University of BRISTOL

Machine Learning

Gaussian Processes

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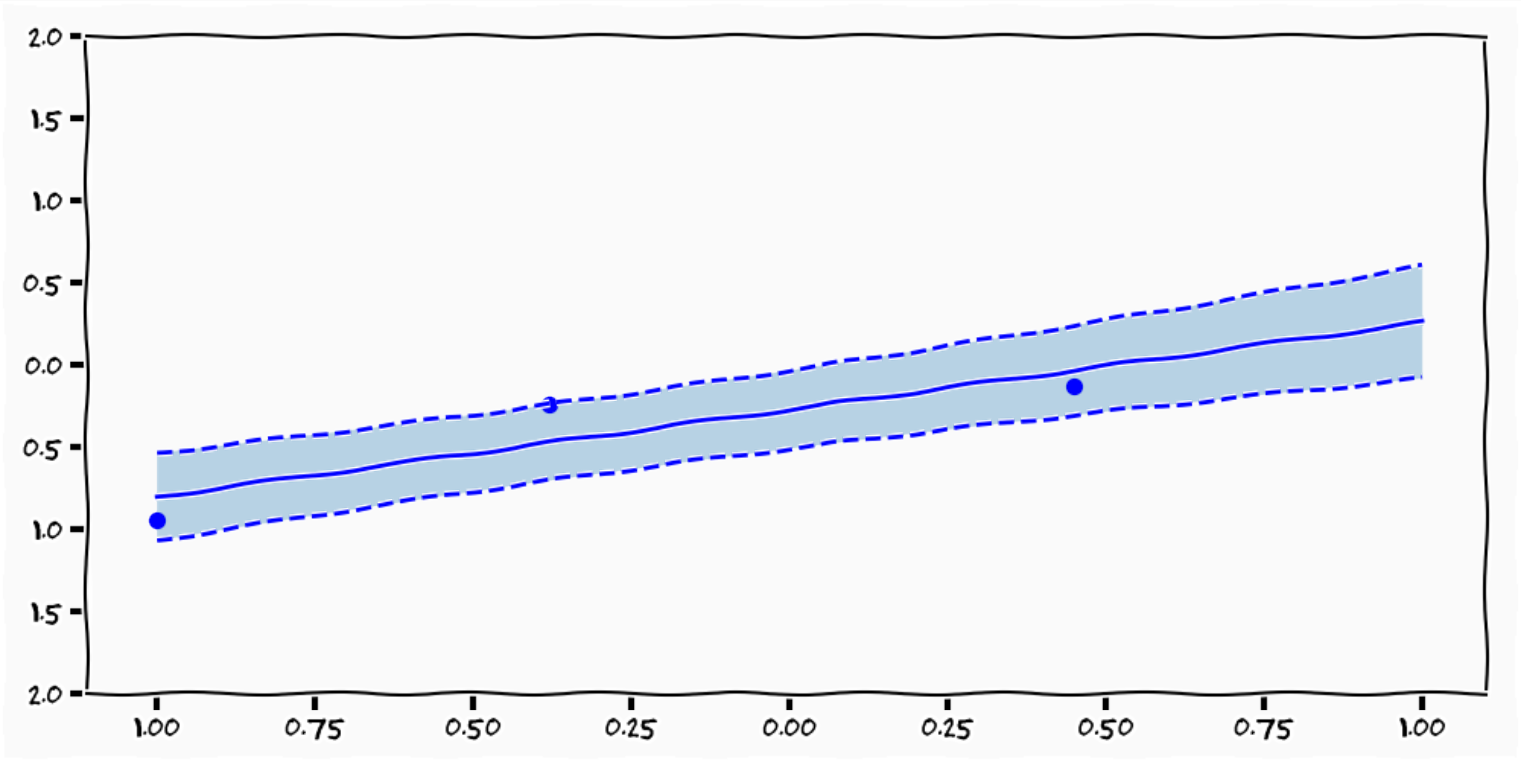
Introduction

Linear Regression

$$
\begin{aligned}
p(\mathbf{t}|\mathbf{w}, \mathbf{x}) &= \prod_{n}^{N} p(t_n|\mathbf{w}, \mathbf{x}) = \prod_{n}^{N} \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\mathbf{x}_n, \sigma^2\mathbf{I}) \\
p(\mathbf{w}) &= \mathcal{N}(\mathbf{0}, \tau^2\mathbf{I}) \\
p(\mathbf{w}|\mathbf{t}, \mathbf{x}) &= \frac{p(\mathbf{t}|\mathbf{w}, \mathbf{x})p(\mathbf{w})}{p(\mathbf{t})} \\
&\propto p(\mathbf{t}|\mathbf{w}, \mathbf{x})p(\mathbf{w})
\end{aligned}
$$

Predictive Posterior



$$p(t_*|\mathbf{x}_*, \mathbf{X}, \mathbf{t}, \beta, \alpha) = \int p(t_*|\mathbf{x}_*, \mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \alpha, \beta) \mathrm{d}\mathbf{w}$$

Dual Linear Regression

$$
\begin{aligned}
\hat{\mathbf{w}} &= \operatorname{argmin}_{\mathbf{w}} - \log\, p(\mathbf{w}|\mathbf{t}, \mathbf{x}) \\
&= \frac{1}{2}(\mathbf{X}\mathbf{w} - \mathbf{t})^{\mathrm{T}}(\mathbf{X}\mathbf{w} - \mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \\
\hat{\mathbf{w}} &= \mathbf{X}^{\mathrm{T}}\left(\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X}) + \lambda\mathbf{I}\right)^{-1}\mathbf{t}
\end{aligned}
$$

Linear Regression

Primal - explicit representation

$$\mathbf{y}(\mathbf{x}_*) = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_*)$$

Dual - implicit representation

$$\mathbf{y}(\mathbf{x}_*) = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_*) = k(\mathbf{x}_*, \mathbf{X})(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}$$
$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{x}')$$

Kernels

$$k(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^{\mathrm{T}} \phi(\mathbf{x}_j)$$

- kernel functions describe inner-products in an induced representation
- induced representation lives in what is called a Hilbert Space
- importantly the space is metric
- *we never need to know the mapping, only the inner-product*

What have we actually done

- Primal
  - See data
  - Encode relationship between variates using parameters $\mathbf{w}$
  - Make predictions using $\mathbf{w}$

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  - *Model complexity depends on data*
  - Non-parametric model

Non-parametrics

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Kernels

Euclidean Distance

$$||\mathbf{x}_i - \mathbf{x}_j||^2 = \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_i - 2\mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j + \mathbf{x}_j^{\mathrm{T}}\mathbf{x}_j$$

Kernelised Euclidean Distance

$$||\phi(\mathbf{x}_i) - \phi(\mathbf{x}_j)||^2 = k(\mathbf{x}_i, \mathbf{x}_j) - 2k(\mathbf{x}_i, \mathbf{x}_j) + k(\mathbf{x}_i, \mathbf{x}_j)$$

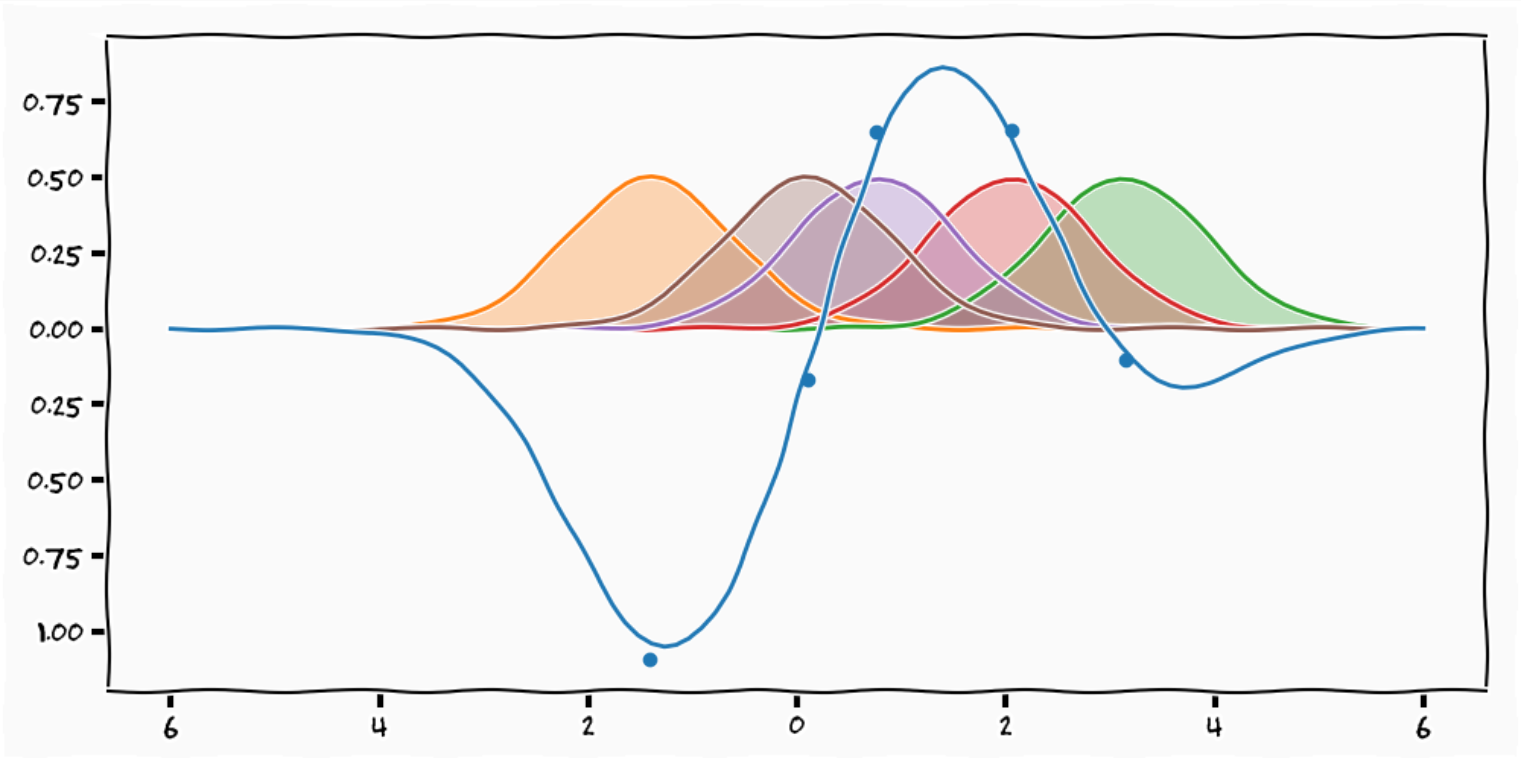
Kernel Example

$$k(\mathbf{x}_i, \mathbf{x}_j) = \sigma^2 e^{-\frac{1}{2\ell^2}(\mathbf{x}_i - \mathbf{x}_j)^{\mathrm{T}}(\mathbf{x}_i - \mathbf{x}_j)}$$

Exponented Quadratic

- How does the data vary along the dimensions spanned by the data
- RBF, Squared Exponential, Exponentiated Quadratic
- Co-variance smoothly decays with distance
- You can build new kernels out of other kernels [1] p. 296

Kernel Regression



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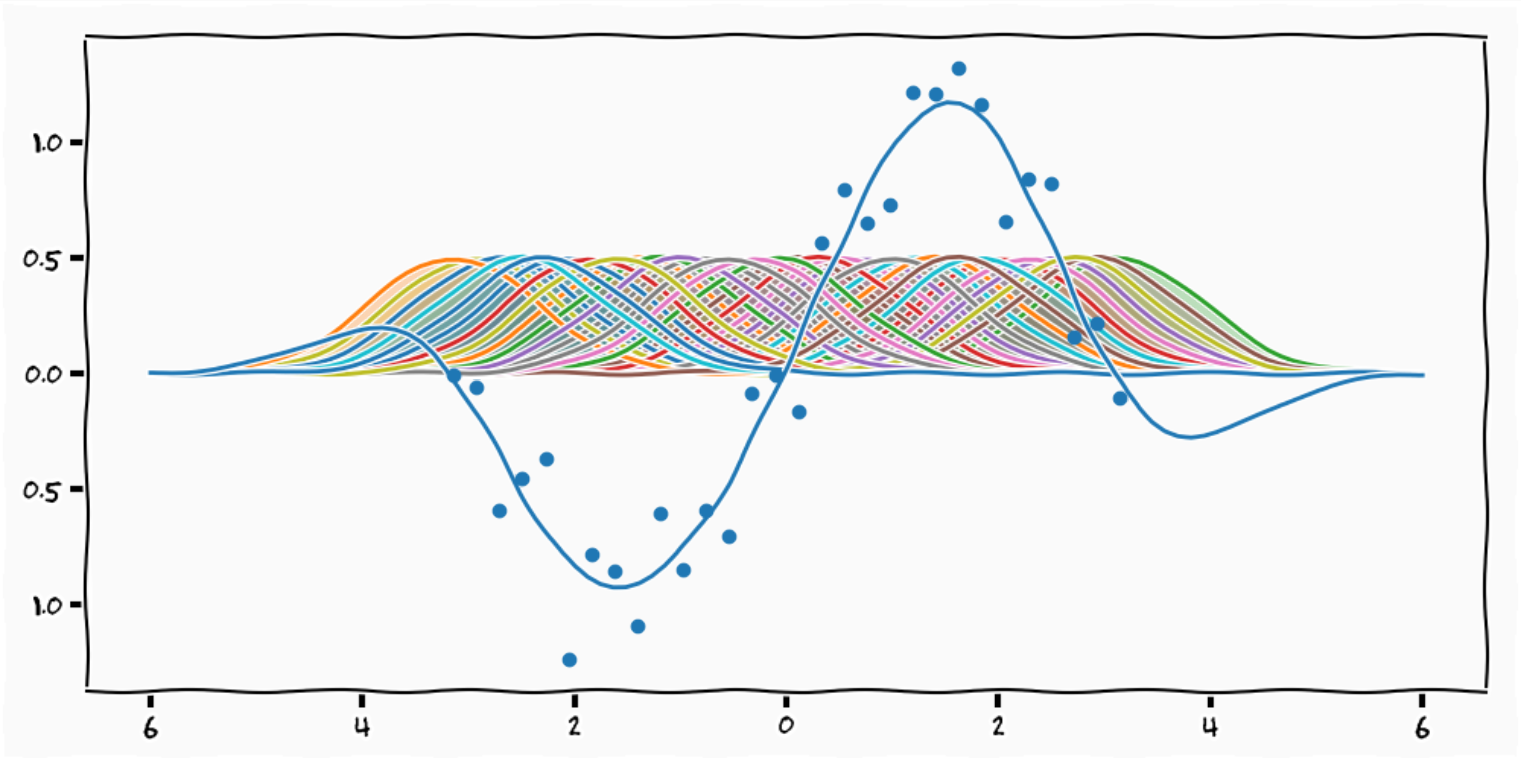

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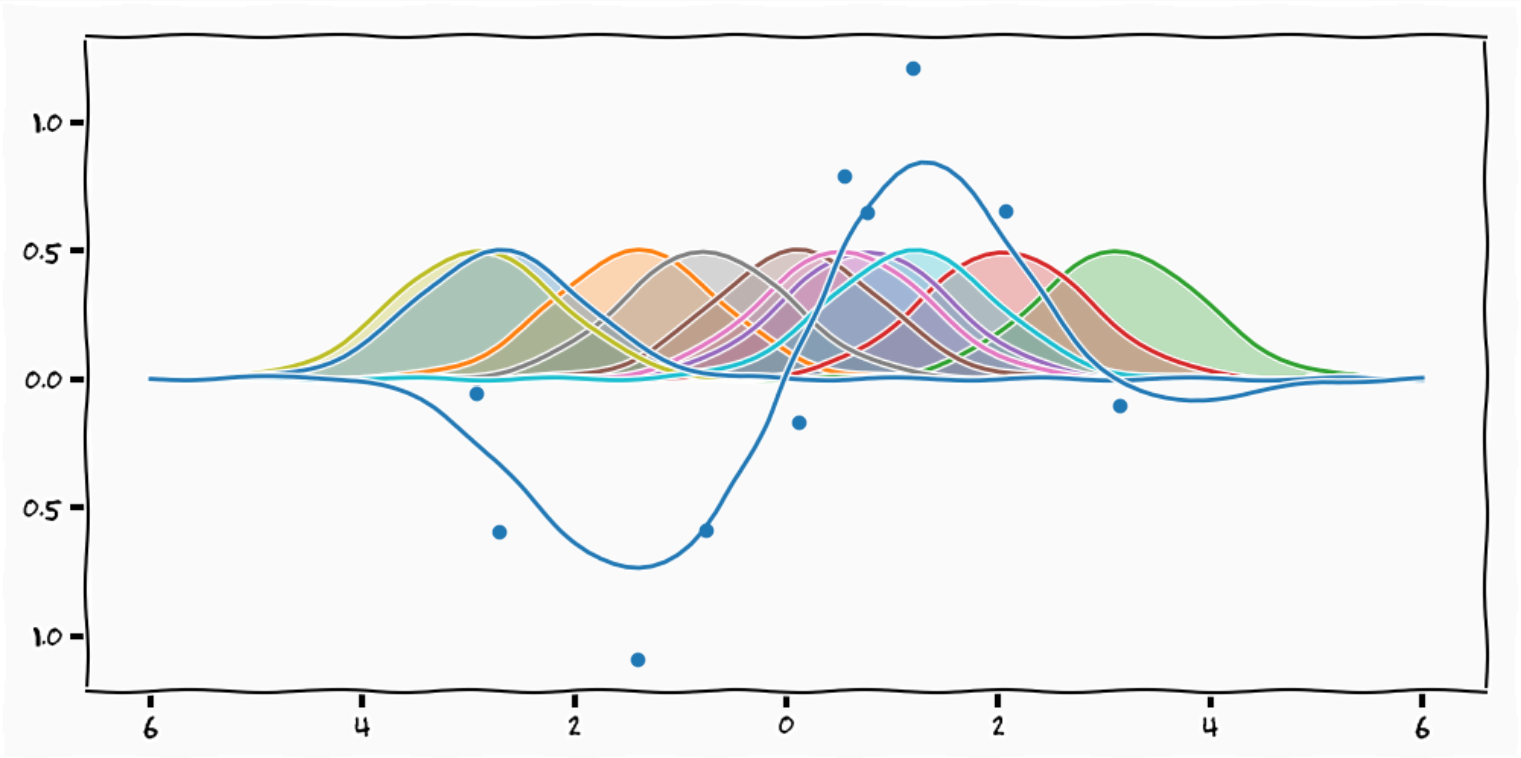

