

Gaussian Processes

a first introduction

Carl Henrik Ek

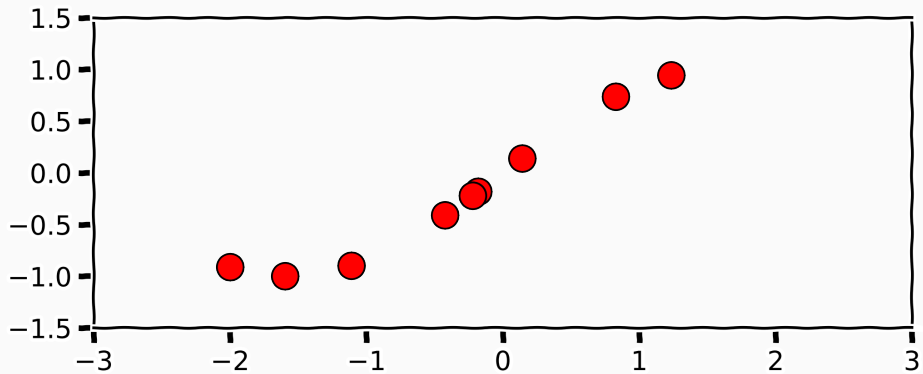
September 8, 2025

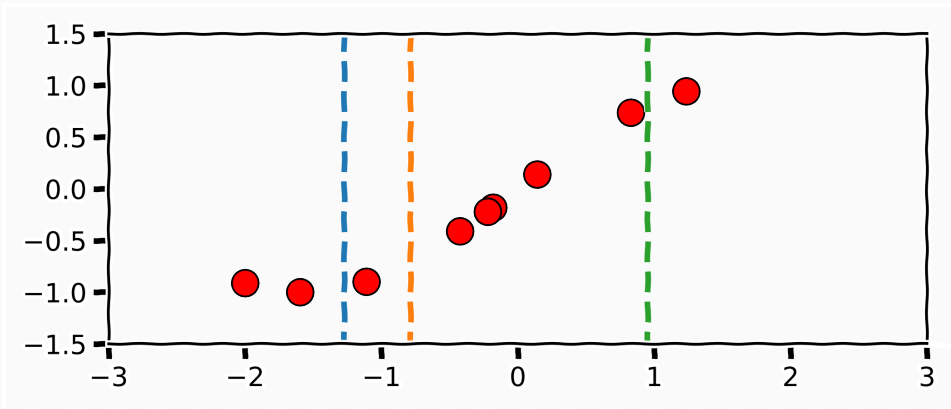
<http://carlhenrik.com>

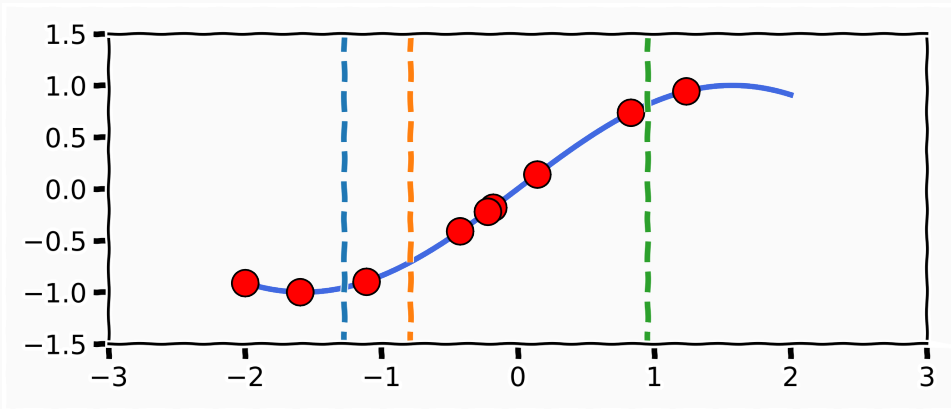
Inductive Reasoning

"In inductive inference, we go from the specific to the general. We make observations, discern a pattern, make a generalization, and infer an explanation or a theory"

– Wassertheil-Smoller

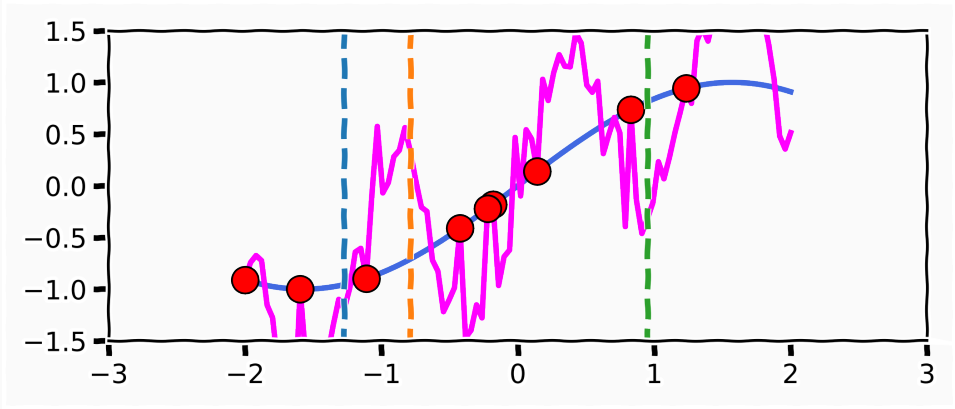




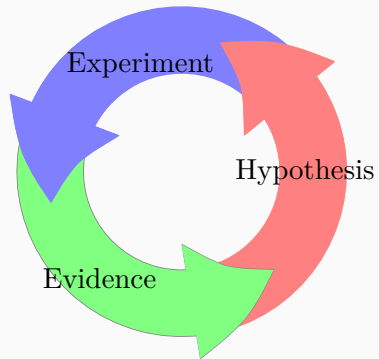


Inductive Reasoning

Unlike deductive arguments, inductive reasoning allows for the possibility that the conclusion is false, even if all of the premises are true.



The Scientific Principle

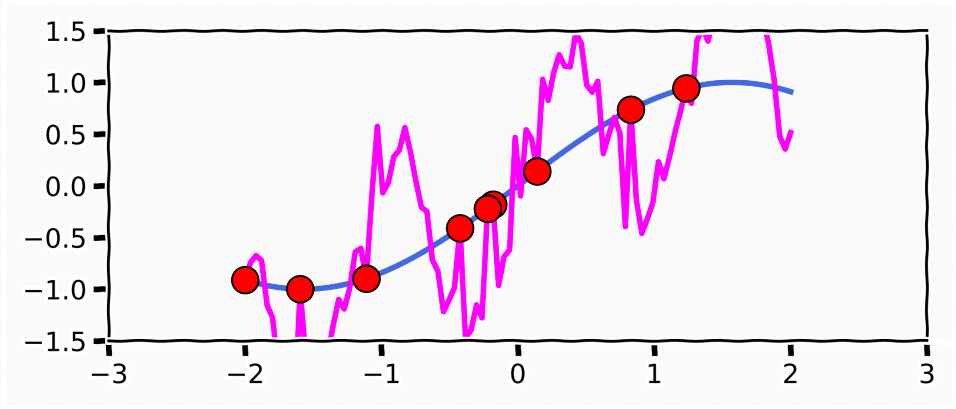


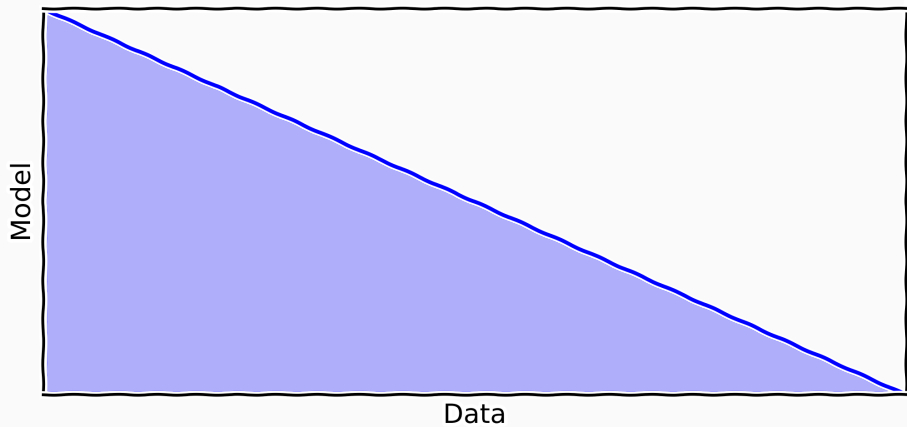
"The Machine Learning Principle"¹

"There is a notion of success ... which I think is novel in the history of science. It interprets success as approximating unanalyzed data."

– Prof. Noam Chomsky

¹Chomsky et al., 1980





What is machine learning?

What is Machine Learning Machine Learning is the task of combining/integrating knowledge with observations to perform predictions using the subset of possible explanations that are consistent with both my knowledge and the observations

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Isn't this Statistics? statistics cares about **parameters** of the knowledge while ML cares about the predictions we get from **using** the parameters we infer by combining knowledge and observations. (It is just a slight but important change of narrative)

Domain Set \mathcal{X} the set of measurements/objects that we want to label
(input)

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Label Set \mathcal{Y} the set of outputs

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Training Data \mathcal{S} a finite sequence of pairs in $\mathcal{X} \times \mathcal{Y}$

Data Distribution \mathcal{D} probability distribution governing the measurements

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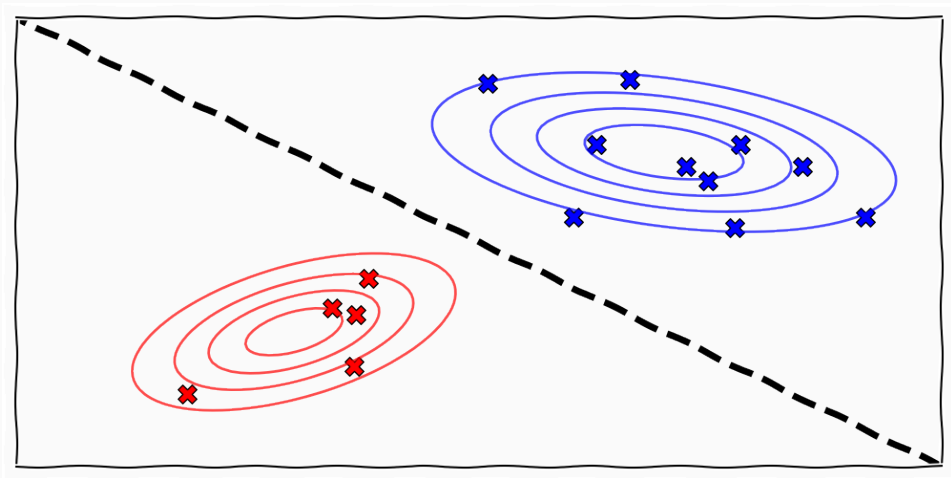
Data Generation $f : \mathcal{X} \rightarrow \mathcal{Y}$ the underlying generating process that we wish to recover

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Data Generation $f : \mathcal{X} \rightarrow \mathcal{Y}$ the underlying generating process that we wish to recover

Prediction Rule $h : \mathcal{X} \rightarrow \mathcal{Y}$ what we wish to recover, the object that encodes the recovered knowledge

Classification



$$L_{\mathcal{D},f}(h) := \mathcal{D}(\{x : h(x) \neq f(x)\})$$

- measure of success as probability of misclassified points (true risk)

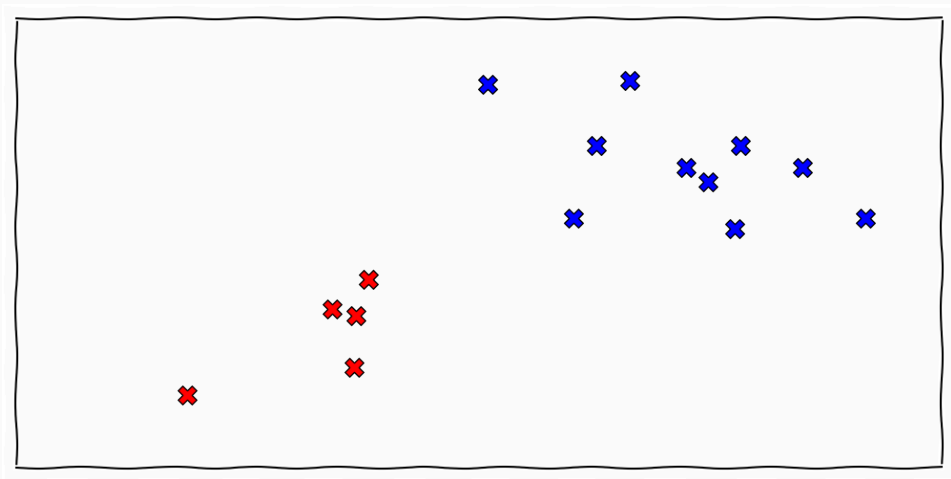
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- we do not have access to \mathcal{D}

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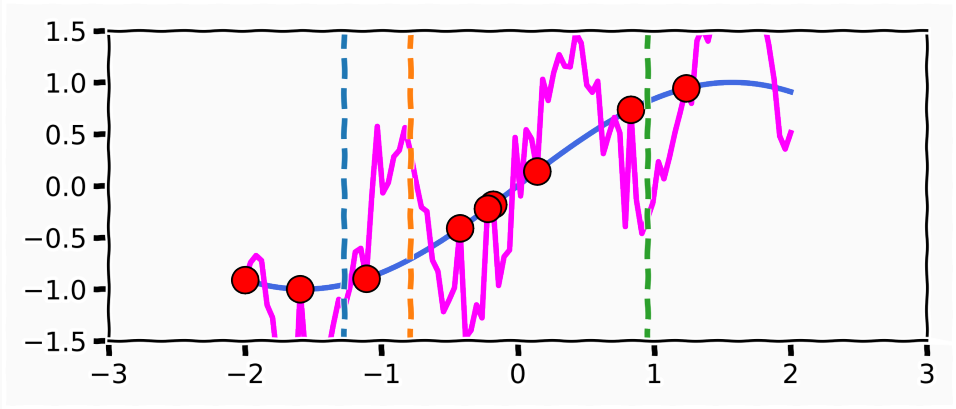
- measure of success as probability of misclassified points (true risk)
- we do not have access to \mathcal{D}
- we do not have access to f

Classification



$$L_{\mathcal{S}}(h) := \frac{|\{i \in [m] : h(x_i) \neq y_i\}|}{m}$$

- We **assume** that $\mathcal{S} \sim \mathcal{D}$
- Empirical measure of risk



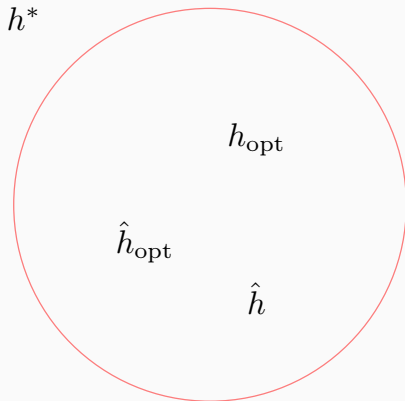
$$L_{\mathcal{S}}(A(\mathcal{S})) := \frac{|\{i \in [m] : h(x_i) \neq y_i\}|}{m}$$

- We use an algorithm $A : \mathcal{S} \rightarrow h$ to find a hypothesis

$$h_{\mathcal{S}} \in \operatorname{argmin}_{h \in \mathcal{H}} L_{\mathcal{S}}(h)$$

- We cannot parametrise **all** possible hypothesis

Error Decomposition



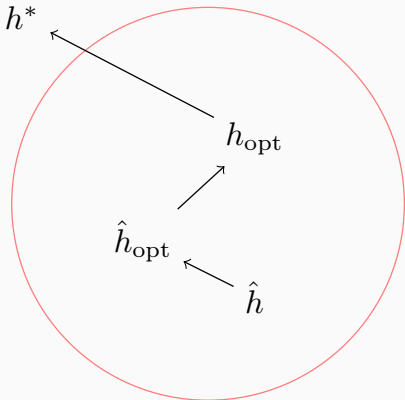
h^* the optimal predictor

h_{opt} the optimal hypothesis

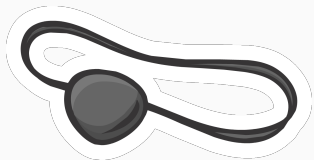
\hat{h}_{opt} the optimal hypothesis
on training data

\hat{h} the hypothesis found by
learning algorithm

Error Decomposition



$$\begin{aligned} & \epsilon(\hat{h}) - \epsilon(h^*) \\ &= \underbrace{\epsilon(h_{\text{opt}}) - \epsilon(h^*)}_{\text{Approximation}} \\ &+ \underbrace{\epsilon(\hat{h}_{\text{opt}}) - \epsilon(h_{\text{opt}})}_{\text{Estimation}} \\ &+ \underbrace{\epsilon(\hat{h}) - \epsilon(\hat{h}_{\text{opt}})}_{\text{Optimisation}} \end{aligned}$$



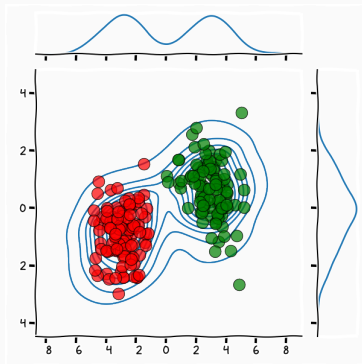
Statistical Learning



$$A_{\mathcal{H}}(\mathcal{S})$$



Assumptions: Biased Sample



Statistical Learning

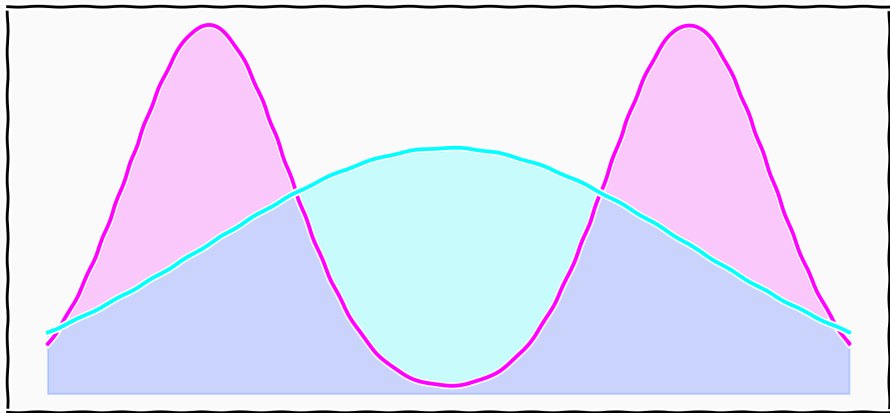
$$\mathcal{A}_{\mathcal{H}}(\mathcal{S})$$

Assumptions: Hypothesis space



Statistical Learning

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



$$p(\theta \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \theta)p(\theta)}{p(\mathcal{D})}$$

