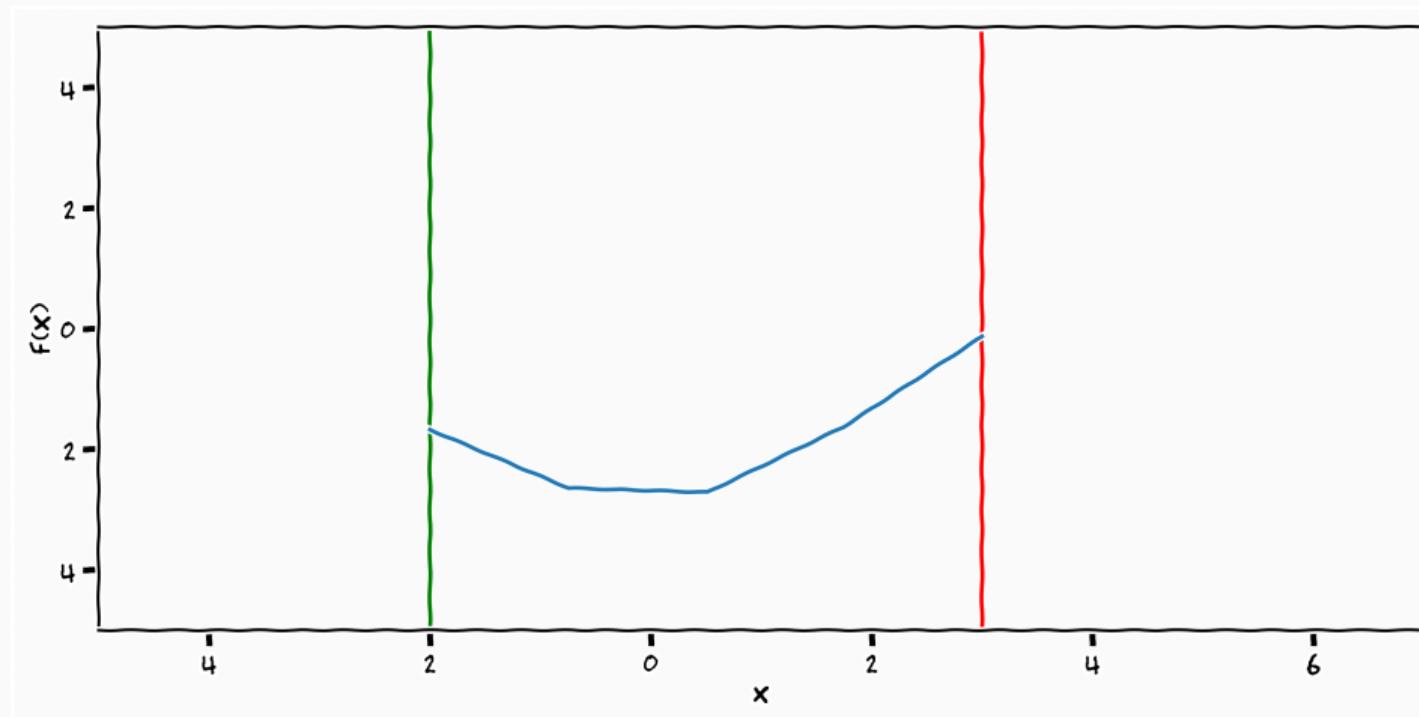
Gaussian Samples



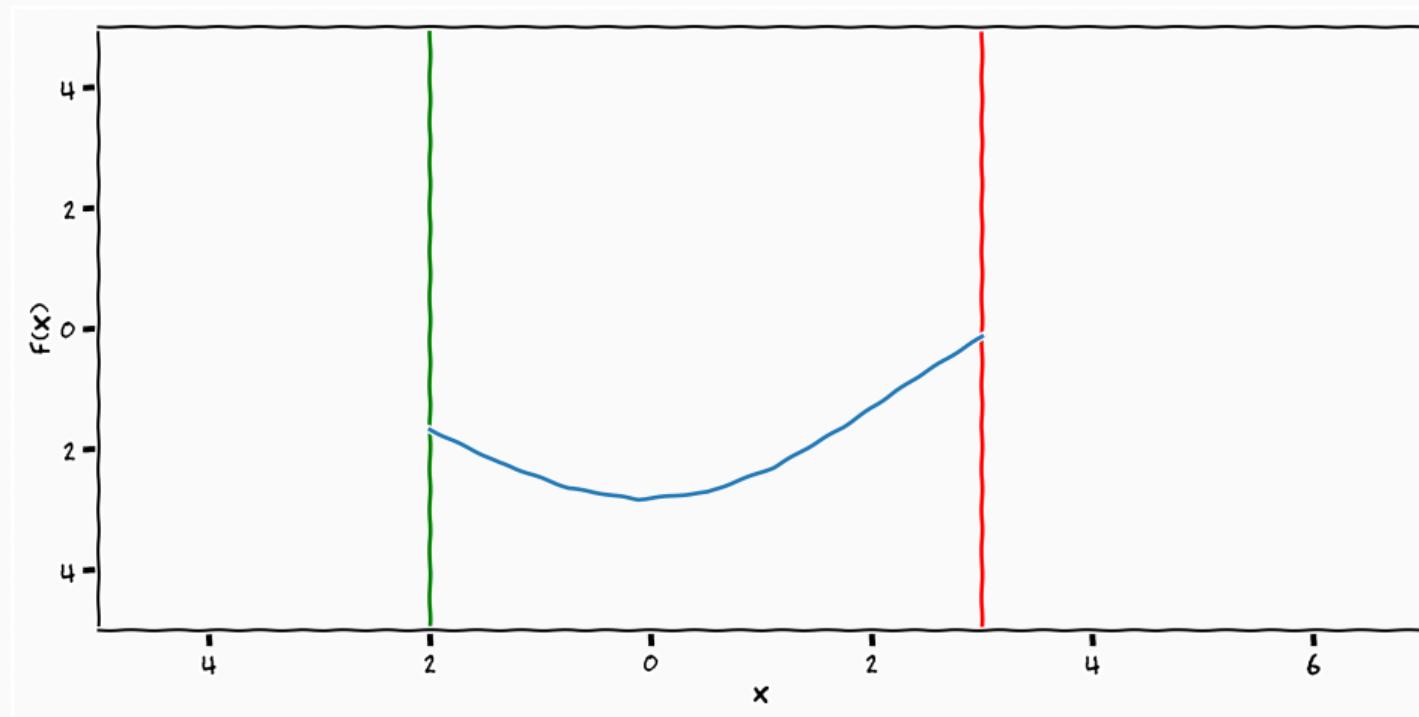
Gaussian Samples



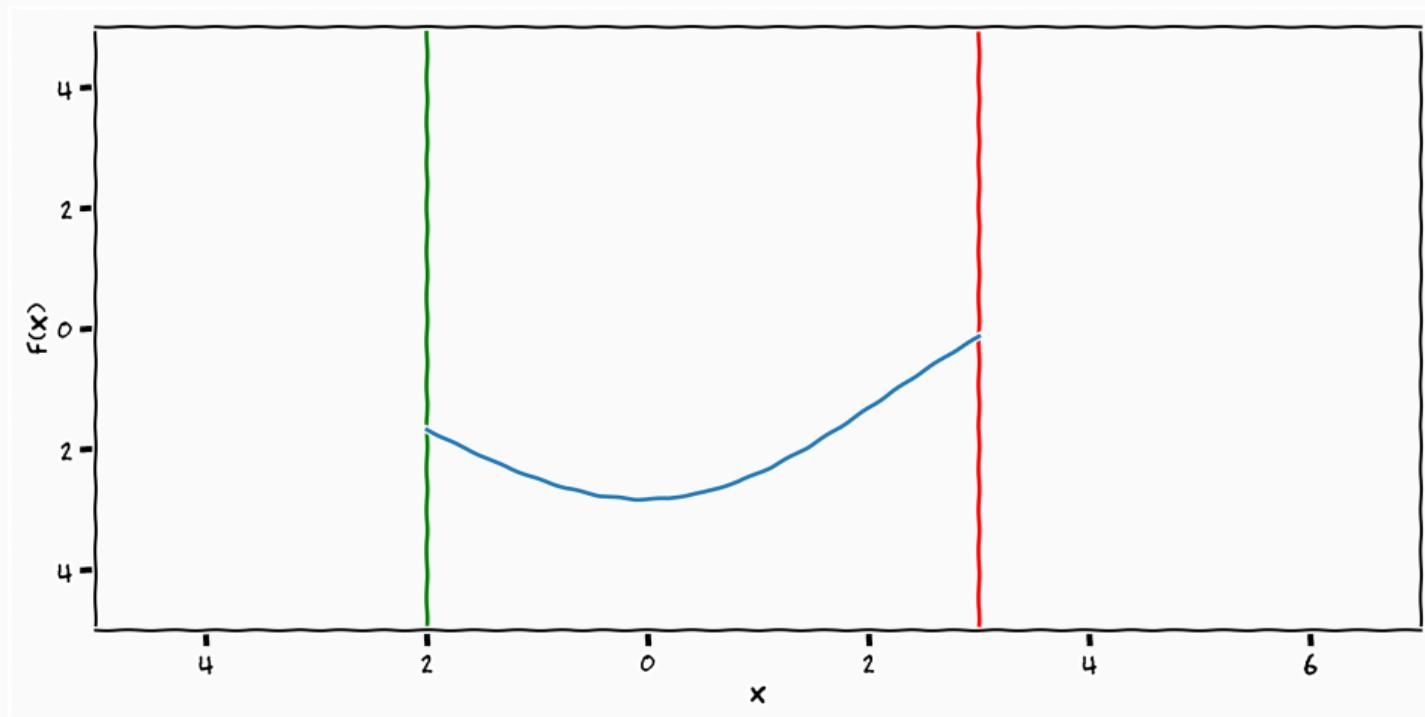
Gaussian Samples



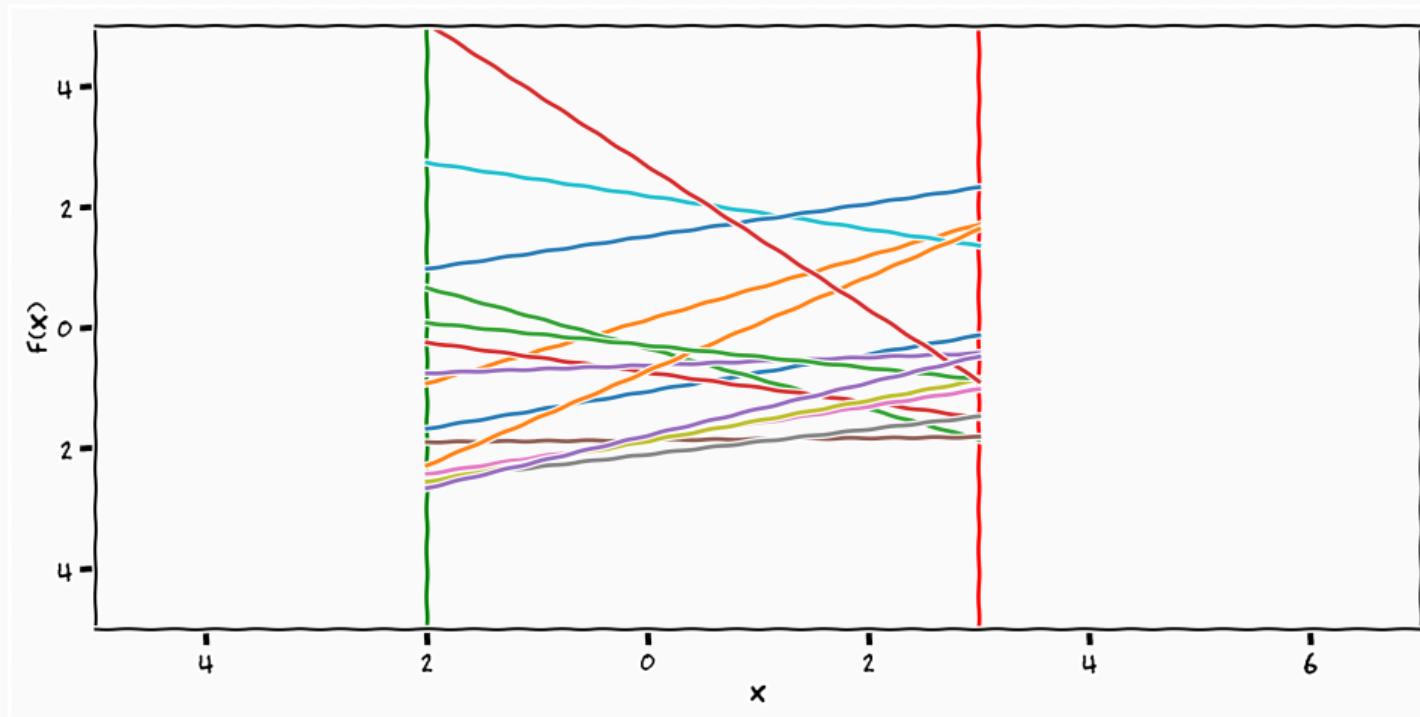
Gaussian Samples



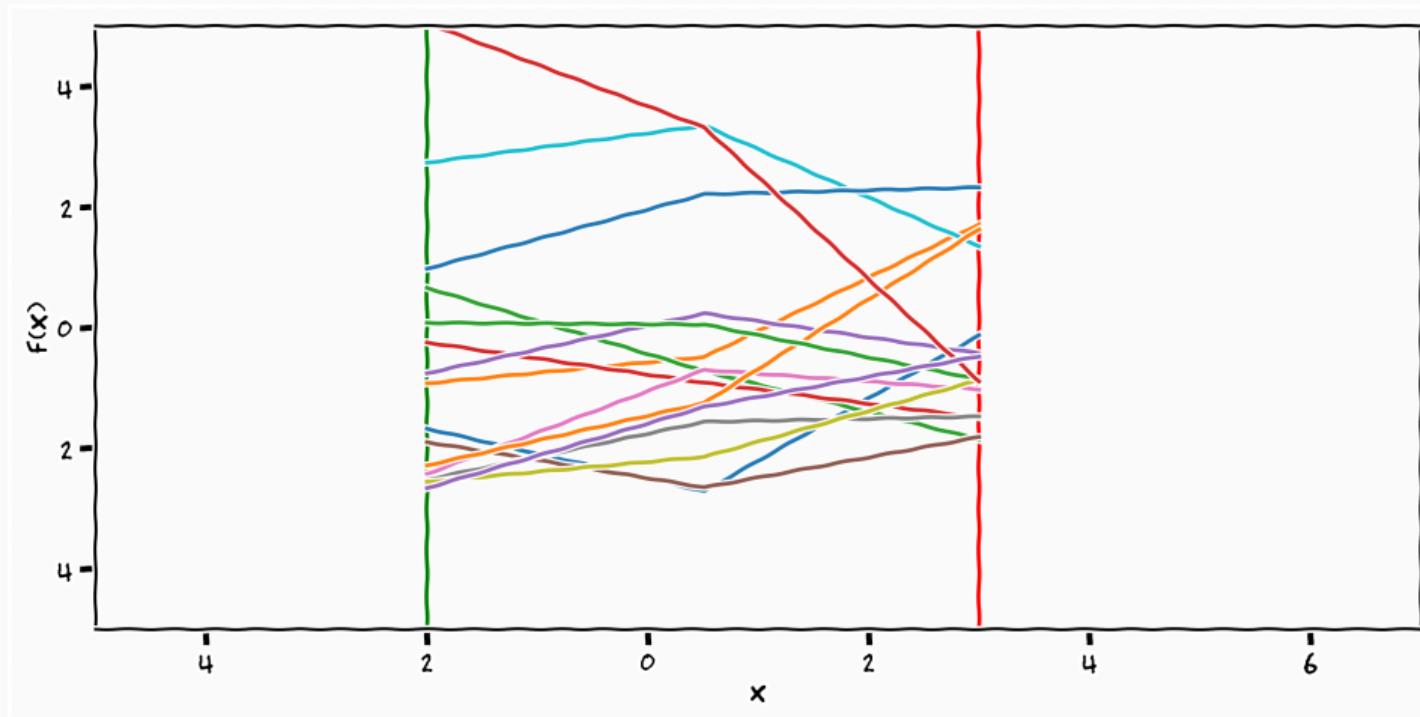
Gaussian Samples



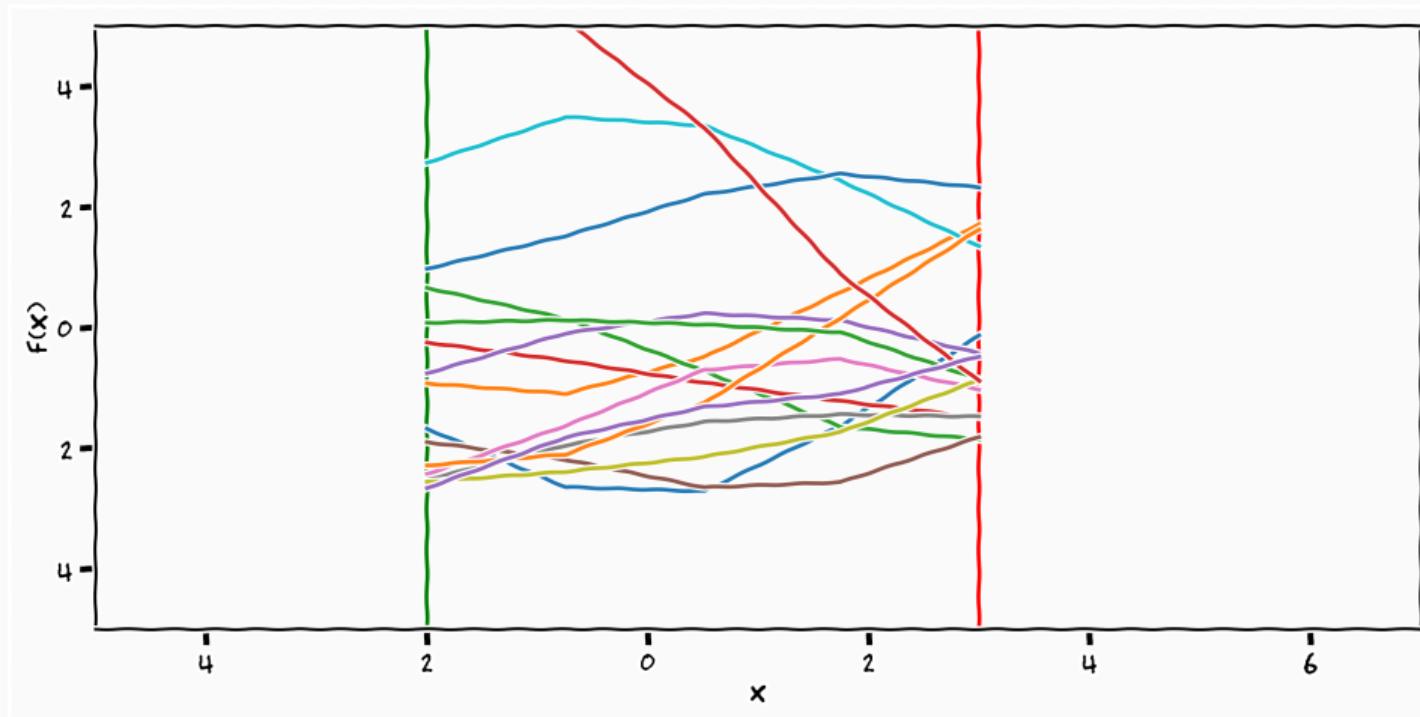
Gaussian Samples



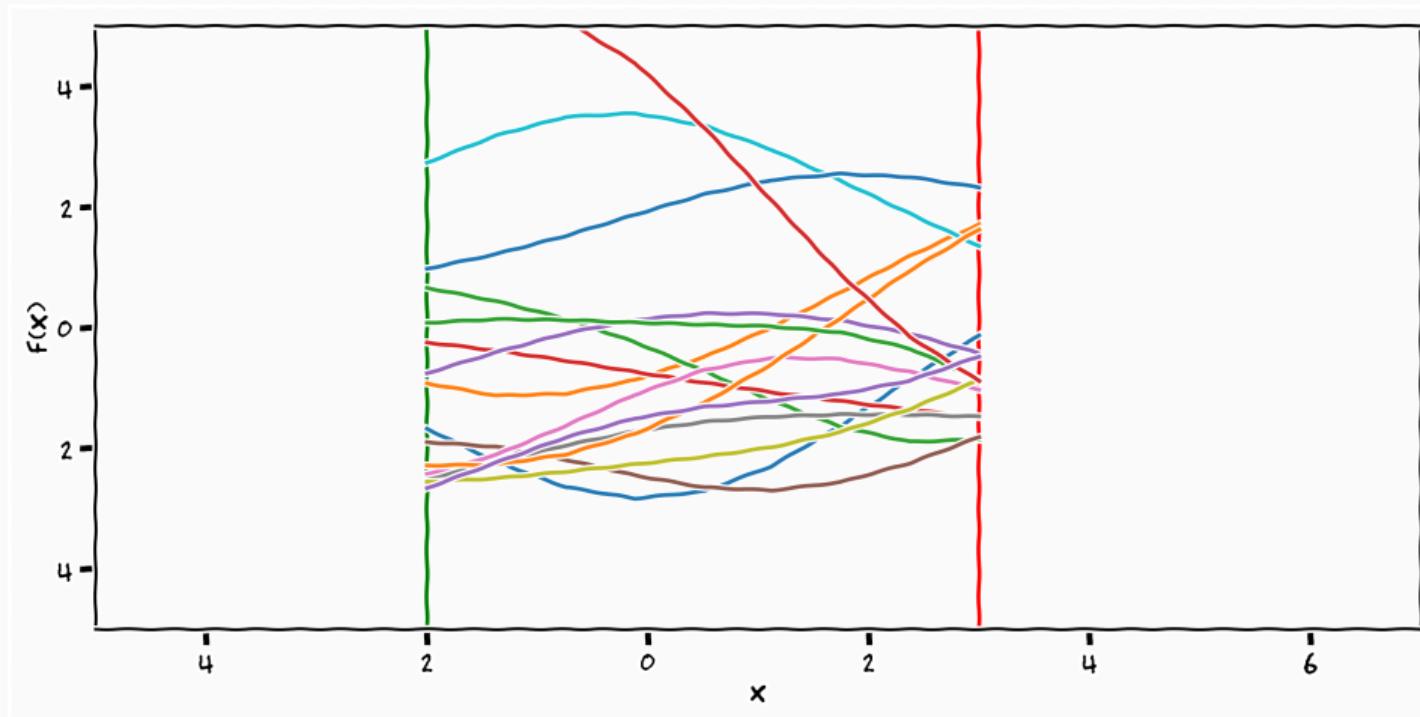
Gaussian Samples



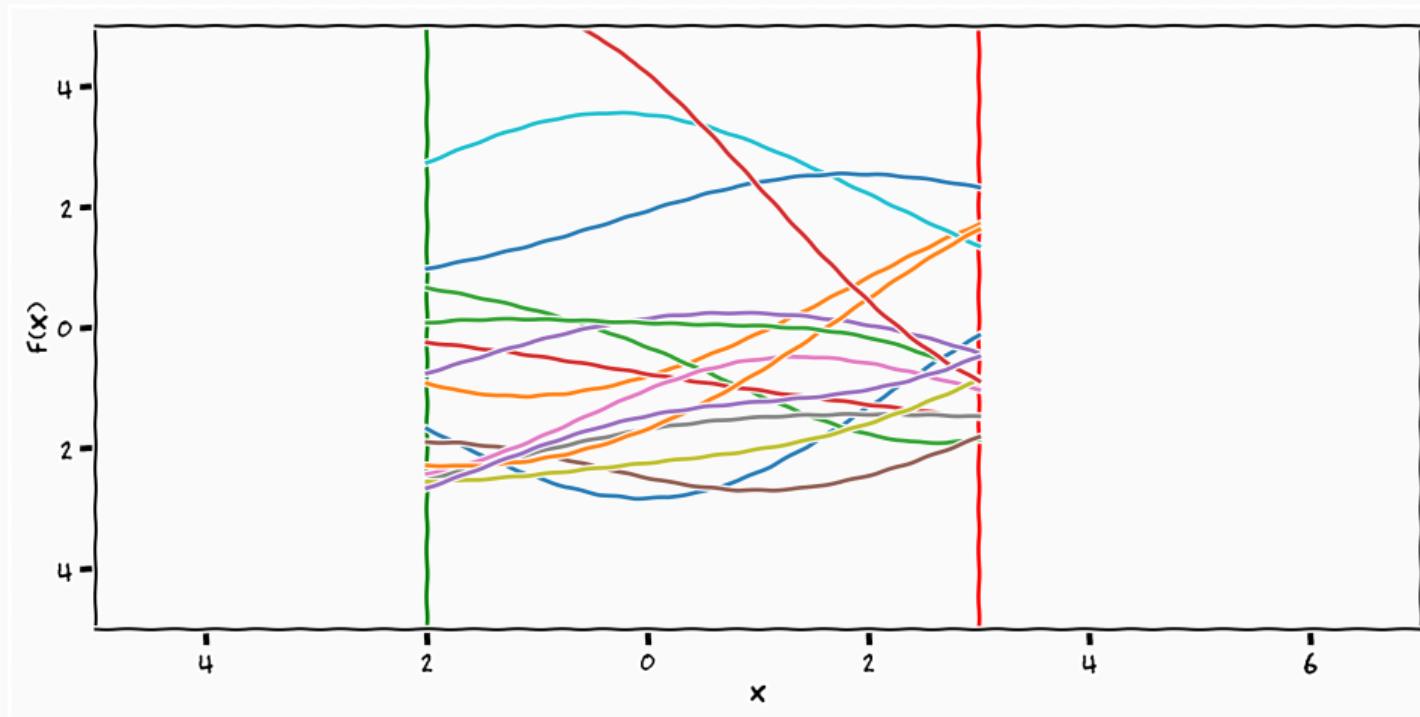
Gaussian Samples



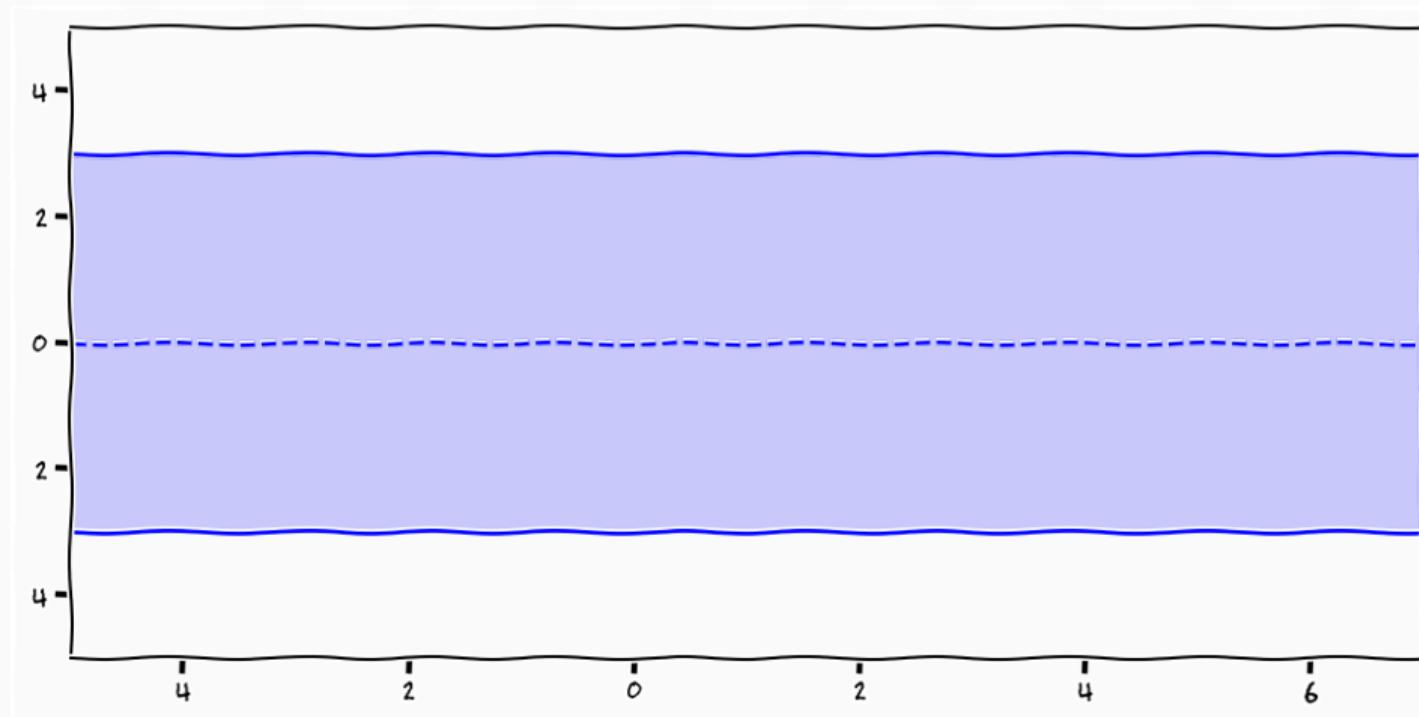
Gaussian Samples



Gaussian Samples



Gaussian Processes



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

$$\begin{array}{ccc} \mathcal{GP}(\cdot, \cdot) & M \in \mathbb{R}^{\infty \times N} & \mathcal{N}(\cdot, \cdot) \\ & \rightarrow & \\ \infty & & N \end{array}$$

The Gaussian distribution is the projection of the infinite Gaussian process