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  - Linear, it is a line
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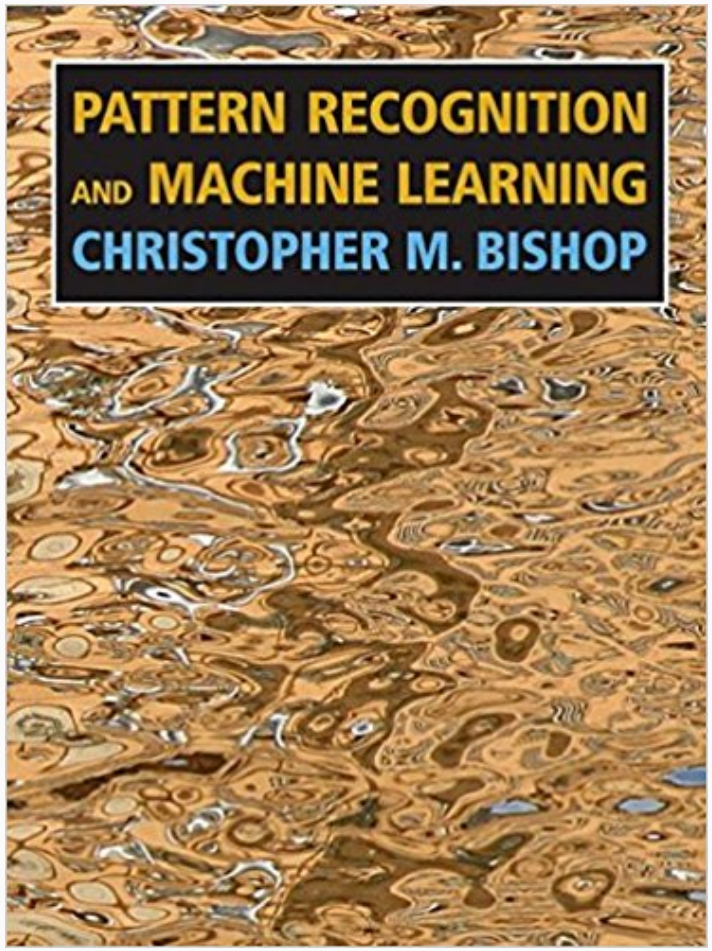
- *need to make assumption over the space of functions*
- A distribution over the space of functions

Gaussian Processes

Book

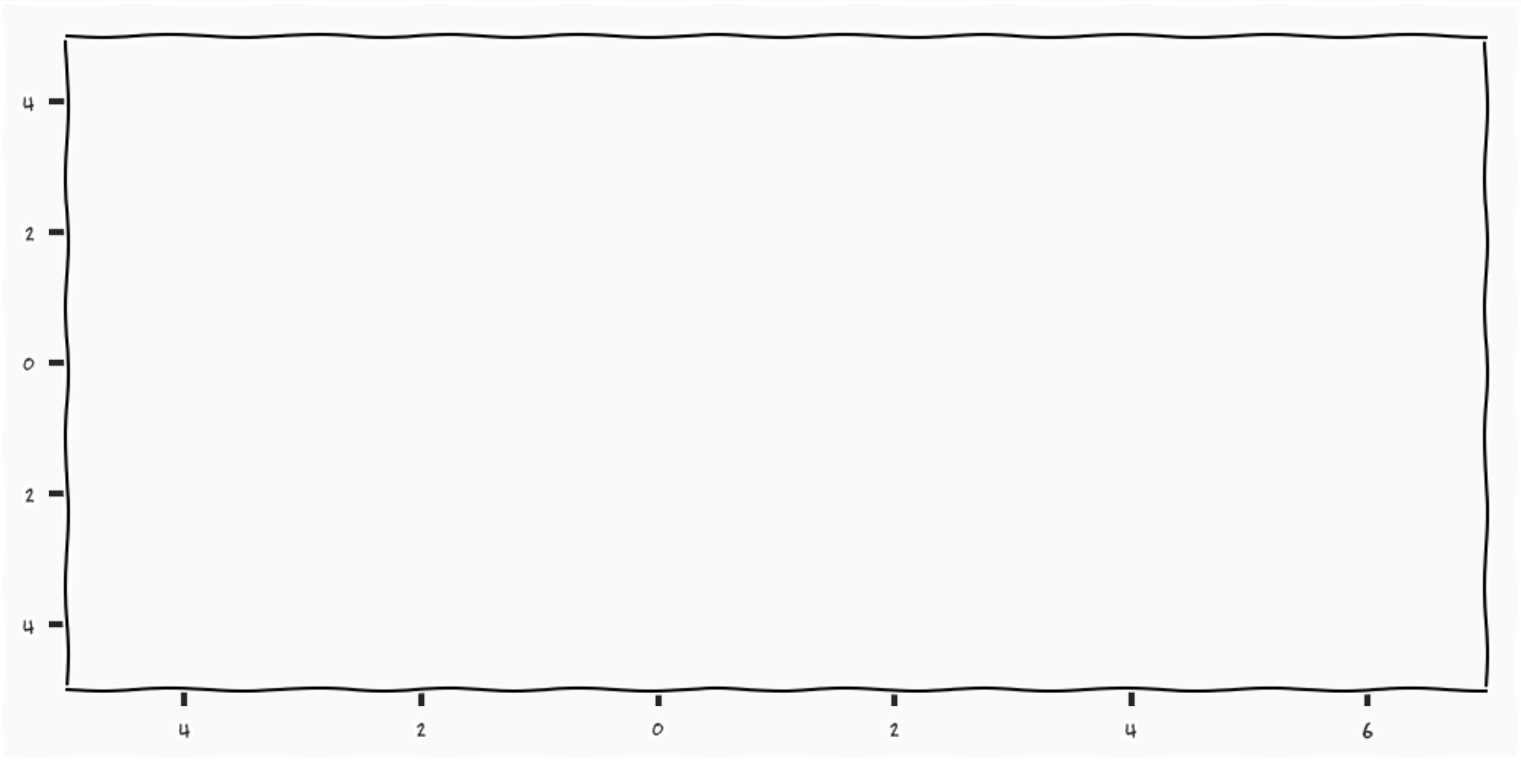

PATTERN RECOGNITION
AND MACHINE LEARNING
CHRISTOPHER M. BISHOP

GPSS[1]

IUDICIUM POSTERIUM DISCIPULUS EST PRIORIS

[1] http://gpss.cc

Gaussian Processes



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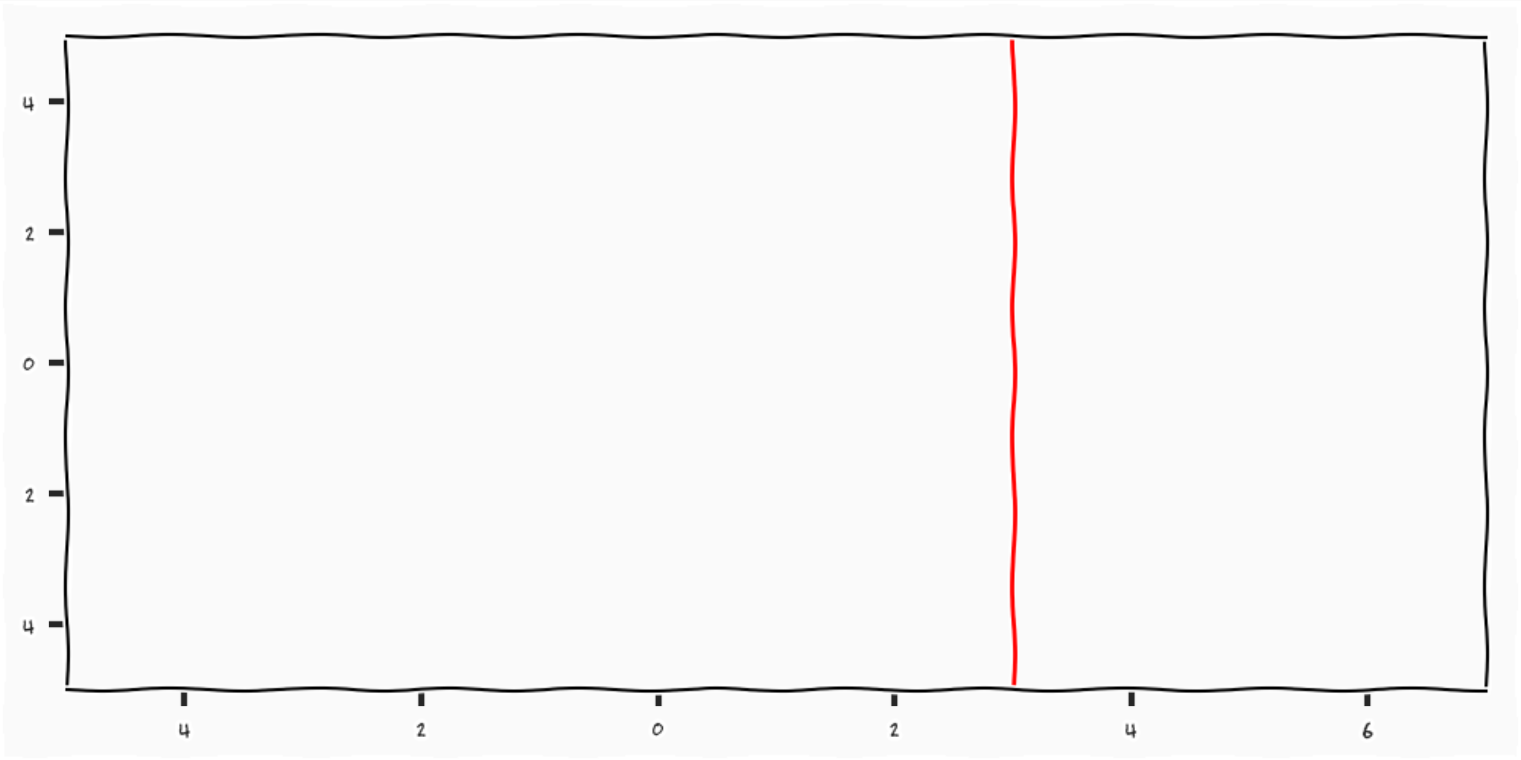

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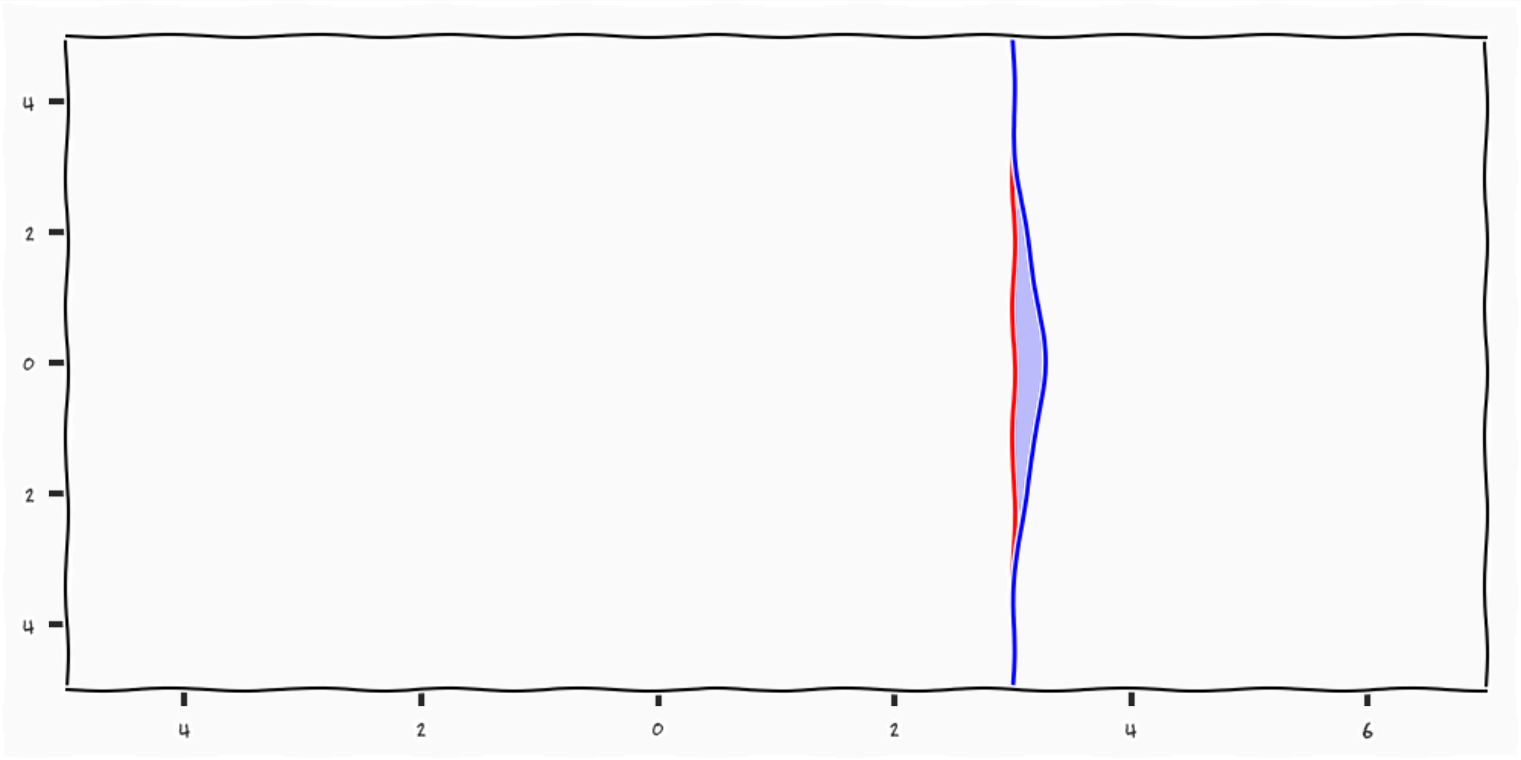

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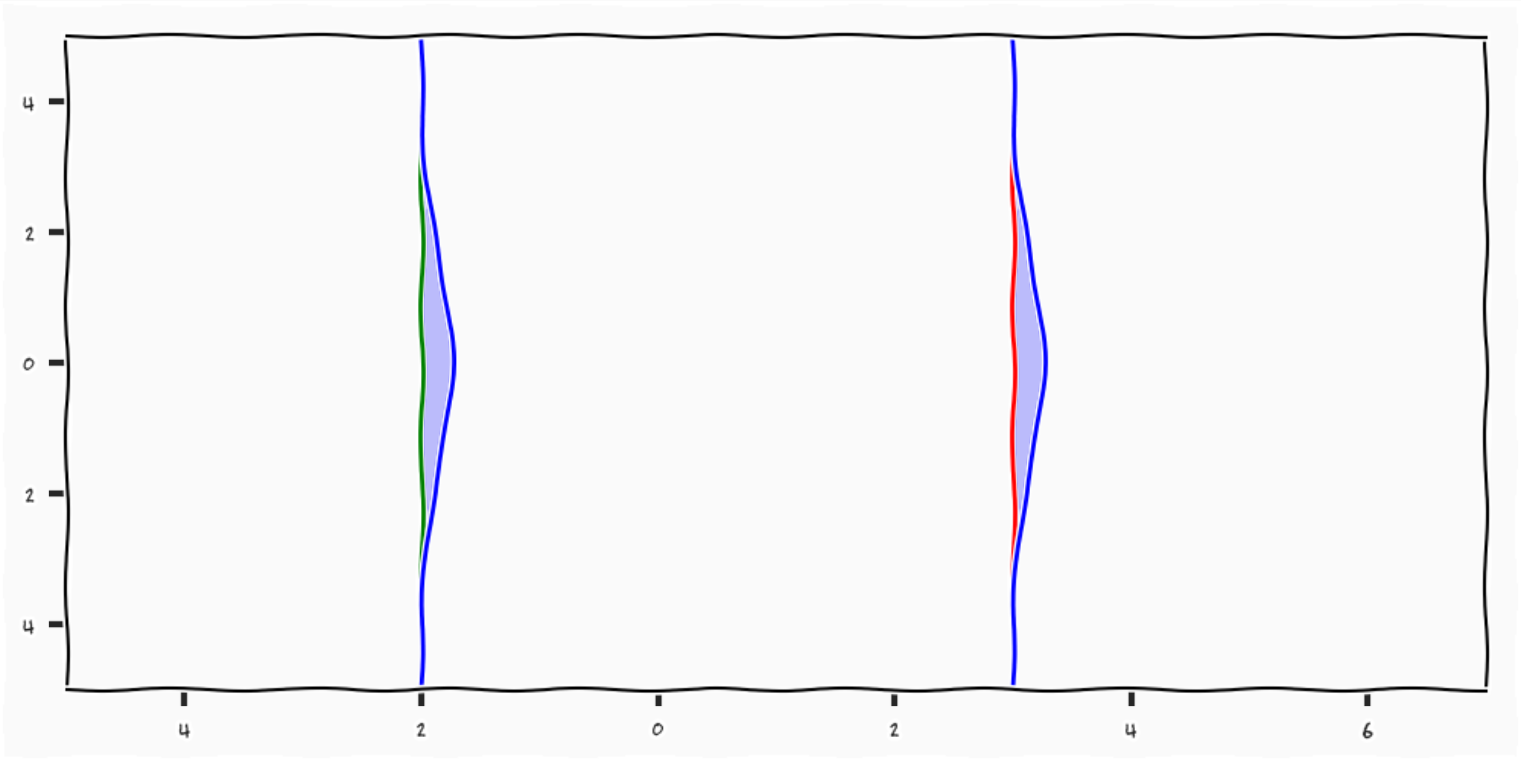

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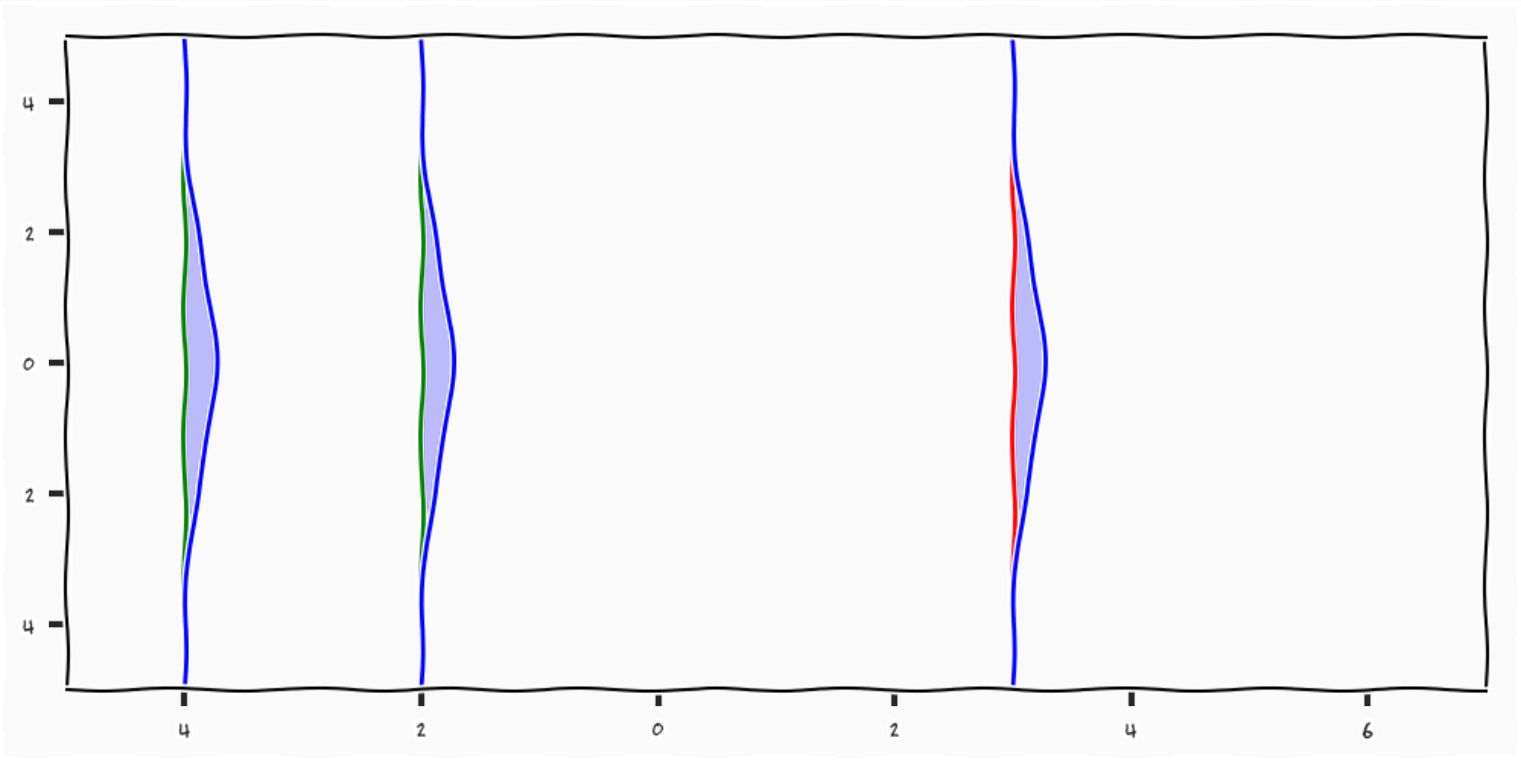