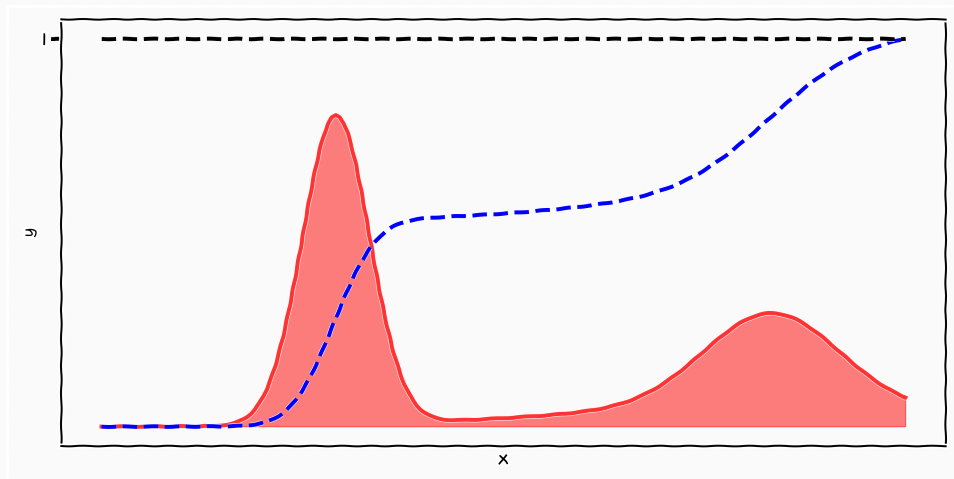
$$p(\mathcal{D}) = \int p(\mathcal{D} \mid \theta) p(\theta) d\theta$$

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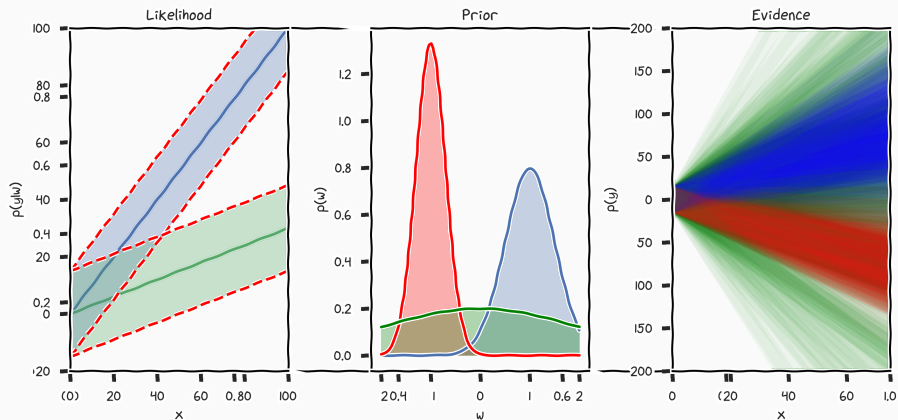
$$p(\mathcal{D}) = \int p(\mathcal{D} \mid \theta) p(\theta) d\theta$$

$$p(\mathcal{D}) = \int p(\mathcal{D} \mid \theta) \underbrace{p(\theta) \mathrm{d}\theta}_{\mathrm{d}t(\theta)}$$

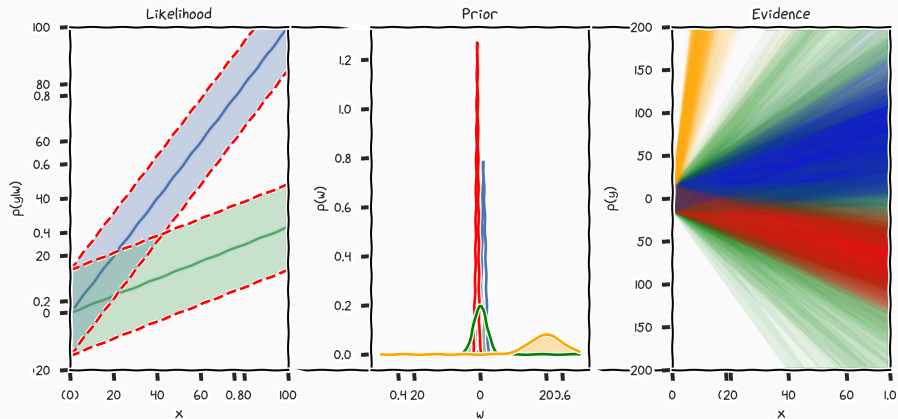
Marginalisation



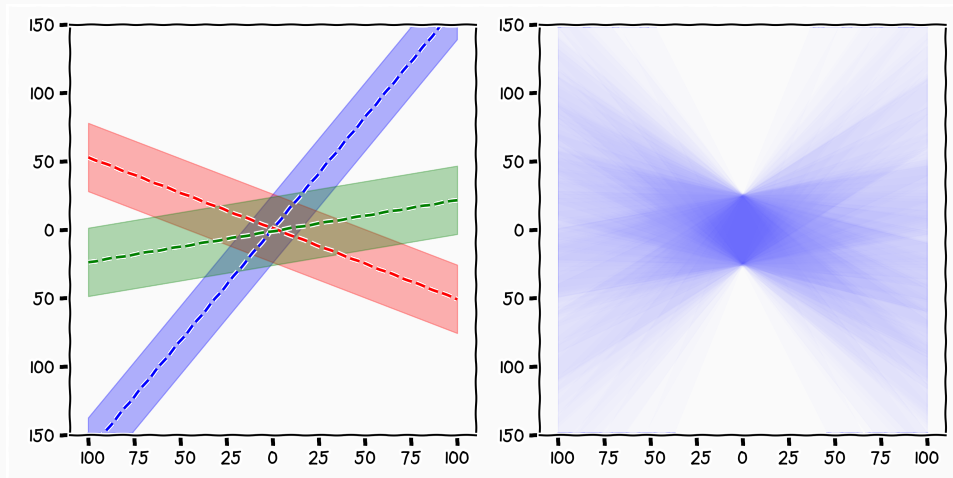
Marginalisation

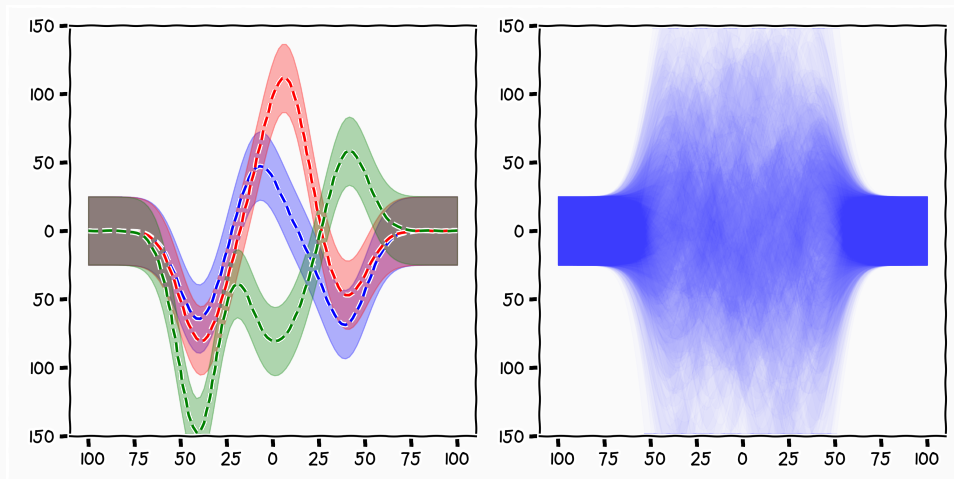


Marginalisation



Model Linear Linear





- The Bayesian argument implies that you try to re-parametrise the hypothesis space to reflect your beliefs

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- A good analogy is to think about "space", the believable parameters gets a bigger space compared to the unlikely ones
- Massive composite models can be thought of as directly altering the parameter space for the optimiser Roy et al., [2024](#)

Flexible such that we do not have to make trade-offs when including beliefs

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Narrow such that we can reduce data-requirements

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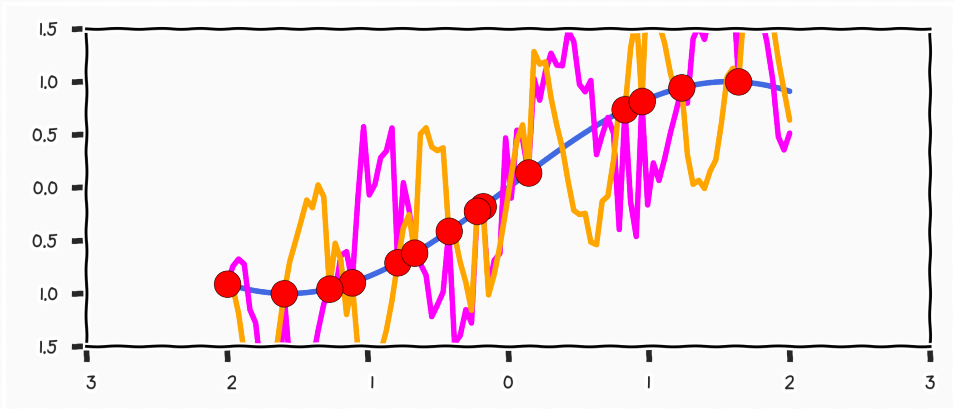
Narrow such that we can reduce data-requirements

Interpretable so that we can translate our knowledge to the parametrisation

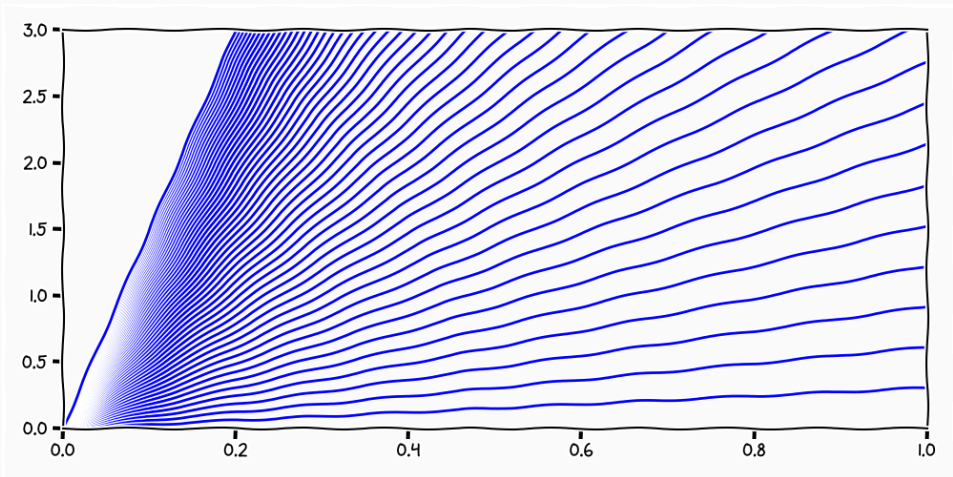


Non-parametrics

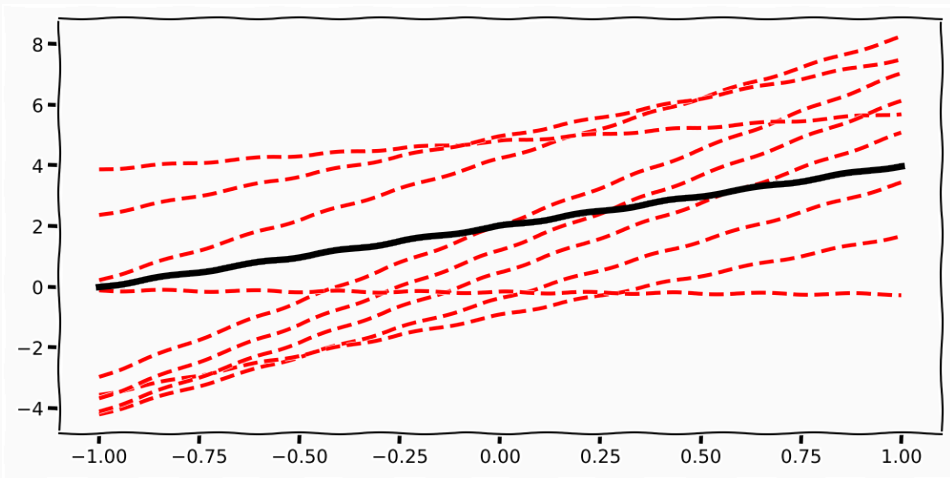
Curve Fitting



$$f(x) = \beta_1 + \beta_2 \cdot x + \beta_3 \cdot x^2 + \dots + \beta_k \sin(x) + \dots$$