- The "function" is completely specified by
 - a mean vector $\mu \in \mathbb{R}^\infty$
 - a co-variance matrix $\mathbf{K}^{\infty \times \infty}$

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 - a mean vector $\mu \in \mathbb{R}^\infty$
 - a co-variance matrix $\mathbf{K}^{\infty \times \infty}$
- They are not without restrictions as they need to parametrise a valid Gaussian
 - $\mathbf{K}_{ii} \geq 0$
 - $\mathbf{K} \succcurlyeq 0$

"Parametrisation"

$$k_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

- We parameterise the covariance as a function of the input

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- *This is your "handle" to input knowledge*

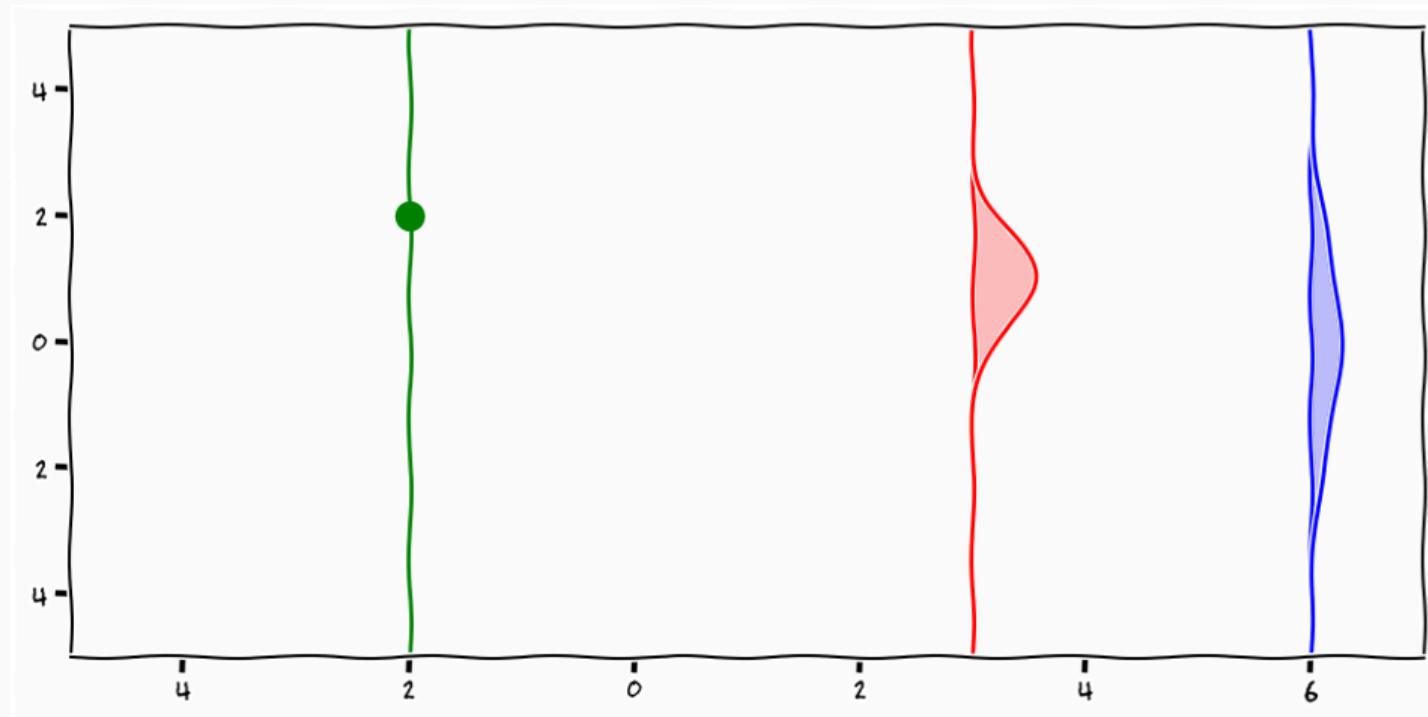
Gaussian Processes: Formalism II

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

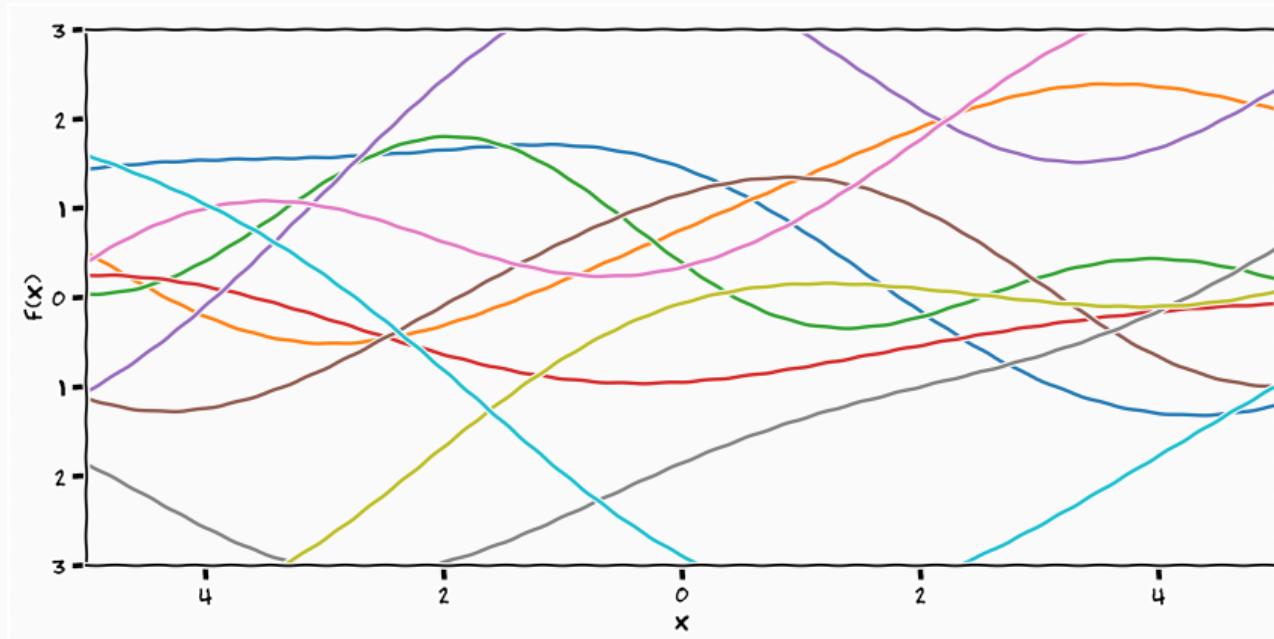
Definition (Gaussian Process)