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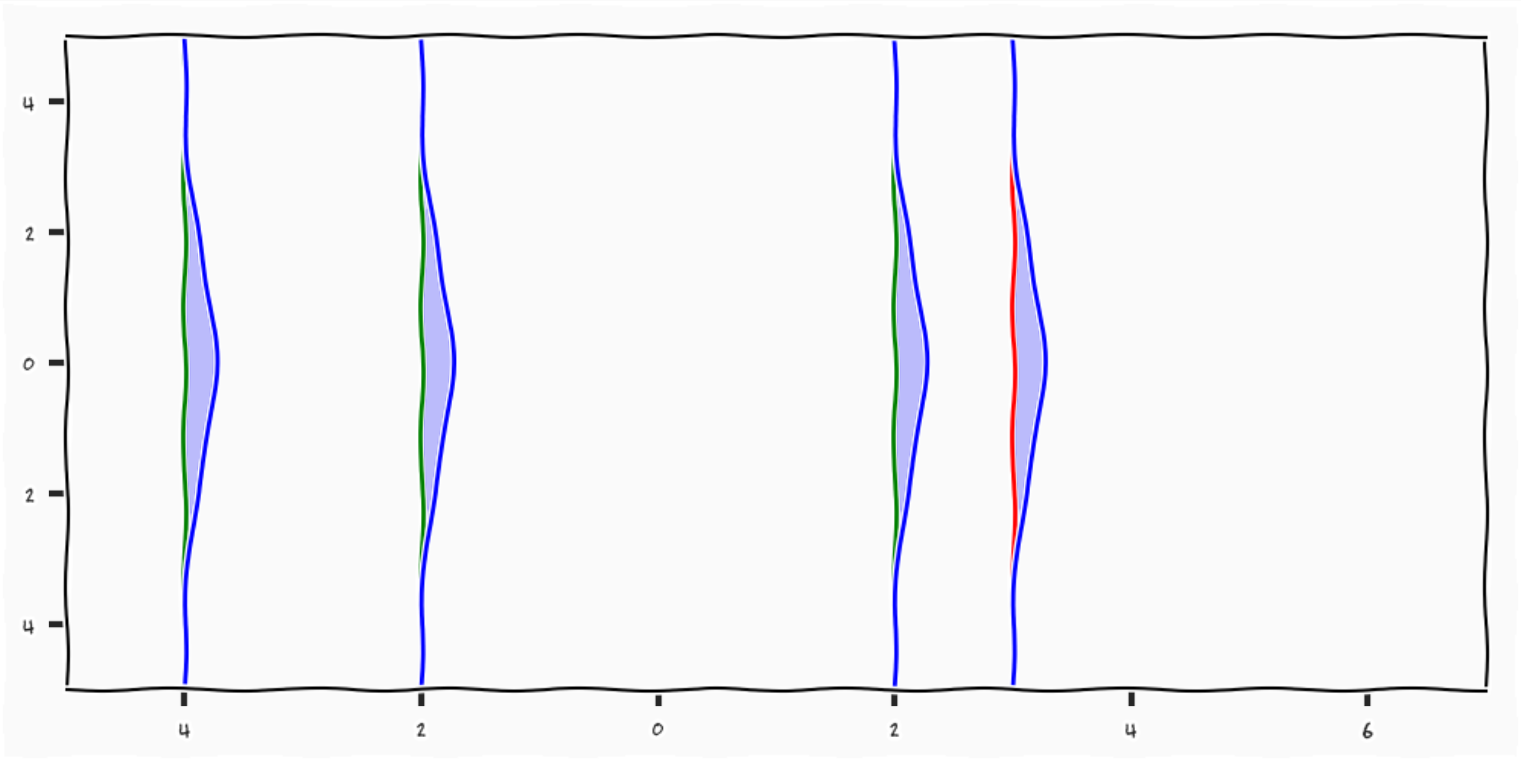

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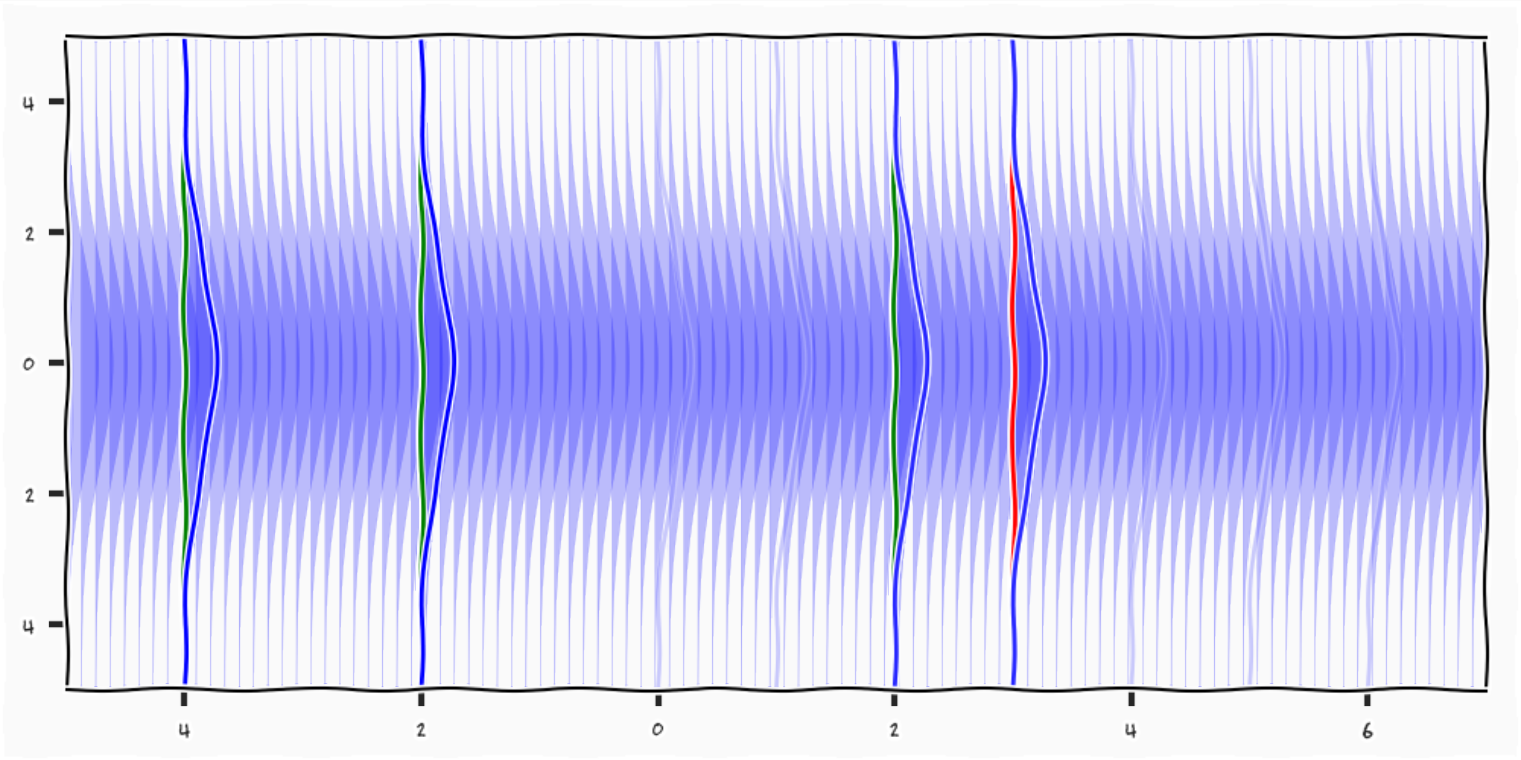

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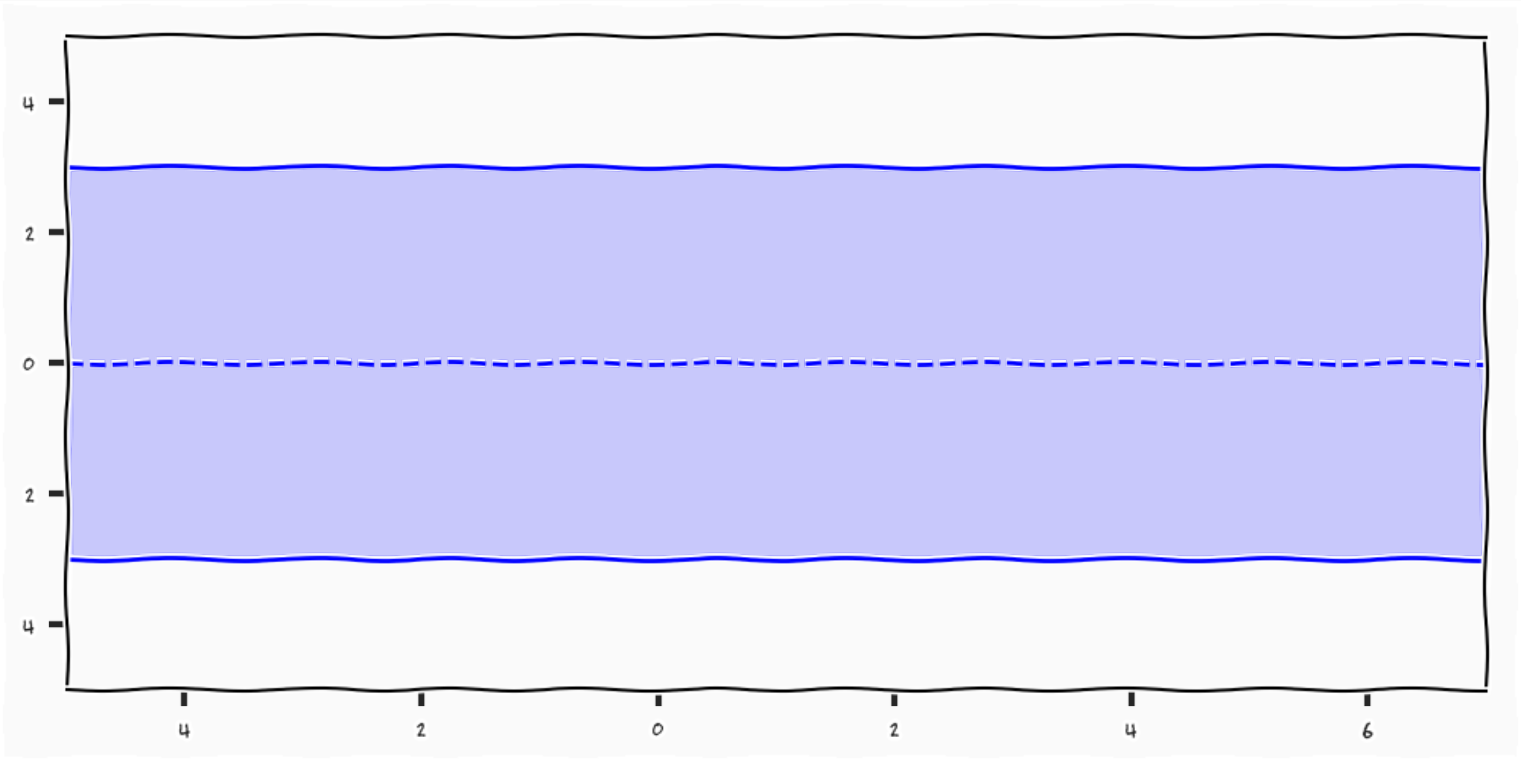

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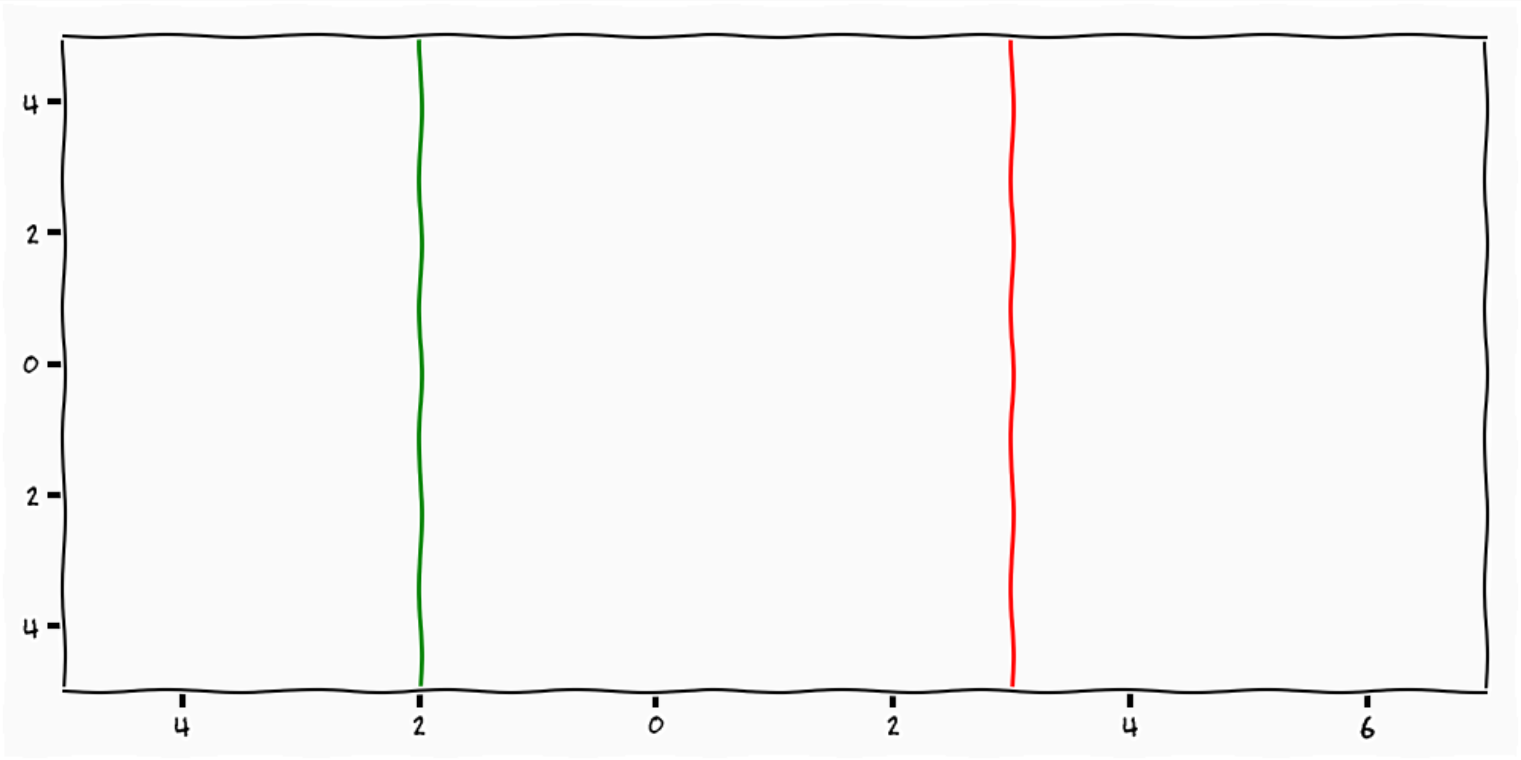

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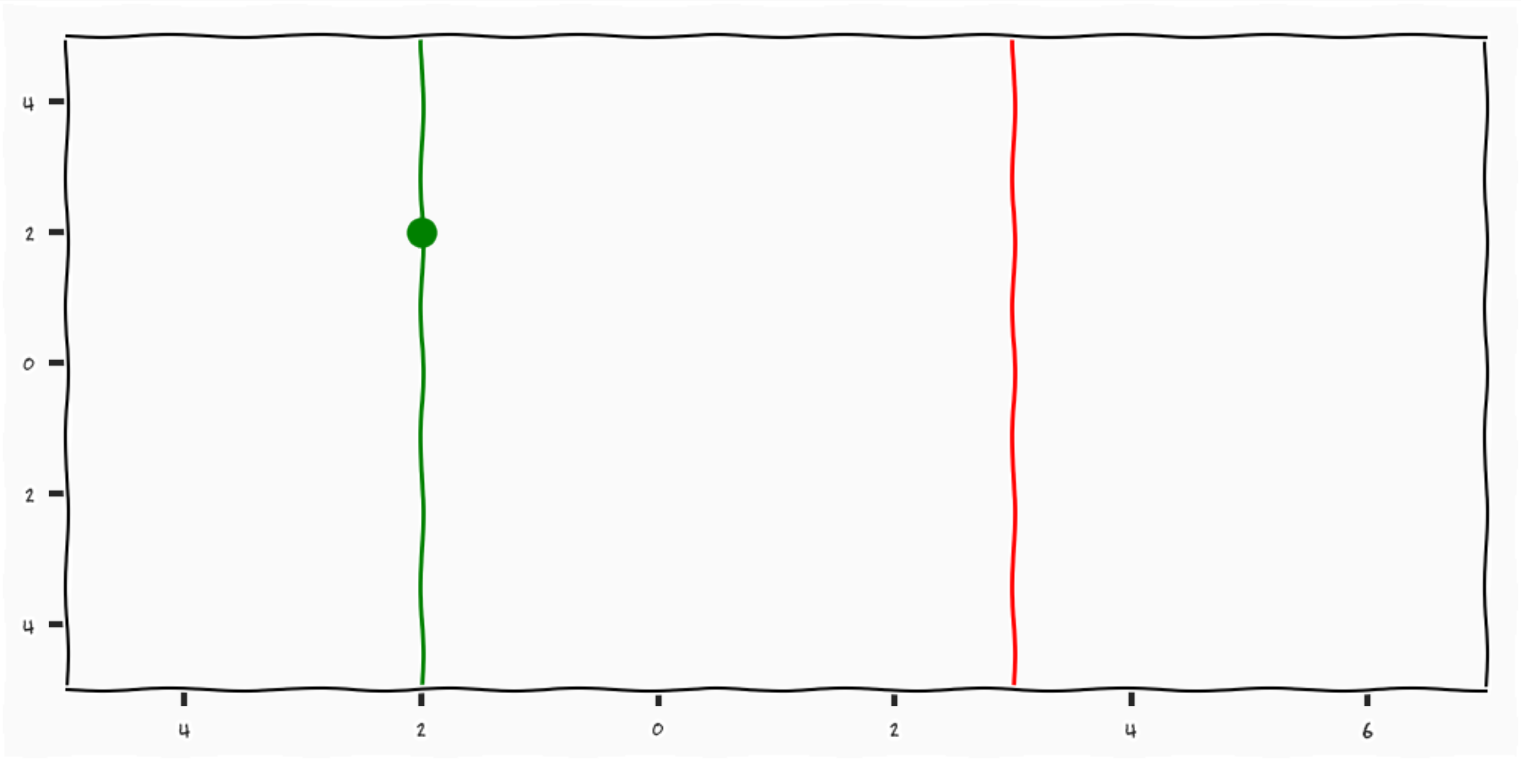