$$f(x) = \beta \cdot x$$



$$f(x) = \beta_1 + \beta_2 \cdot x$$



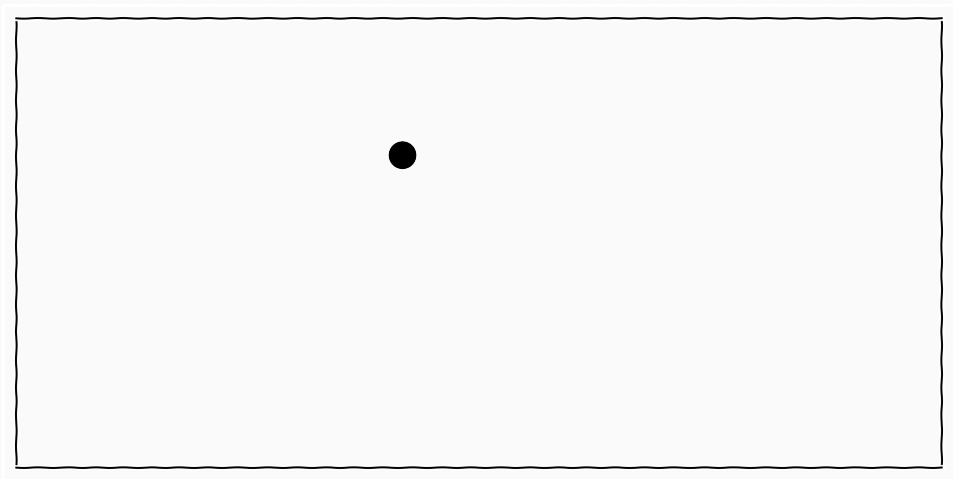




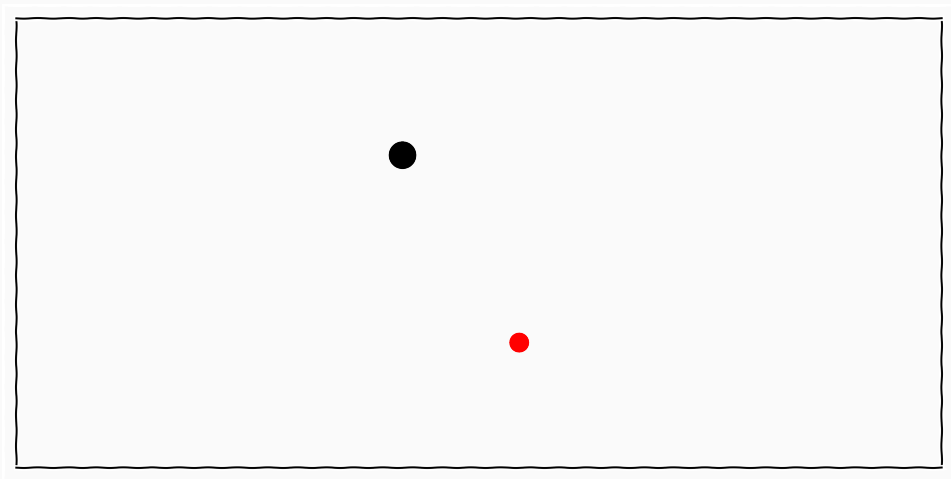
Non-parametrics



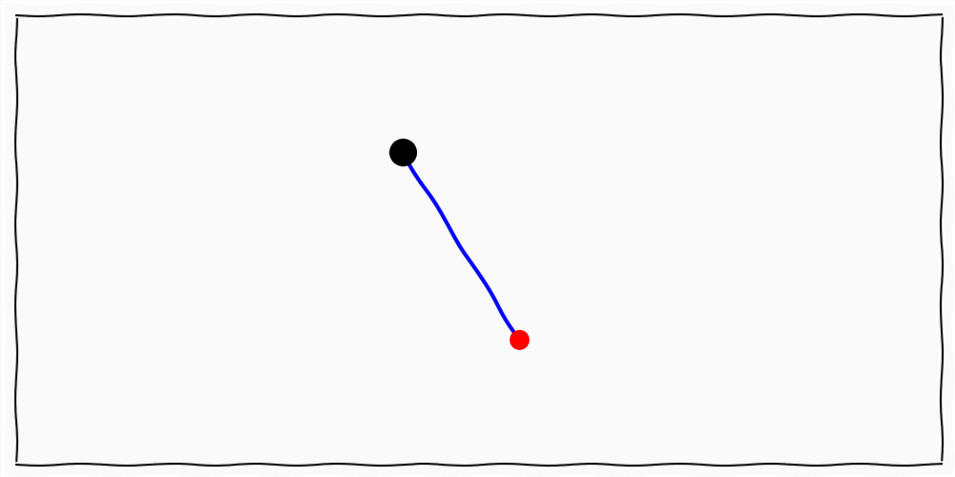
Example



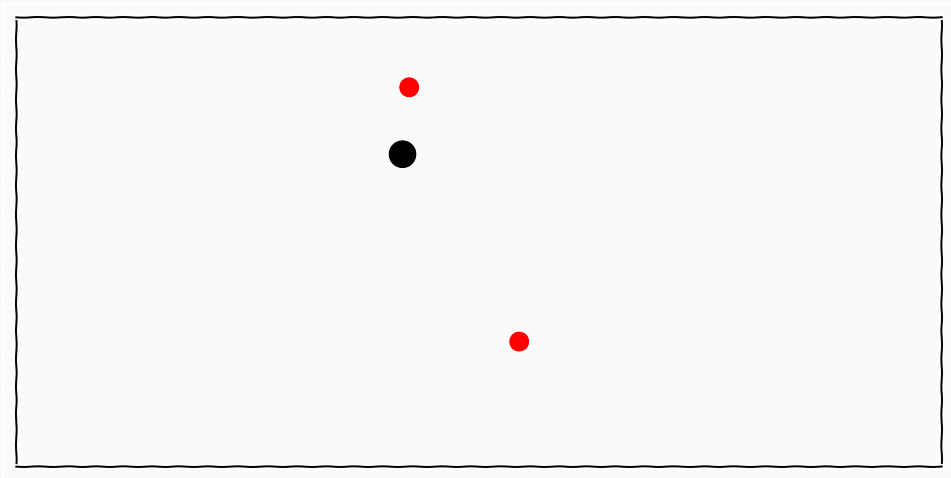
Example



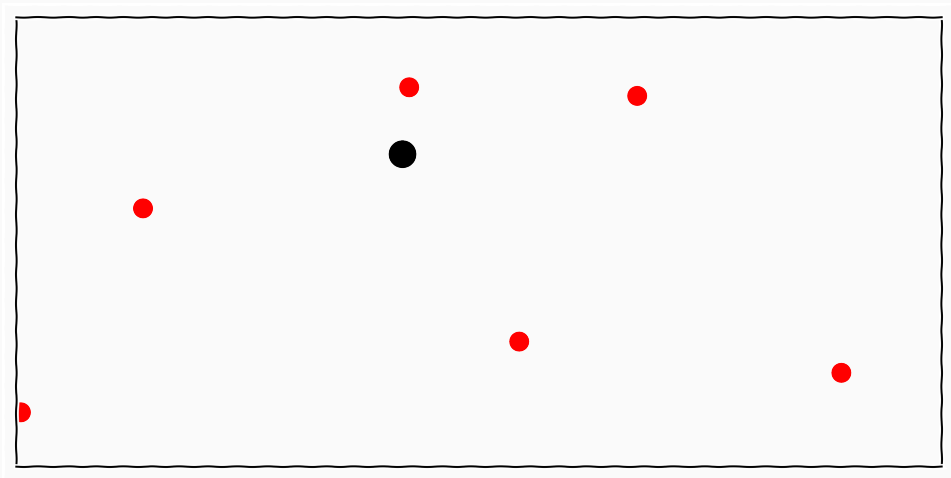
Example



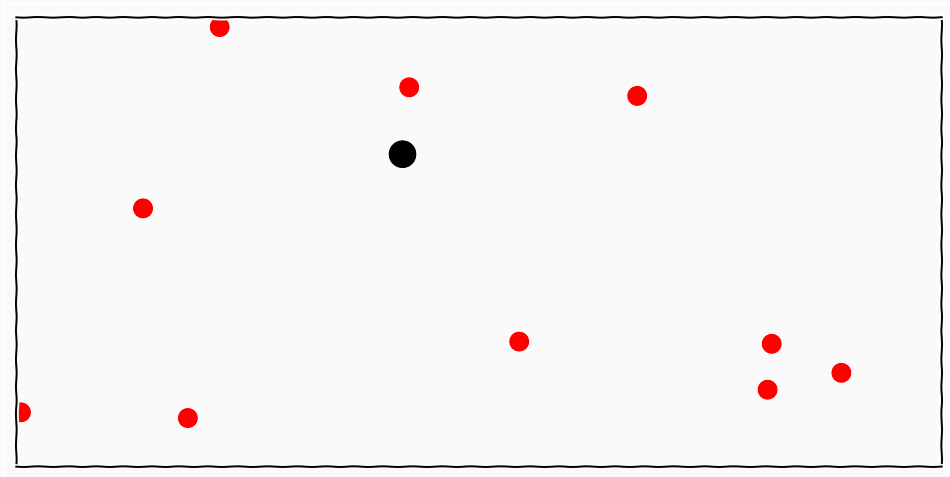
Example



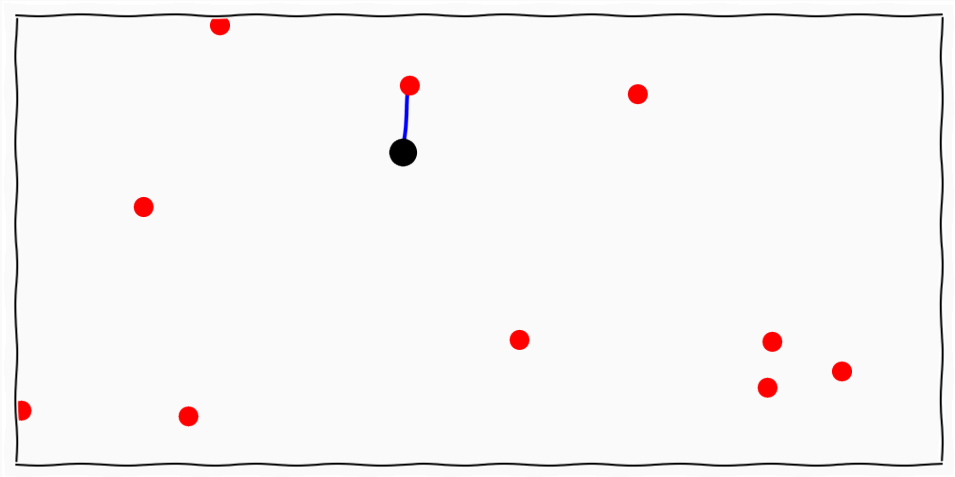
Example



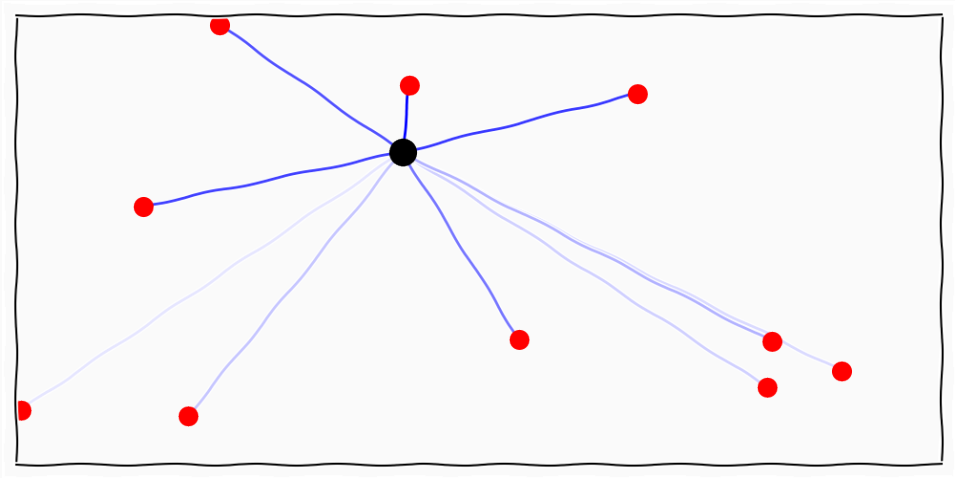
Example



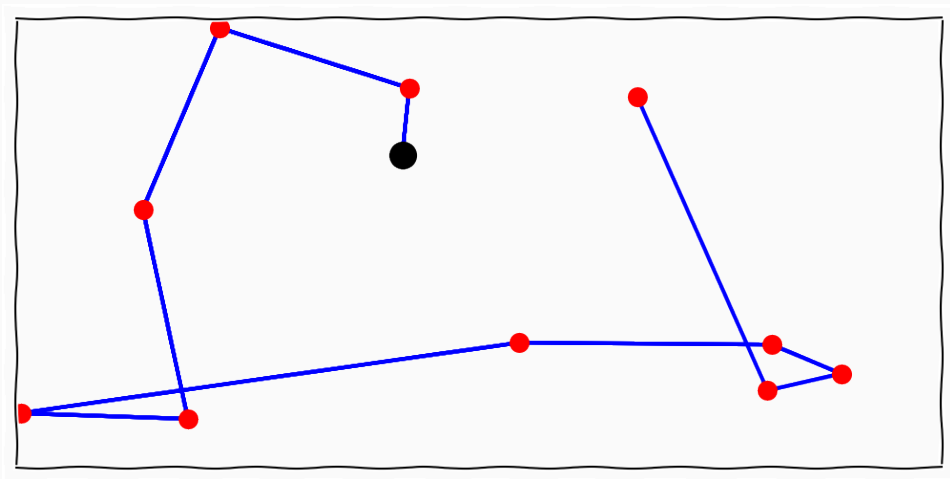
Example



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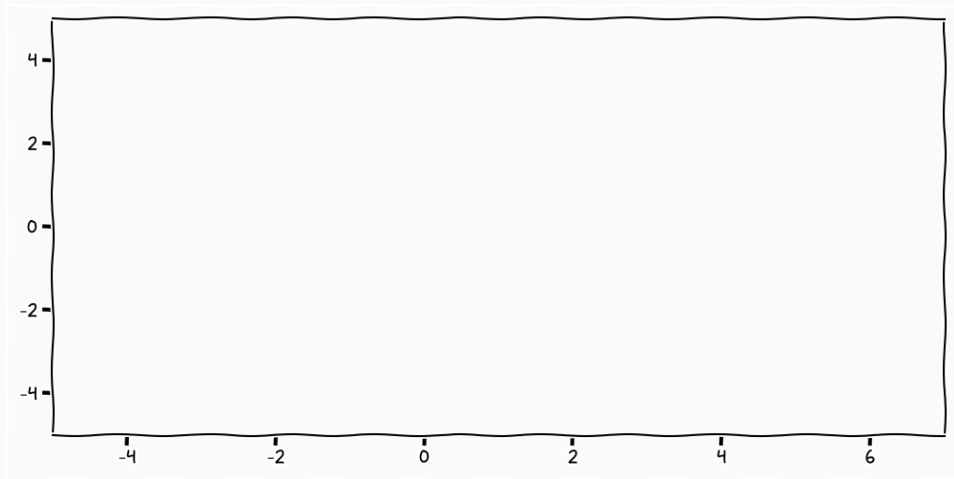


Example

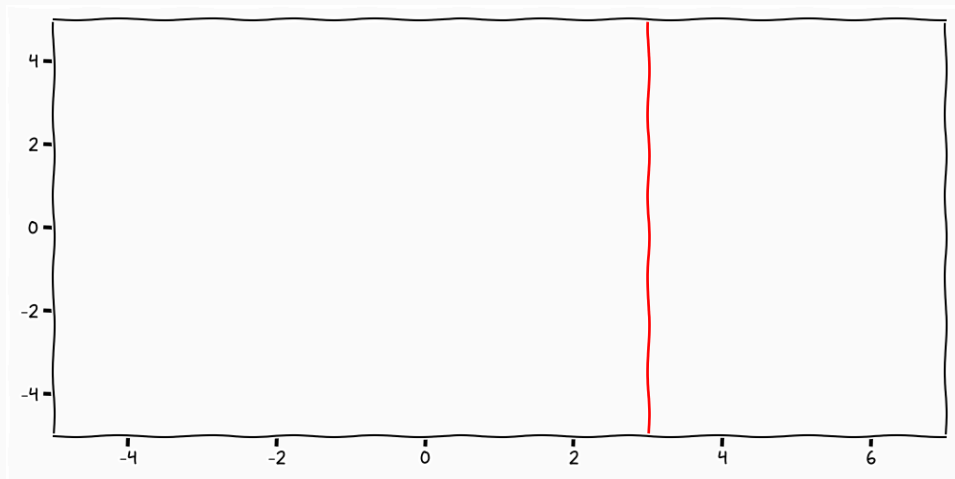


Non-parametric Models

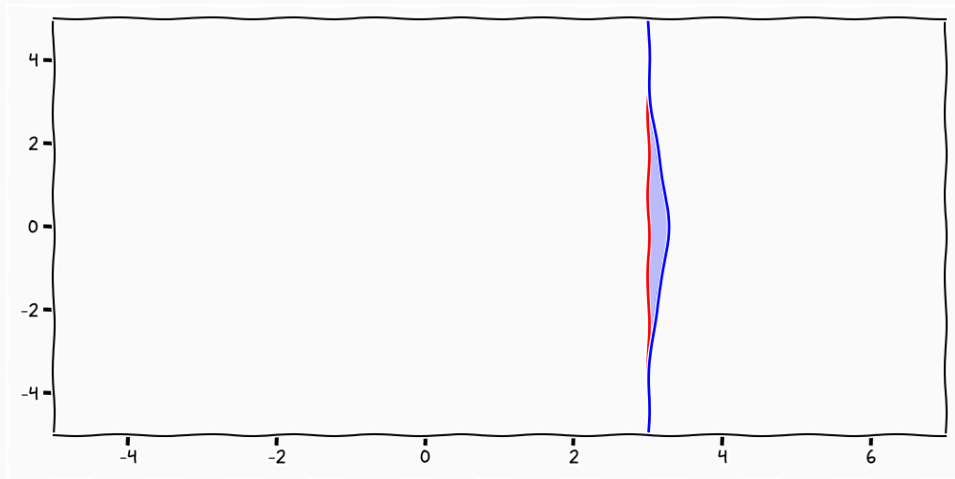
Lets talk about functions



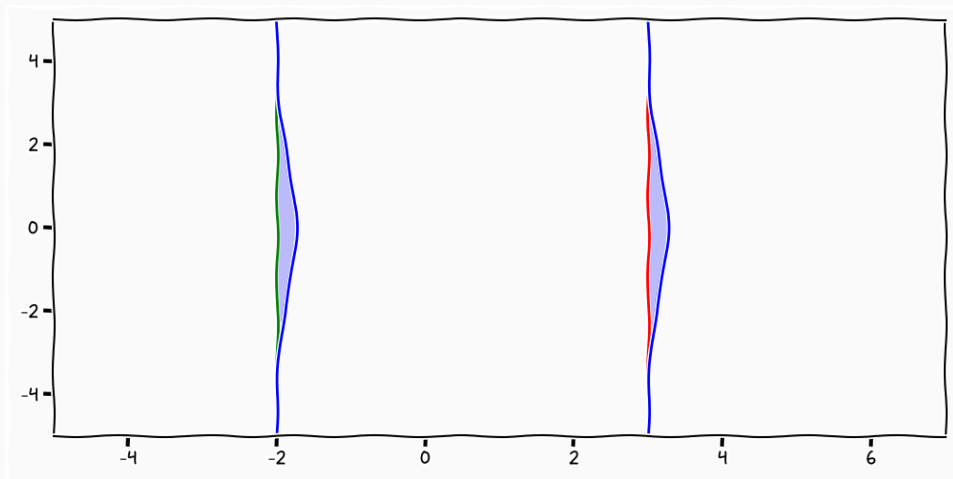
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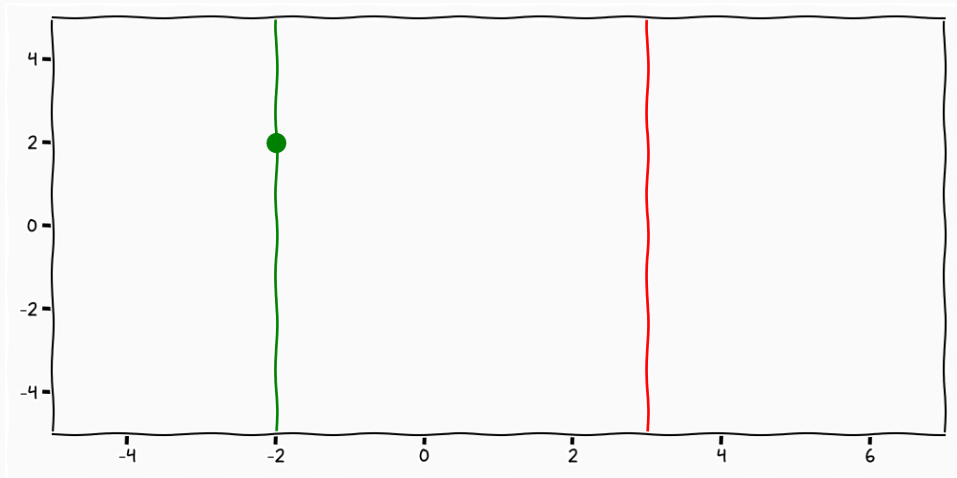
Lets talk about functions



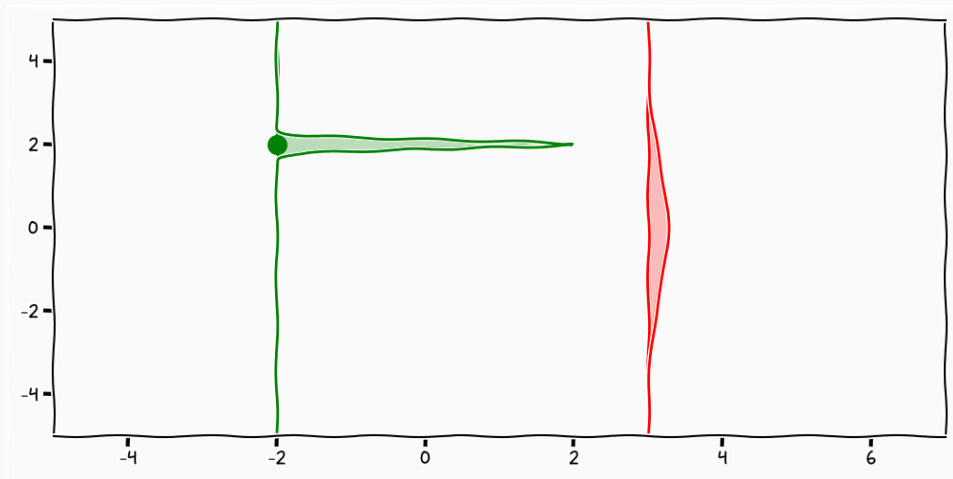
$$f_1 = \mathcal{N}(\mu_1, k_1)$$

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

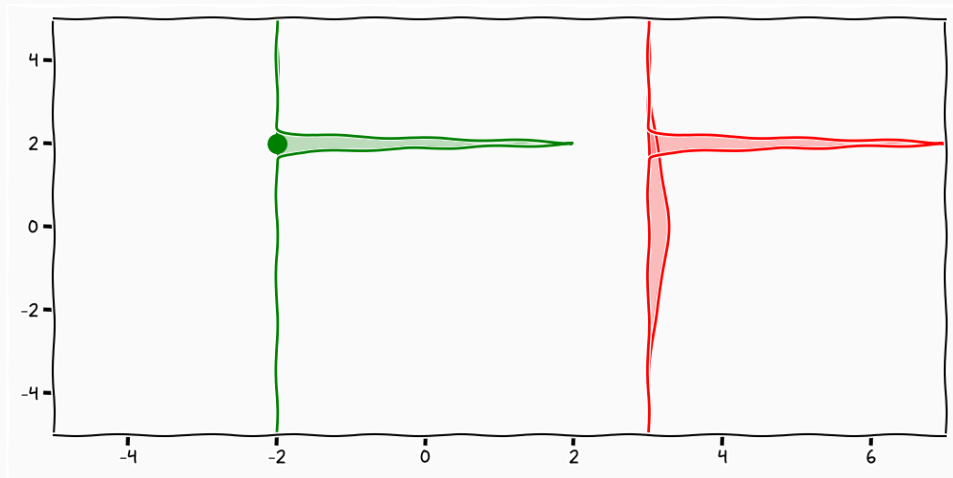
Non-parametric functions



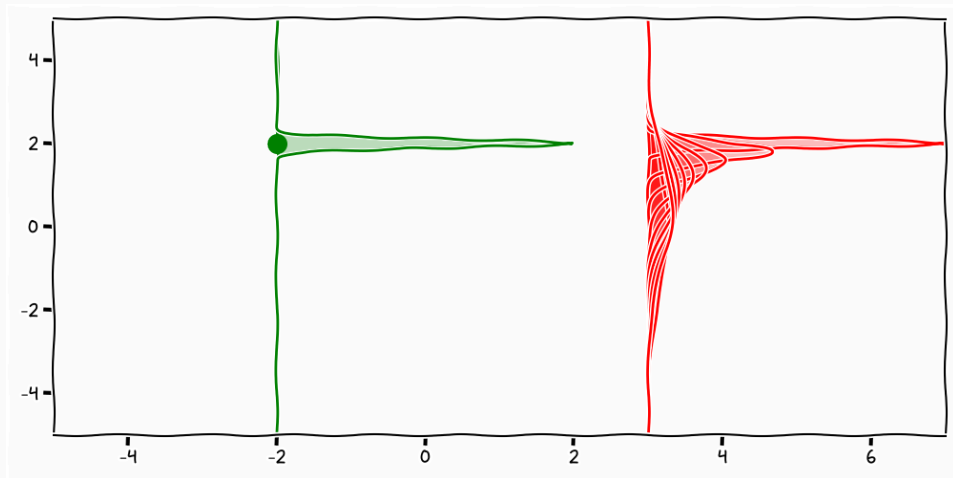
Non-parametric functions



Non-parametric functions

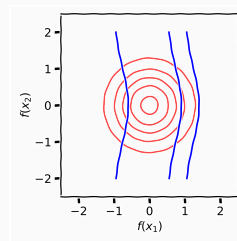
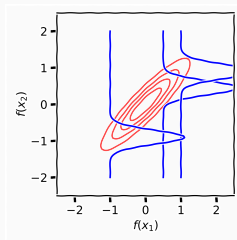
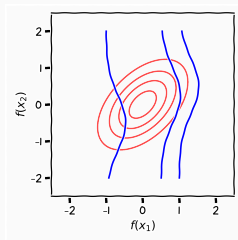