A Gaussian process is a collection of random variables who are **jointly** Gaussian distributed index by a **infinite** index set

Gaussian Processes

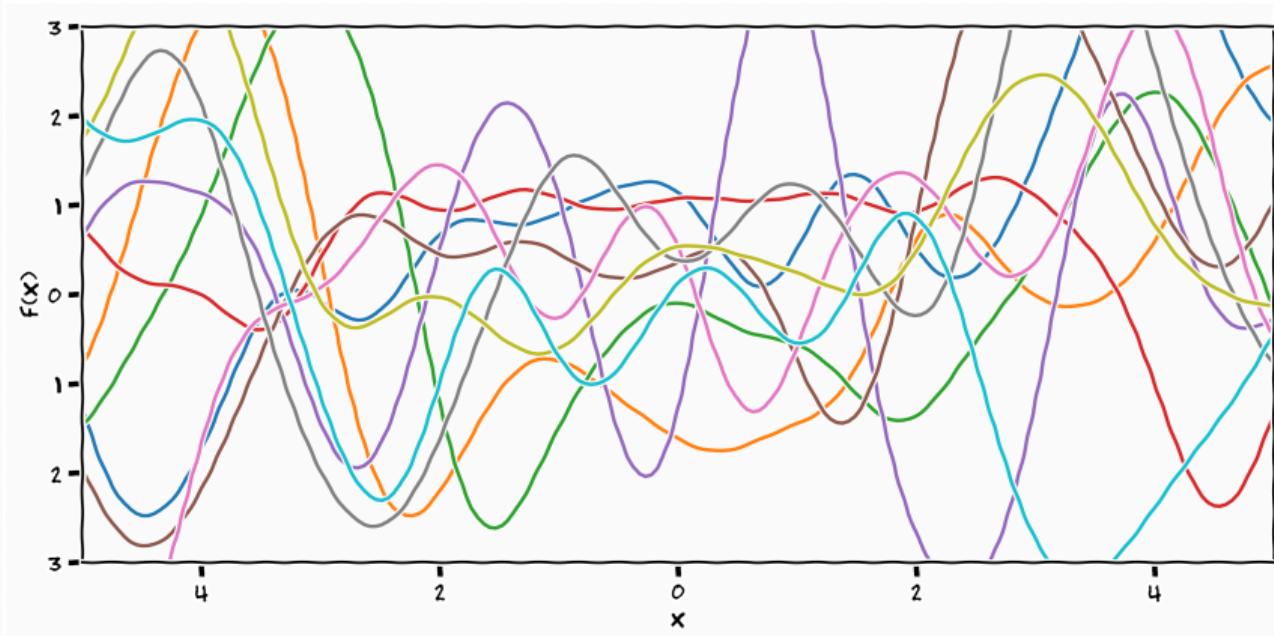


Gaussian Processes Samples



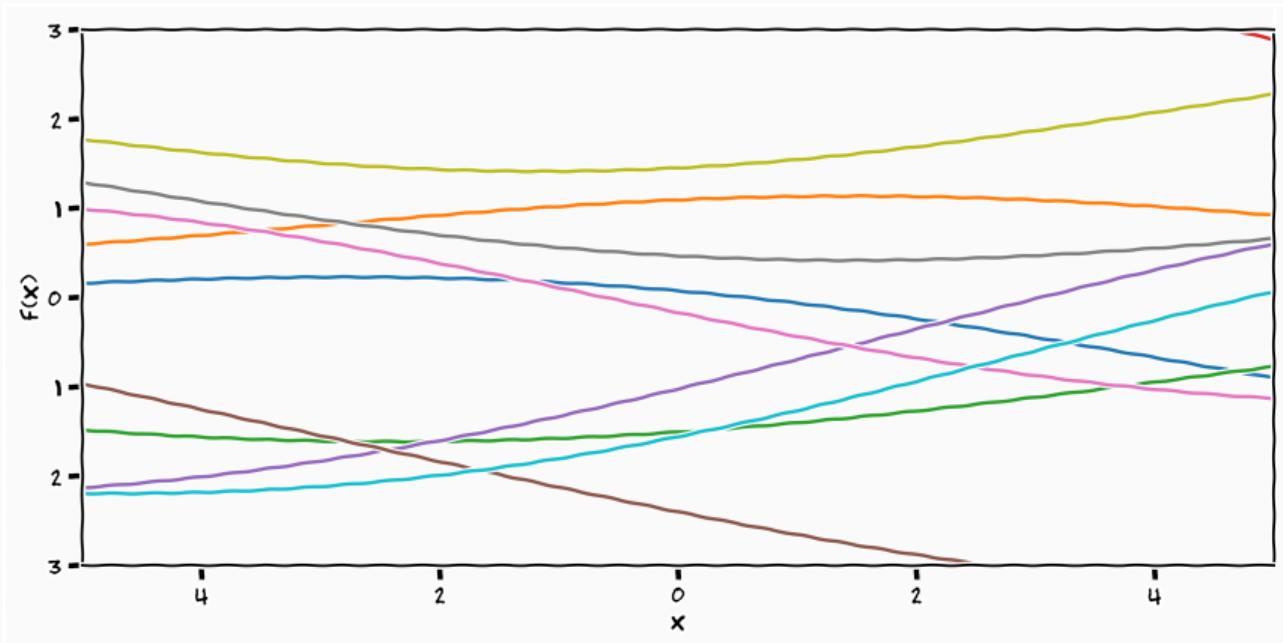
$$k(x_i, x_j) = 3 \cdot e^{-\frac{(x_i - x_j)^2}{15}}$$

Gaussian Processes Samples



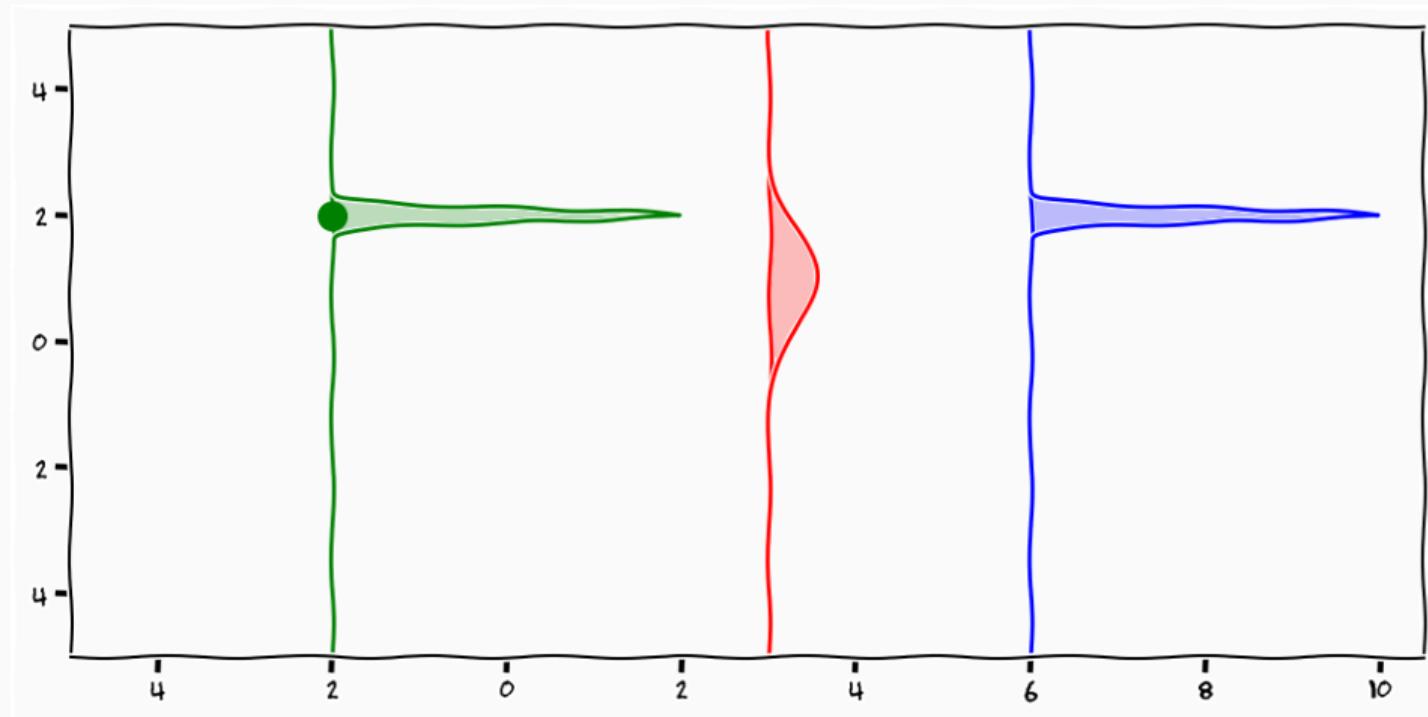
$$k(x_i, x_j) = 3 \cdot e^{-\frac{(x_i - x_j)^2}{1}}$$

Gaussian Processes Samples



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

Gaussian Processes



Bayesian Inference

Bayes' Rule

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

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

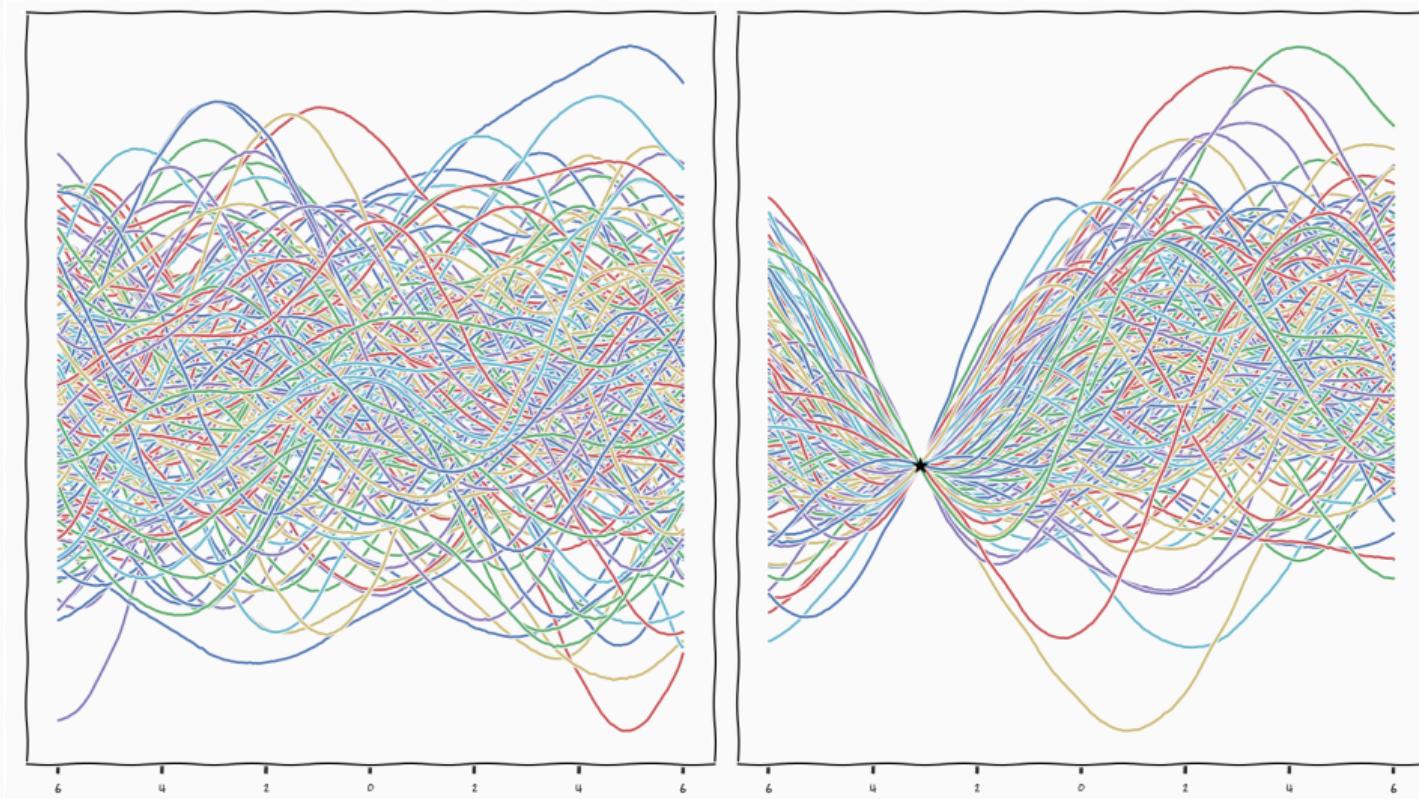
- Take every possible function value/marginal \mathbf{f}_* at location \mathbf{x}_* according to their probability, at every location

Marginal Likelihood

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

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

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

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

Gaussian Process: "Predictive Posterior"

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

Gaussian Process: "Predictive Posterior"

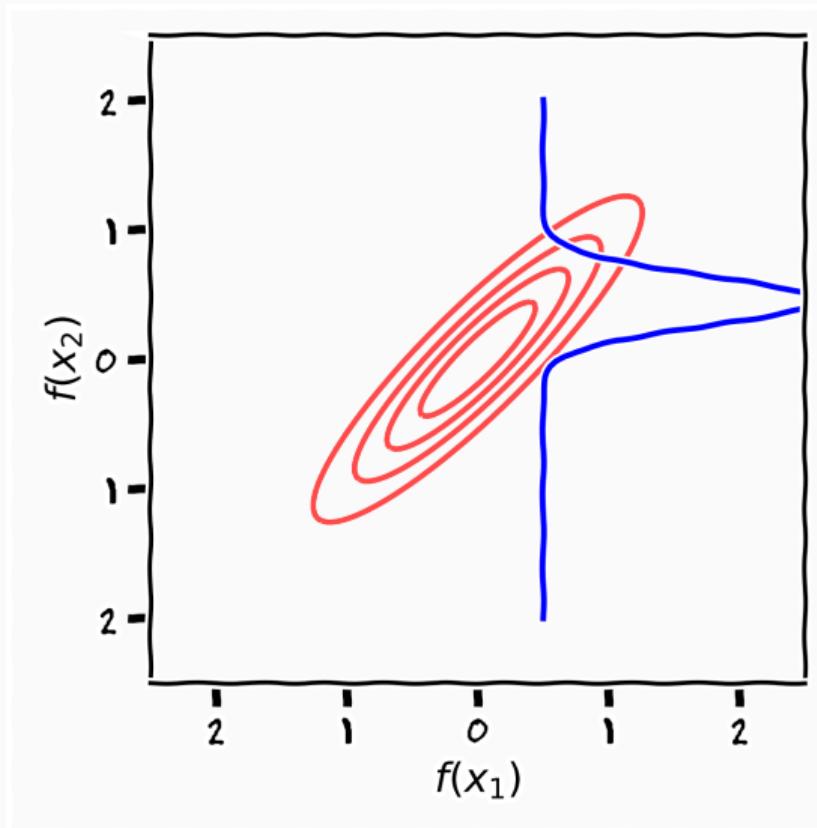
- All instantiations are jointly Gaussian

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}, \mathbf{x}) & k(\mathbf{x}, \mathbf{x}_*) \\ k(\mathbf{x}_*, \mathbf{x}) & k(\mathbf{x}_*, \mathbf{x}_*) \end{bmatrix} \right)$$