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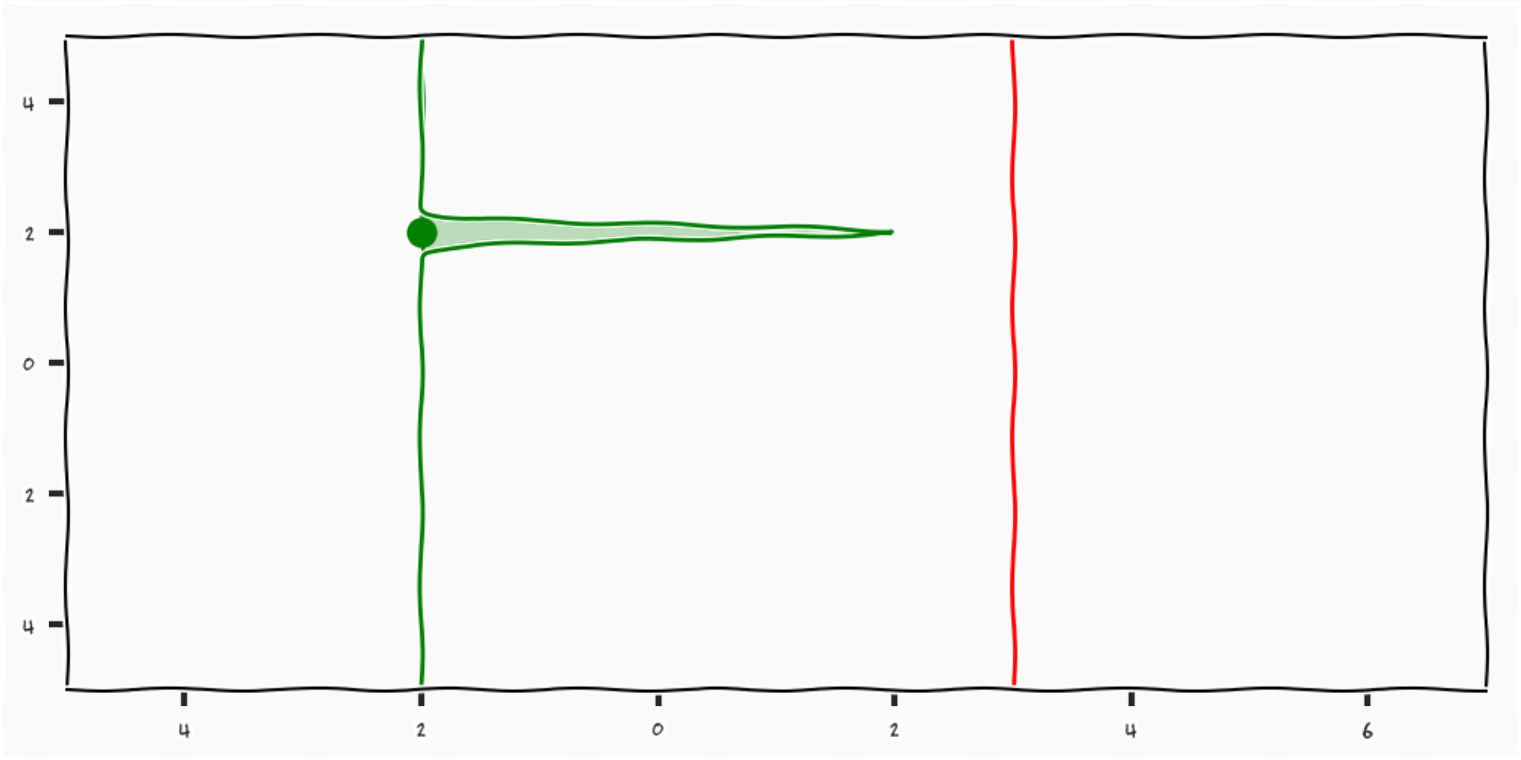

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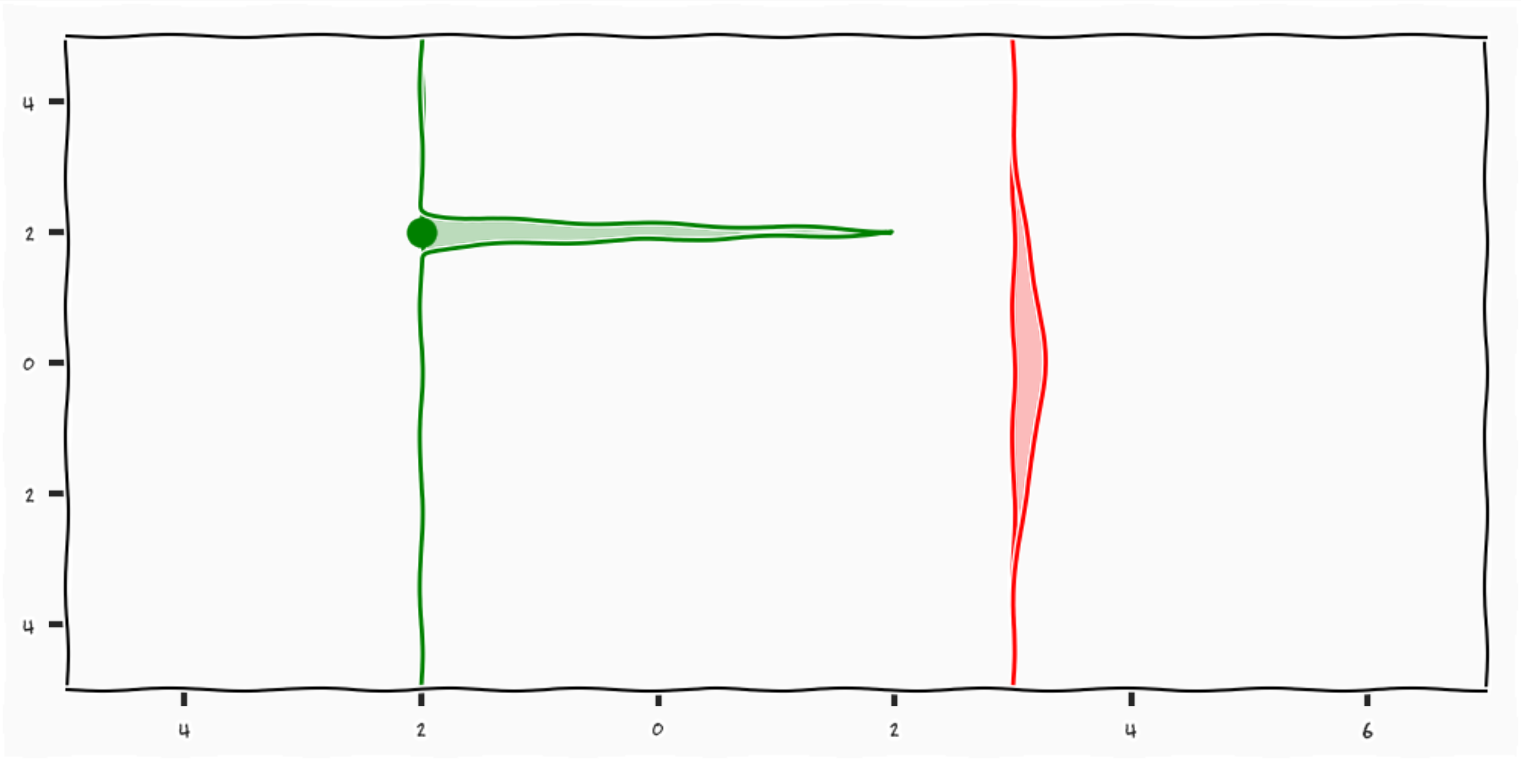

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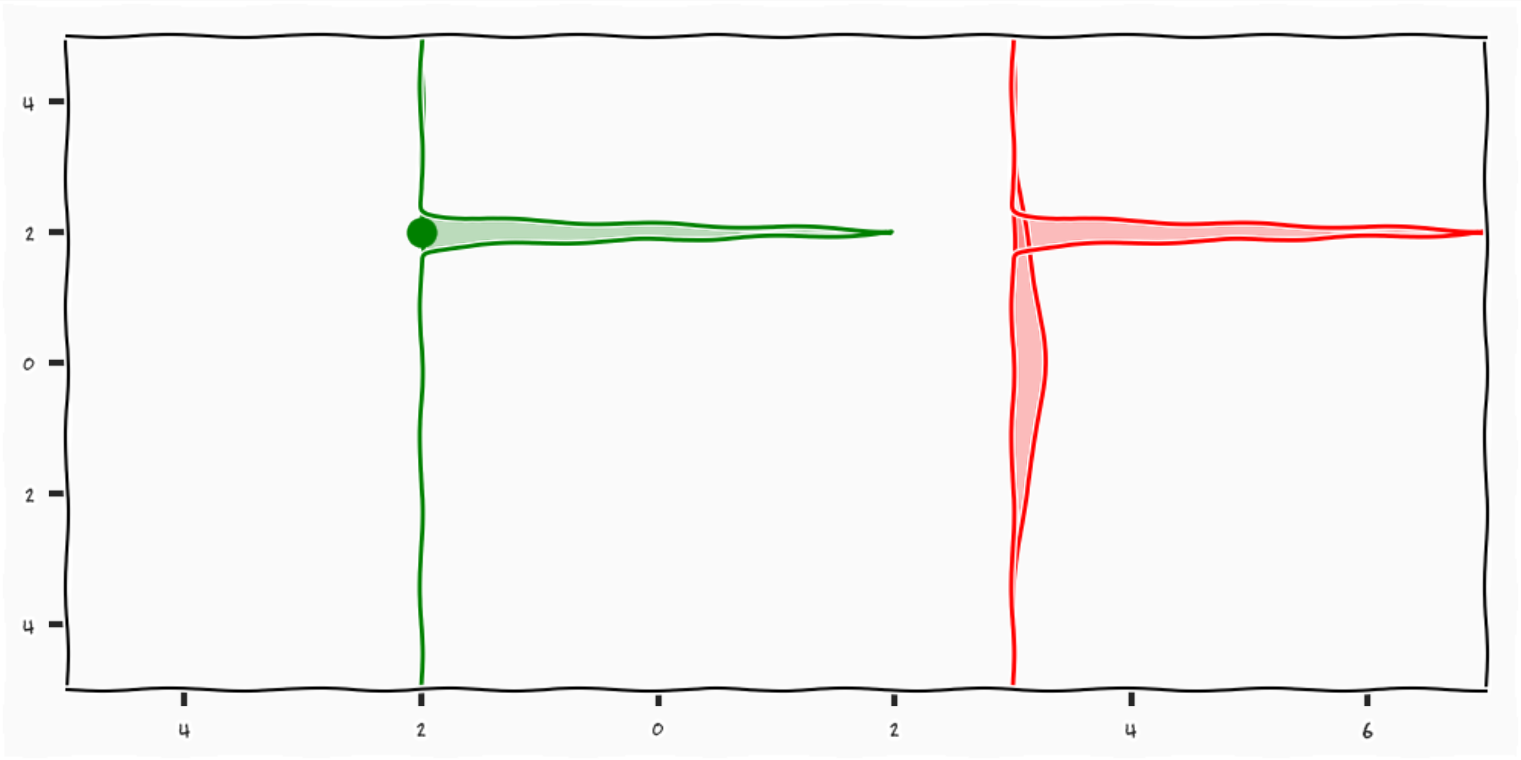

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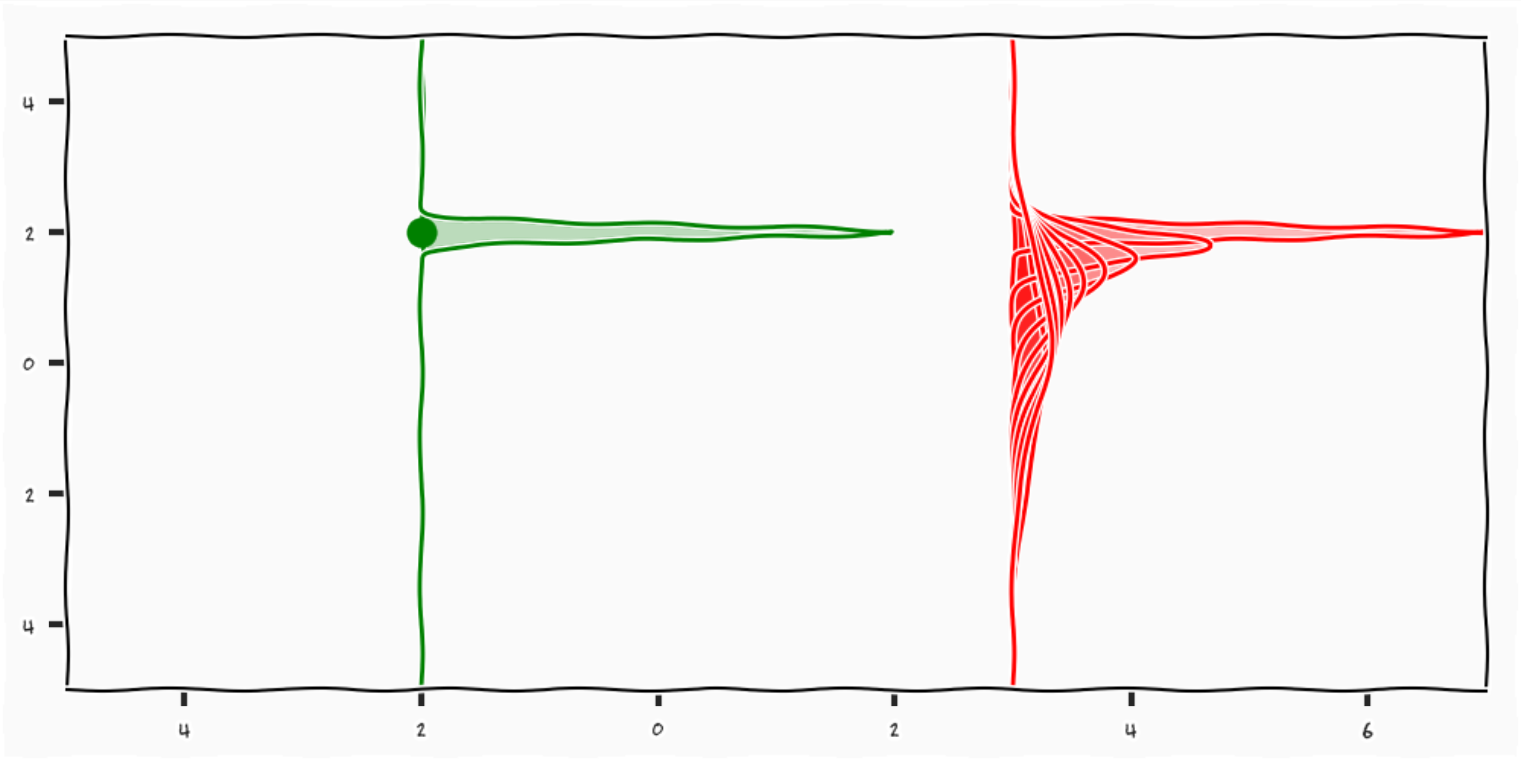
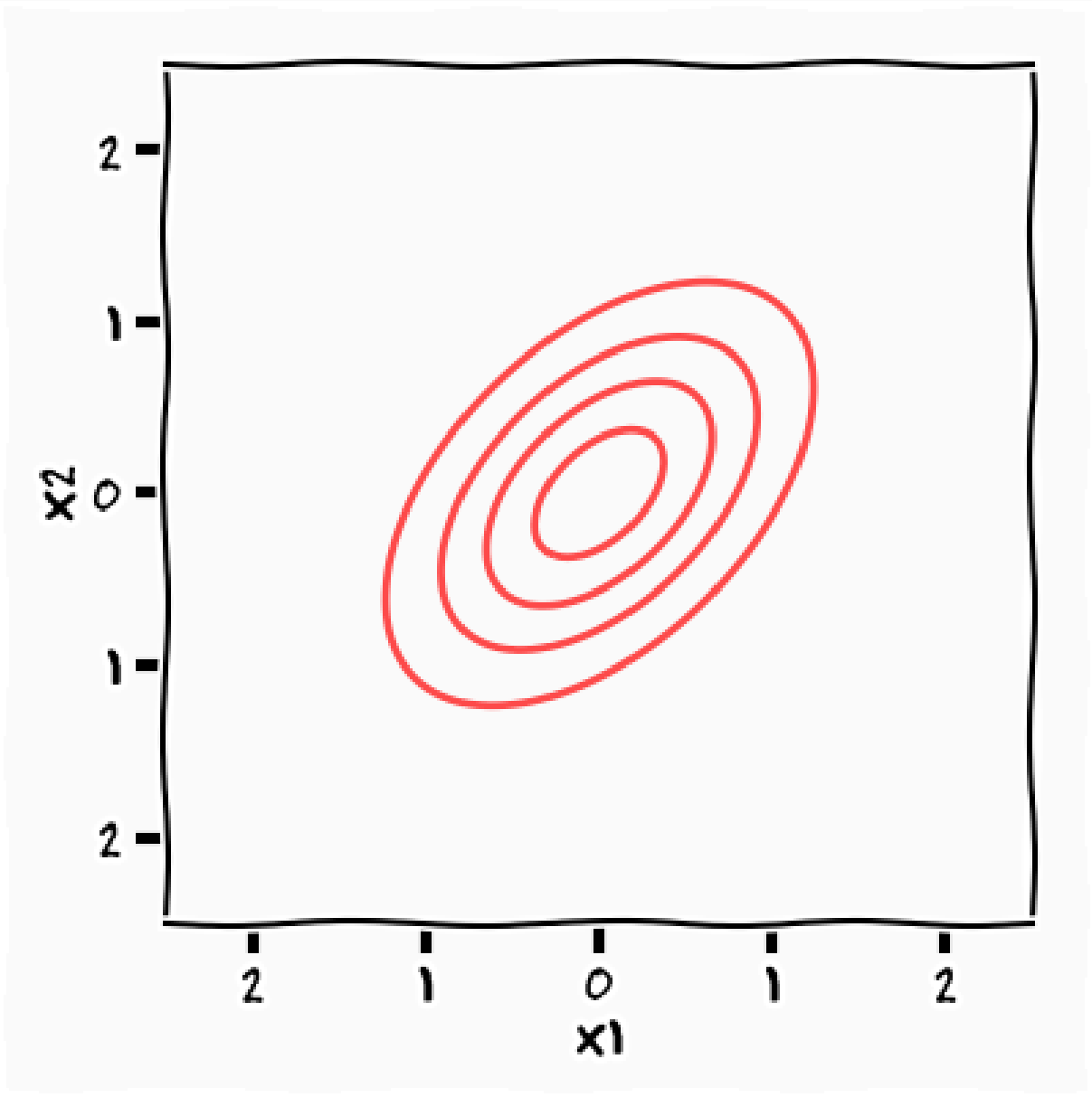