Non-parametric functions



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

Conditional Gaussians

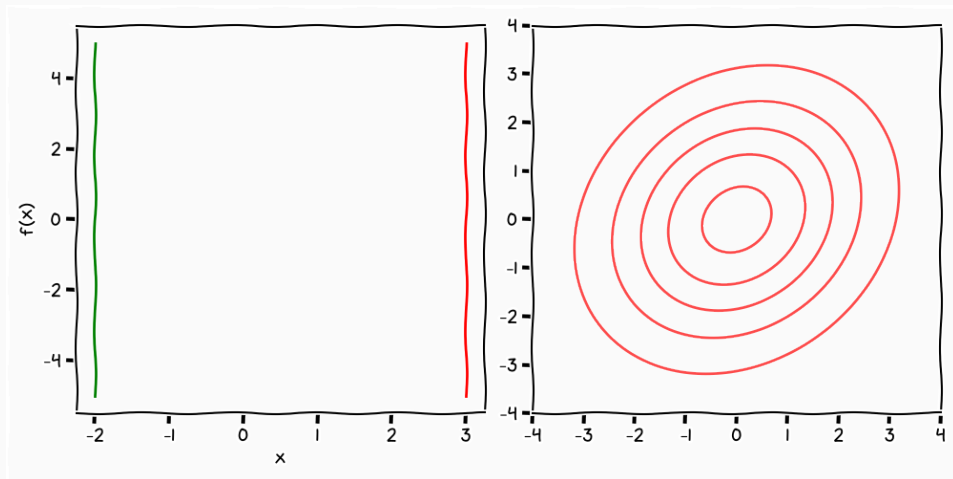


$$N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}\right)$$

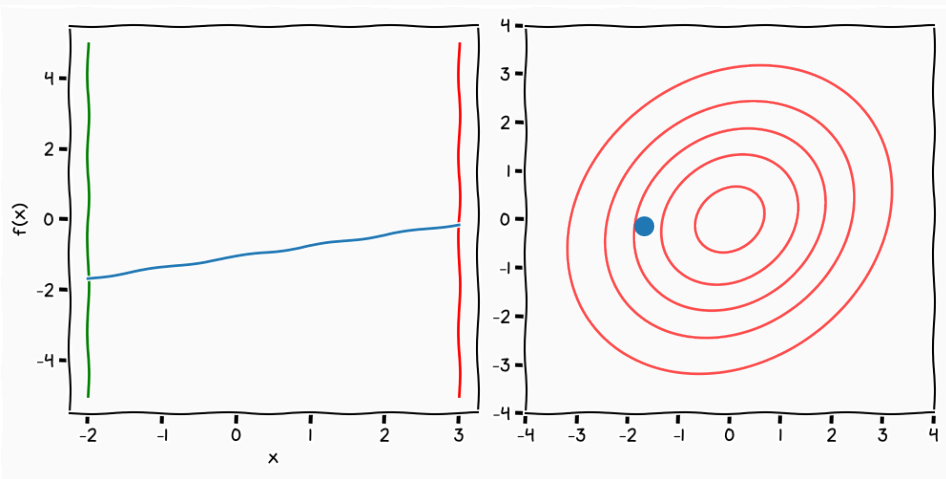
$$N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.9 \\ 0.9 & 1 \end{bmatrix}\right)$$

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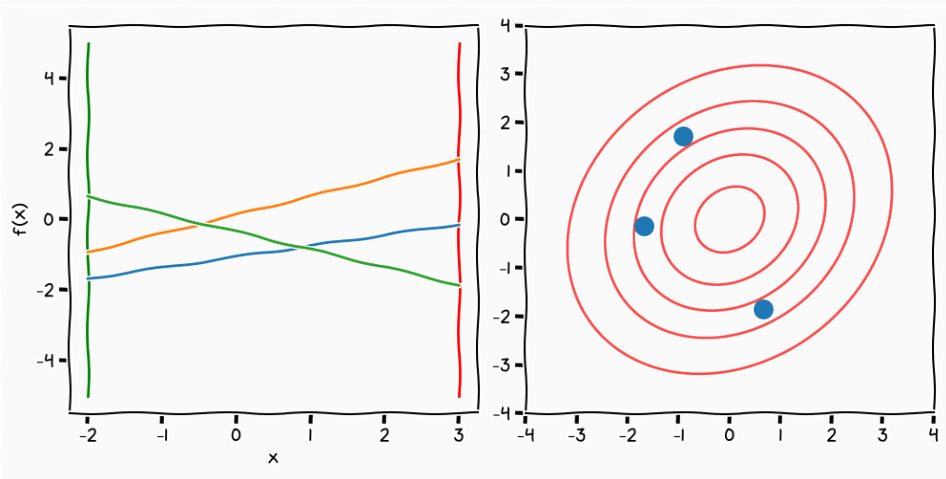
Gaussian Samples



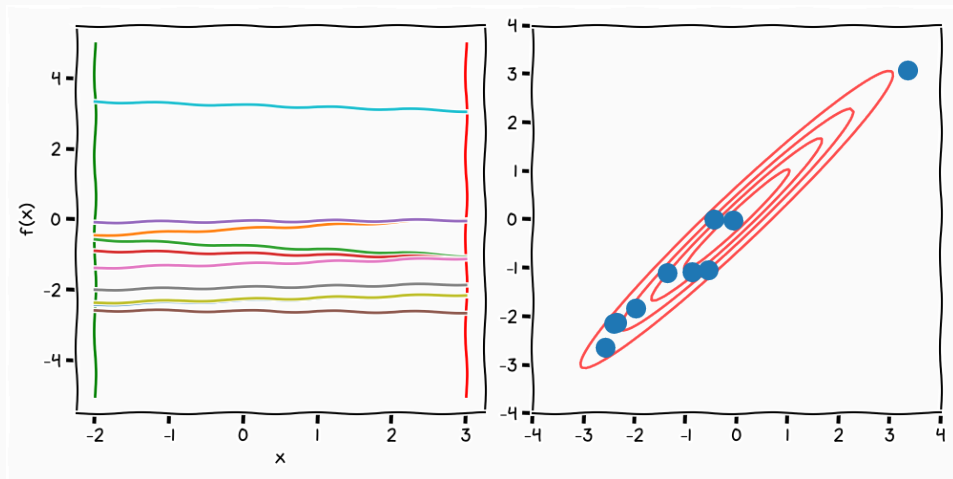
Gaussian Samples



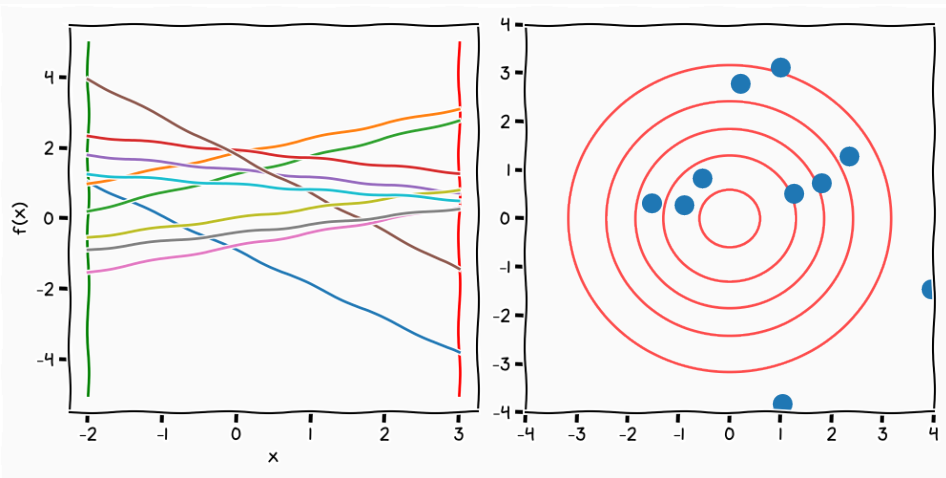
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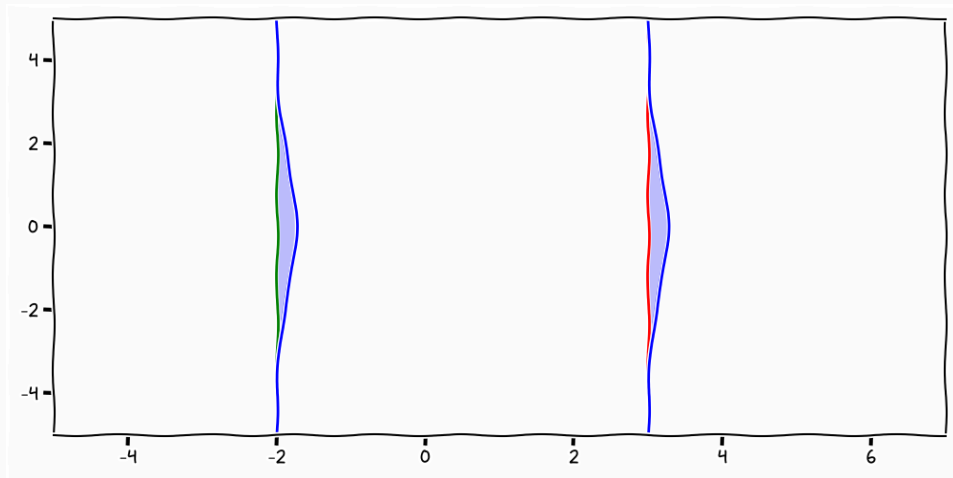
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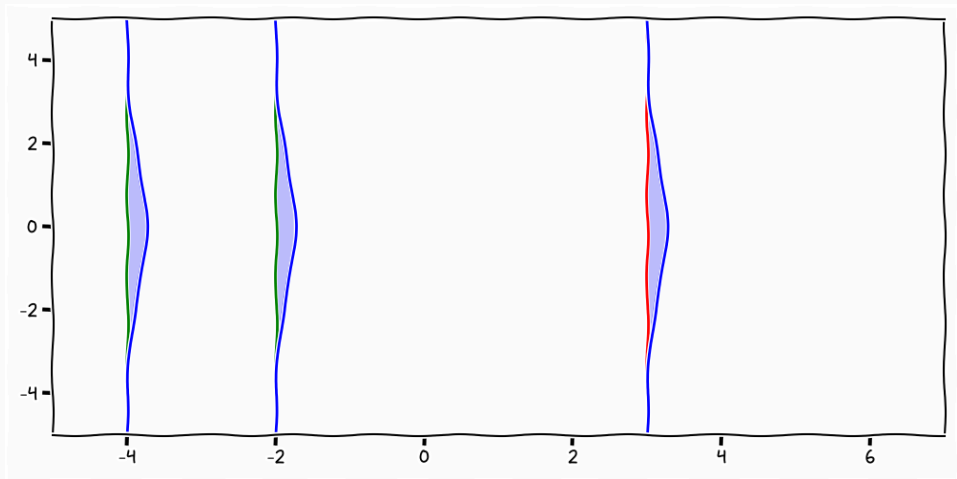
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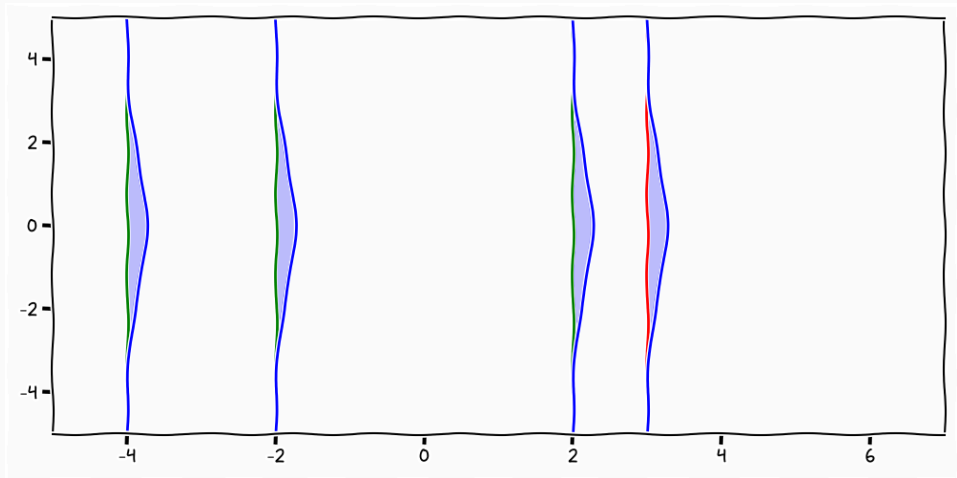
Lets talk about functions



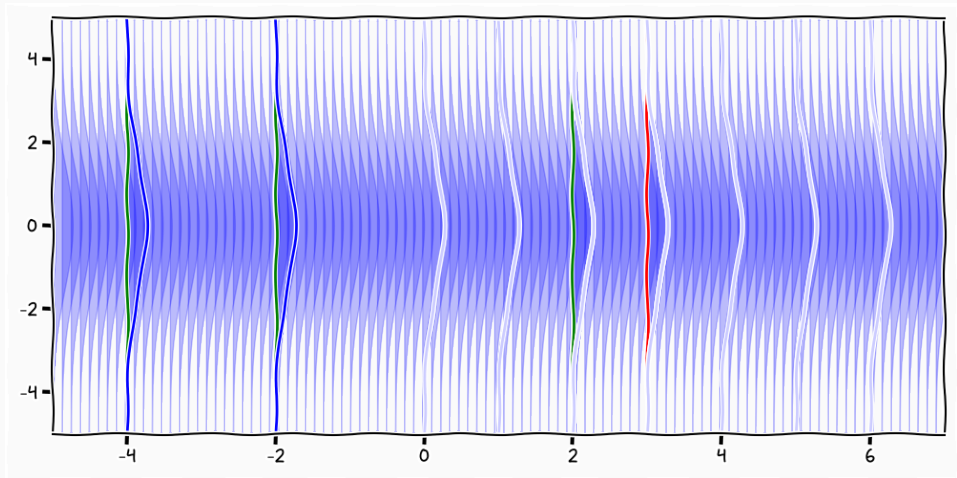
Non-parametric functions



Non-parametric functions



Non-parametric functions



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

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

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

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

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

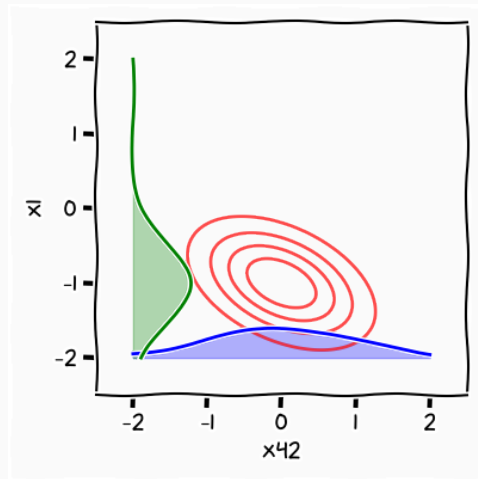
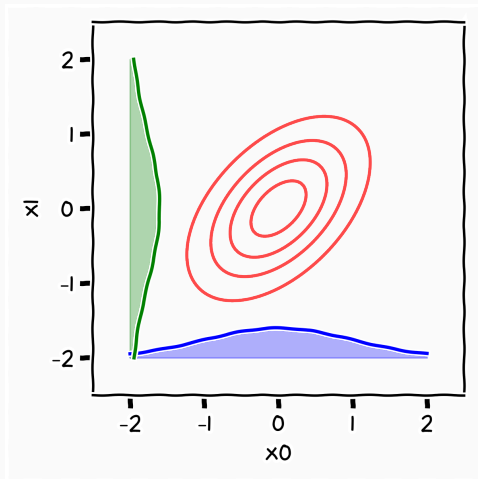
$$p(\mathbf{x}_1, x_2) = \mathcal{N} \left(\begin{array}{c|cc} \mathbf{x}_1 & \mu_1 & k_{11} & k_{12} \\ x_2 & \mu_2 & k_{21} & k_{22} \end{array} \right)$$