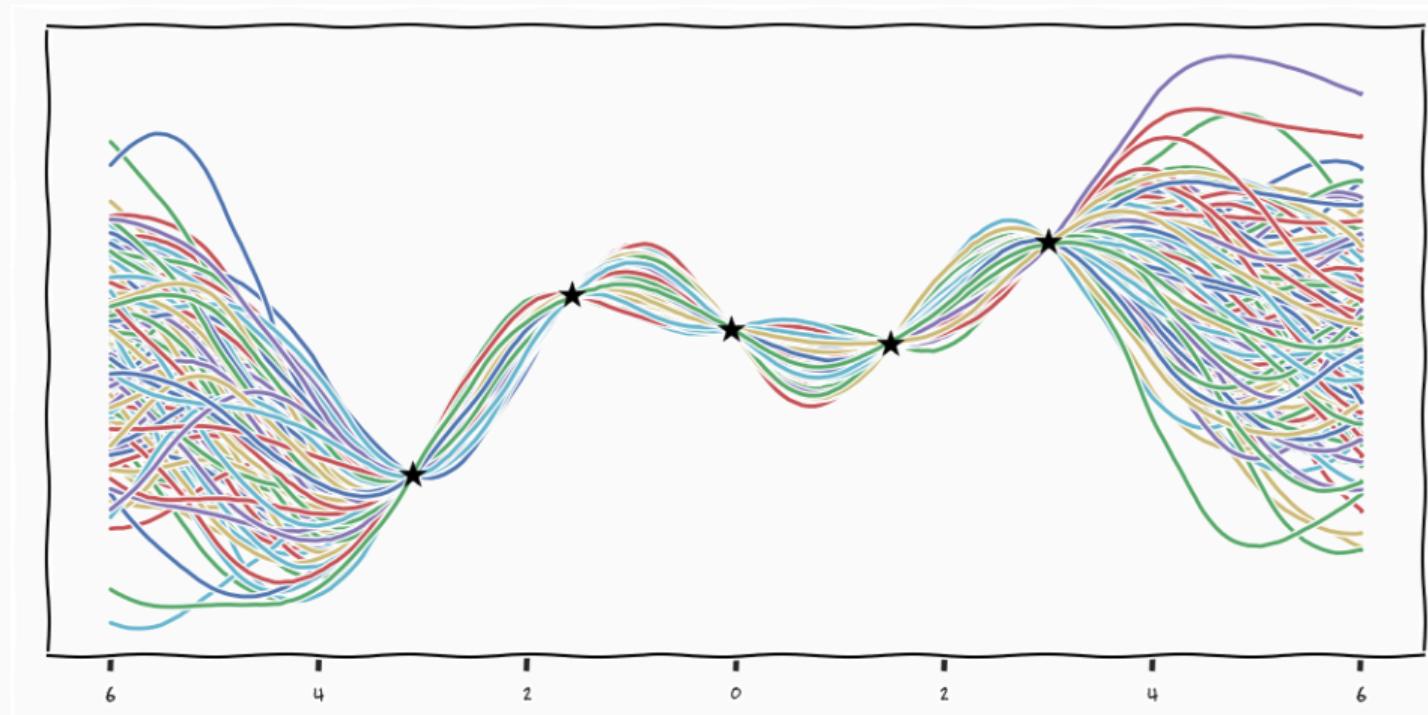
- Conditional Gaussian

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

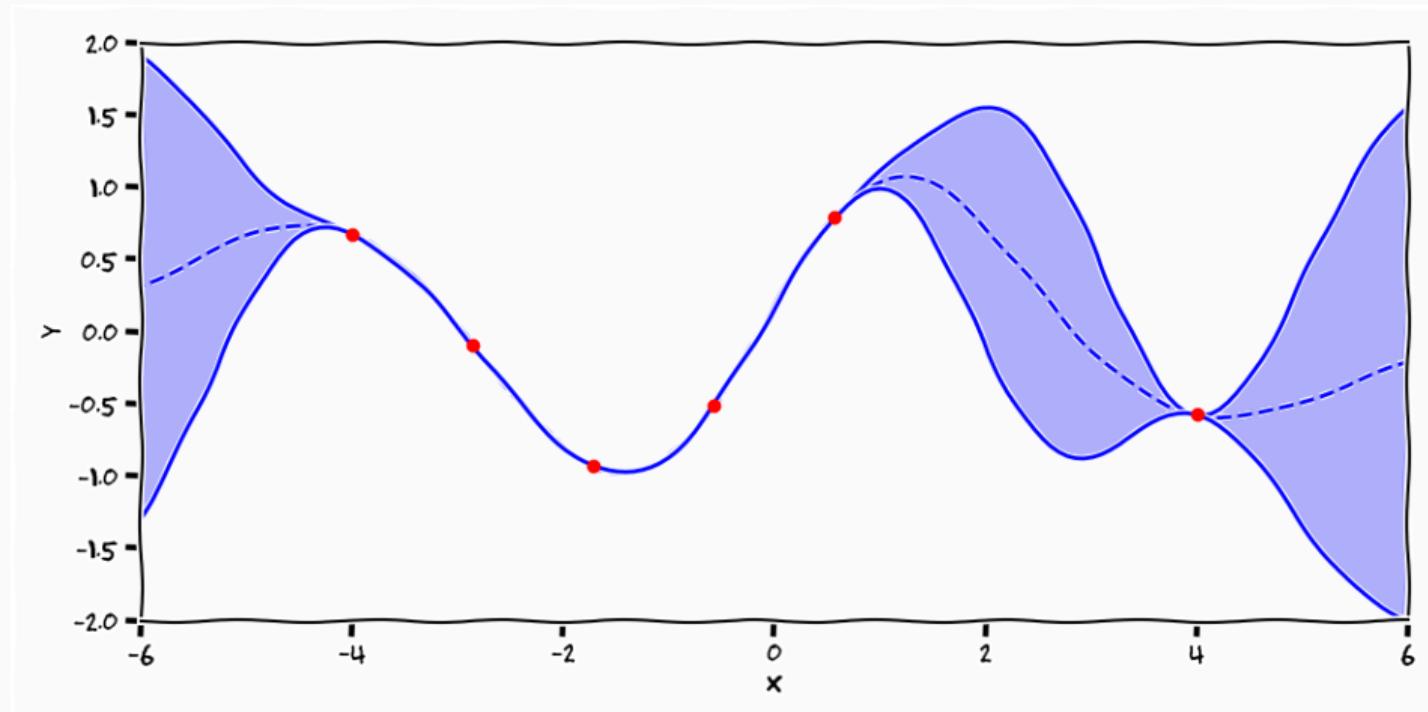
Conditional Gaussians



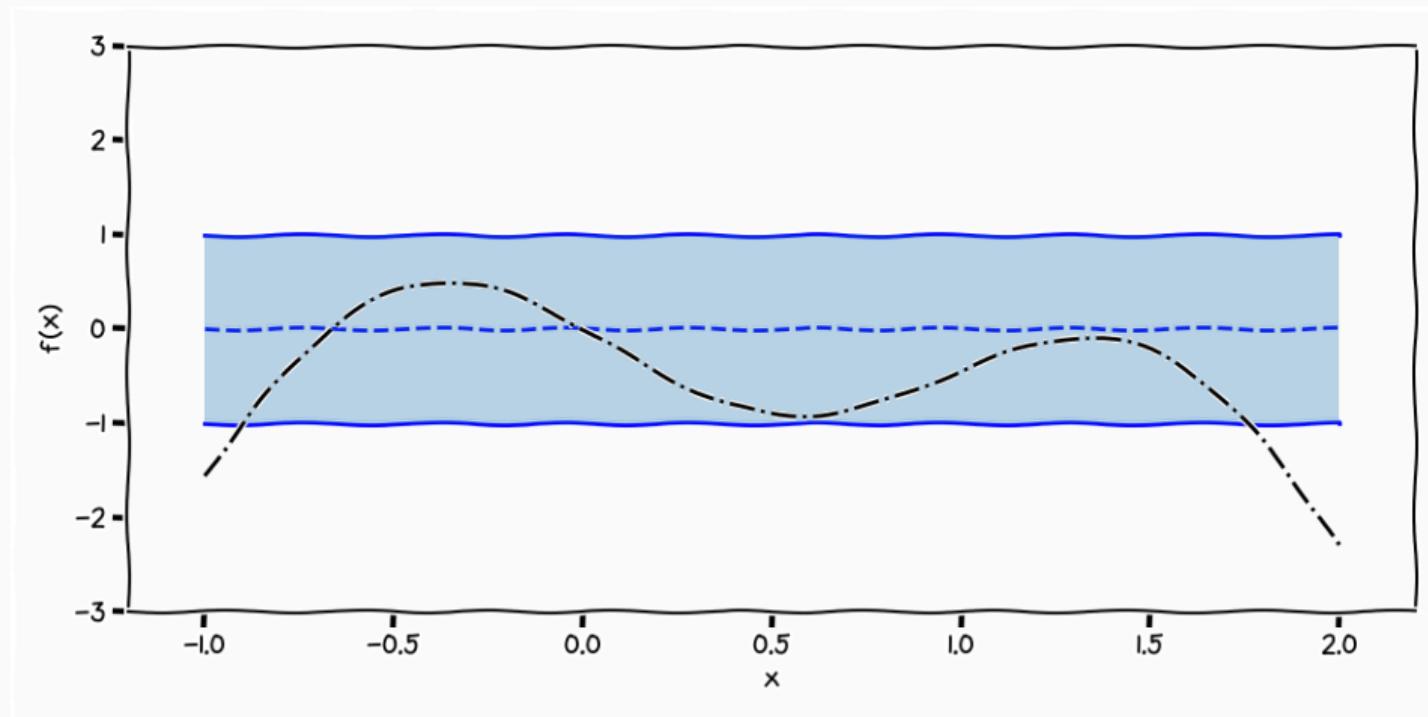
Gaussian Processes: "Predictive Posterior Samples"



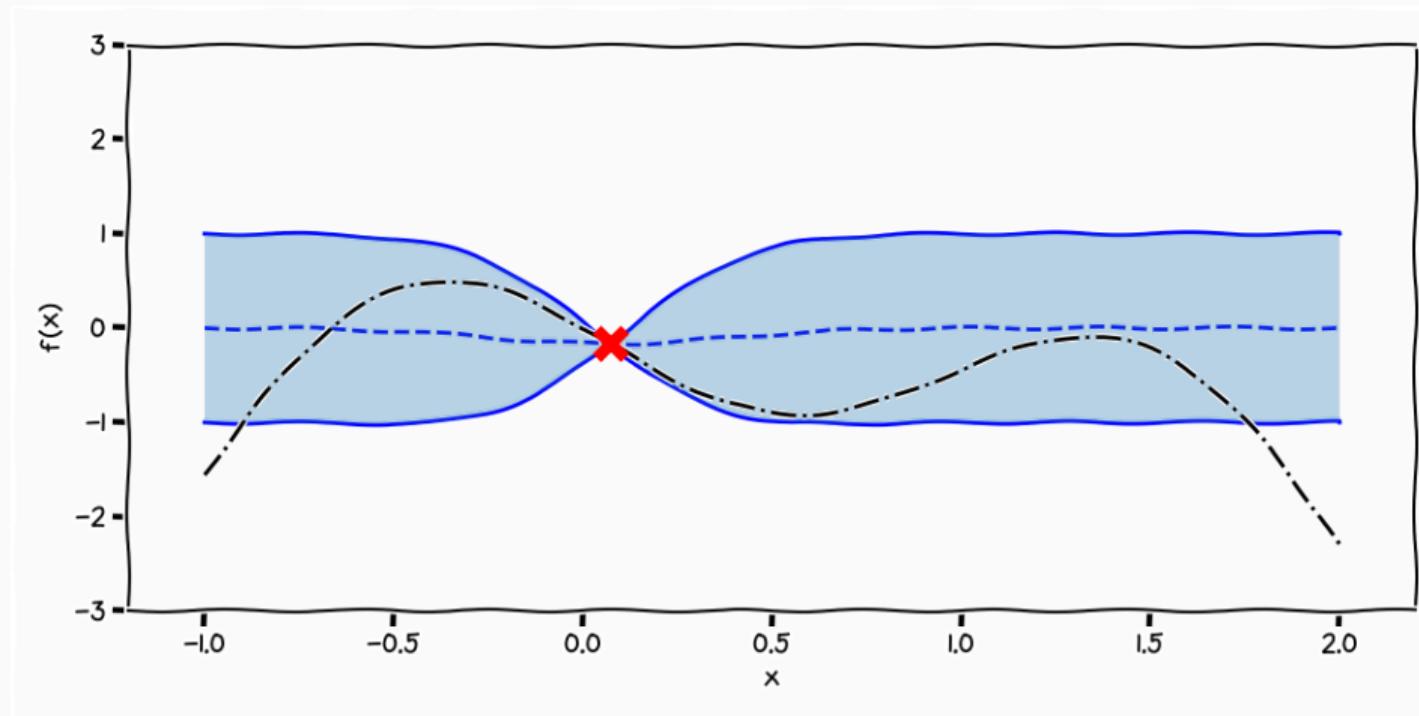
Gaussian Processes: "Predictive Posterior Process"