Conditional Gaussians

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

Conditional Gaussians



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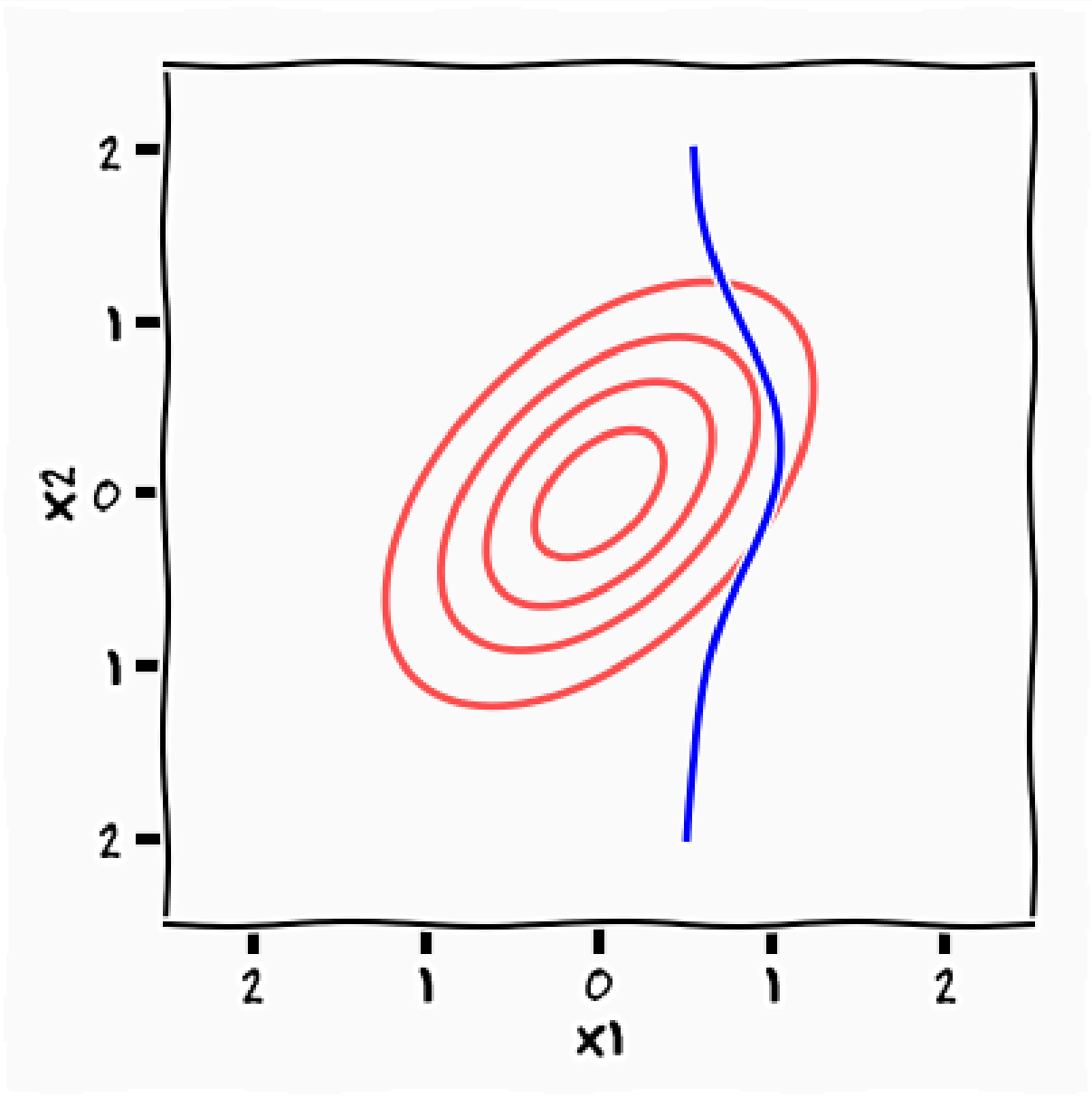

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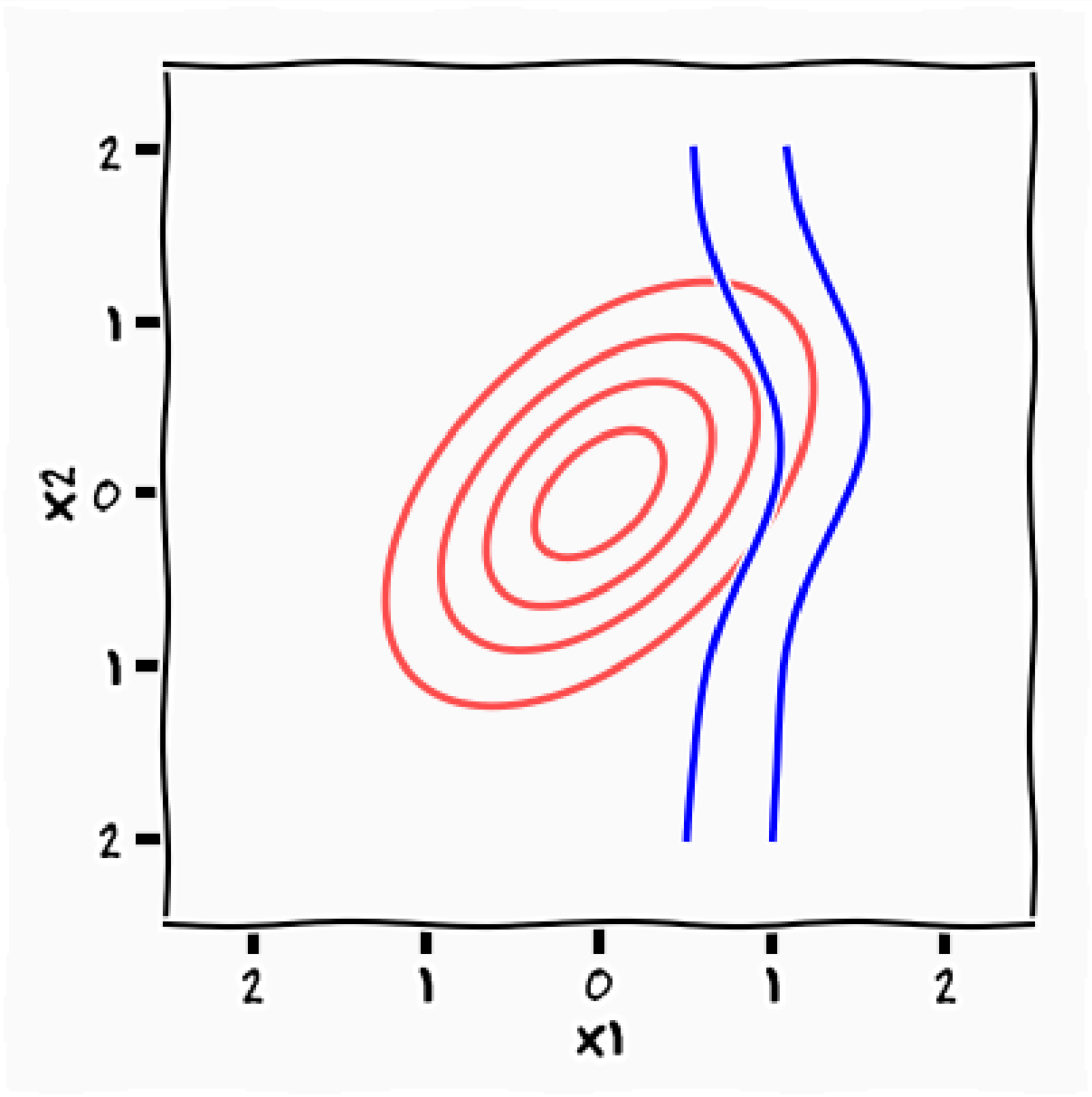

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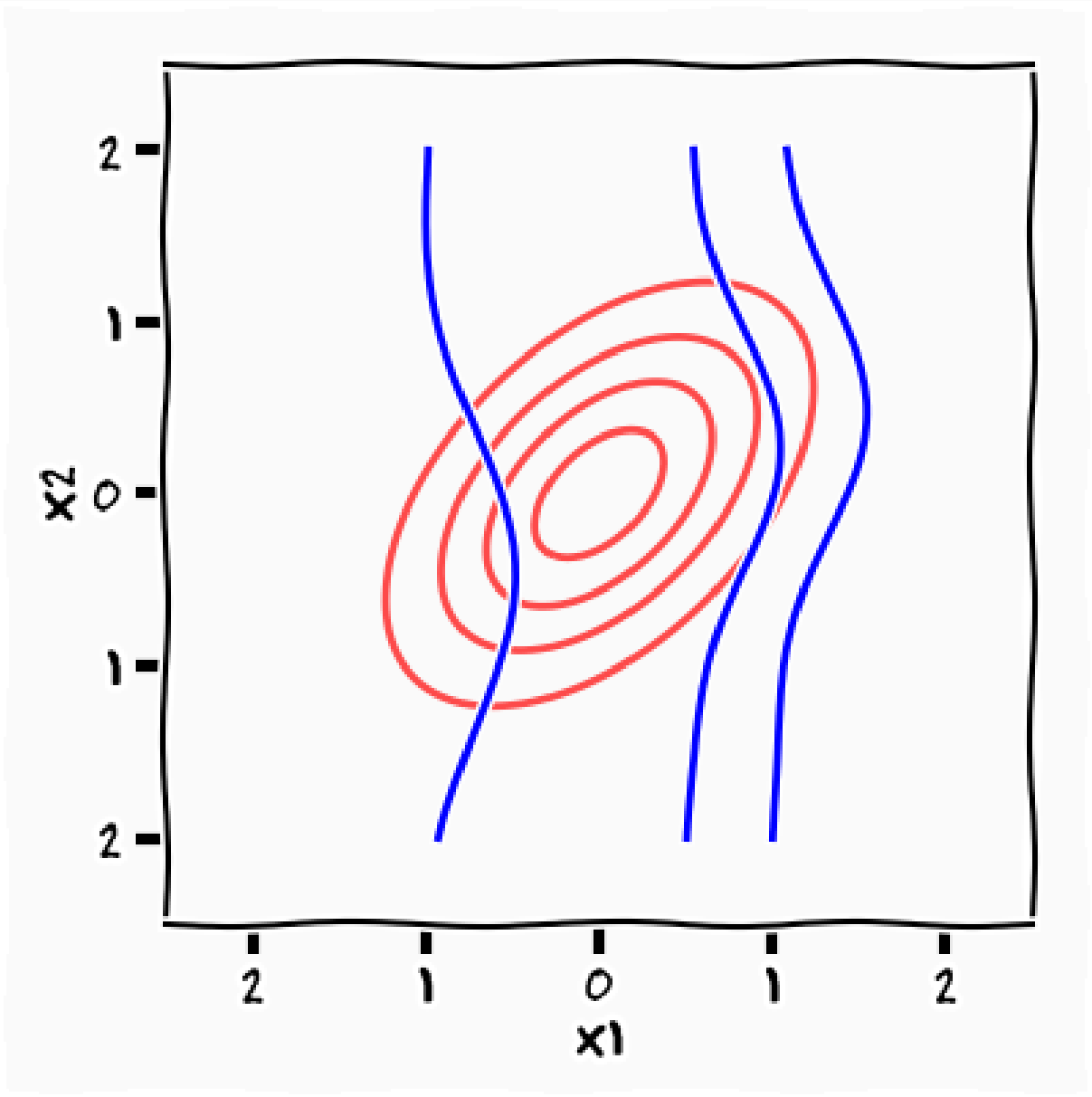

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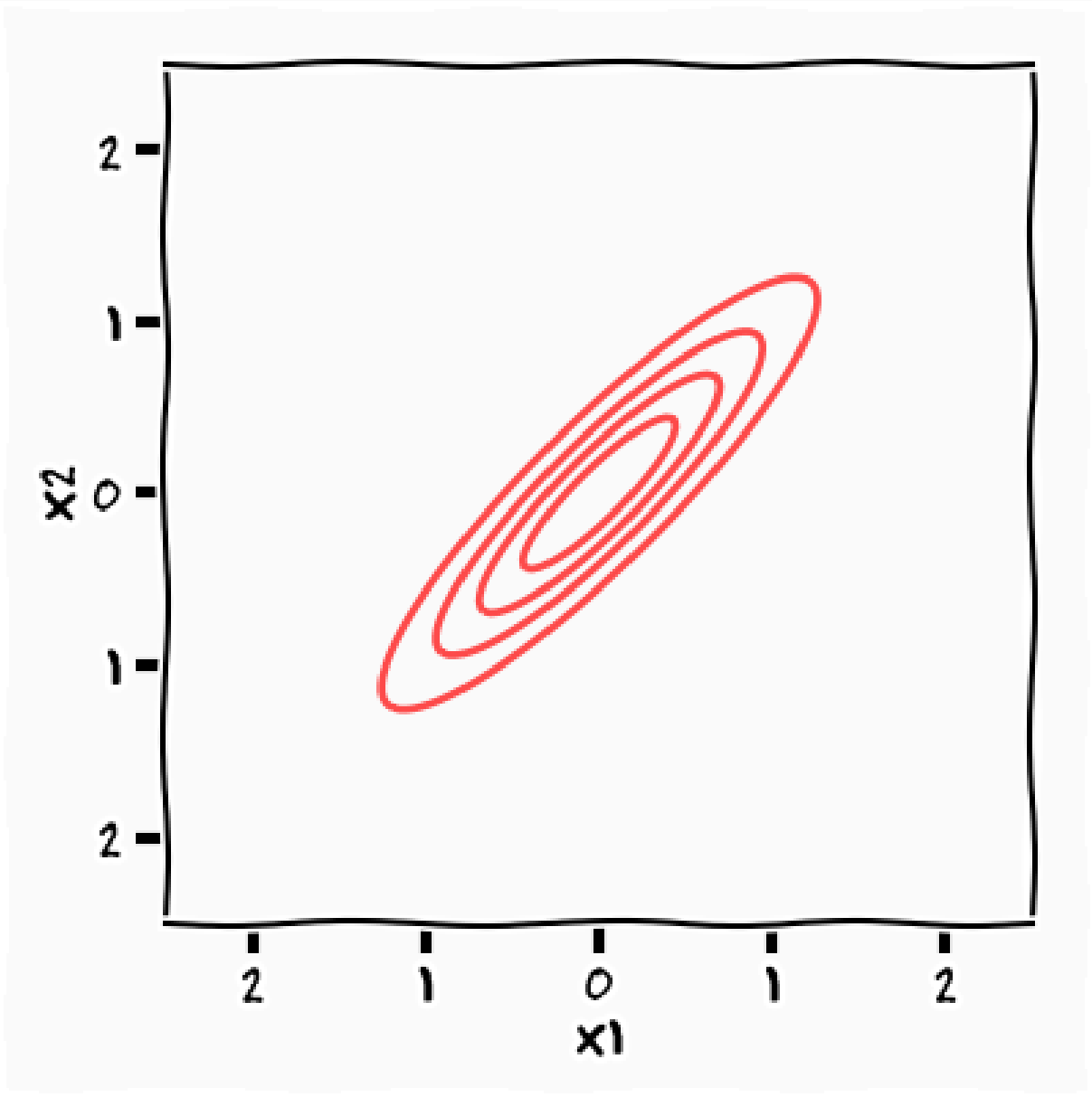

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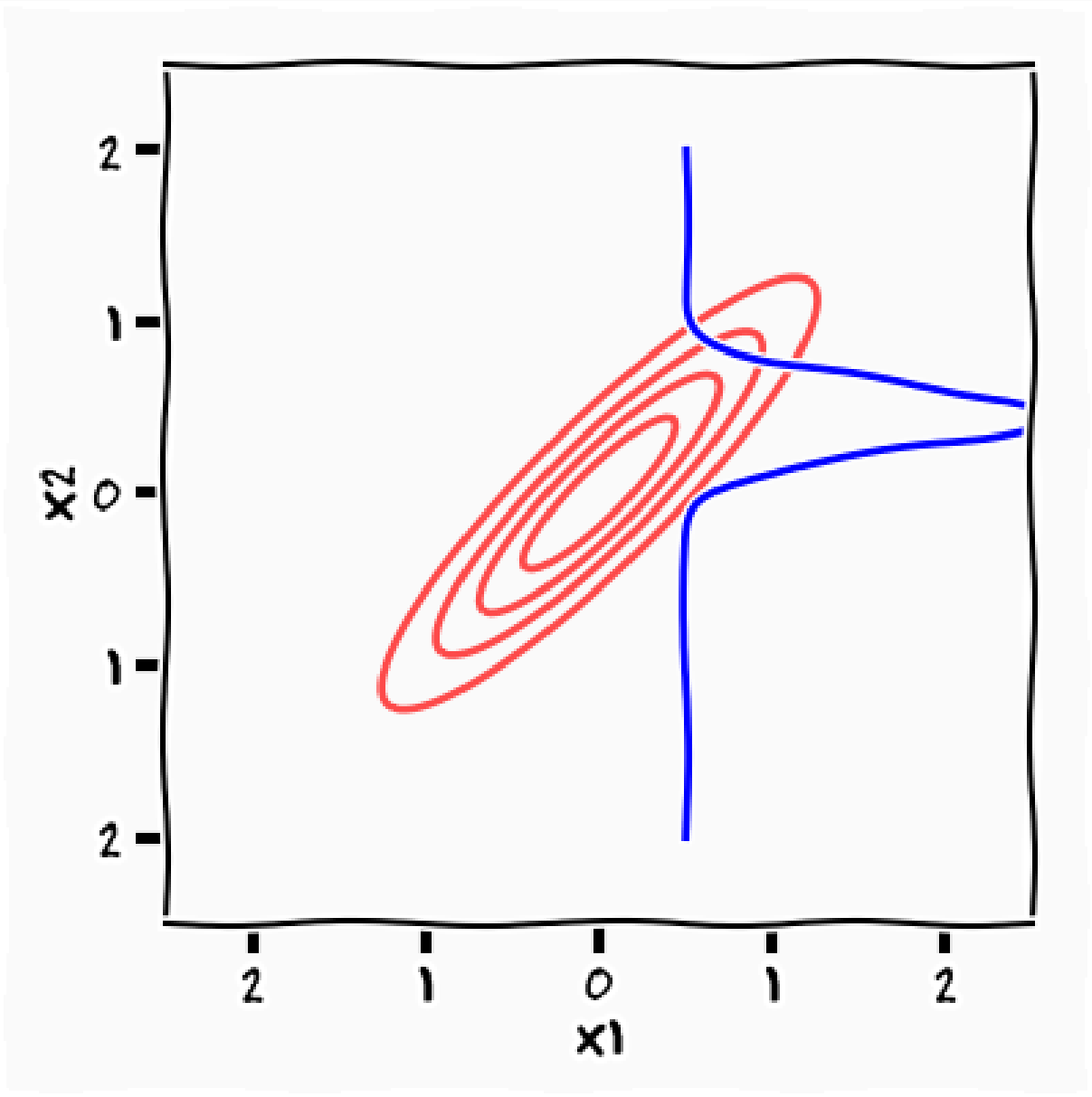