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

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

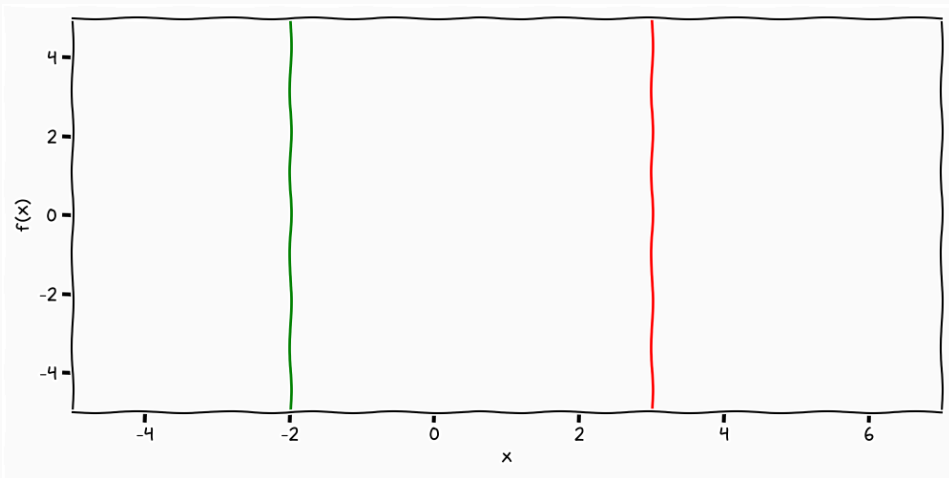
Gaussian Distribution - Marginal



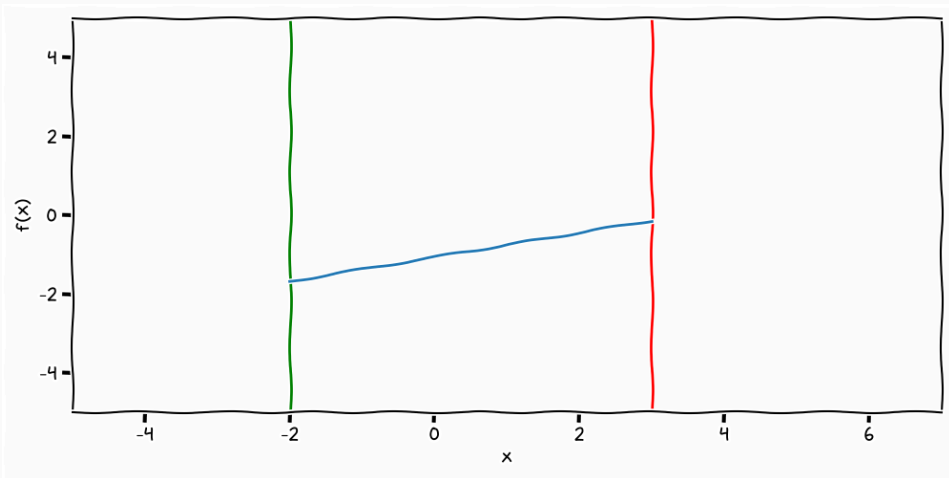
For all measurable sets $F_i \subseteq \mathbb{R}^n$ and probability measure \mathcal{N}

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

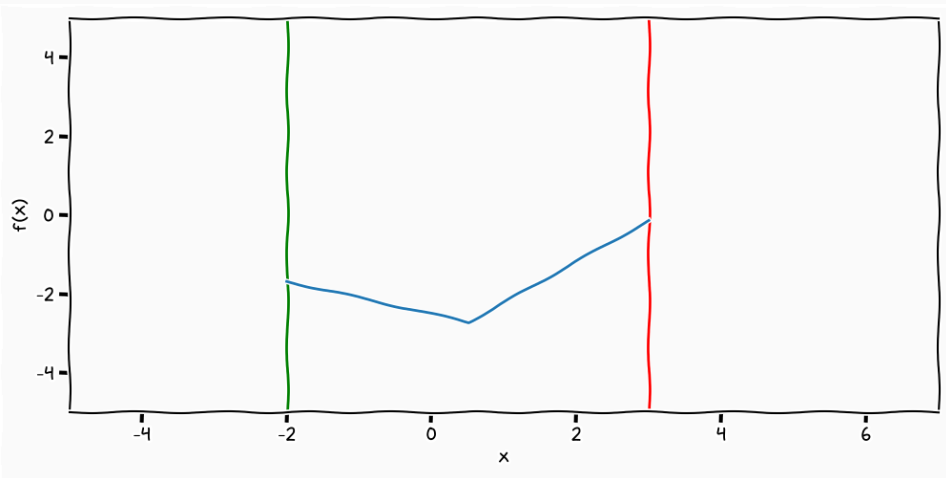
Gaussian Samples



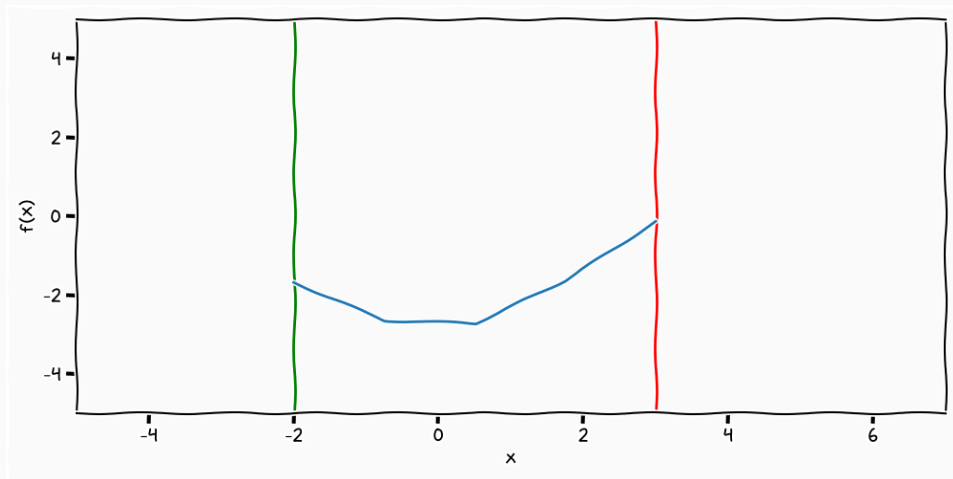
Gaussian Samples



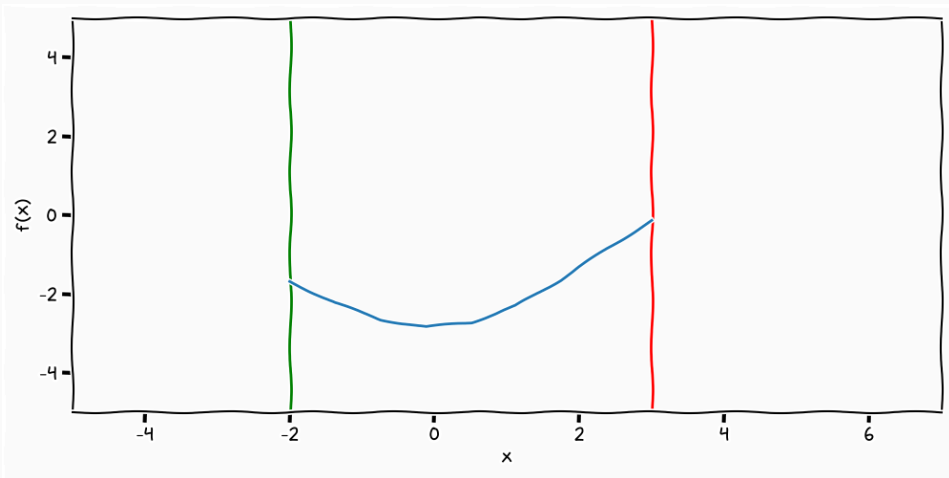
Gaussian Samples



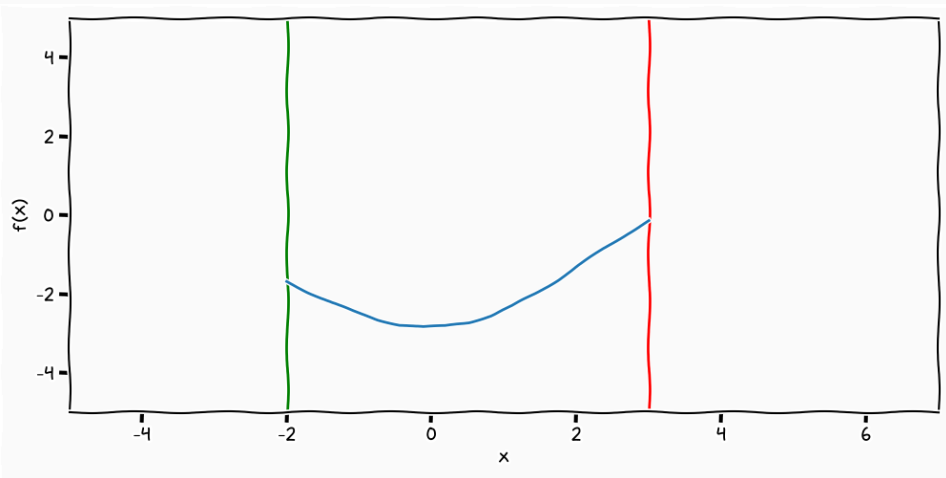
Gaussian Samples



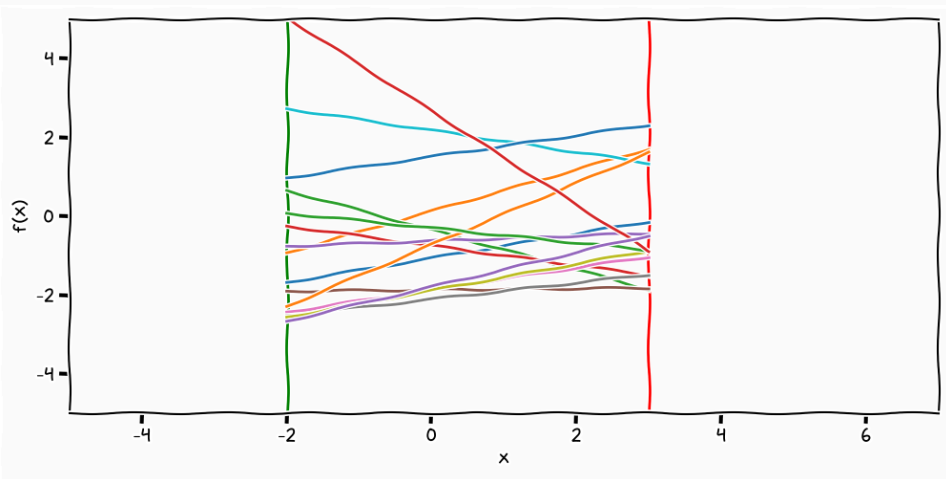
Gaussian Samples



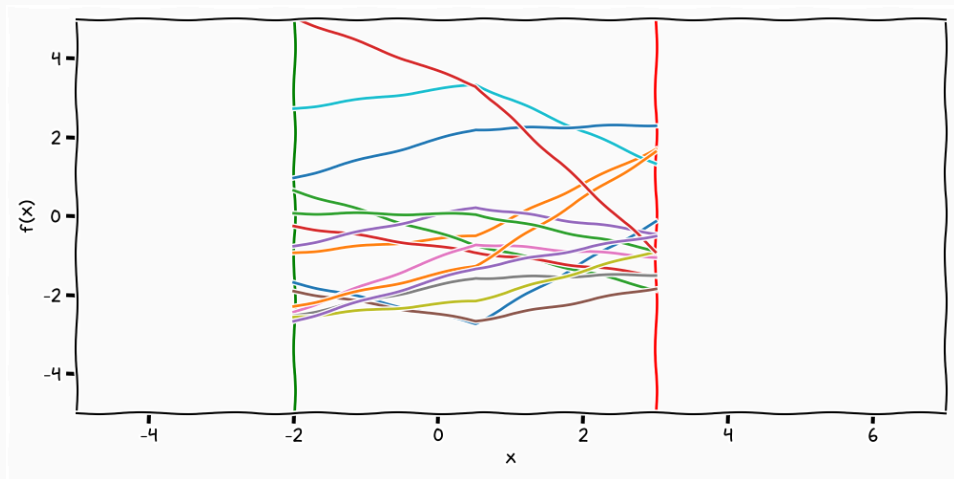
Gaussian Samples



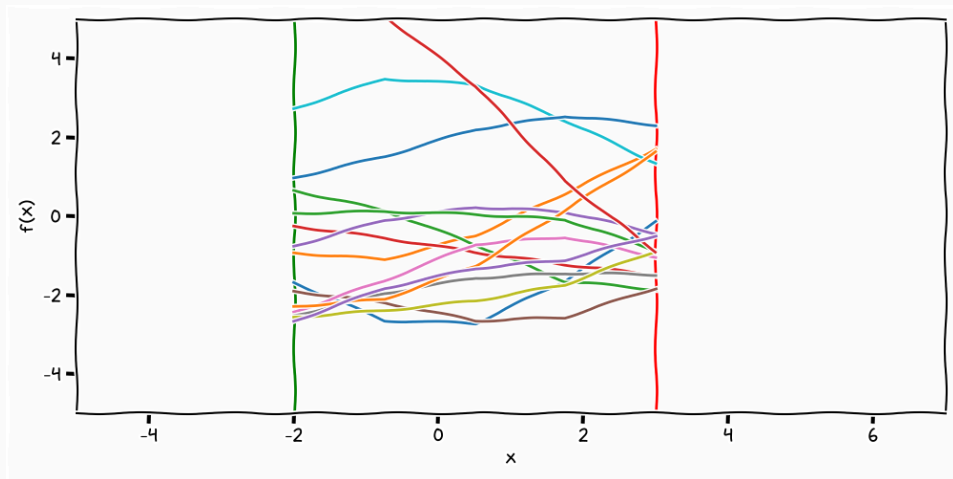
Gaussian Samples



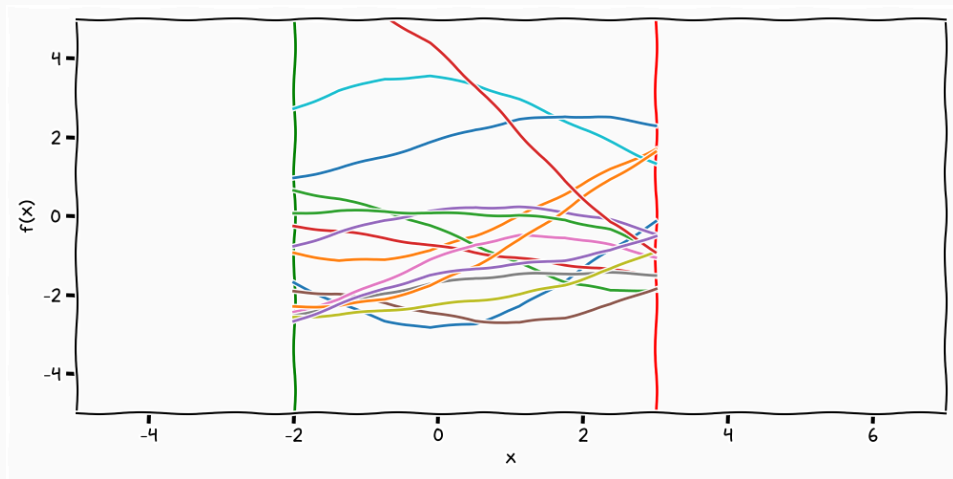
Gaussian Samples



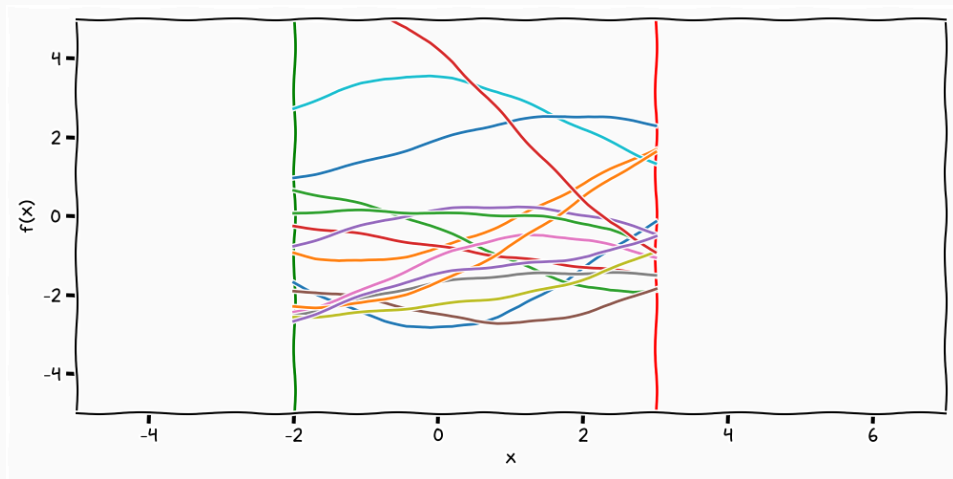
Gaussian Samples



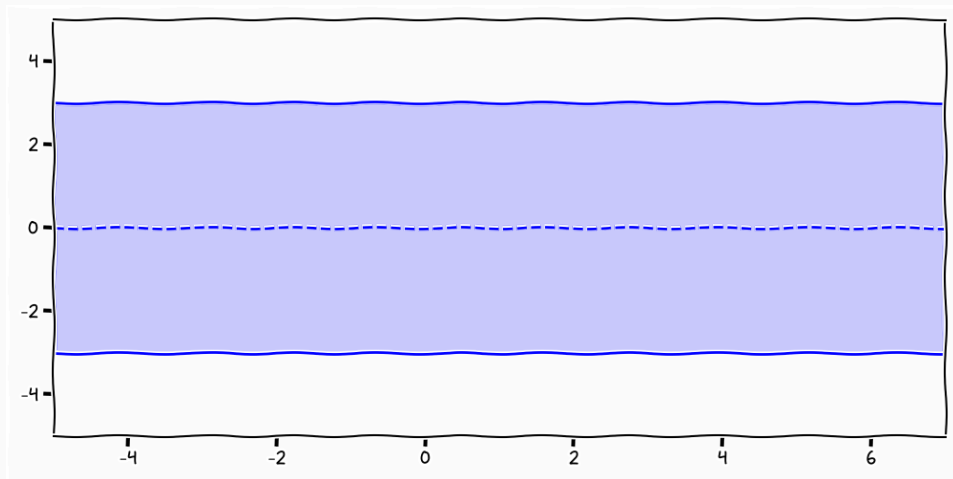
Gaussian Samples



Gaussian Samples



Gaussian Processes



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

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

The Gaussian distribution is the projection of the infinite 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