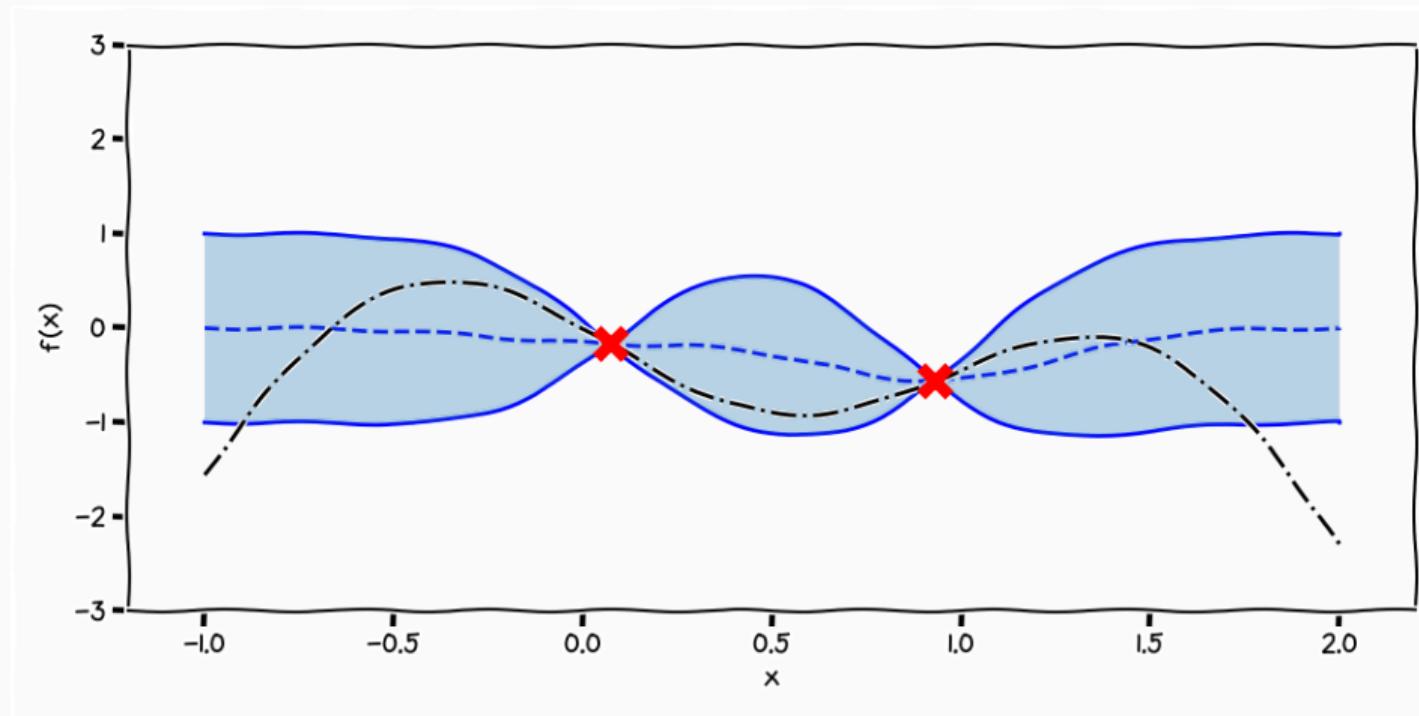
Posterior Processes



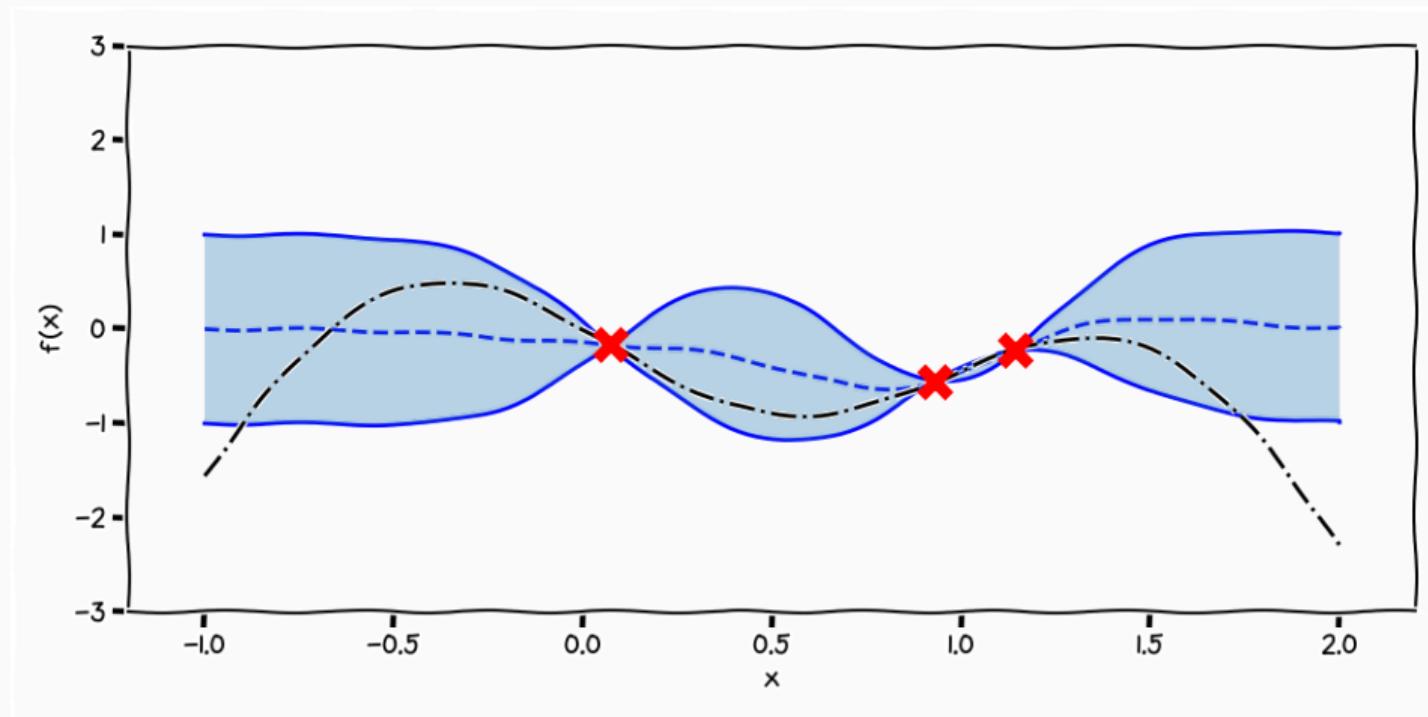
Posterior Processes



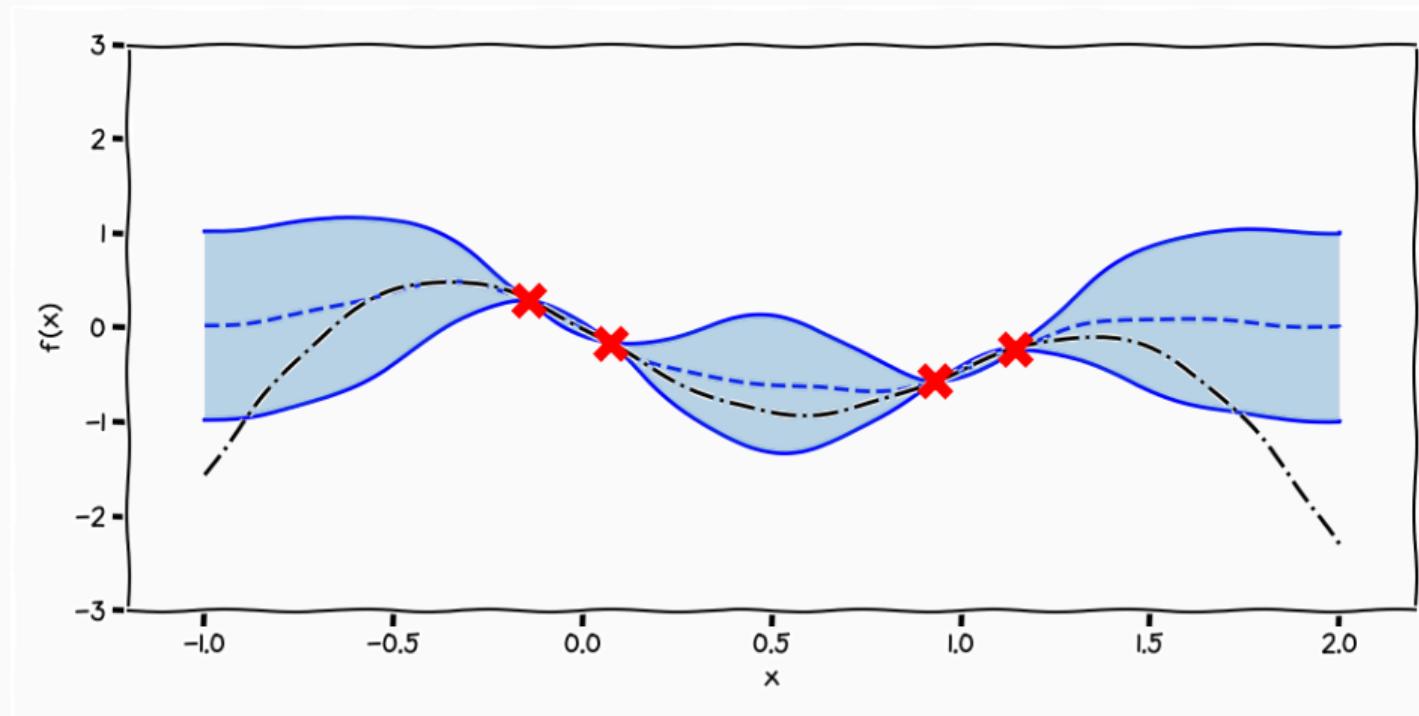
Posterior Processes



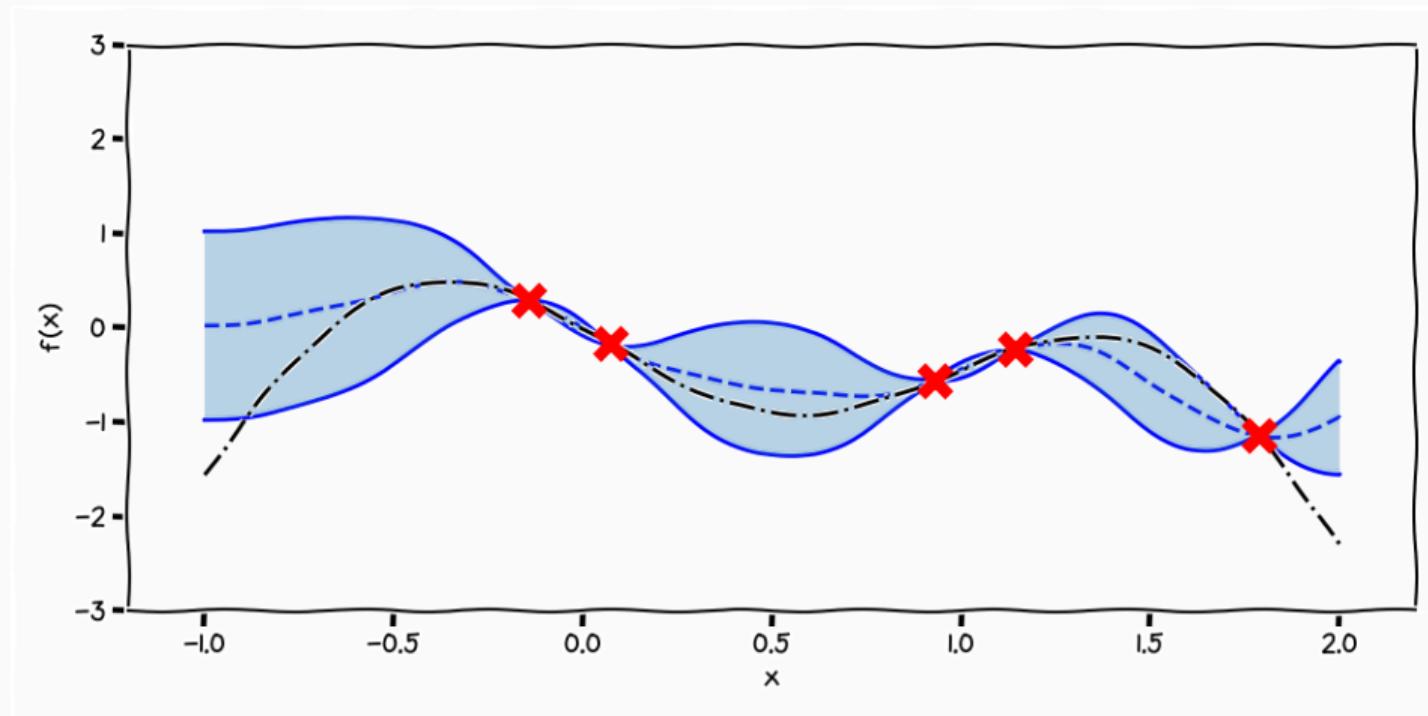
Posterior Processes



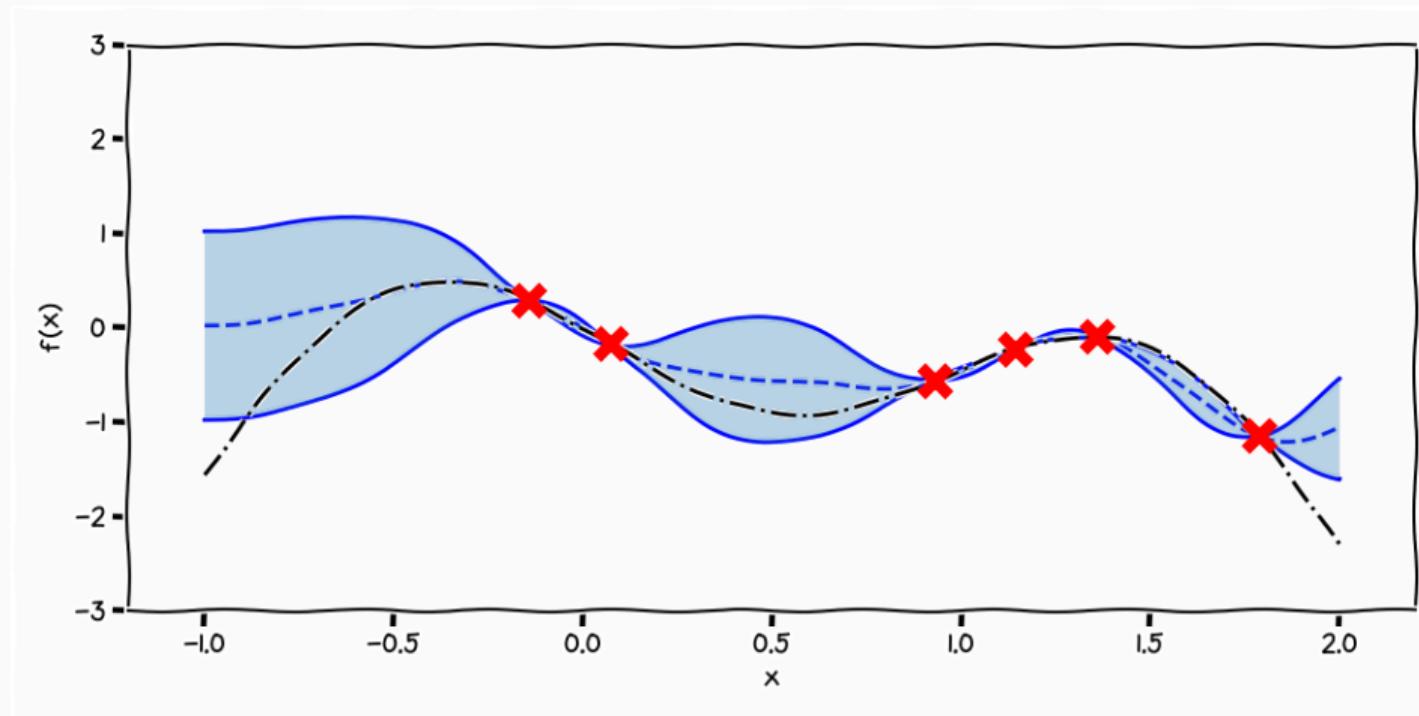
Posterior Processes



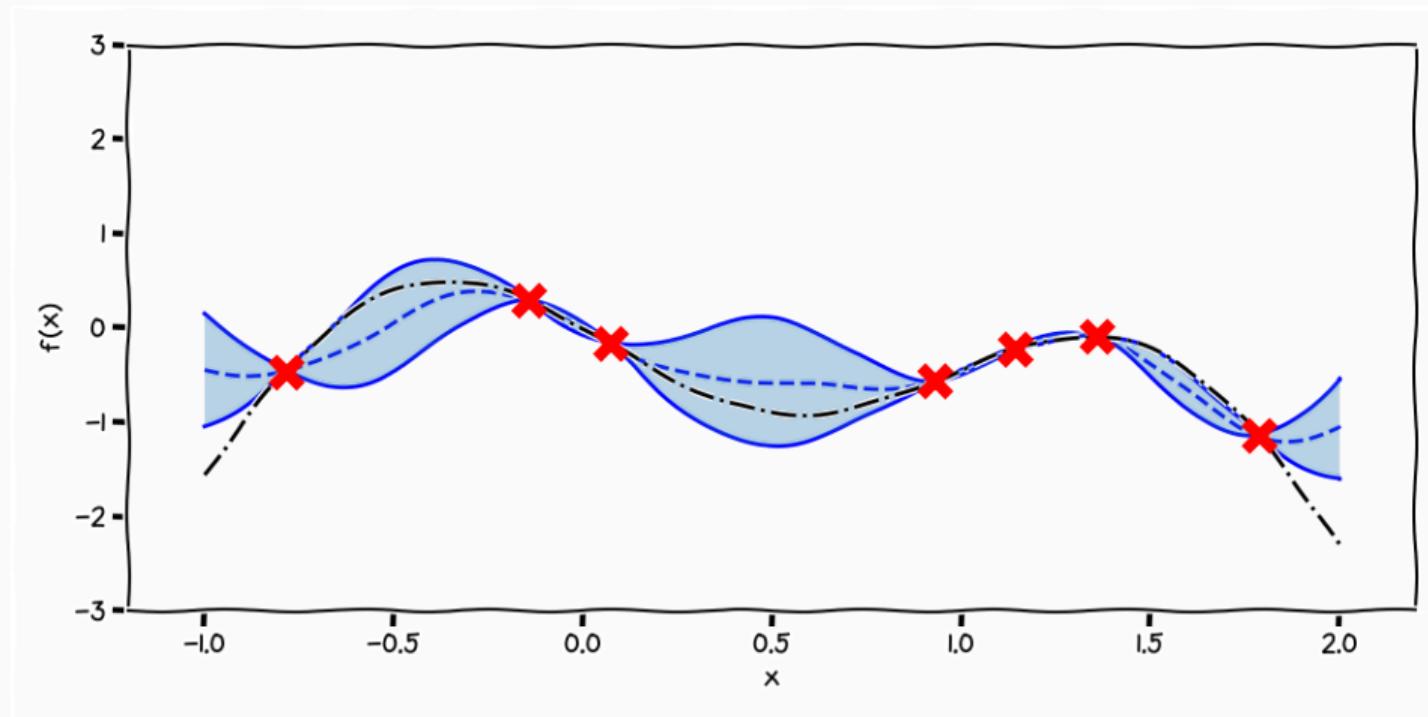
Posterior Processes



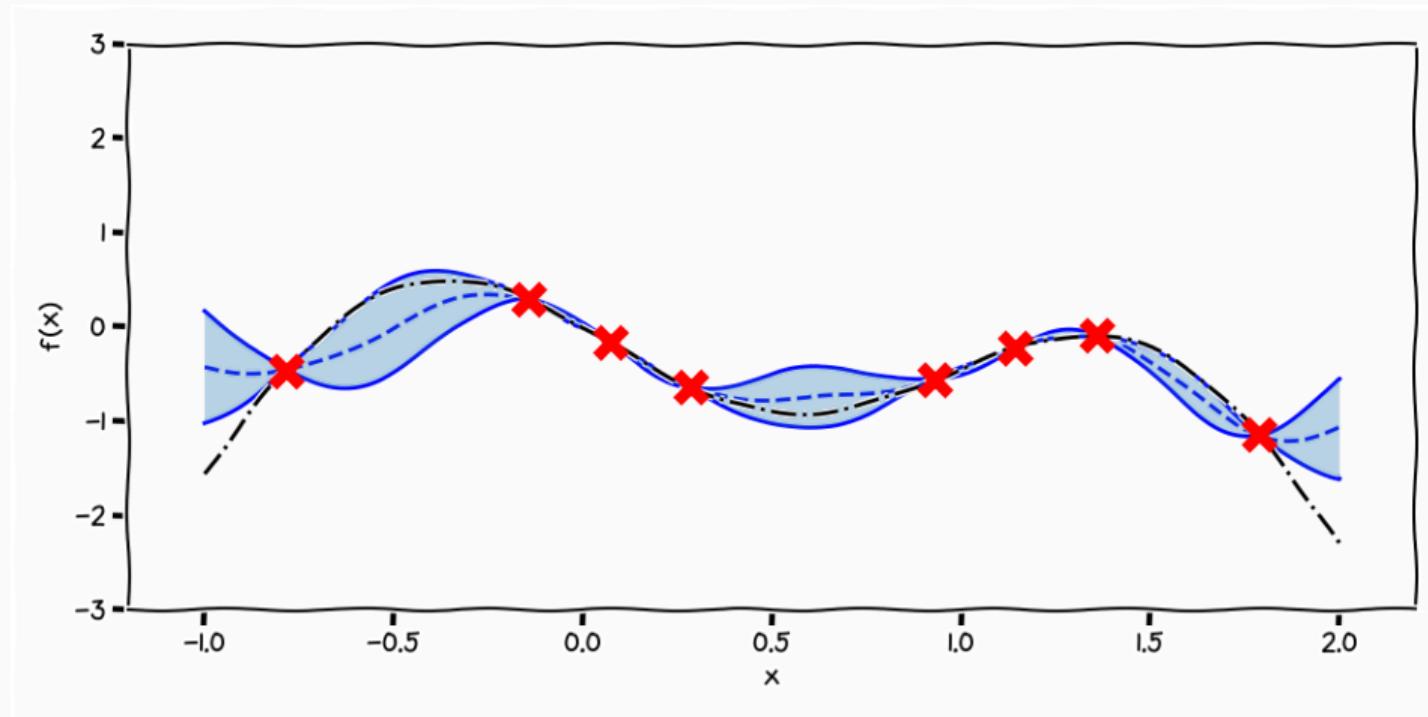
Posterior Processes



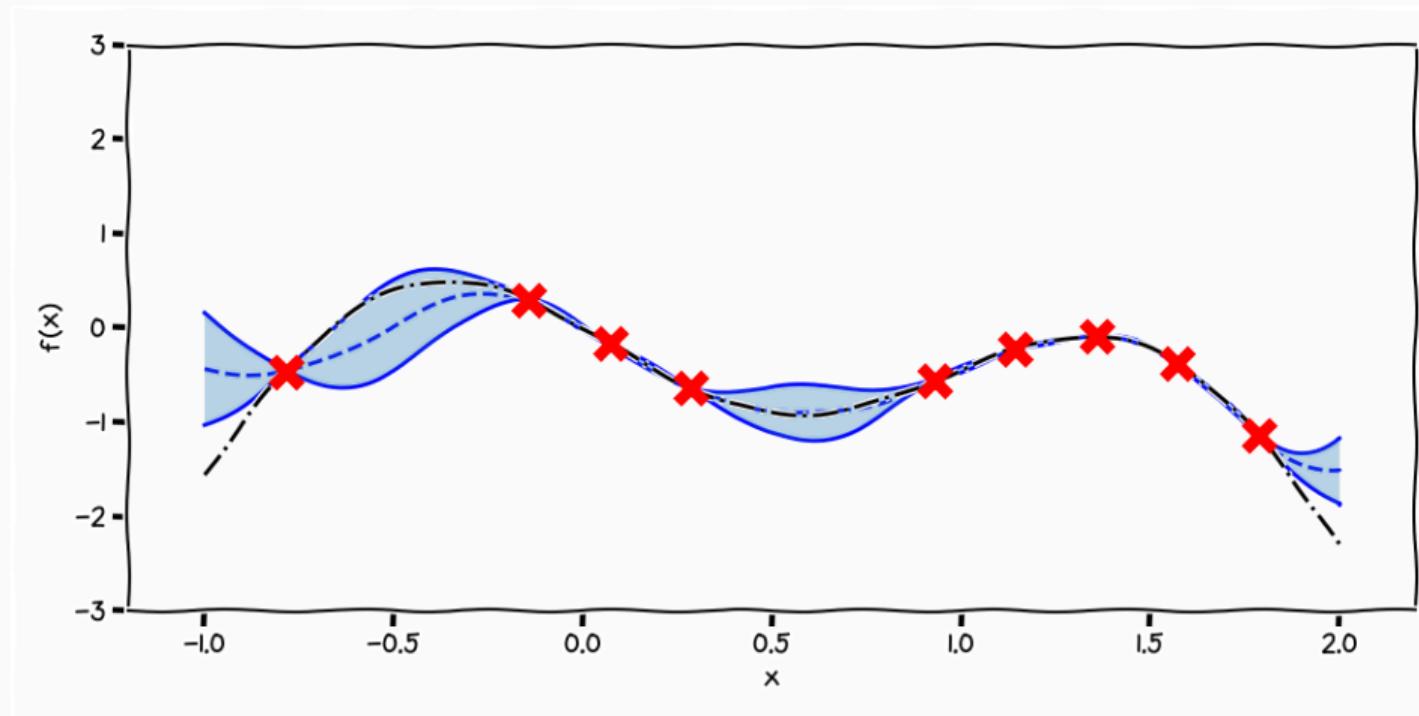
Posterior Processes



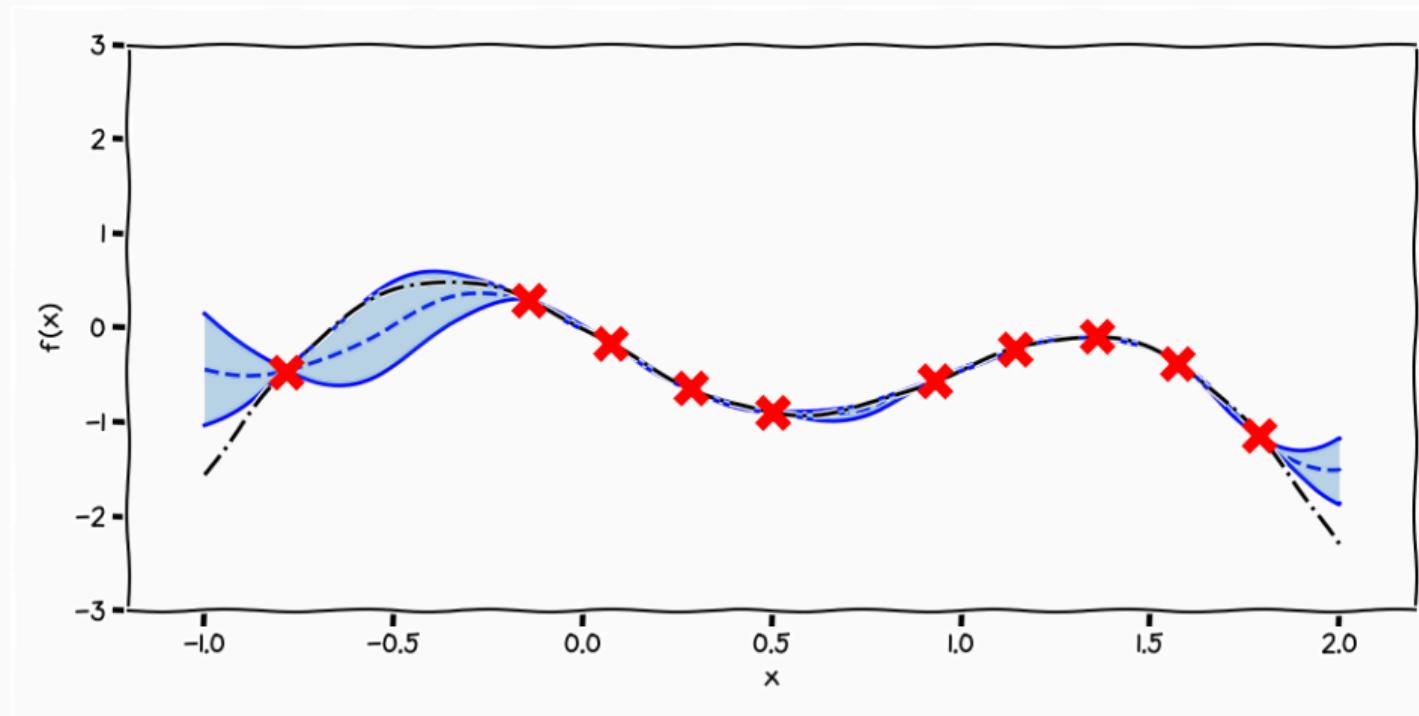