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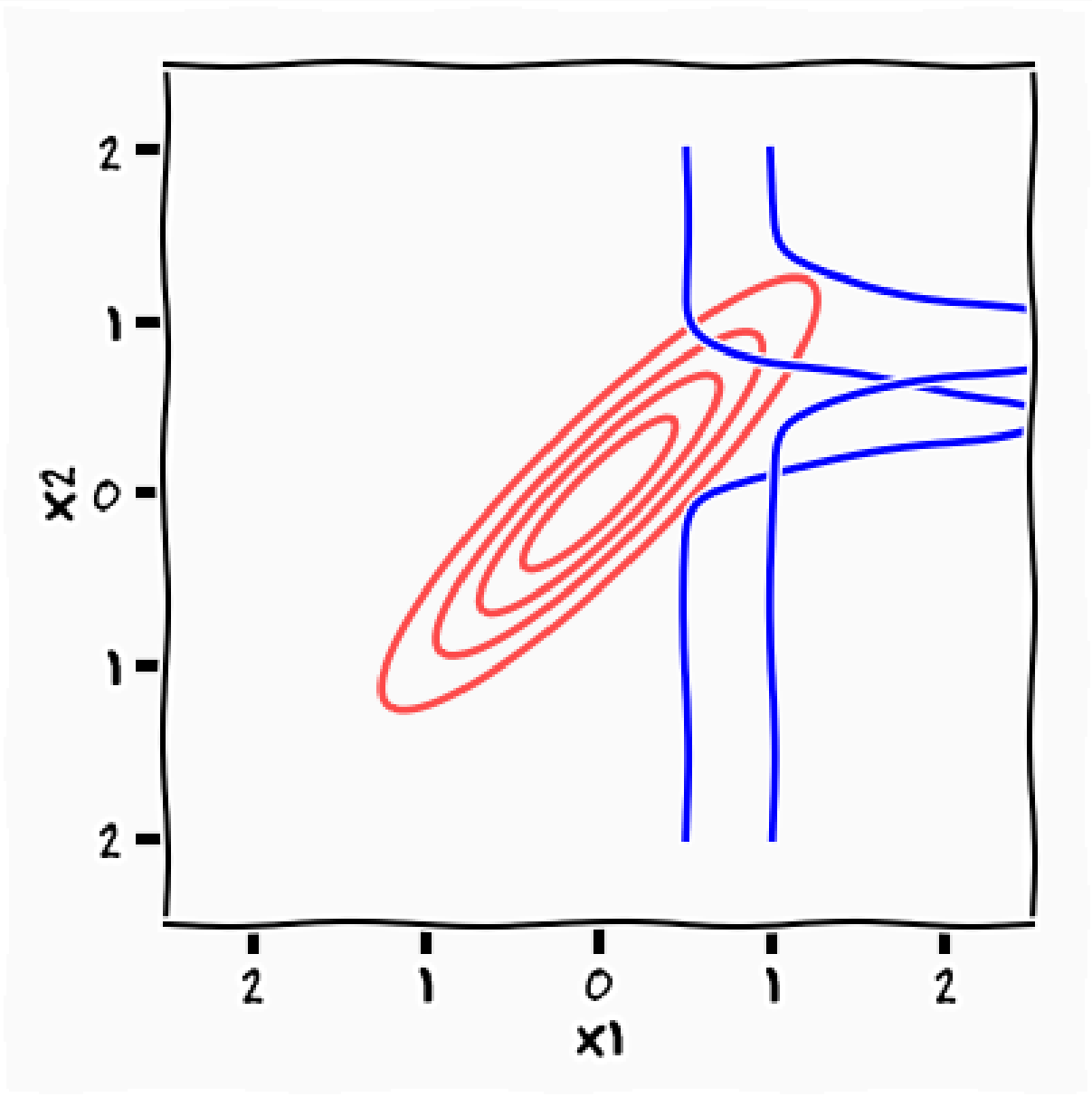

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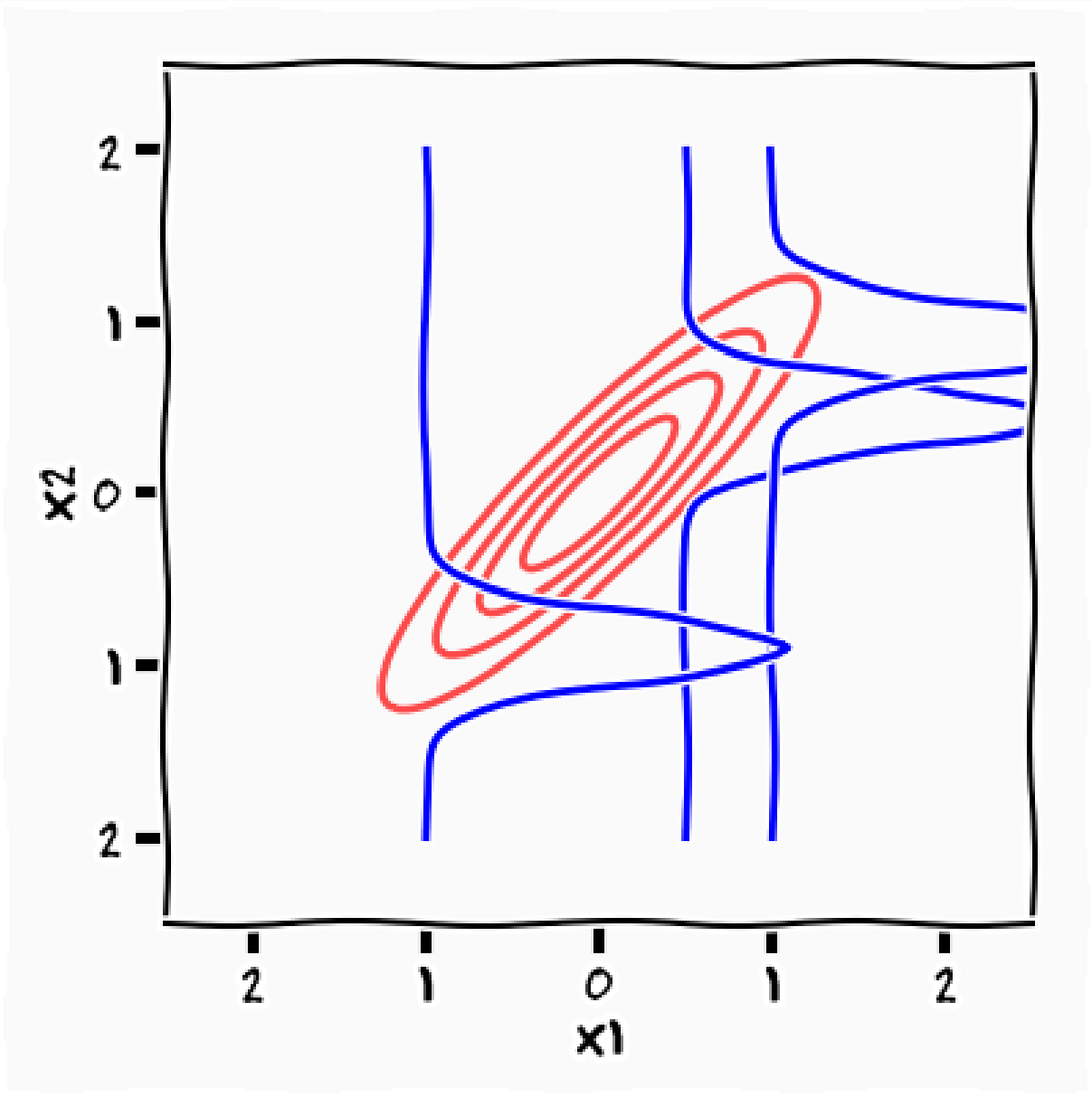

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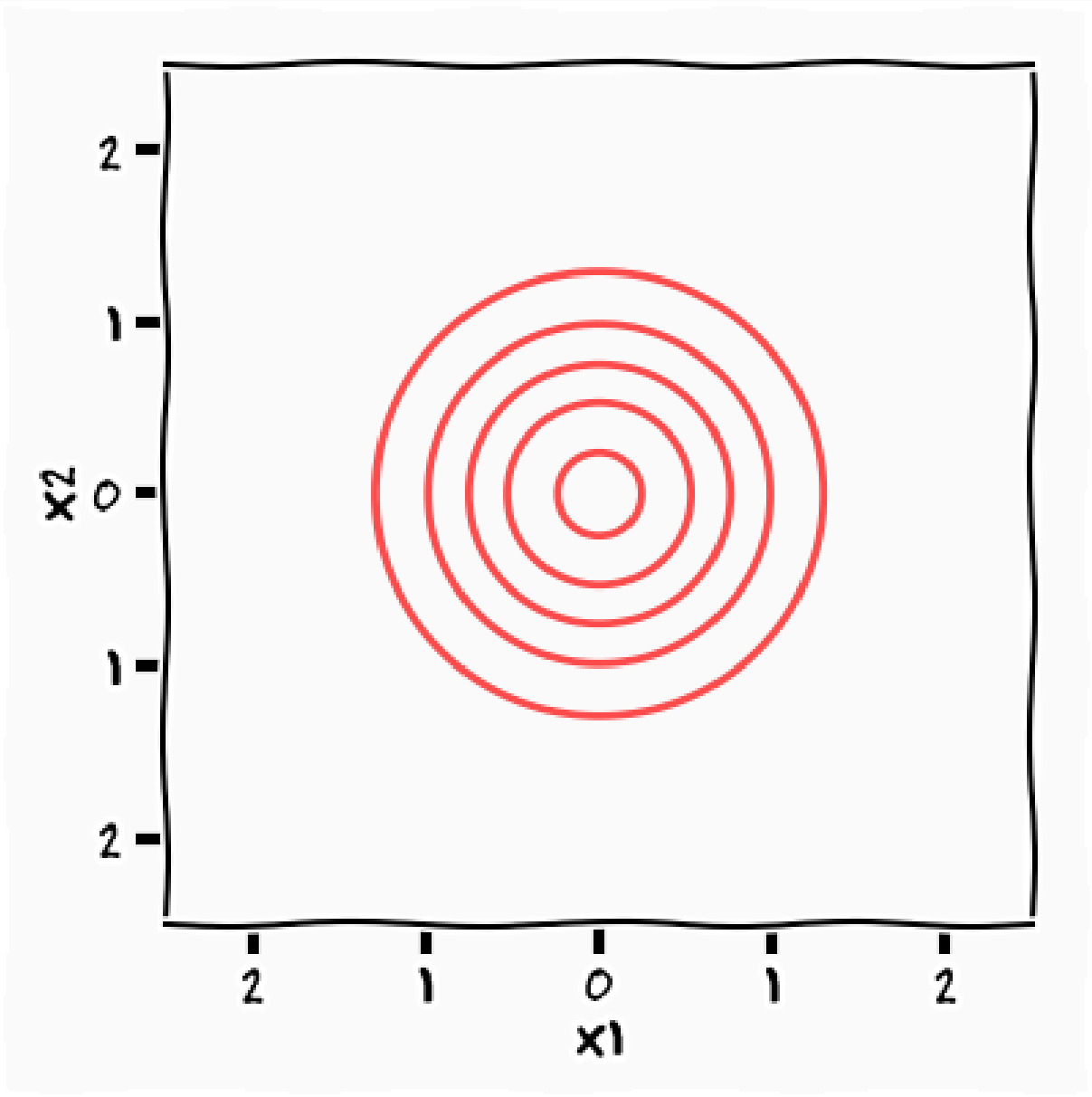

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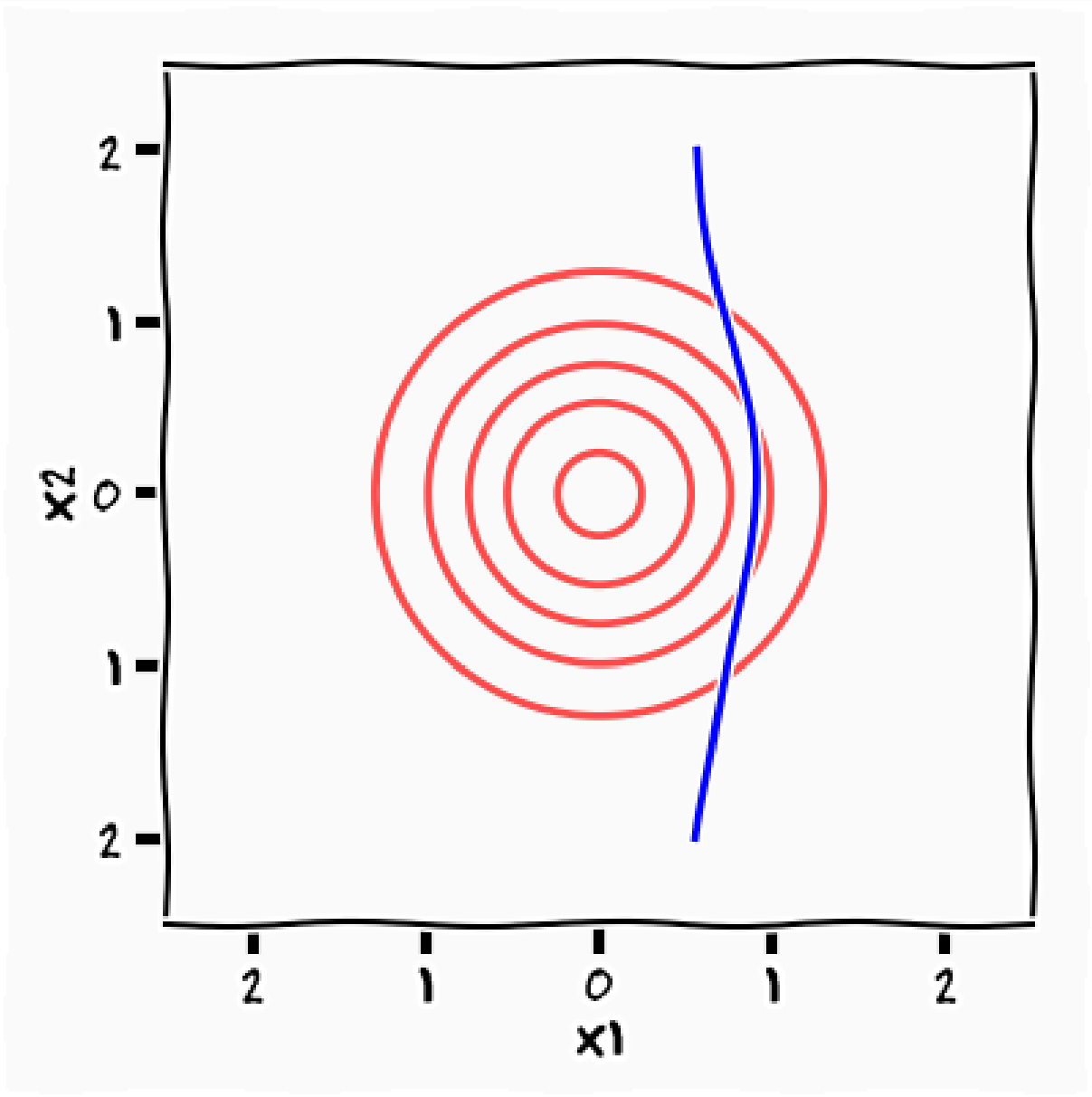

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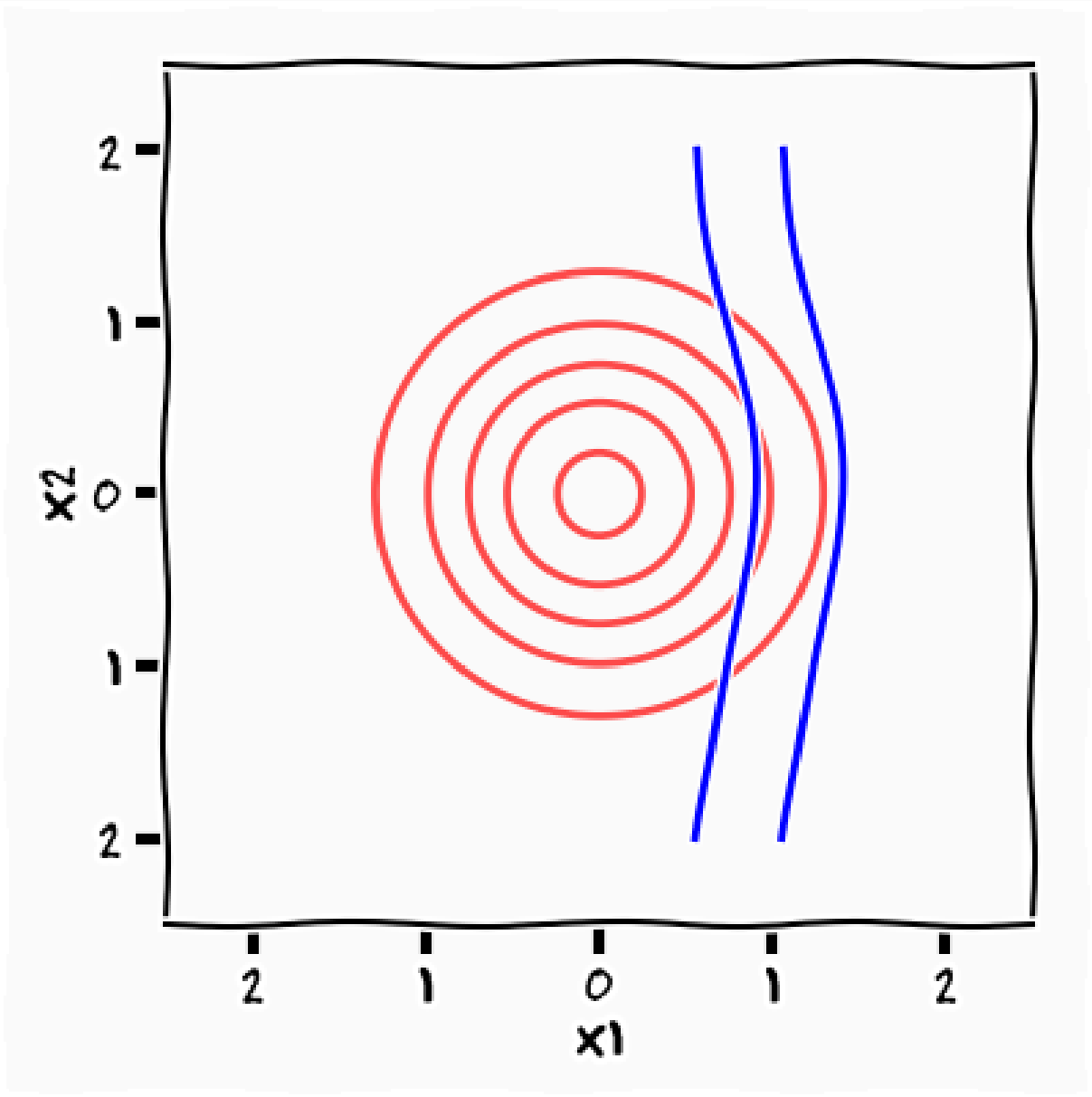