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

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

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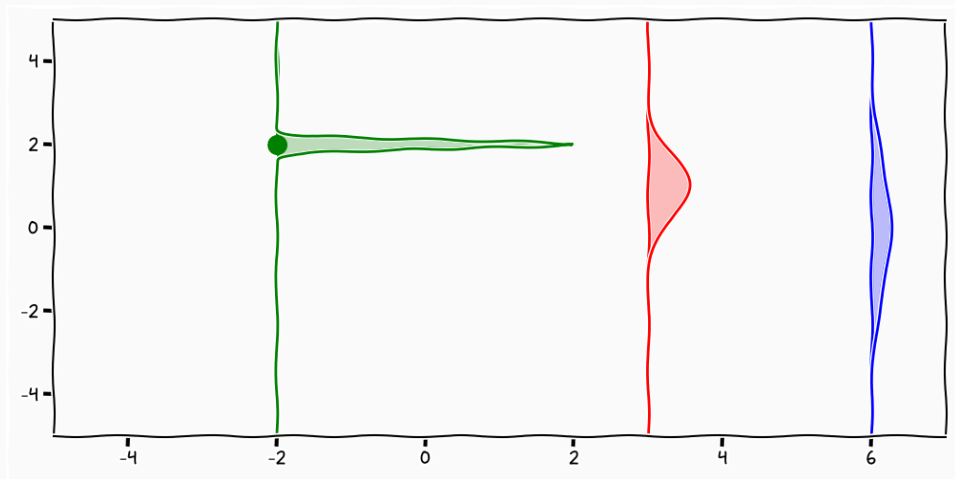
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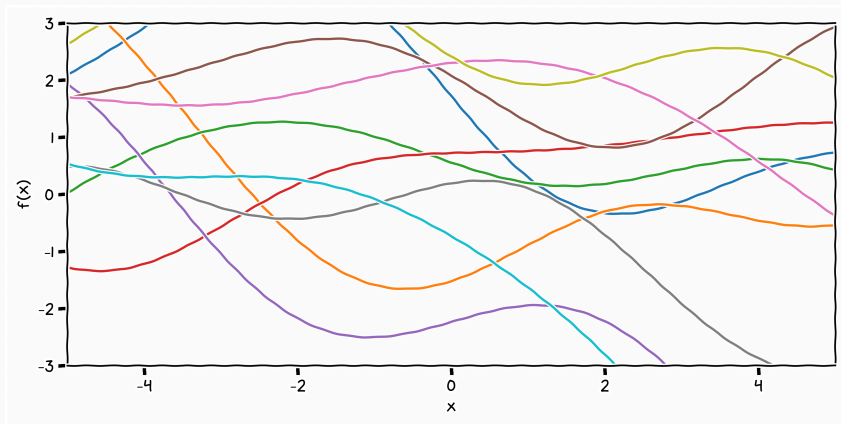
$$k_{ij} = k(x_i, x_j)$$

- 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

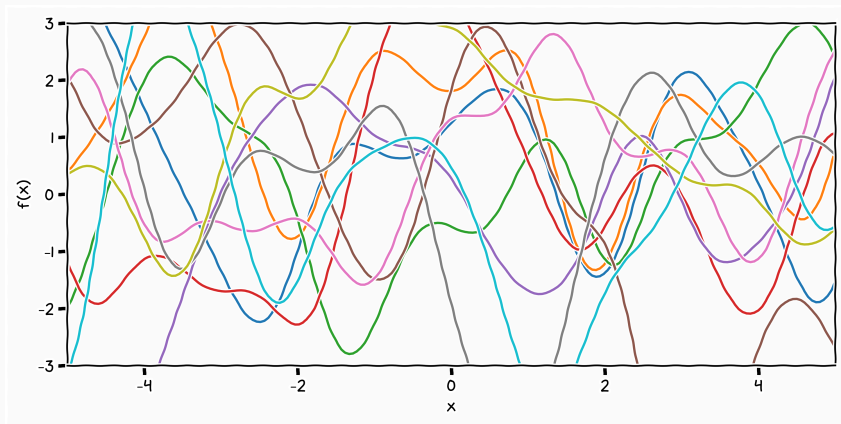


Gaussian Processes Samples



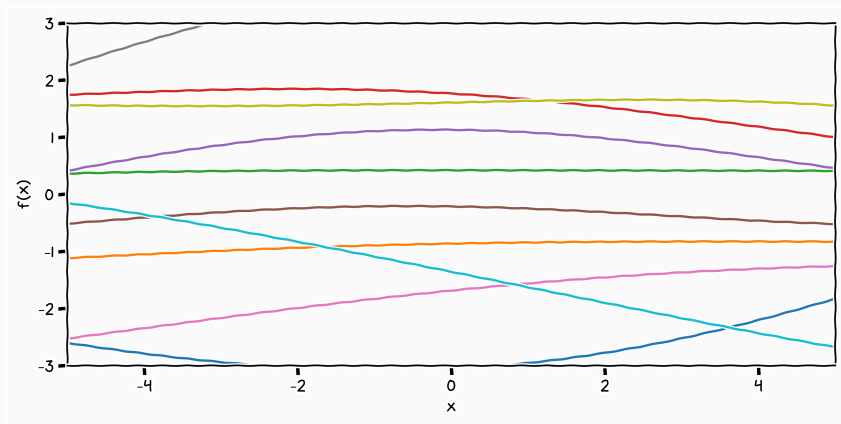
$$k(x_i, x_j) = 3 \cdot e^{-\frac{(x_i - x_j)^2}{15}}$$

Gaussian Processes Samples



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

Gaussian Processes Samples



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

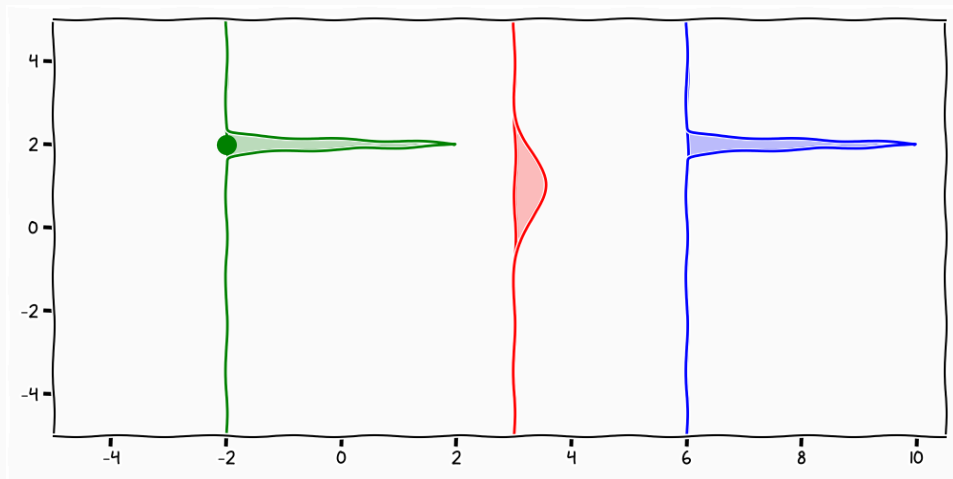
Code

```
x = np.linspace(-5,5,200)
x = x.reshape((-1,1))

Sigma = 3.0*np.exp(-np.power(cdist(x,x),2)/lengthScale)
mu = np.zeros(x.shape)

y = np.random.multivariate_normal(mu.flatten(),Sigma,10)
ax.plot(x,y.T)
```

Gaussian Processes



Choosing Covariances²

$$k(x, x') = ck_1(x, x')$$

$$k(x, x') = f(x)k_1(x, x')f(x')$$

$$k(x, x') = q(k_1(x, x'))$$

$$k(x, x') = \exp(k_1(x, x'))$$

$$k(x, x') = k_1(x, x') + k_2(x, x')$$

$$k(x, x') = k_1(x, x')k_2(x, x')$$

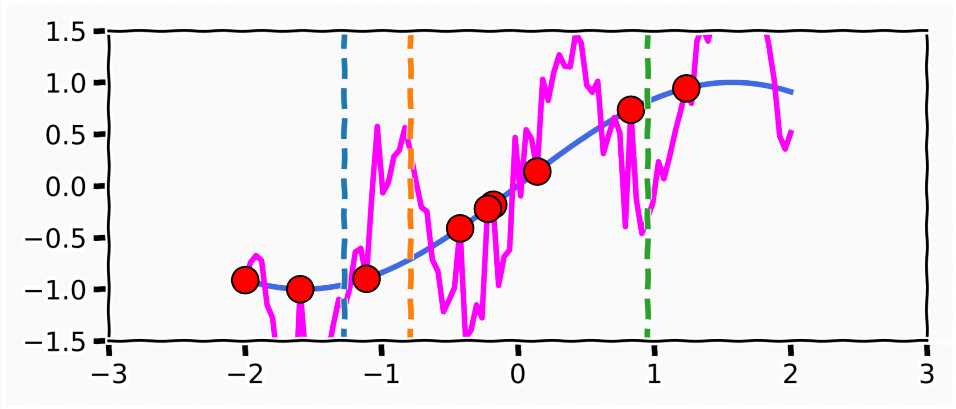
$$k(x, x') = k_3(\phi(x), \phi(x'))$$

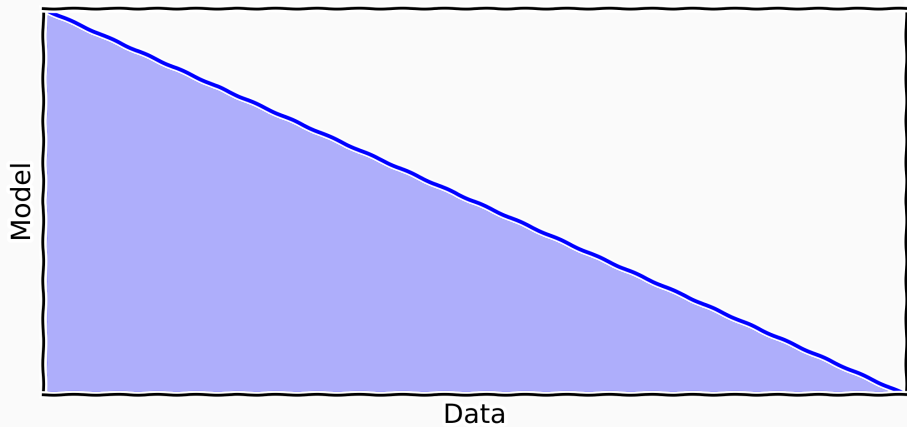
$$k(x, x') = x^T \mathbf{A} x'$$

$$k(x, x') = k_a(x_a, x'_a) + k_b(x_b, x'_b)$$

$$k(x, x') = k_a(x_a, x'_a)k_b(x_b, x'_b)$$

²Bishop, 2006.





Inference

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

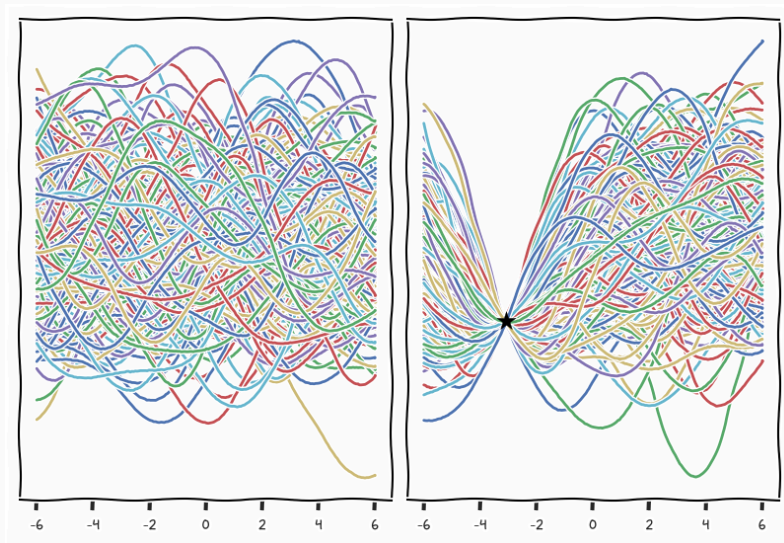
$$\int p(\mathbf{f}, \mathbf{f}_*) d\mathbf{f}_* = \int p(\mathbf{f} | \mathbf{f}_*) p(\mathbf{f}_*) d\mathbf{f}_*$$

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

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- 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



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

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

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

- All instantiations are jointly Gaussian

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

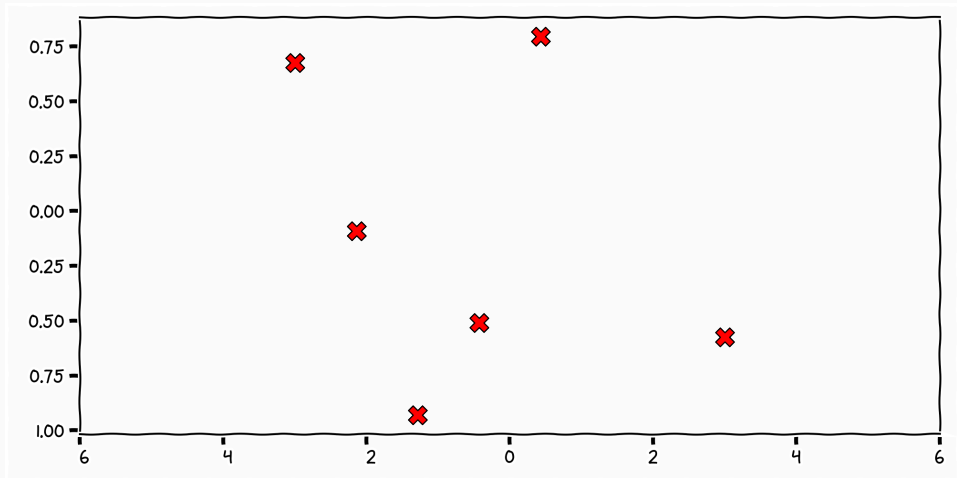
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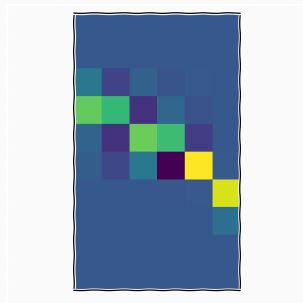
- Conditional Gaussian

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

Intuition

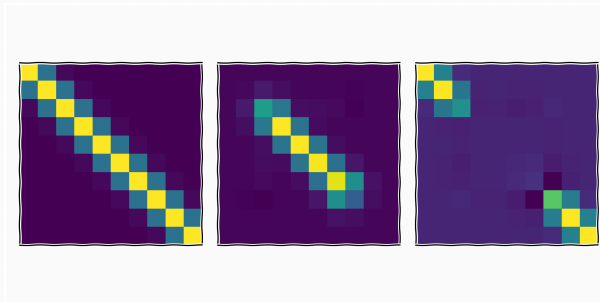


Does it make sense: Mean



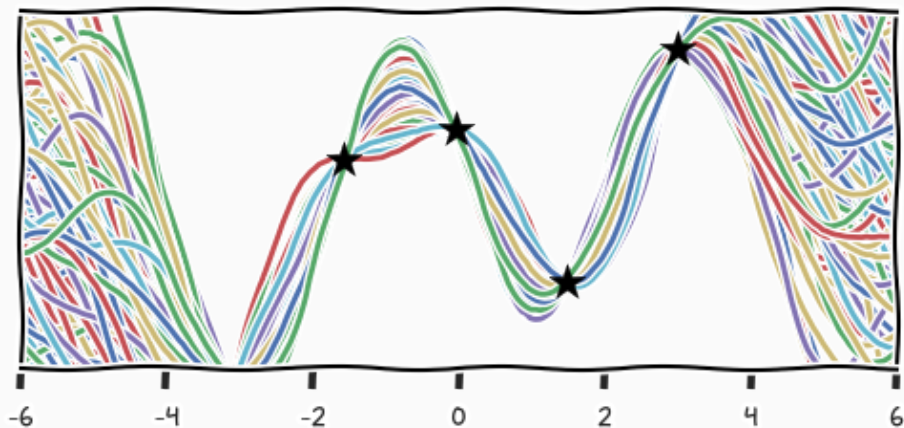
$$k(\mathbf{x}_*, \mathbf{X})^T k(\mathbf{X}, \mathbf{X})^{-1} \mathbf{f}$$

Does it make sense: Covariance

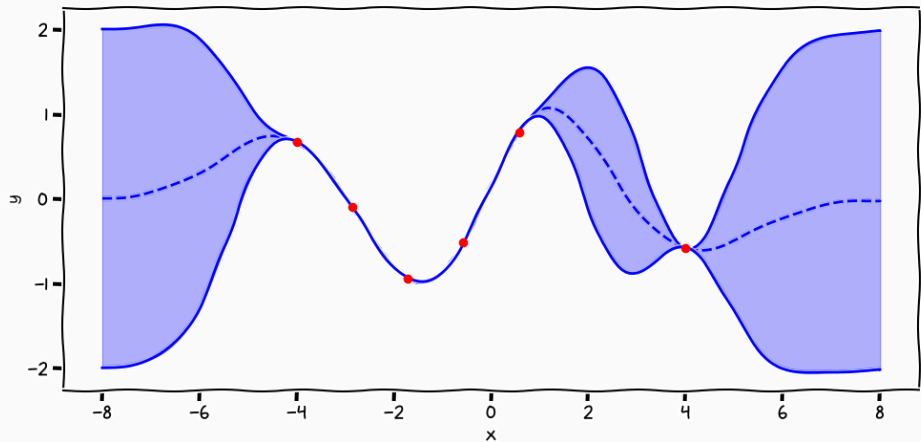


$$k(\mathbf{x}_*, \mathbf{x}_*) - k(\mathbf{x}_*, \mathbf{x})^T k(\mathbf{x}, \mathbf{x})^{-1} k(\mathbf{x}, \mathbf{x}_*)$$

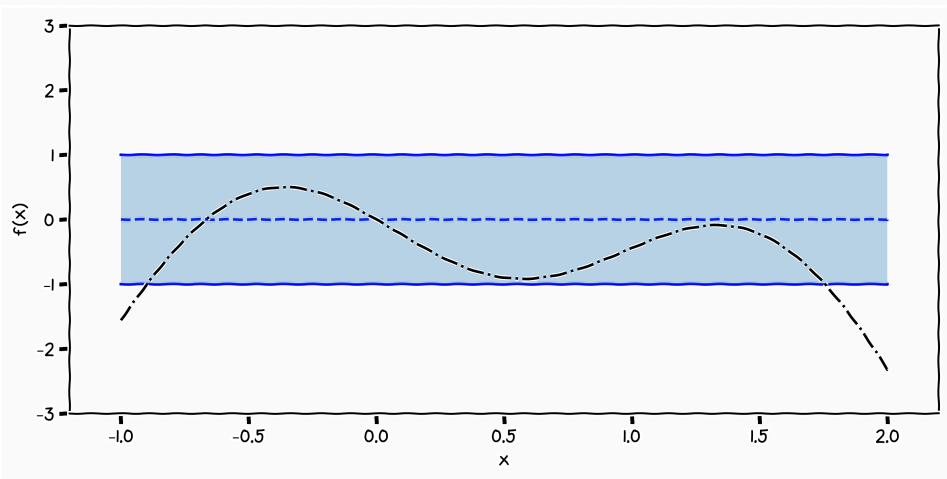
Gaussian Processes: "Predictive Posterior Samples"