Posterior Processes



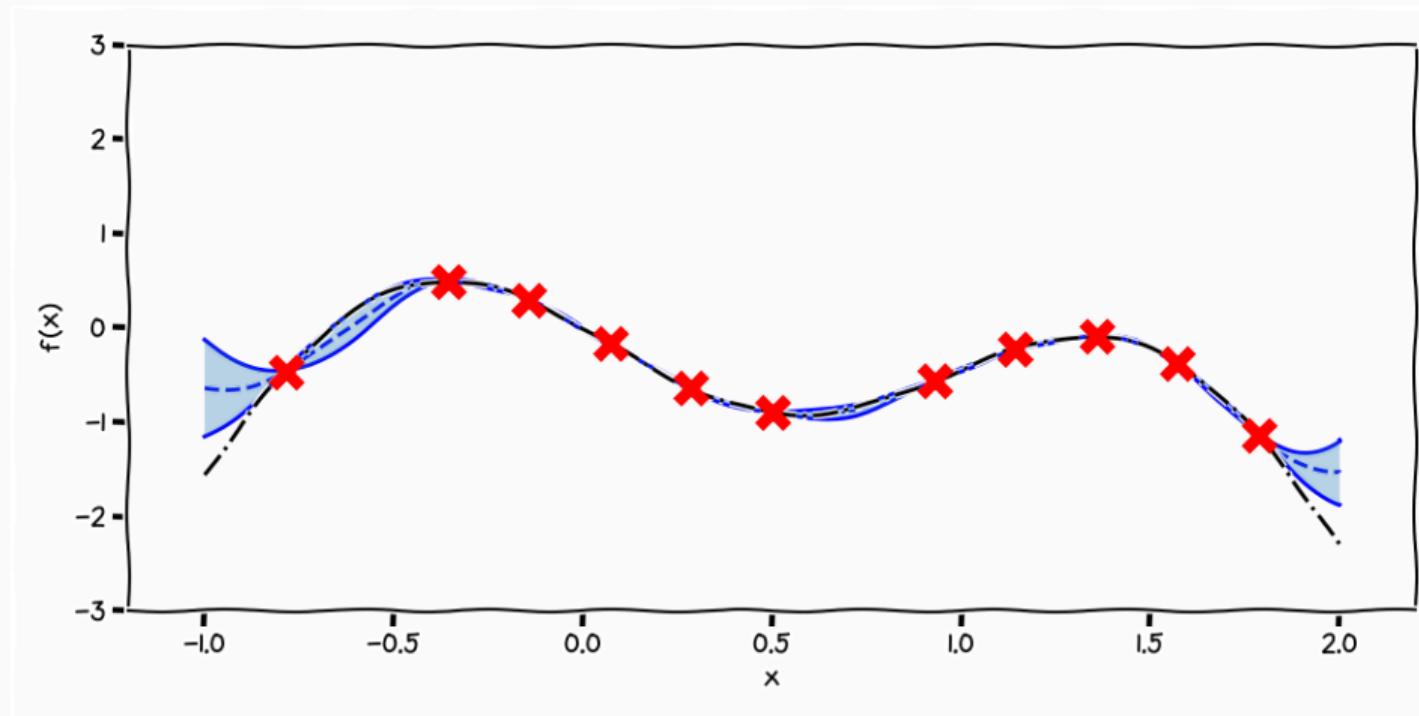
Posterior Processes



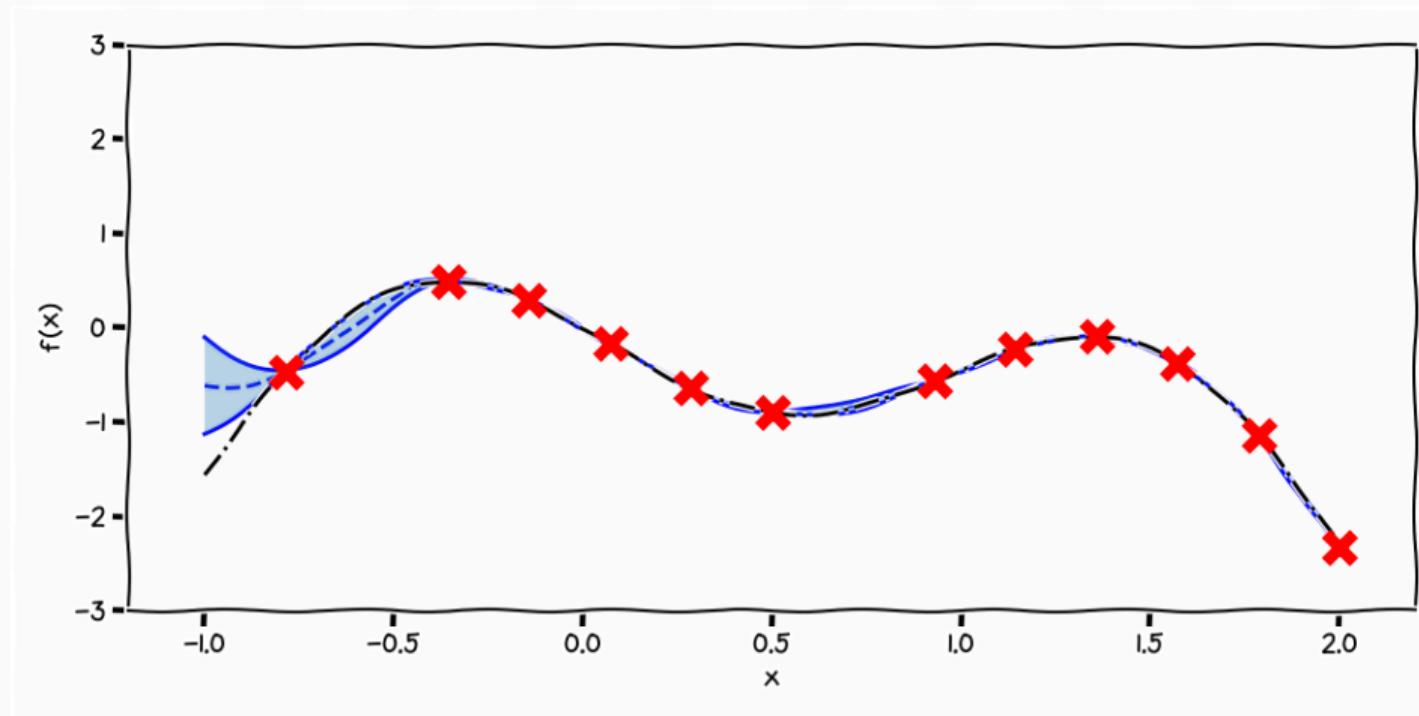
Posterior Processes



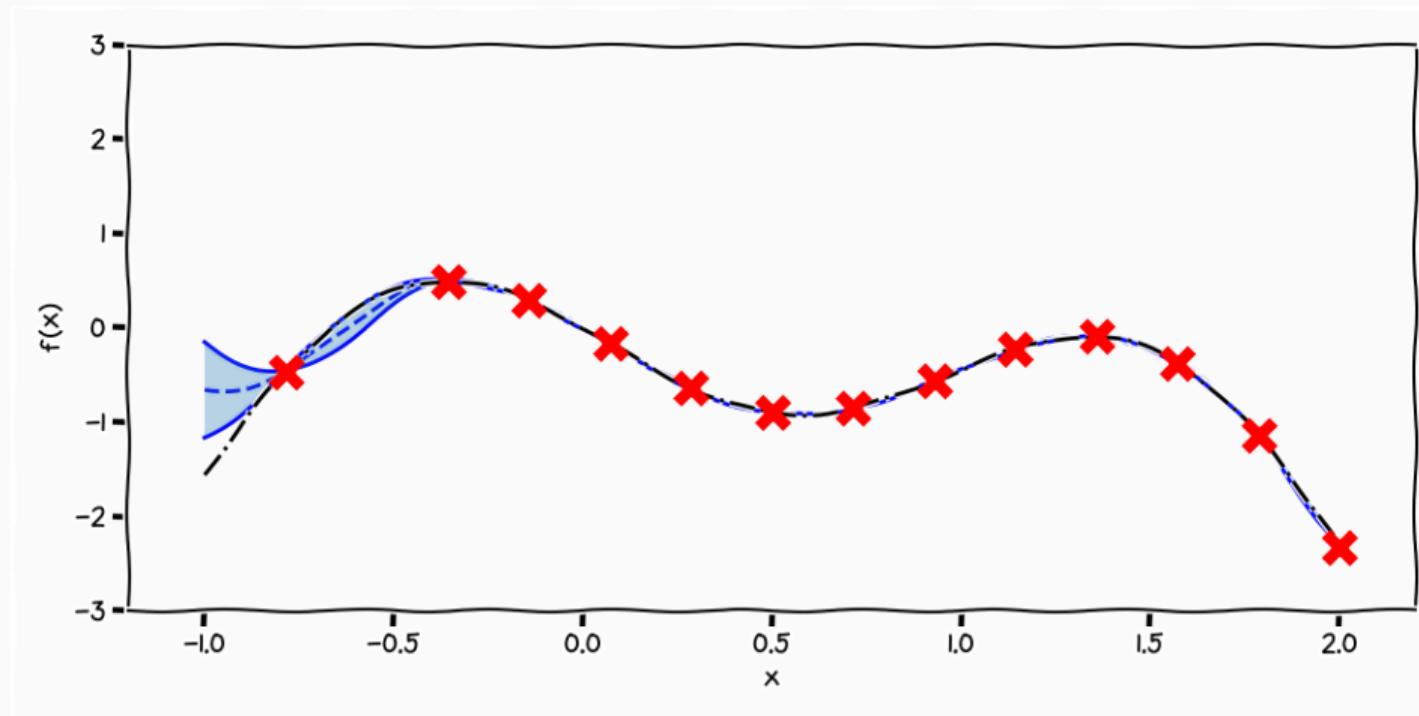
Posterior Processes



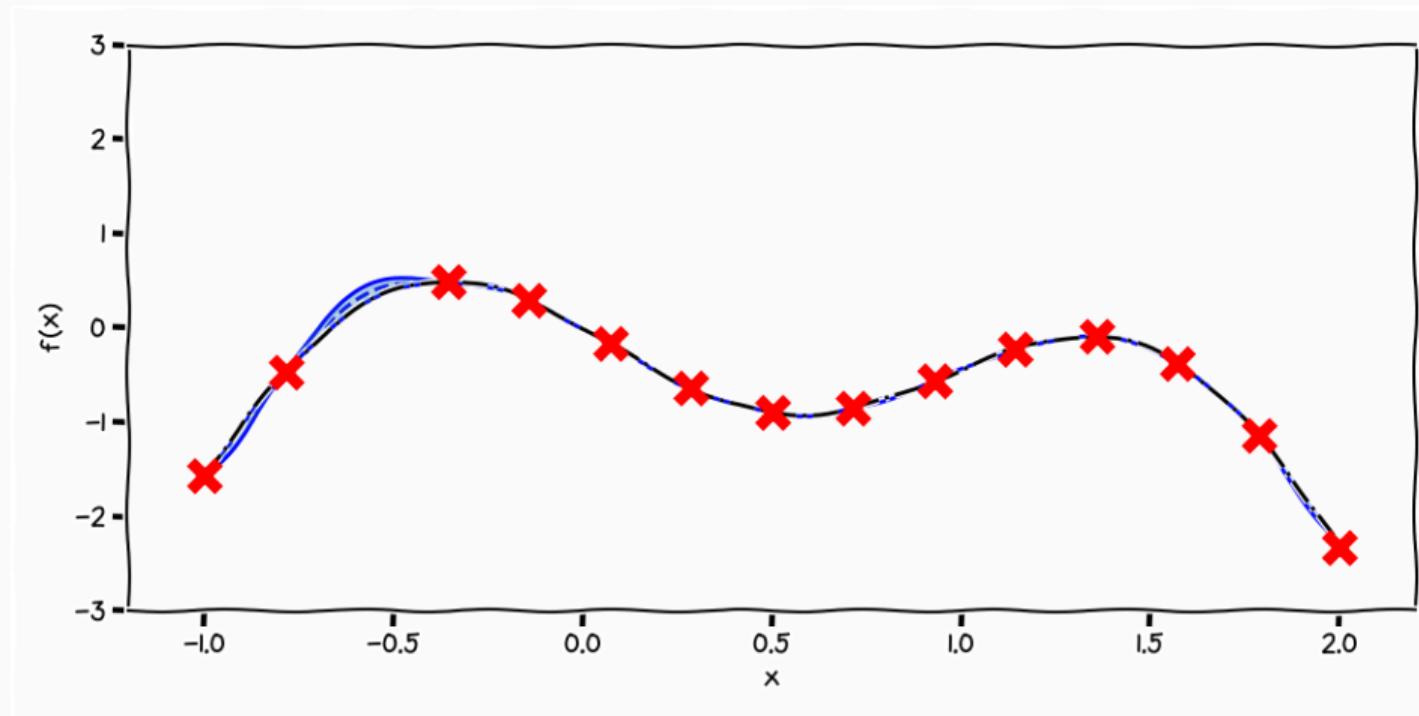
Posterior Processes



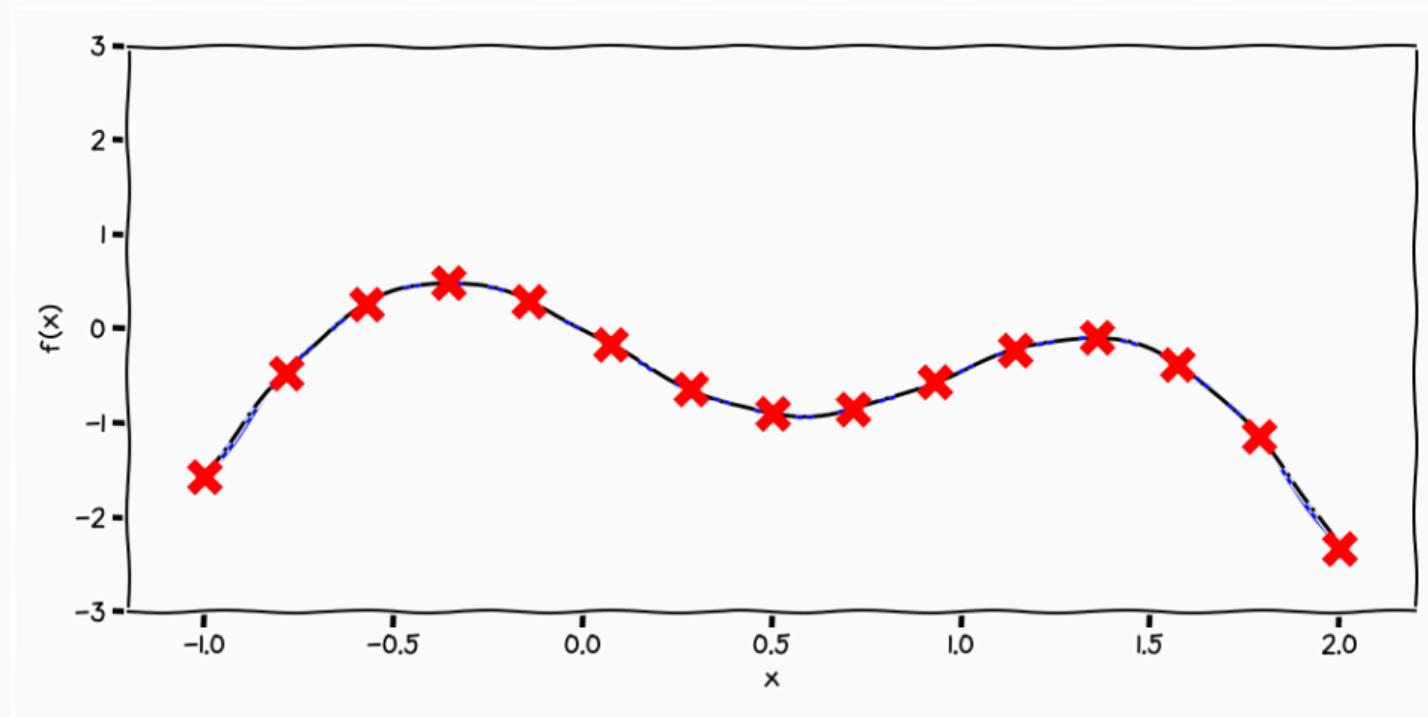
Posterior Processes



Posterior Processes



Posterior Processes



- 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

$$p(\mathbf{y}, \mathbf{f}) = p(\mathbf{y} \mid \mathbf{f})p(\mathbf{f}) = p(\mathbf{f}) \prod_{i=1} p(y_i \mid f_i)$$