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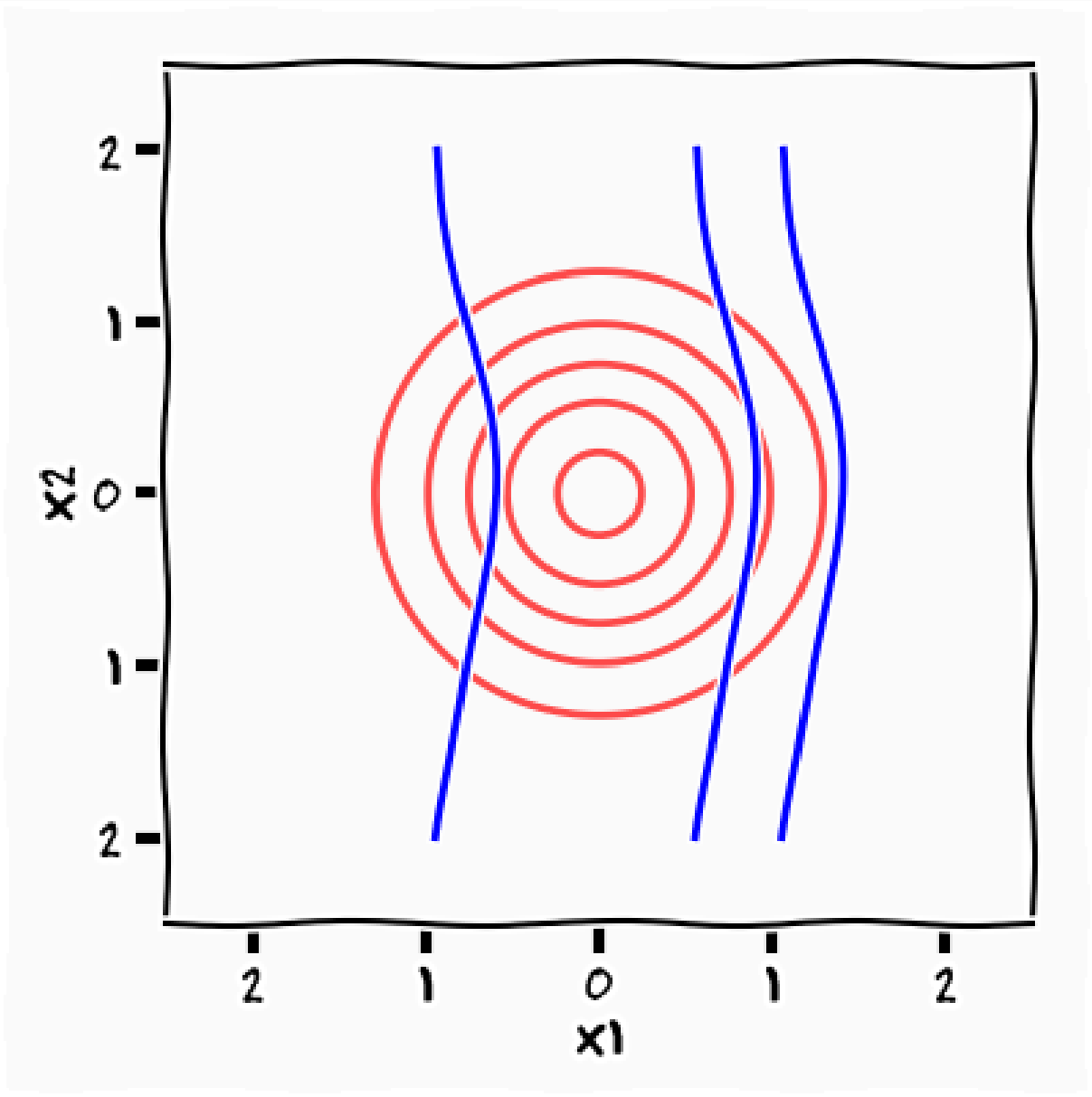

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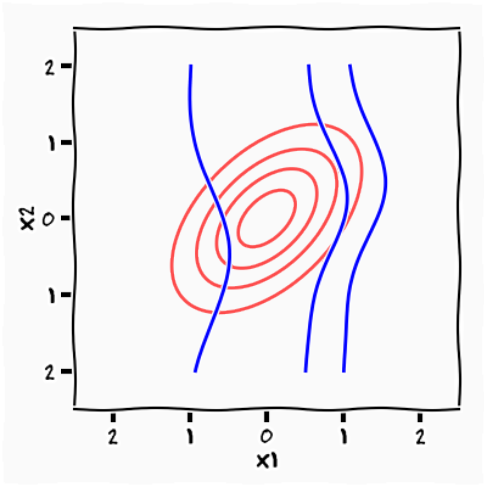

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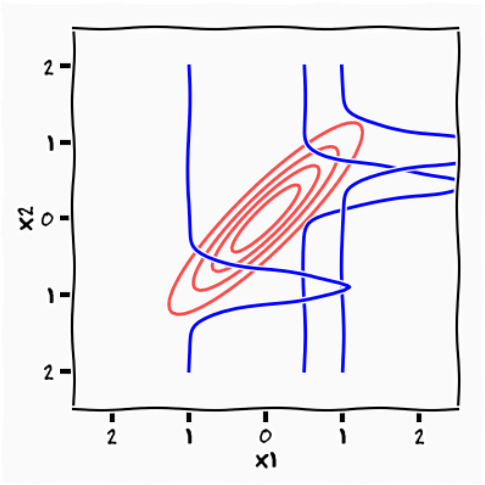

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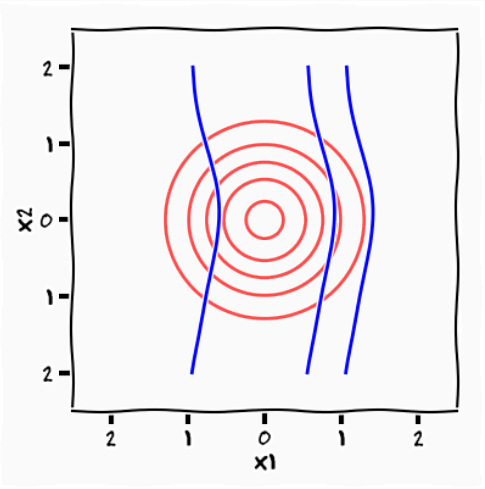

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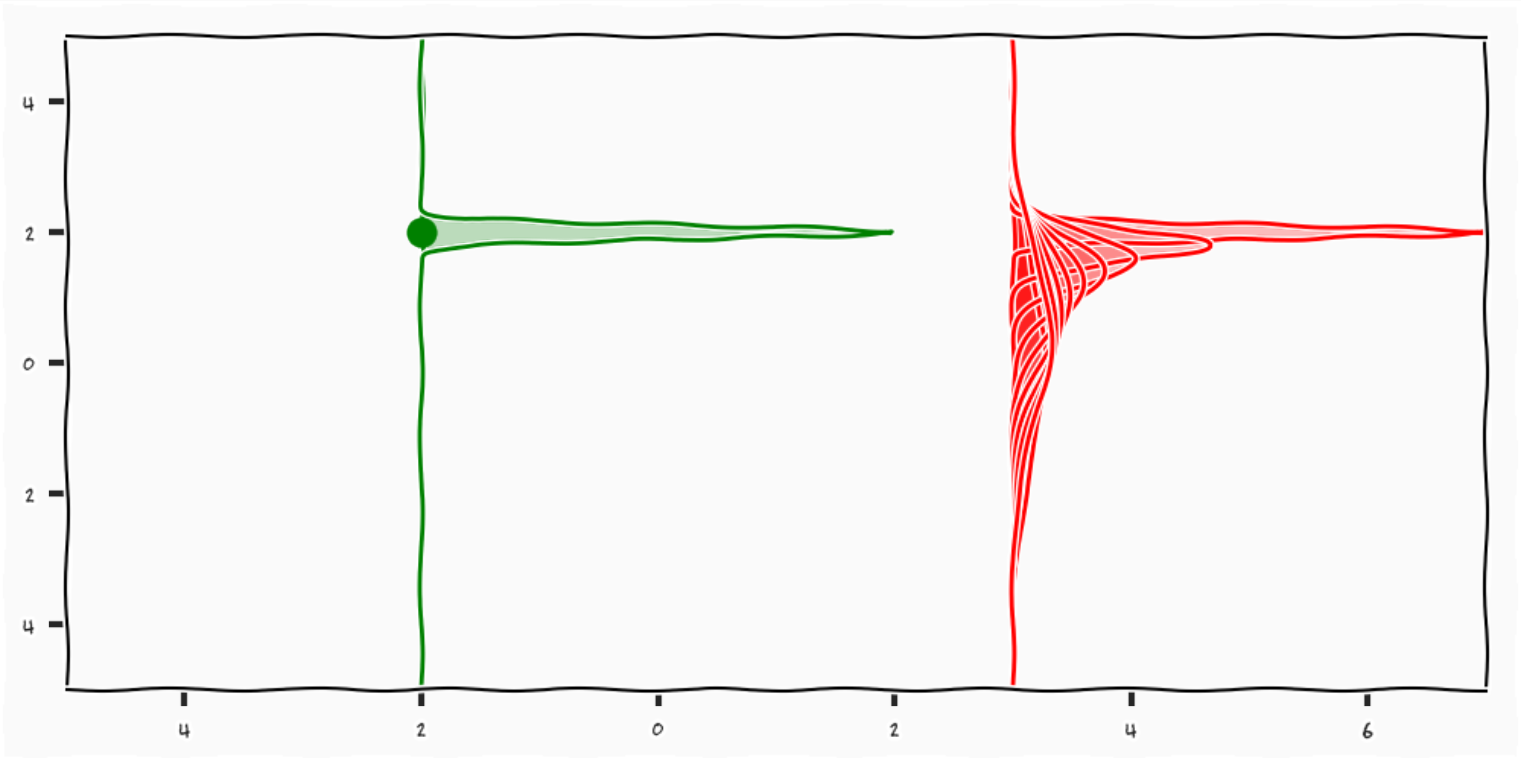
Gaussian Processes



Gaussian Processes [1] Ch 6.4.2

$$p(\mathbf{f}|\mathbf{x}, \boldsymbol{\theta}) \sim \mathcal{GP}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x}))$$

Definition (Gaussian Process)

A Gaussian Process is an infinite collection of random variables who any subset is jointly gaussian. The process is specified by a mean function $\mu(\cdot)$ and a co-variance function $k(\cdot, \cdot)$

Gaussian Marginal

$$p(f_1, f_2, \ldots, f_N, \ldots | \mathbf{x}, \boldsymbol{\theta}) = \mathcal{GP}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x}))$$

$$= \mathcal{N}\left(\begin{bmatrix} \mu(x_1) \\ \mu(x_2) \\ \vdots \\ \mu(x_N) \\ \vdots \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \cdots & k(x_1, x_N) & \cdots \\ k(x_2, x_1) & k(x_2, x_2) & \cdots & k(x_2, x_N) & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ k(x_N, x_1) & k(x_N, x_2) & \cdots & k(x_N, x_N) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \right)$$

Gaussian Processes

$$
\begin{aligned}
p(\mathbf{f}|\mathbf{x}, \boldsymbol{\theta}) &\sim \mathcal{GP}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x})) \\
\mathbf{y}_i &= f_i + \boldsymbol{\epsilon} \\
\boldsymbol{\epsilon} &\sim \mathcal{N}(\mathbf{0}, \sigma^2 \boldsymbol{I}) \\
p(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}) &= \int p(\mathbf{y}|\mathbf{f}) p(\mathbf{f}|\mathbf{x}, \boldsymbol{\theta}) \mathrm{d}f
\end{aligned}
$$

$\mathcal{GP}$ is infinite, but we only observe finite amount of data. This means conditioning on a subset of the data, the $\mathcal{GP}$ is a just a Gaussian distribution

Uncertainty over functions

- Regression model,

$$\mathbf{y}_i = f(\mathbf{x}_i) + \boldsymbol{\epsilon}$$
$$\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \boldsymbol{I})$$

- Introduce f_i as *instantiation* of function at location x_i

$$f_i = f(\mathbf{x}_i),$$

- as a new random variable.
- now we have a "handle" to specify our assumptions over

Uncertainty over functions

Joint

$$p(\mathbf{y}, \mathbf{f}|\mathbf{x}, \boldsymbol{\theta}) = p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{x}, \boldsymbol{\theta})$$

Prior

$$p(\mathbf{f}|\mathbf{x}, \boldsymbol{\theta}),$$

Likelihood

$$p(\mathbf{y}|\mathbf{f}) = \prod_{i}^{N} p(y_i|f_i)$$

The Mean Function

- Function of only the input location
- What do I expect the function value to be only accounting for the input location

The Covariance Function

- Function of two input locations
- How should the information from other locations with known function value observations effect my estimate

The Mean Function

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- What do I expect the function value to be only accounting for the input location
- We will assume this to be constant

The Covariance Function

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- How should the information from other locations with known function value observations effect my estimate

Gaussian Processes

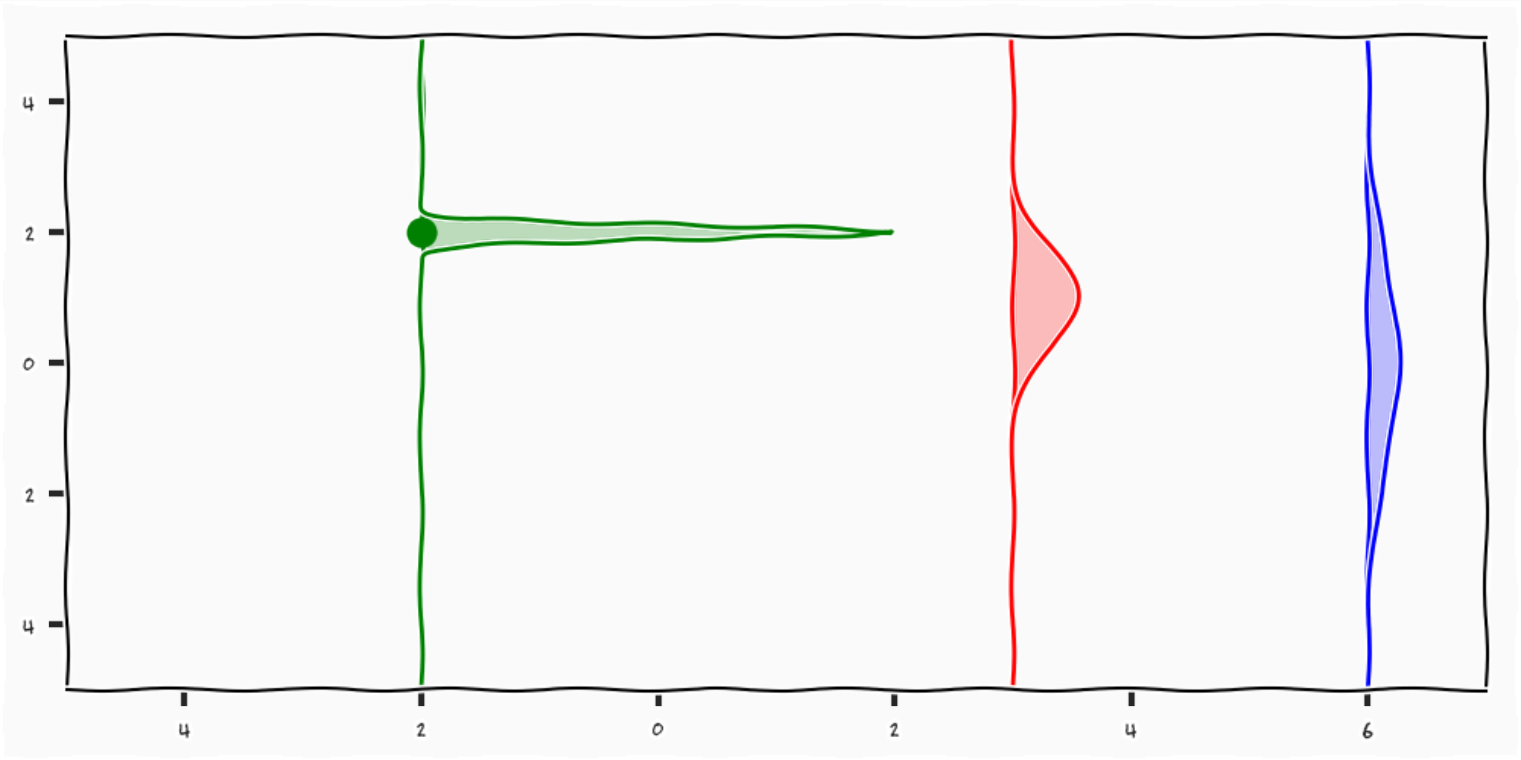
The Mean Function

- Function of only the input location
- What do I expect the function value to be only accounting for the input location
- We will assume this to be constant

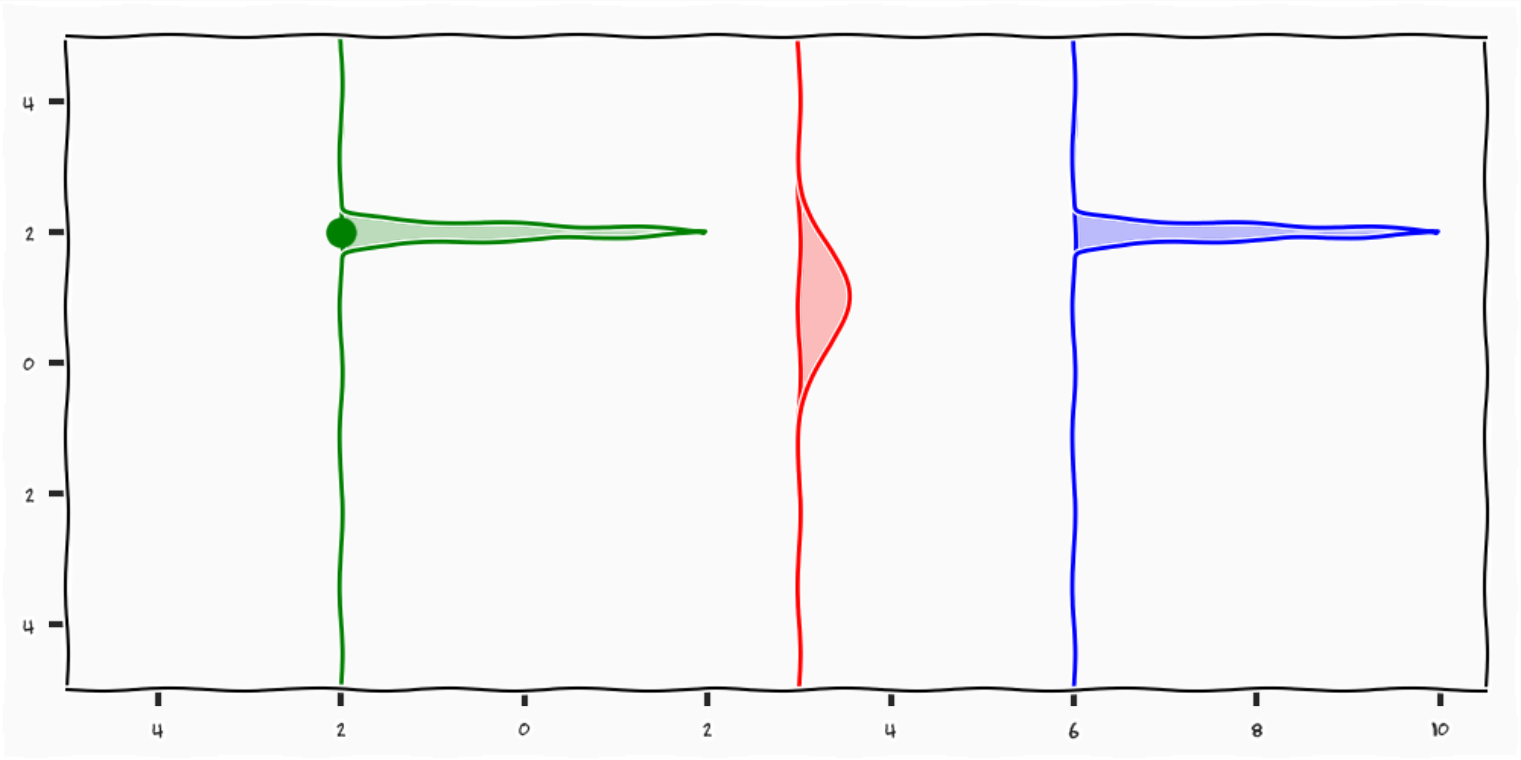
The Covariance Function

- Function of two input locations
- How should the information from other locations with known function value observations effect my estimate
- Encodes the behavior of the function