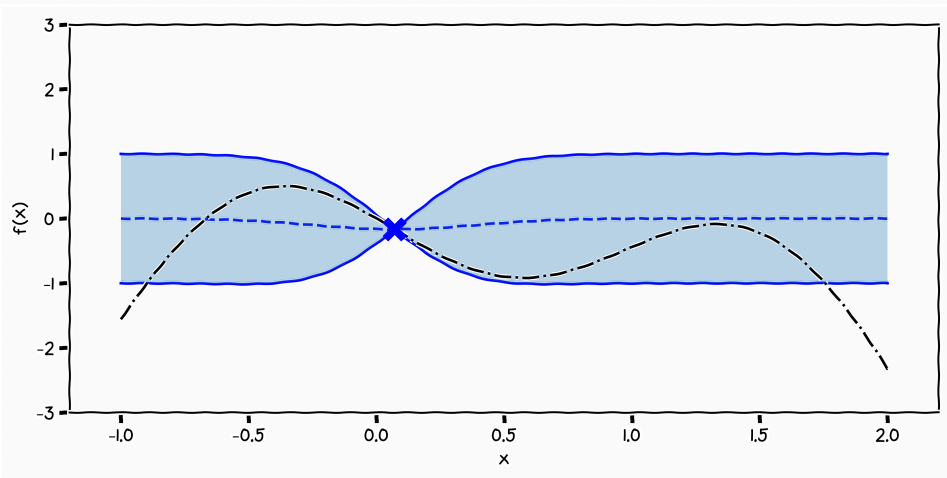
Gaussian Processes: "Predictive Posterior Process"



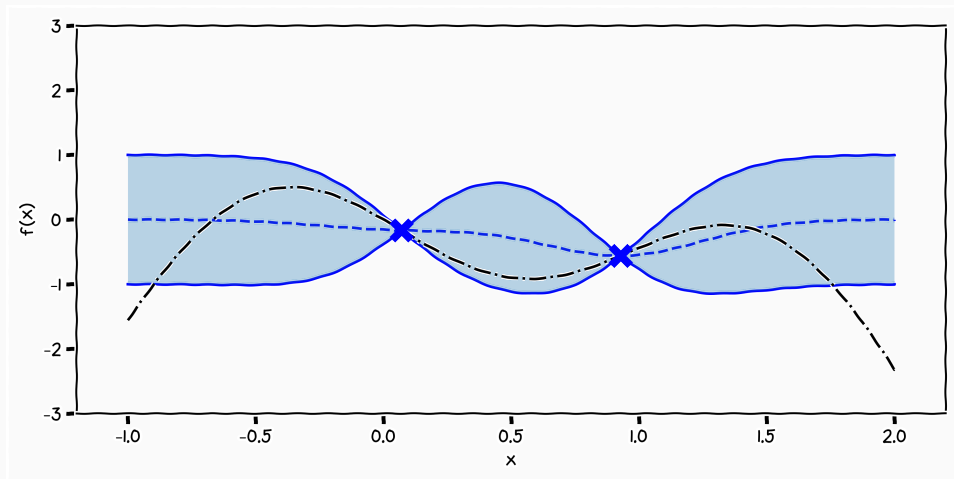
Posterior Processes



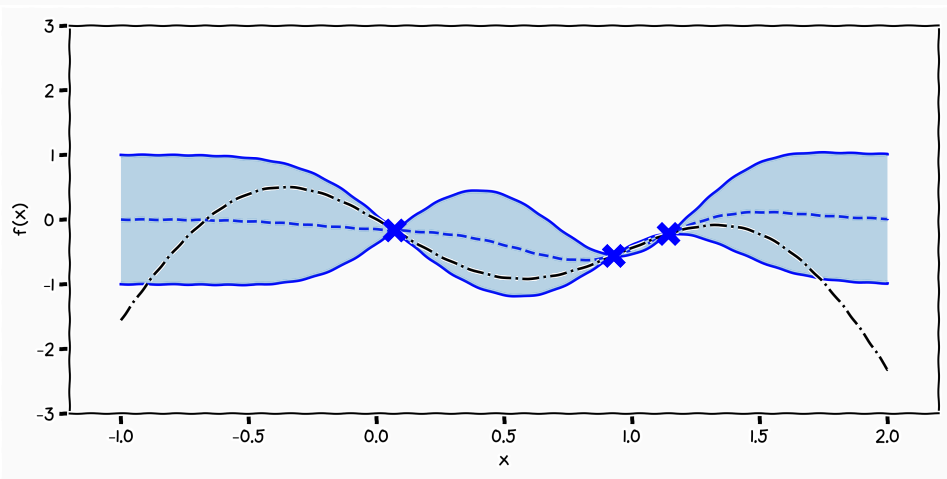
Posterior Processes



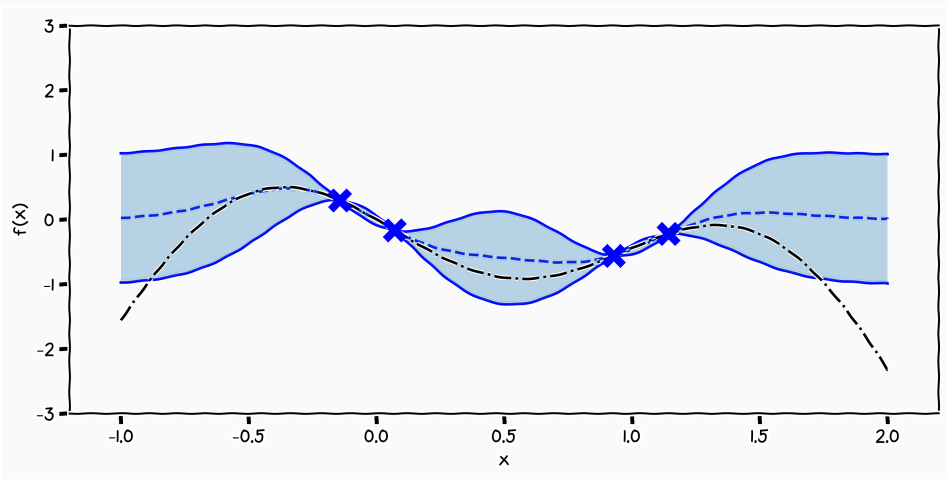
Posterior Processes



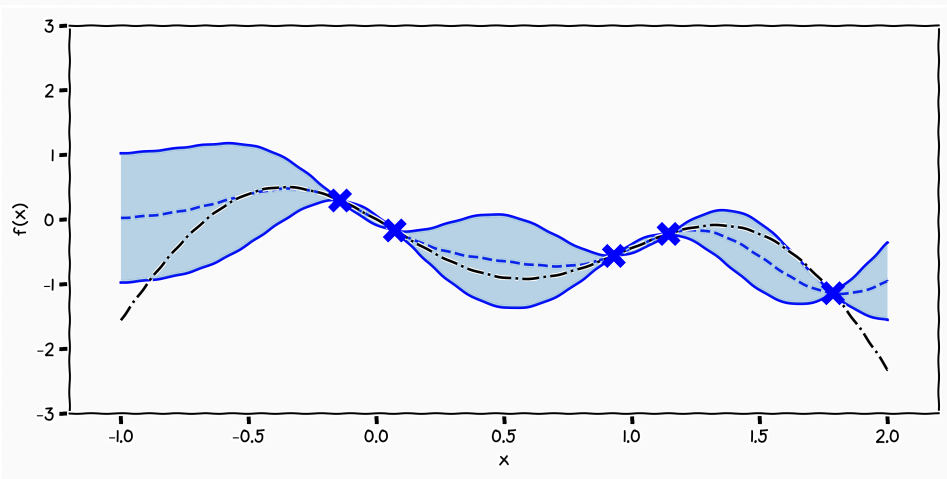
Posterior Processes



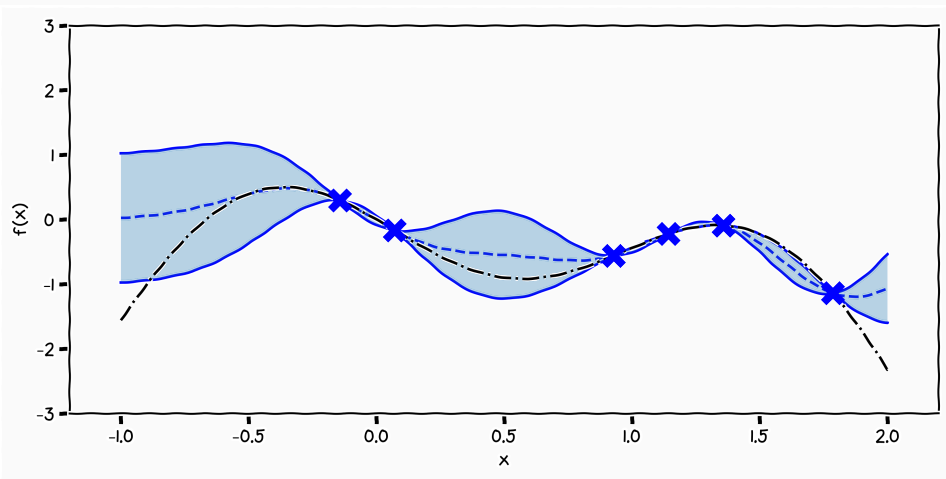
Posterior Processes



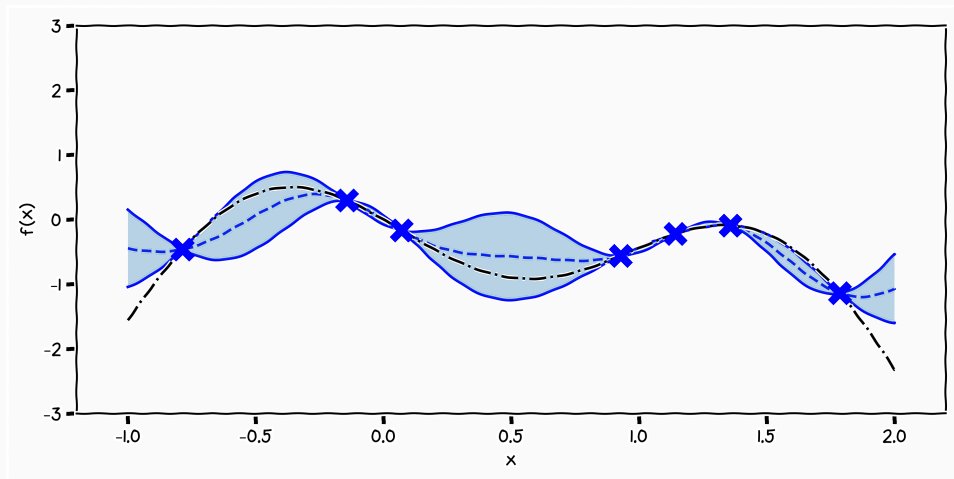
Posterior Processes



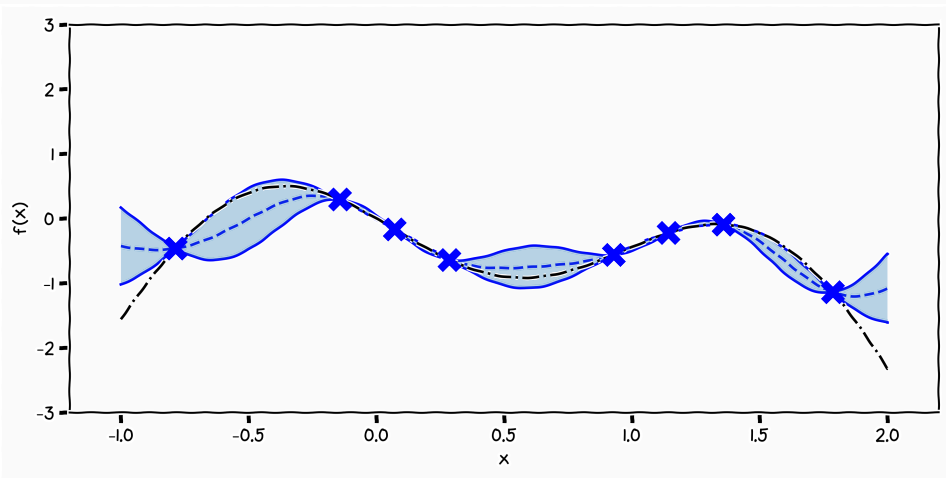
Posterior Processes



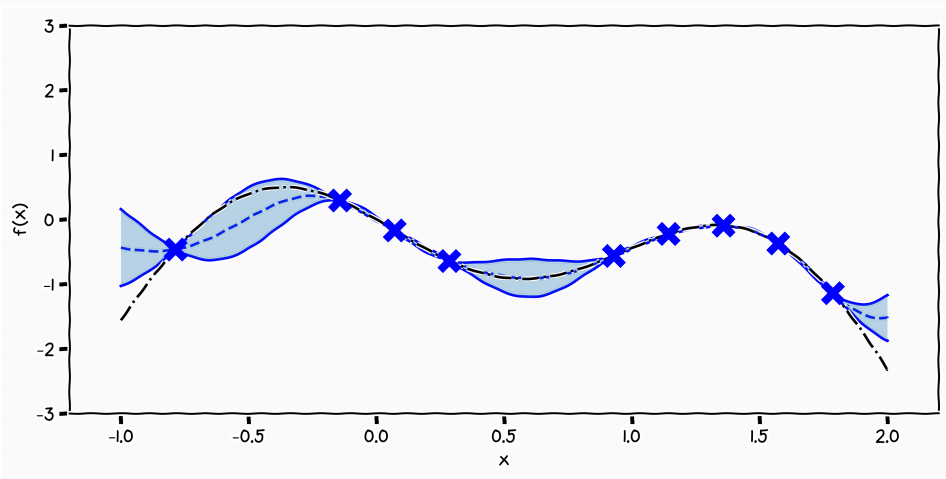
Posterior Processes



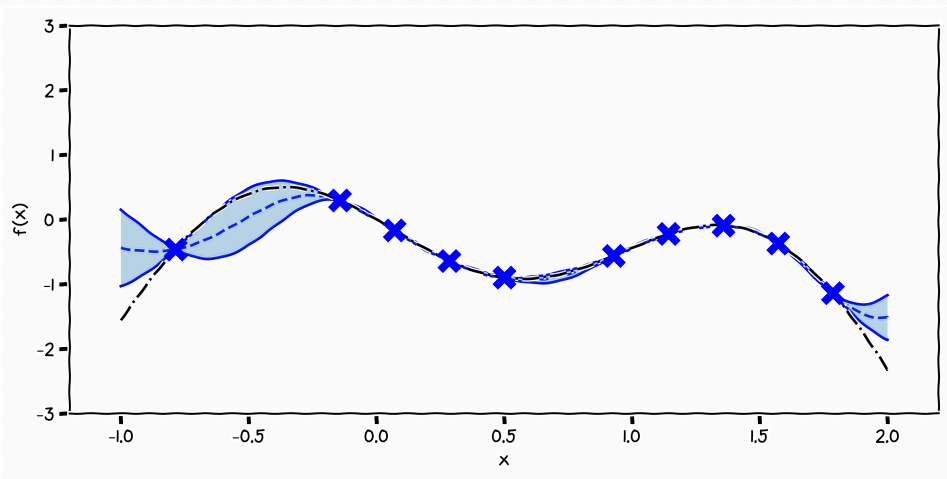
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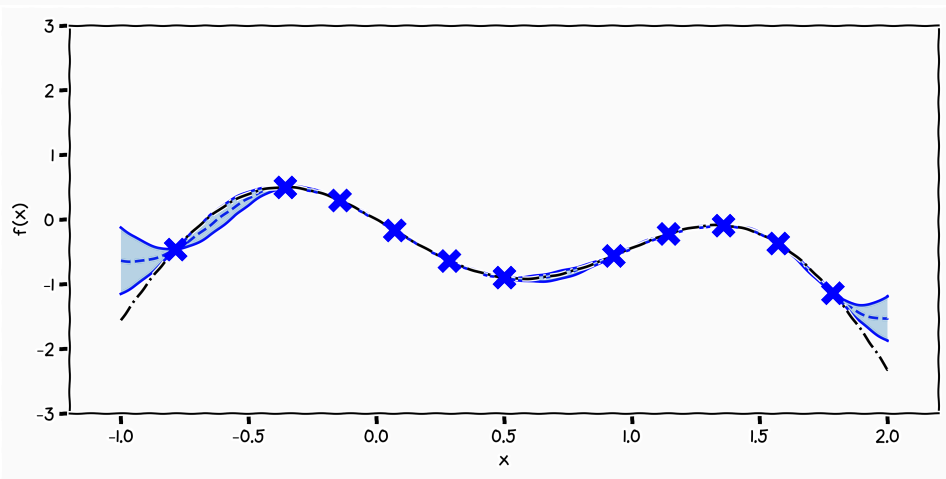
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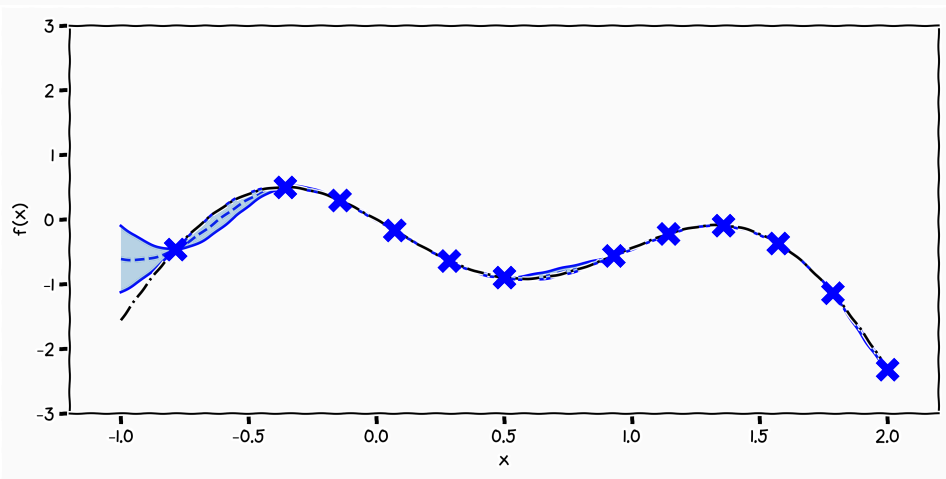
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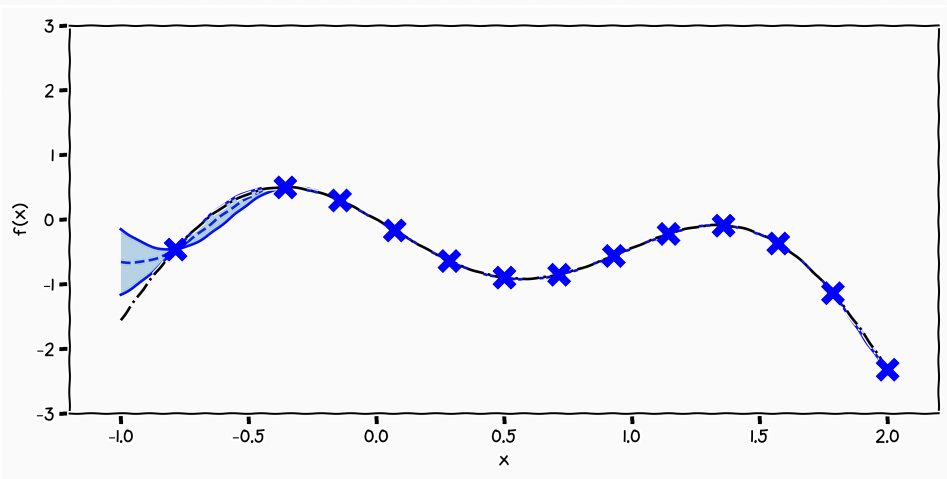
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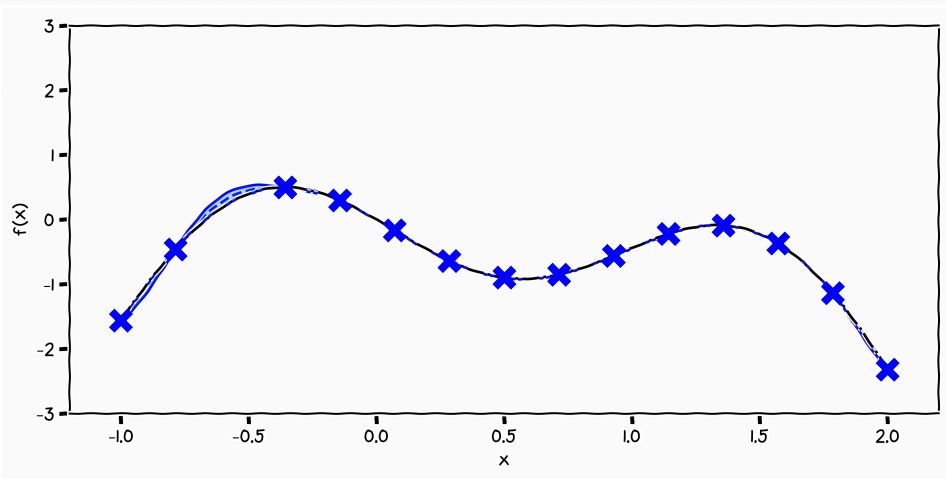
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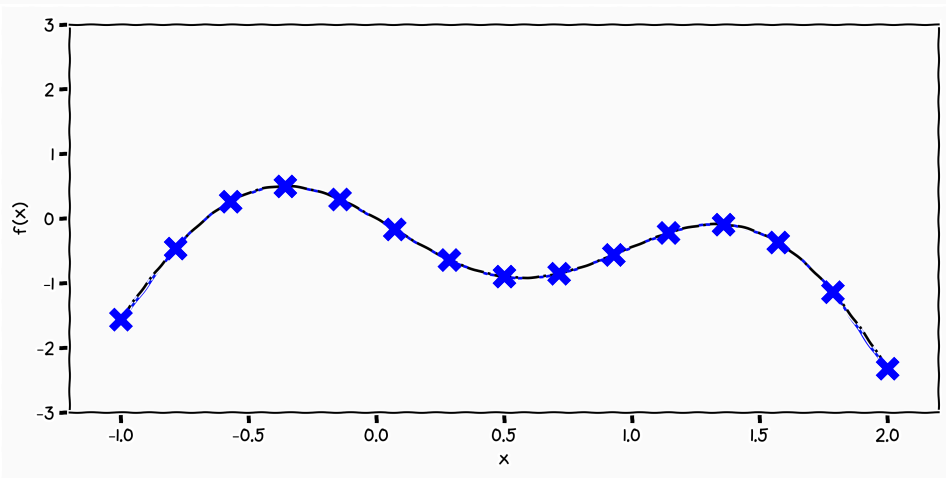
Posterior Processes