$$p(\mathbf{y} \mid \mathbf{f}) = \mathcal{N}(\mathbf{y} \mid \mathbf{f}, \sigma^2 \mathbf{I})$$

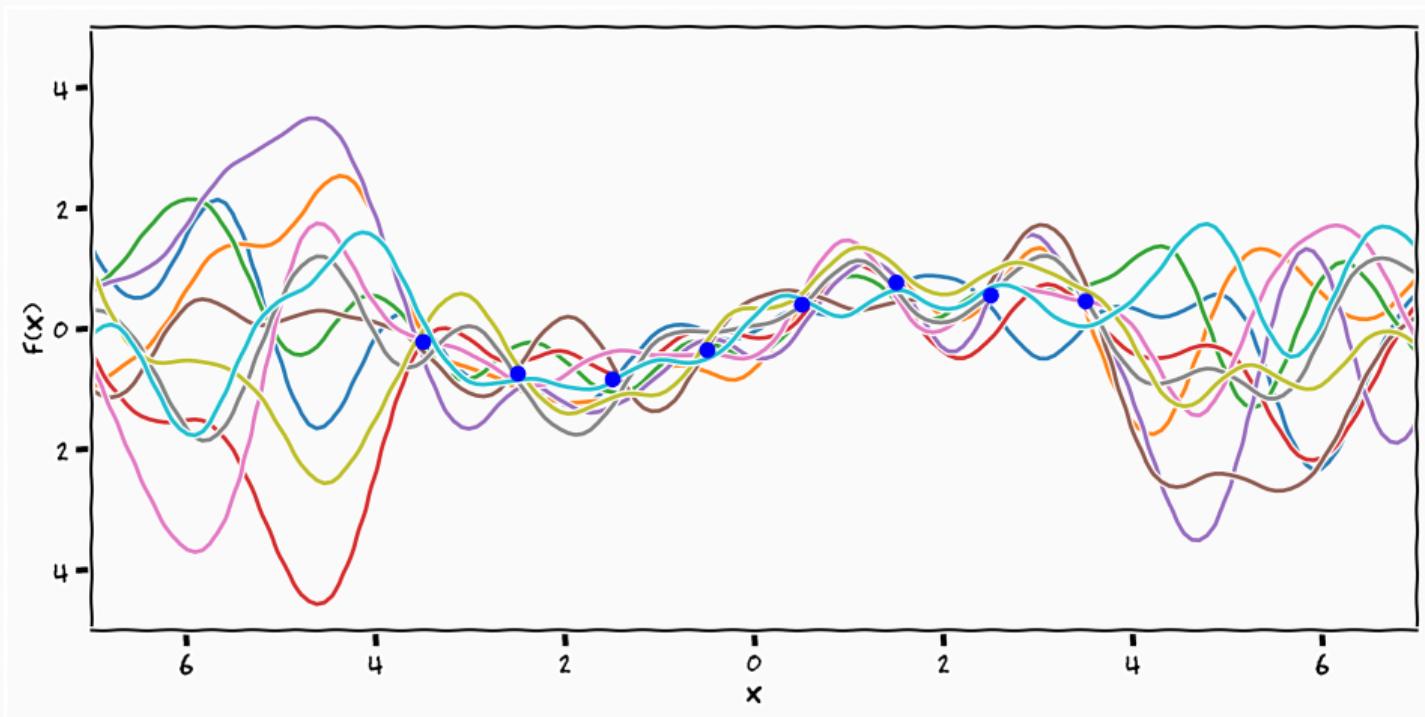
- Same motivation as with linear regression
- we want to **explain away** our ignorance from the data using σ

Predictive Posterior Process

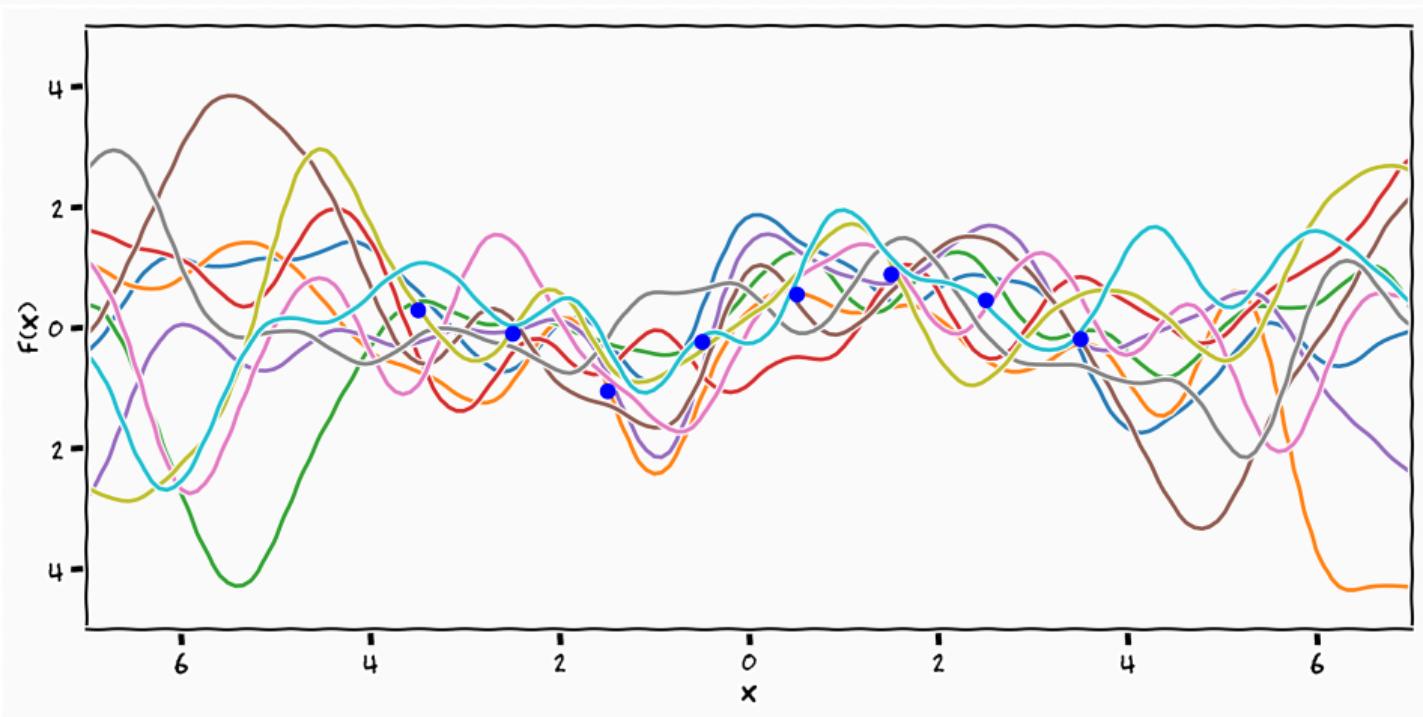
$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}, \mathbf{x}) + \sigma^2 \mathbf{I} & k(\mathbf{x}, \mathbf{x}_*) \\ k(\mathbf{x}_*, \mathbf{x}) & k(\mathbf{x}_*, \mathbf{x}_*) \end{bmatrix}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

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

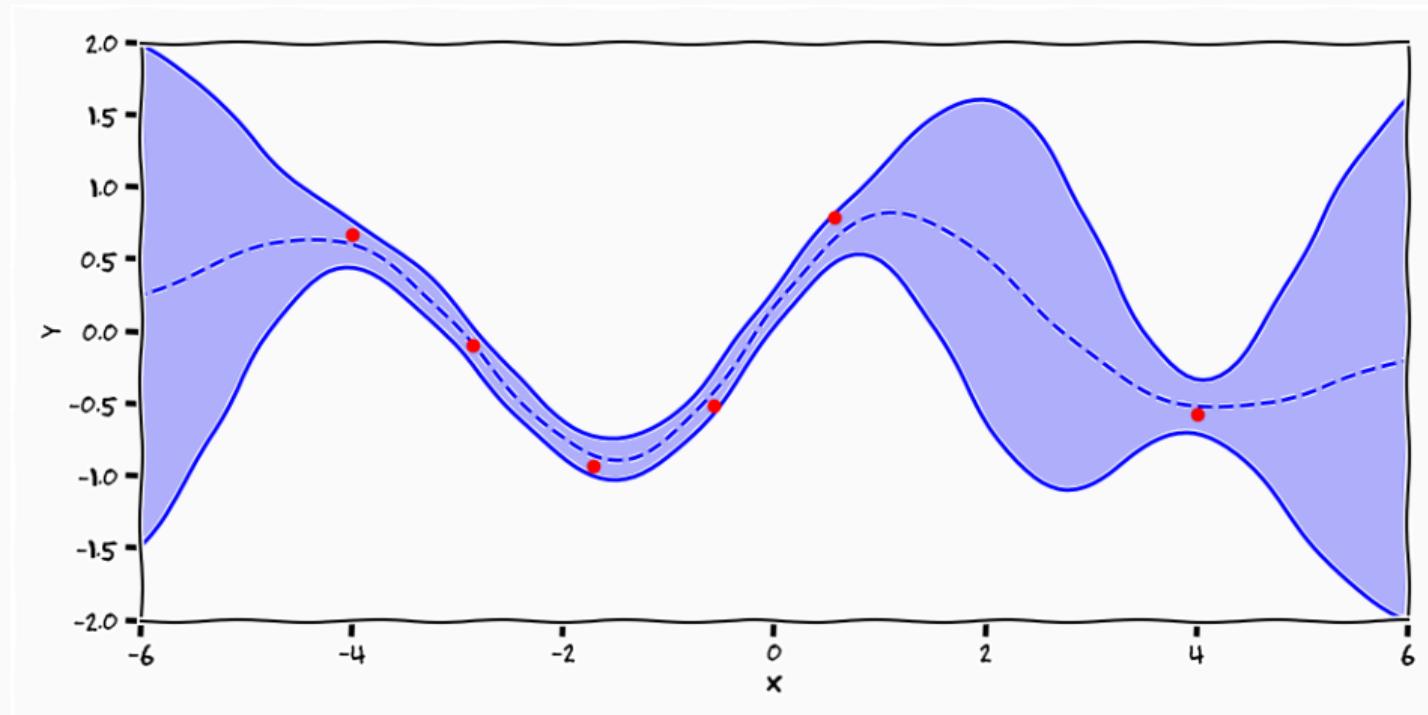
Posterior Samples



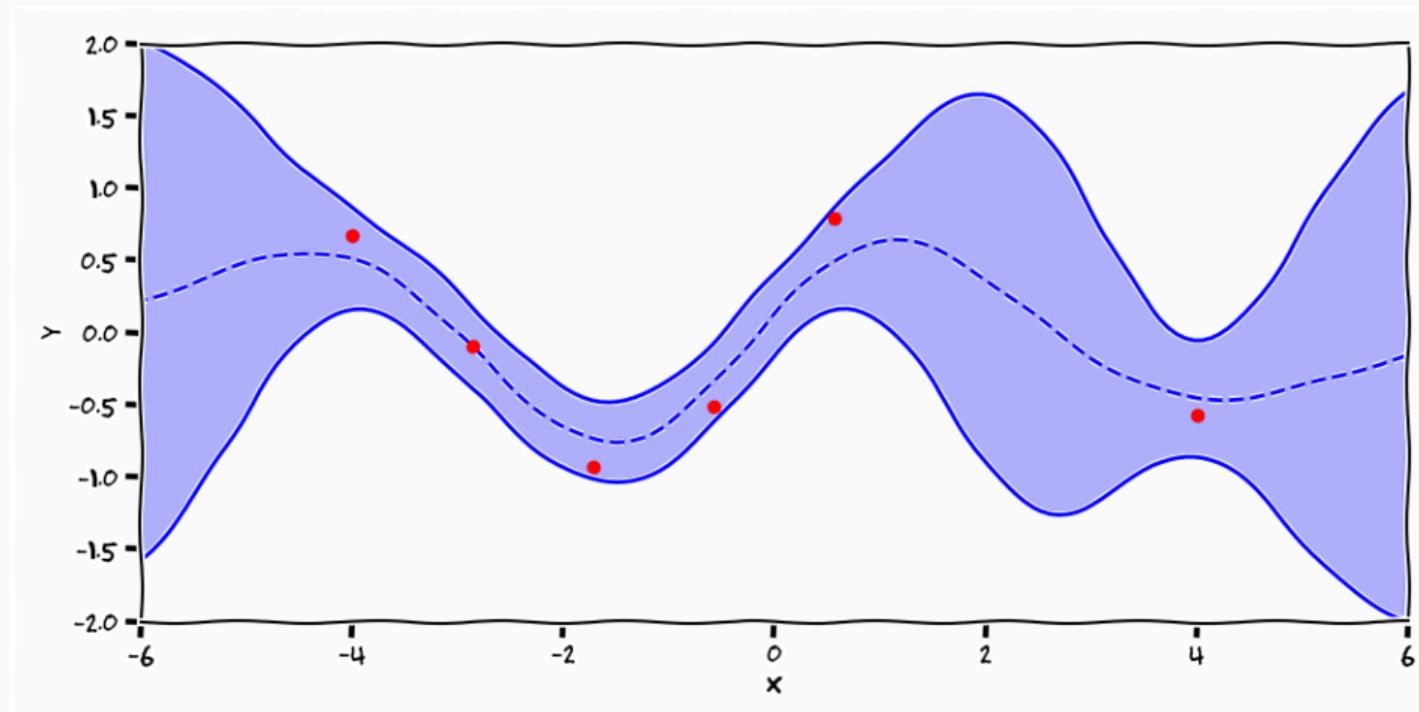
Posterior Samples



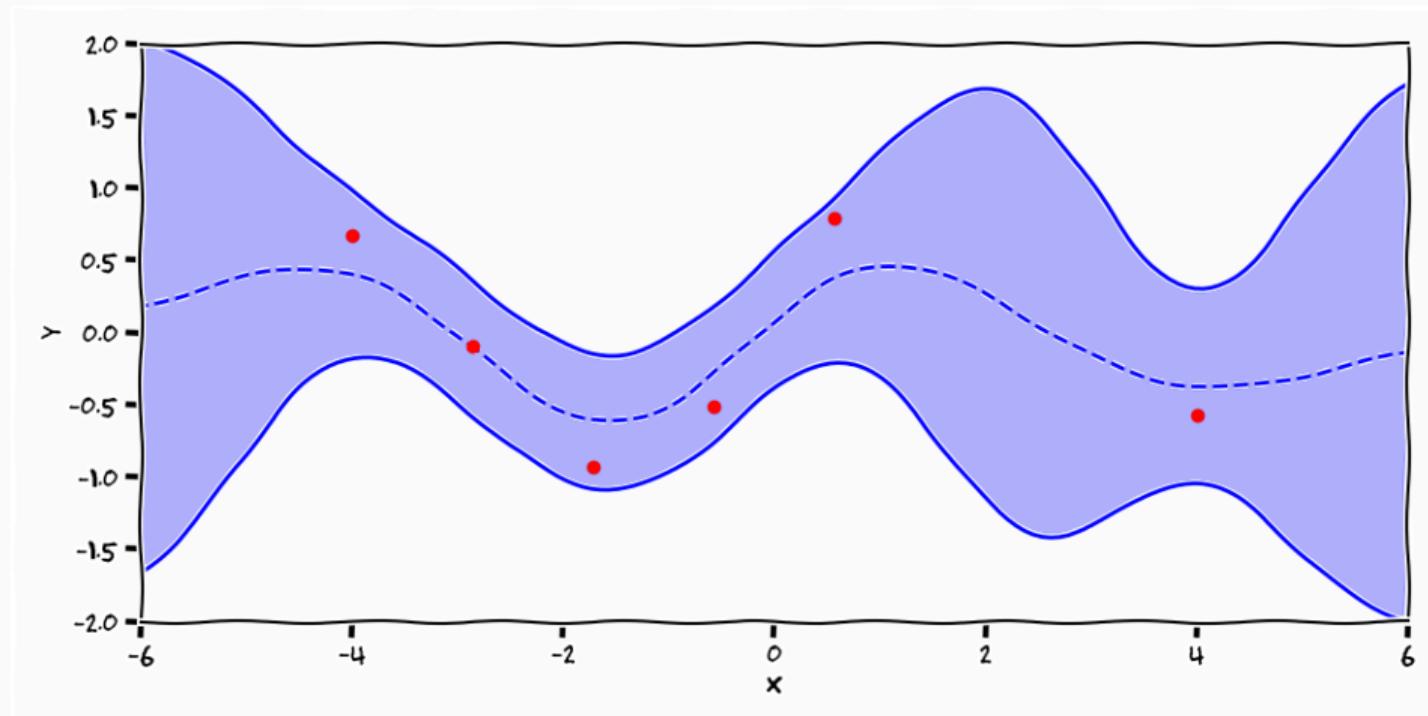
Gaussian Processes: Predictive Posterior Process



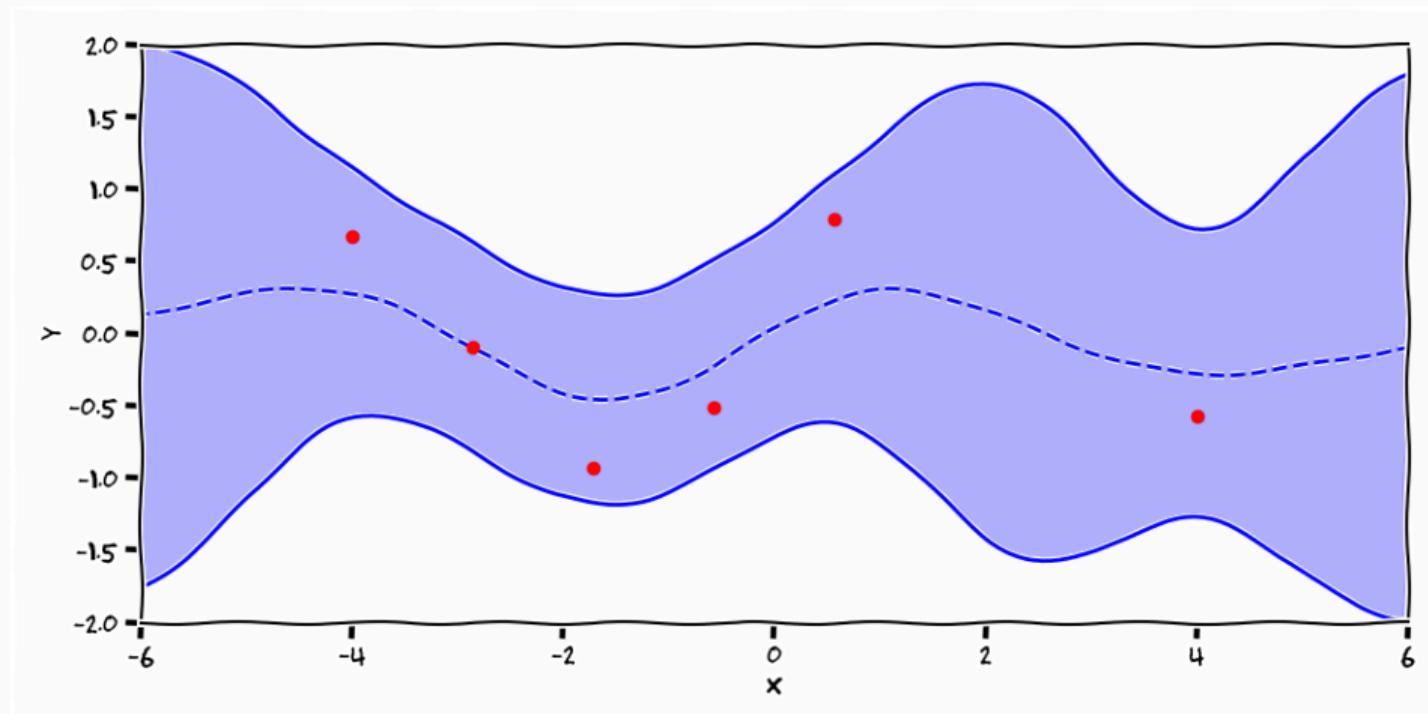
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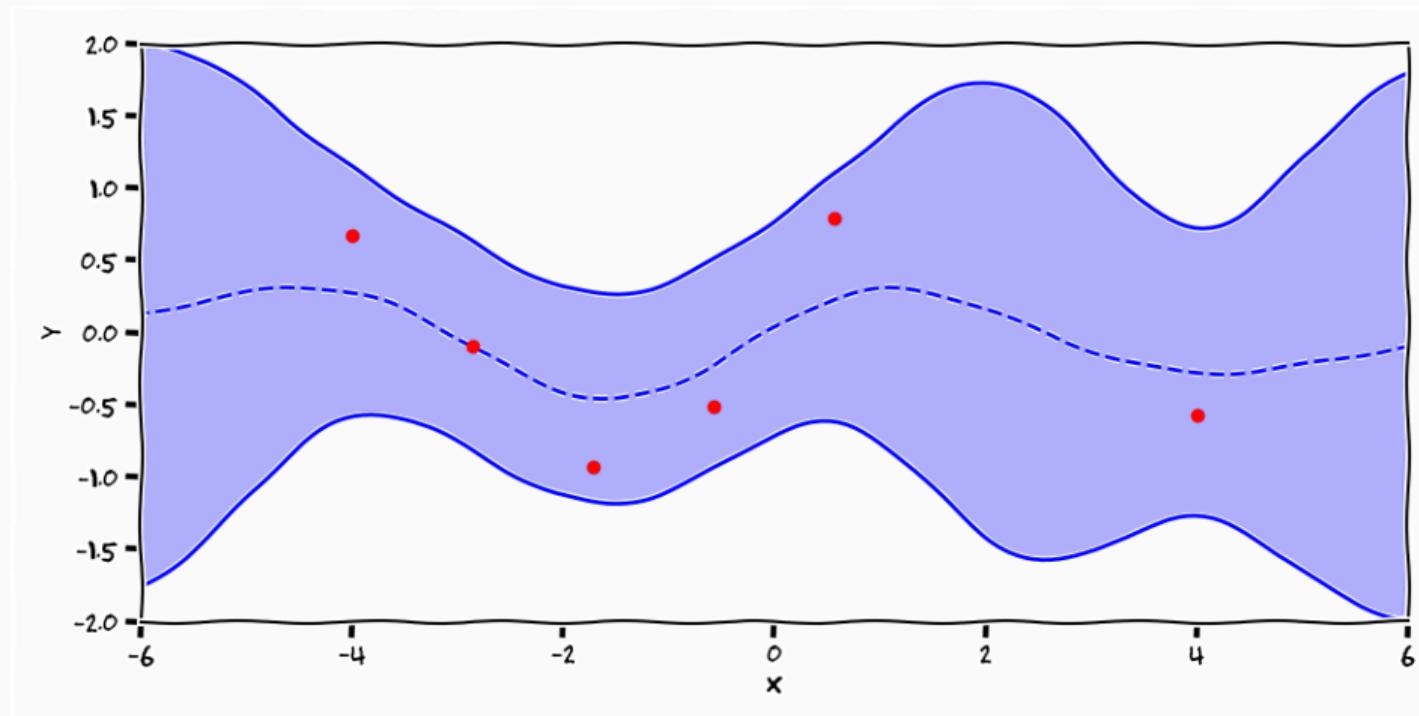
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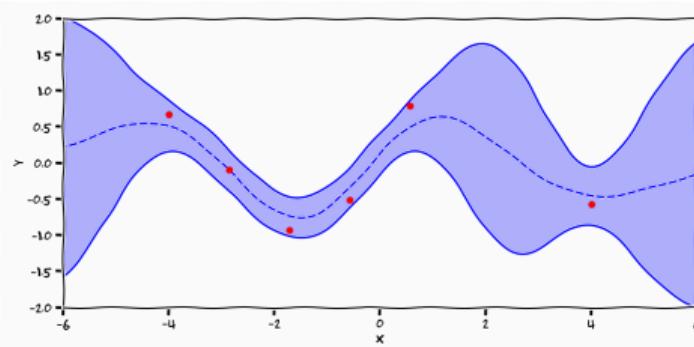
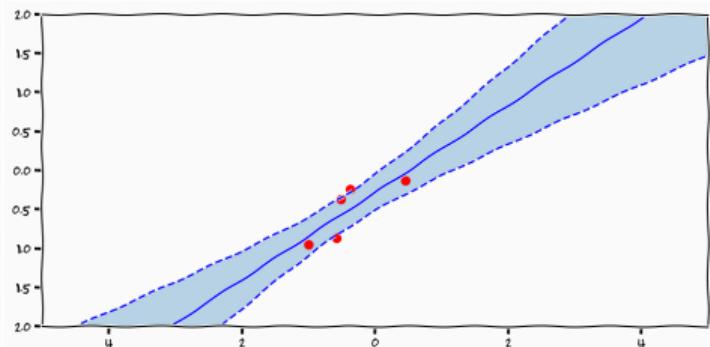
Gaussian Processes: Predictive Posterior Process



Gaussian Processes: Predictive Posterior Process



Two views



- Gaussian Process - *Non-parametric formulation*

$$p(y_* \mid \mathbf{y}, \mathbf{x}_*, \mathbf{X}, \theta) = \mathcal{N}(y_* \mid \mu_*, K_*)$$

$$\mu_* = k(\mathbf{x}_*, \mathbf{x}) (\sigma^2 \mathbf{I} + k(\mathbf{x}, \mathbf{x}))^{-1} \mathbf{y}$$

$$K_* = k(\mathbf{x}_*, \mathbf{x}_*) - k(\mathbf{x}_*, \mathbf{x}) (k(\mathbf{x}, \mathbf{x}) + \sigma^2 \mathbf{I})^{-1} k(\mathbf{x}, \mathbf{x}_*)$$

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- Linear Regression - *Parametric formulation*

$$\begin{aligned} p(y_* | \mathbf{y}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) &= \int p(y_* | \mathbf{x}_*, \mathbf{w}, \beta) p(\mathbf{w} | \mathbf{y}, \mathbf{X}, \alpha, \beta) d\mathbf{w} \\ &= \mathcal{N}(y_* \mid \mu_*(x_*), \Sigma_*(x_*)) \end{aligned}$$

$$\mu_* = (\beta(\alpha \mathbf{I} + \beta \mathbf{x}^T \mathbf{x})^{-1} \mathbf{x} \mathbf{y}^T \mathbf{x}_* = \mathbf{x}_*^T \mathbf{x} (\beta(\alpha \mathbf{I} + \beta \mathbf{x}^T \mathbf{x}))^{-1} \mathbf{y}$$

$$\Sigma_* = \frac{1}{\beta} + \mathbf{x}_*^T (\alpha \mathbf{I} + \beta \mathbf{x}^T \mathbf{x})^{-1} \mathbf{x}$$

Regression Models: Mean

$$\mu_*^{\text{GP}} = k(\mathbf{x}_*, \mathbf{x}) (\sigma^2 \mathbf{I} + k(\mathbf{x}, \mathbf{x}))^{-1} \mathbf{y} \quad \mu_*^{\text{Lin}} = \mathbf{x}_*^T \mathbf{x} (\beta(\alpha \mathbf{I} + \beta \mathbf{x}^T \mathbf{x}))^{-1} \mathbf{y}$$

- both means are linear with respect to the output data

¹or use a kernel $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}$

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- if we could parametrise $\Phi(\mathbf{x}_*)^T \Phi(\mathbf{x}) = k(\mathbf{x}_*, \mathbf{x})$ as a function
- this leads to the interpretation of GPs as infinite basis functions

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Summary

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- Non-parametrics
 - parametrise relationship between data

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- 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

$$\nu_{t_{\pi(1)} \dots t_{\pi(k)}} (F_{\pi(1)} \times \dots \times F_{\pi(k)}) = \nu_{t_1 \dots t_k} (F_1 \times \dots \times F_k)$$

2. Marginal

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

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

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