Posterior Processes



Posterior Processes



$$p(\mathbf{f}) \sim \mathcal{N}(\mathbf{f} \mid \mu(\cdot), k(\cdot, \cdot)), p(\mathbf{f}_* \mid \mathbf{f}) = \mathcal{N}(\mathbf{f}_*(\mathbf{x}_*, \mathbf{x})^T k(\mathbf{x}, \mathbf{x})^{-1} \mathbf{f}, \\ k(\mathbf{x}_*, \mathbf{x}_*) - k(\mathbf{x}_*, \mathbf{x})^T k(\mathbf{x}, \mathbf{x})^{-1} k(\mathbf{x}, \mathbf{x}_*))$$

- we have defined a measure over functions

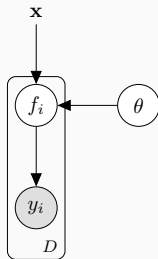
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- we have defined a measure over functions
- we can parametrise this measure to reflect our knowledge

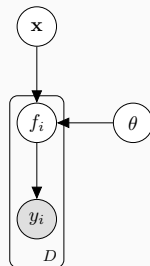
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- we have defined a measure over functions
- we can parametrise this measure to reflect our knowledge
- we can get an updated measure that combines our knowledge with data

Models

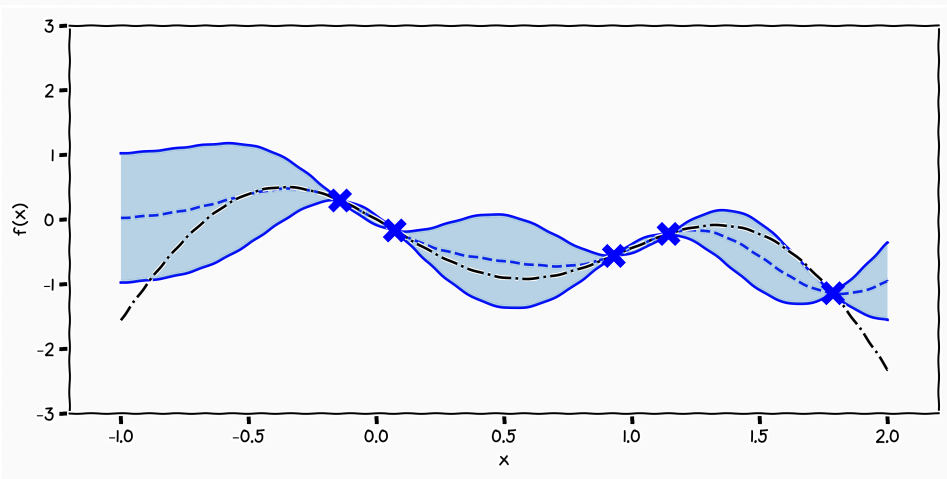


$$p(y|x) = \int p(y | f) p(f | x) df$$

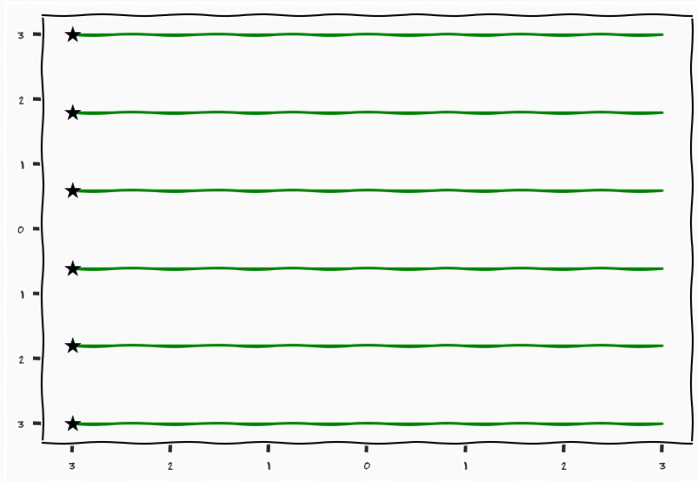


$$p(y) = \int p(y | f) p(f | x) p(x) df dx$$

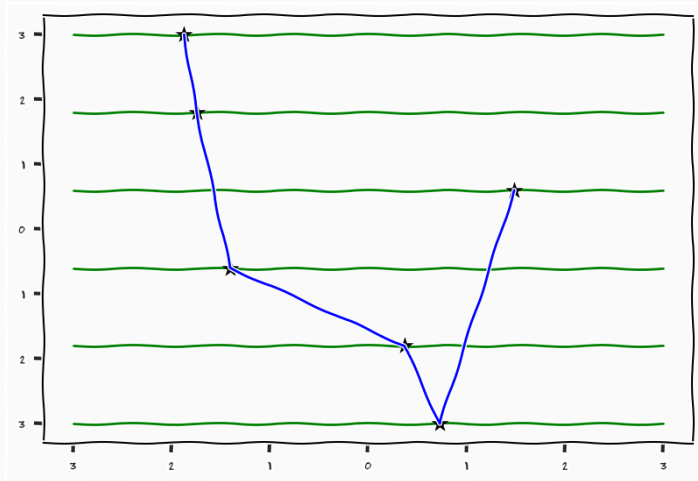
Posterior Processes



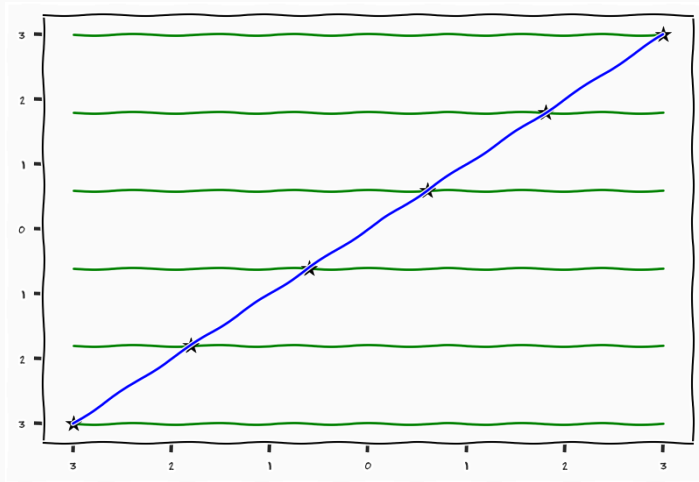
Unsupervised Learning



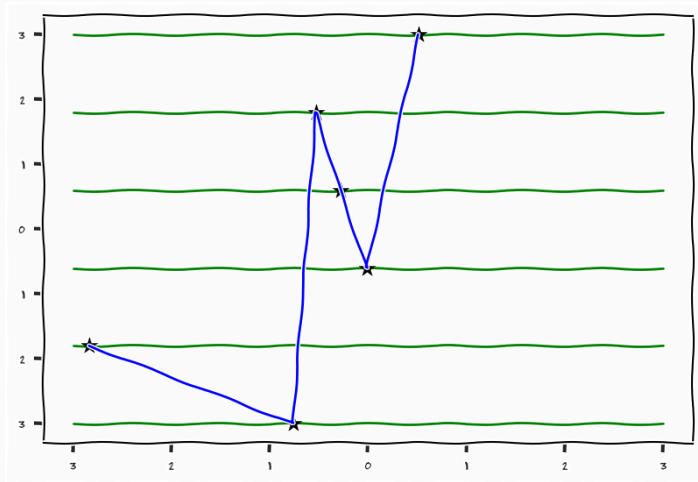
Unsupervised Learning



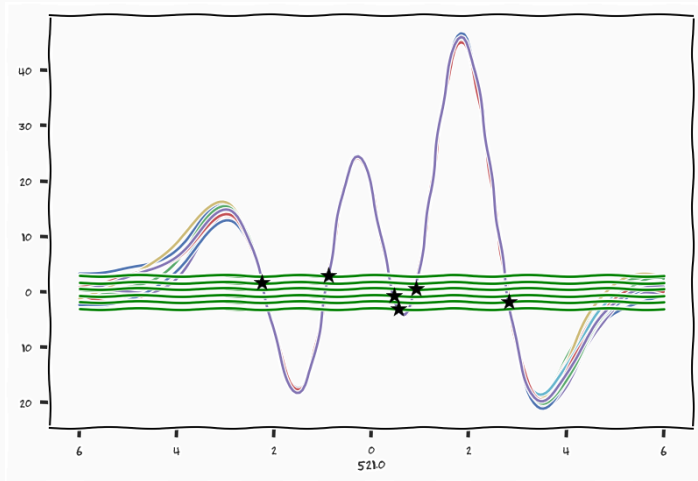
Unsupervised Learning



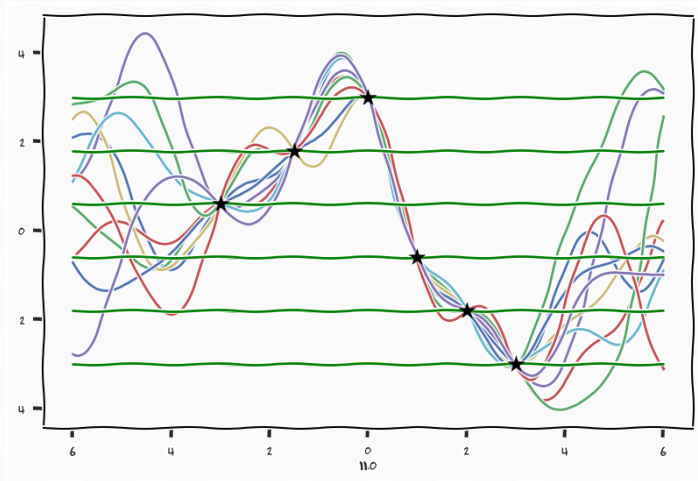
Unsupervised Learning



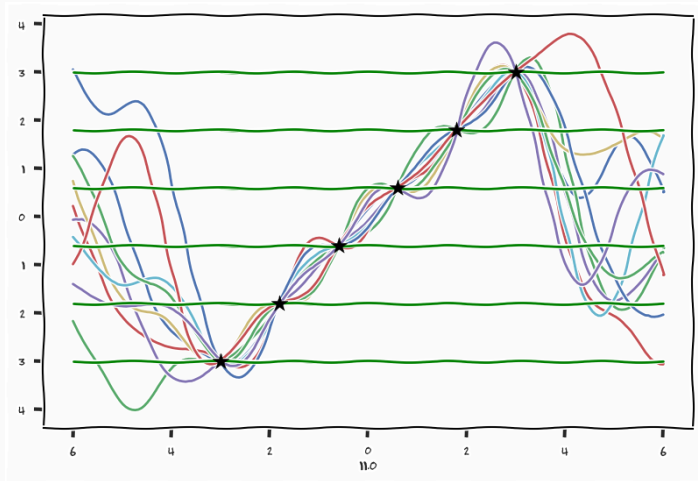
Unsupervised Learning



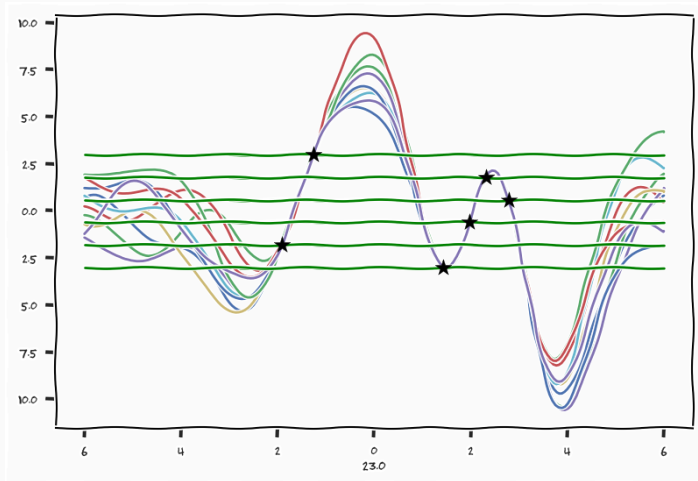
Unsupervised Learning



Unsupervised Learning



Unsupervised Learning



$$p(y) = \int p(y | f_2)p(f_2 | f_1)df_2df_1$$

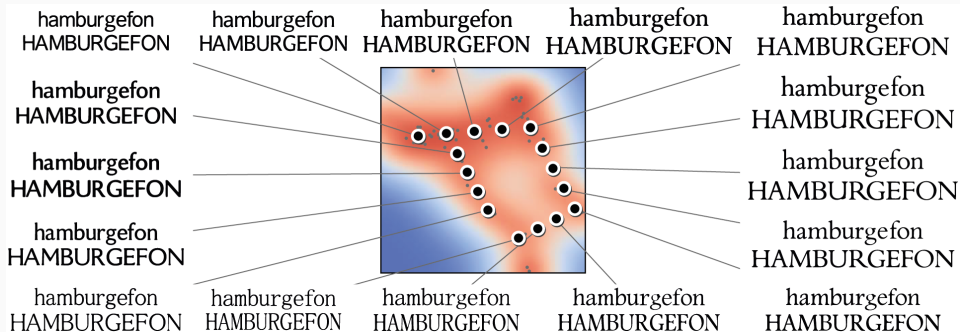
- The process of Marginalisation allows me to convert one measure to another measure

Regression there are infinite number of possible functions that connects the data equally well. A GP provides a measure over these solutions that makes the problem "well-posed".

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Unsupervised Learning there are infinite number of possible combinations of input locations and functions that generate the data equally well. A GP and a latent space prior jointly provides a measure over these solutions to make the problem "well-posed"

Fonts “Learning a manifold of fonts”



URL

Summary

- There is no such thing as a free lunch, anything that learns something does so by being biased

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- Any explanation of a result can only ever be interpreted relative to the bias that has been included
- Arguing religiously about being Bayesian or not boils down to do if you agree with the process of marginalisation
 - I believe you can be pragmatically non-bayesian, but it is very hard to motivate philosophically

- infinite capacity by parametrising the model through relationship between data

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- model of non-parametric parametrisation leads to stochastic processes

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- practical use** simple manipulation with multi-variate normals

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practical use simple manipulation with multi-variate normals

theoretically beautiful semantic in terms of stochastic processes

Kolmogorov's Extension Theorem

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

1. Exchangeable

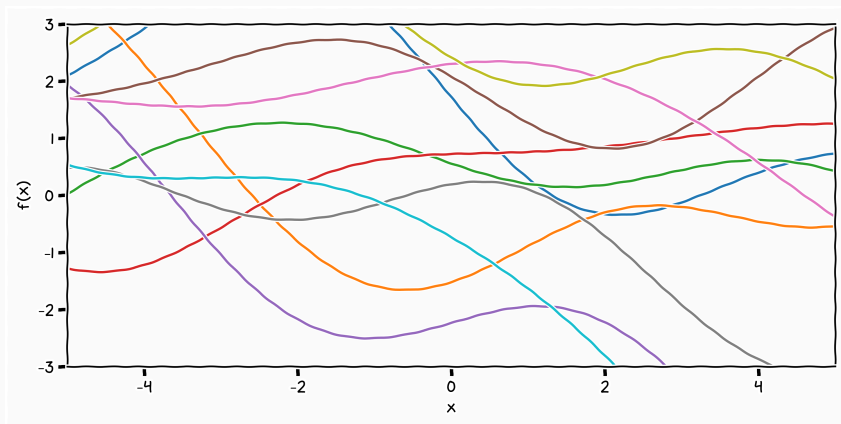
$$\nu_{t_{\pi(1)} \dots t_{\pi(k)}} (F_{\pi(1)} \times \dots \times F_{\pi(k)}) = \nu_{t_1 \dots t_k} (F_1 \times \dots \times F_k)$$

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

Are Gaussian Processes good parametrisations?



Are Gaussian Processes good parametrisations?

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Are Gaussian Processes good parametrisations?




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- Yes** they are incredibly "narrow" but have infinite coverage

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