Gaussian Processes



Gaussian Processes

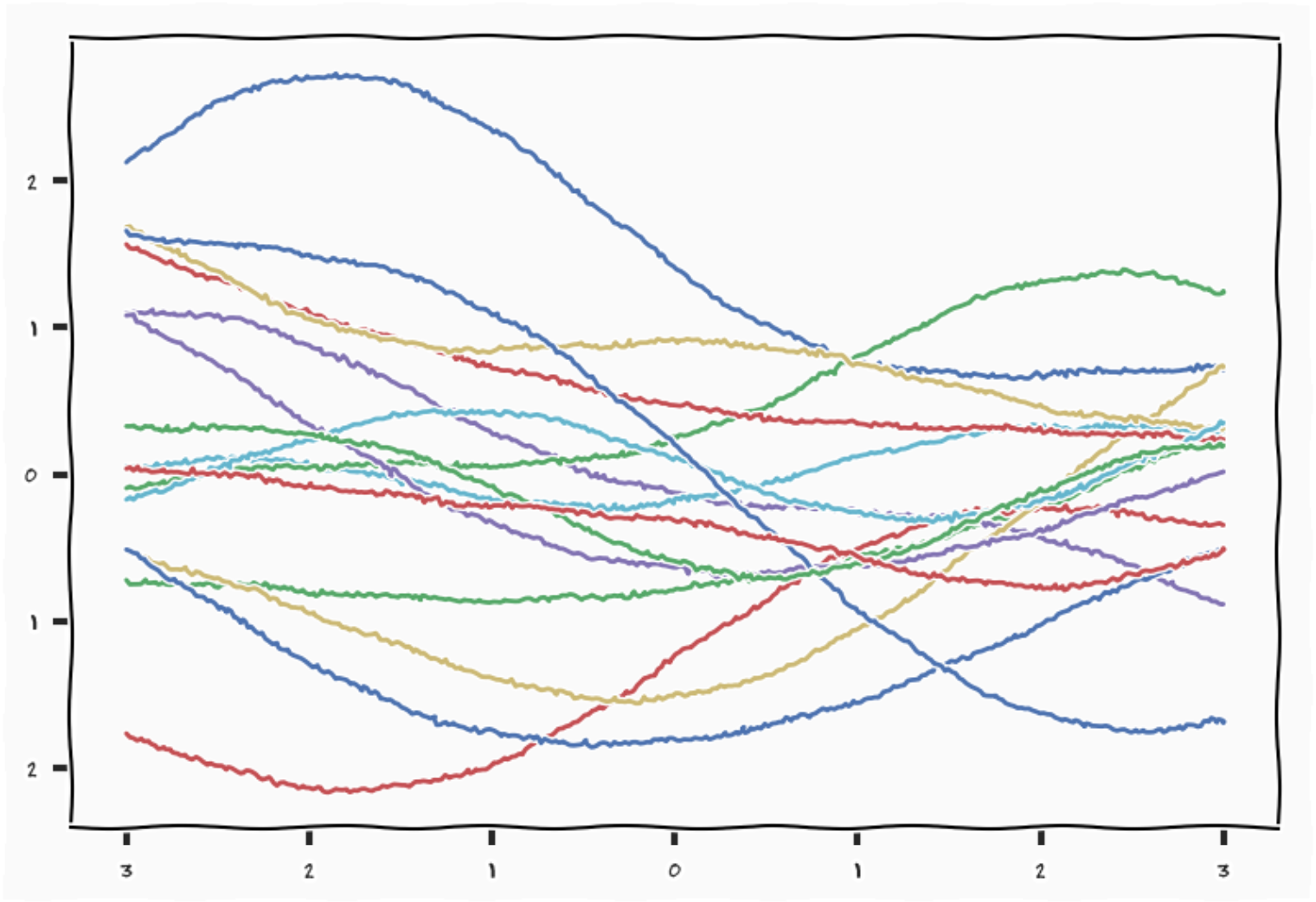


Gaussian Process: Samples

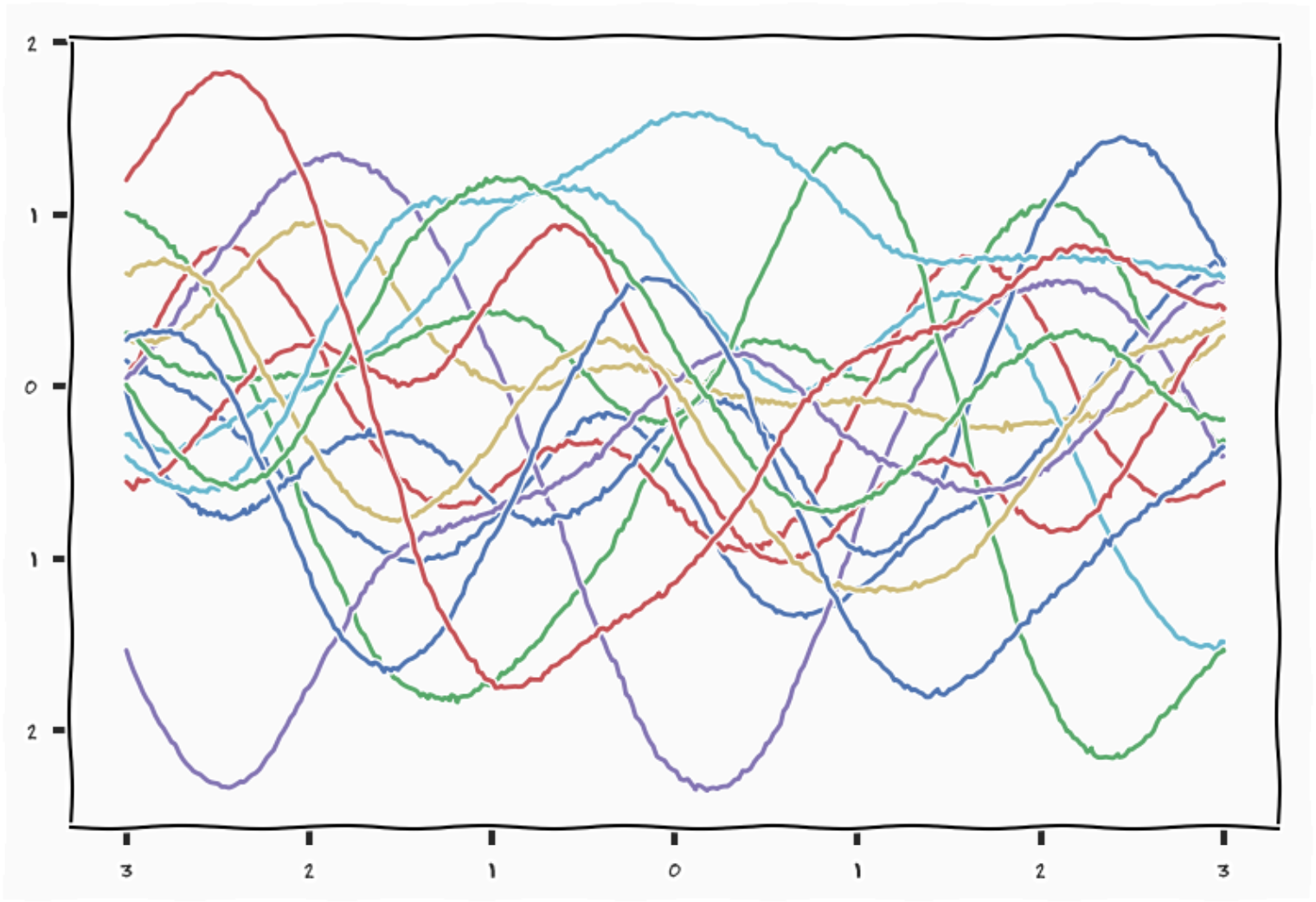
$$p(f_1, f_2, \ldots, f_N, \ldots | \mathbf{x}, \boldsymbol{\theta}) = \mathcal{GP}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x}))$$

$$= \mathcal{N}\left(\begin{bmatrix} \mu(x_1) \\ \mu(x_2) \\ \vdots \\ \mu(x_N) \\ t \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \cdots & k(x_1, x_N) & \cdots \\ k(x_2, x_1) & k(x_2, x_2) & \cdots & k(x_2, x_N) & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ k(x_N, x_1) & k(x_N, x_2) & \cdots & k(x_N, x_N) & \cdots \end{bmatrix} \right)$$

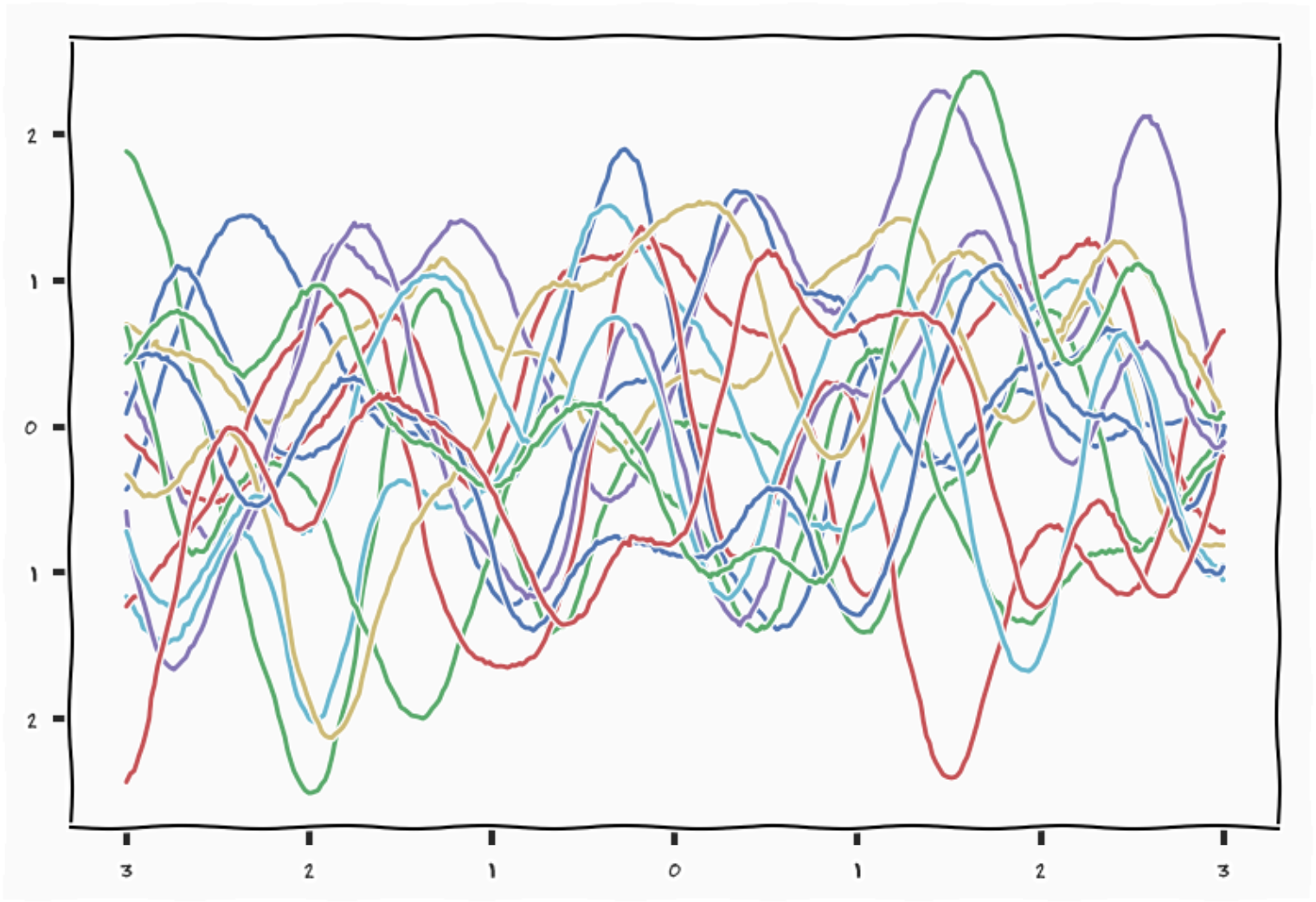
Gaussian Processes: Samples



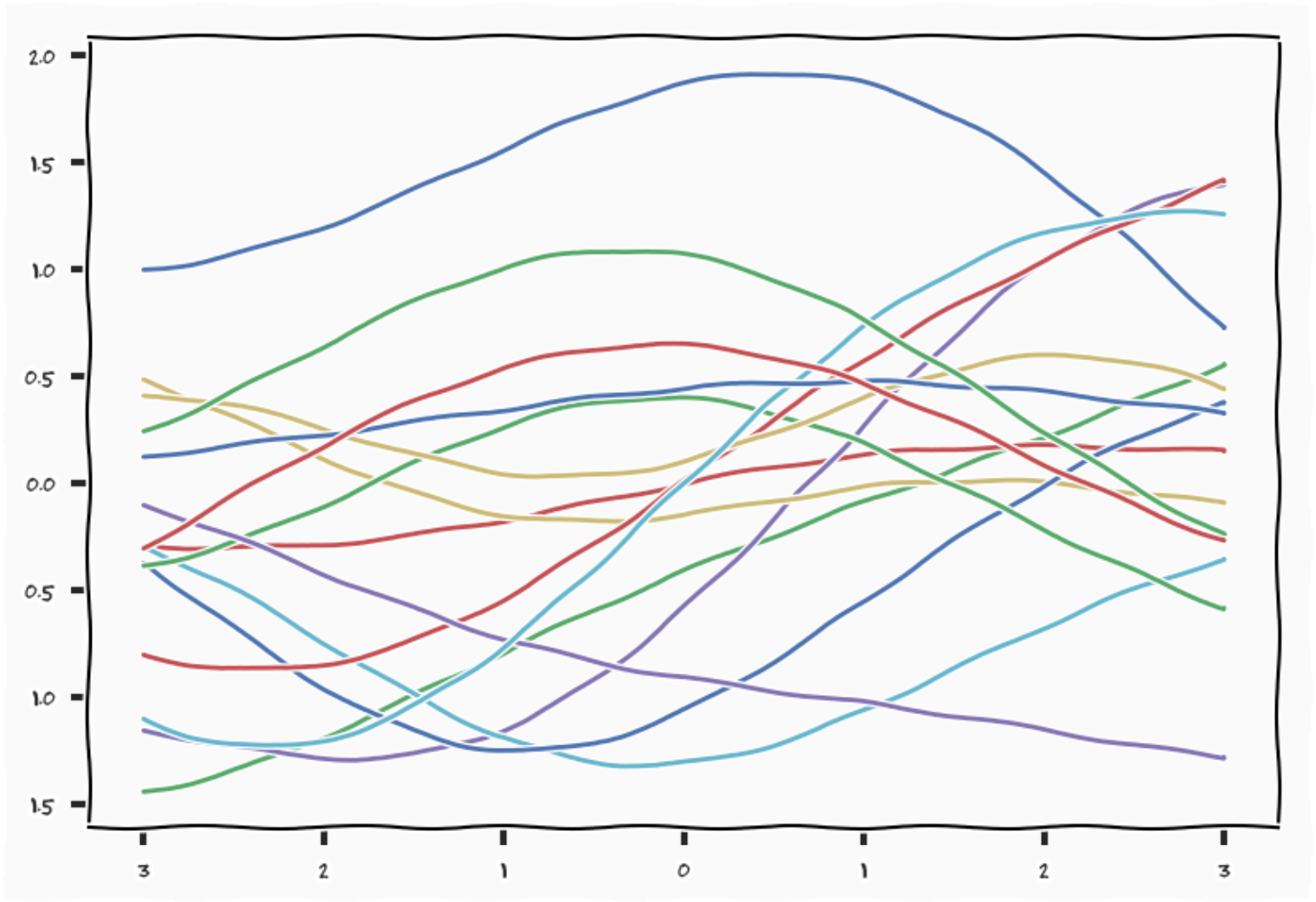
Gaussian Processes: Samples



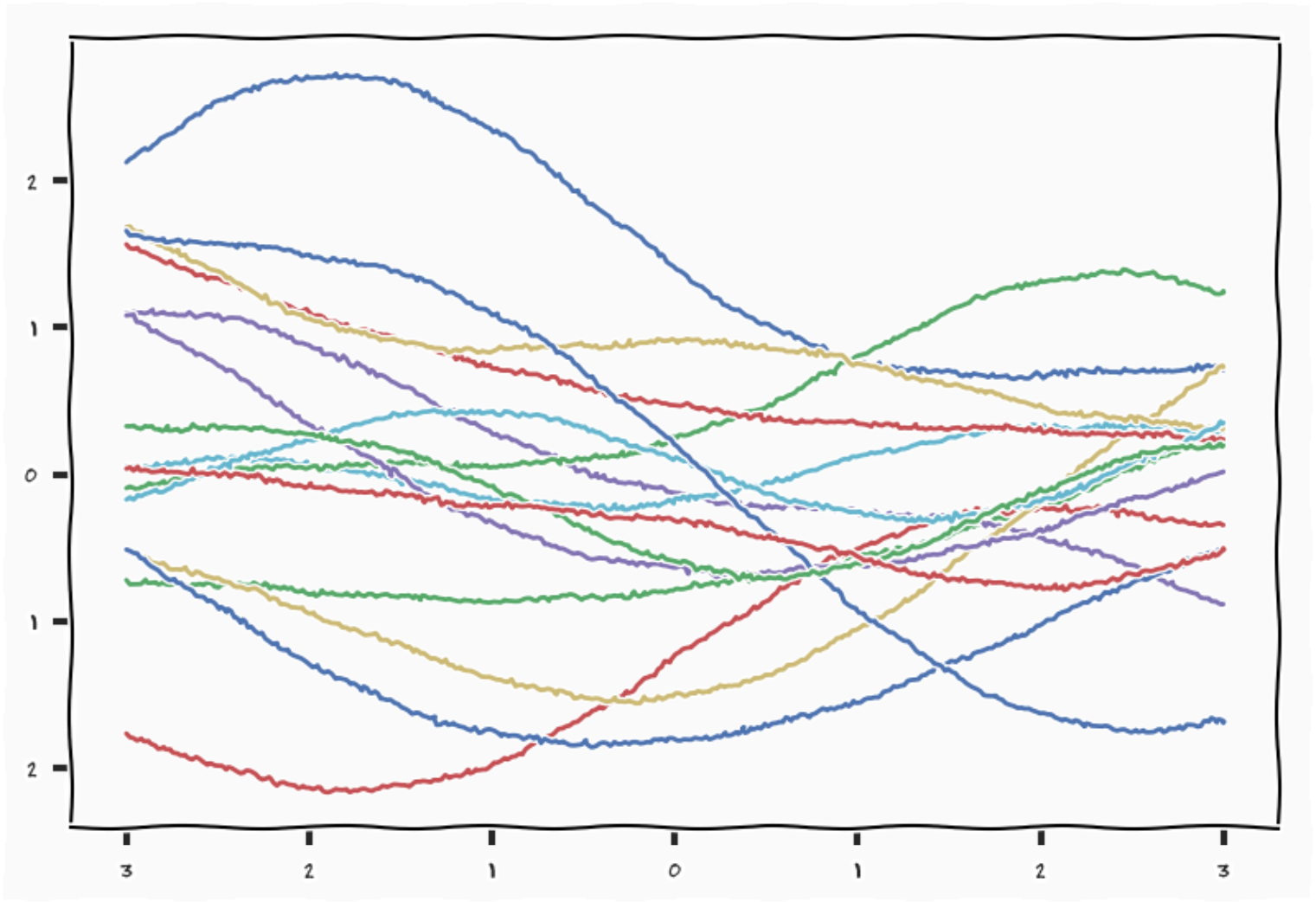
Gaussian Processes: Samples



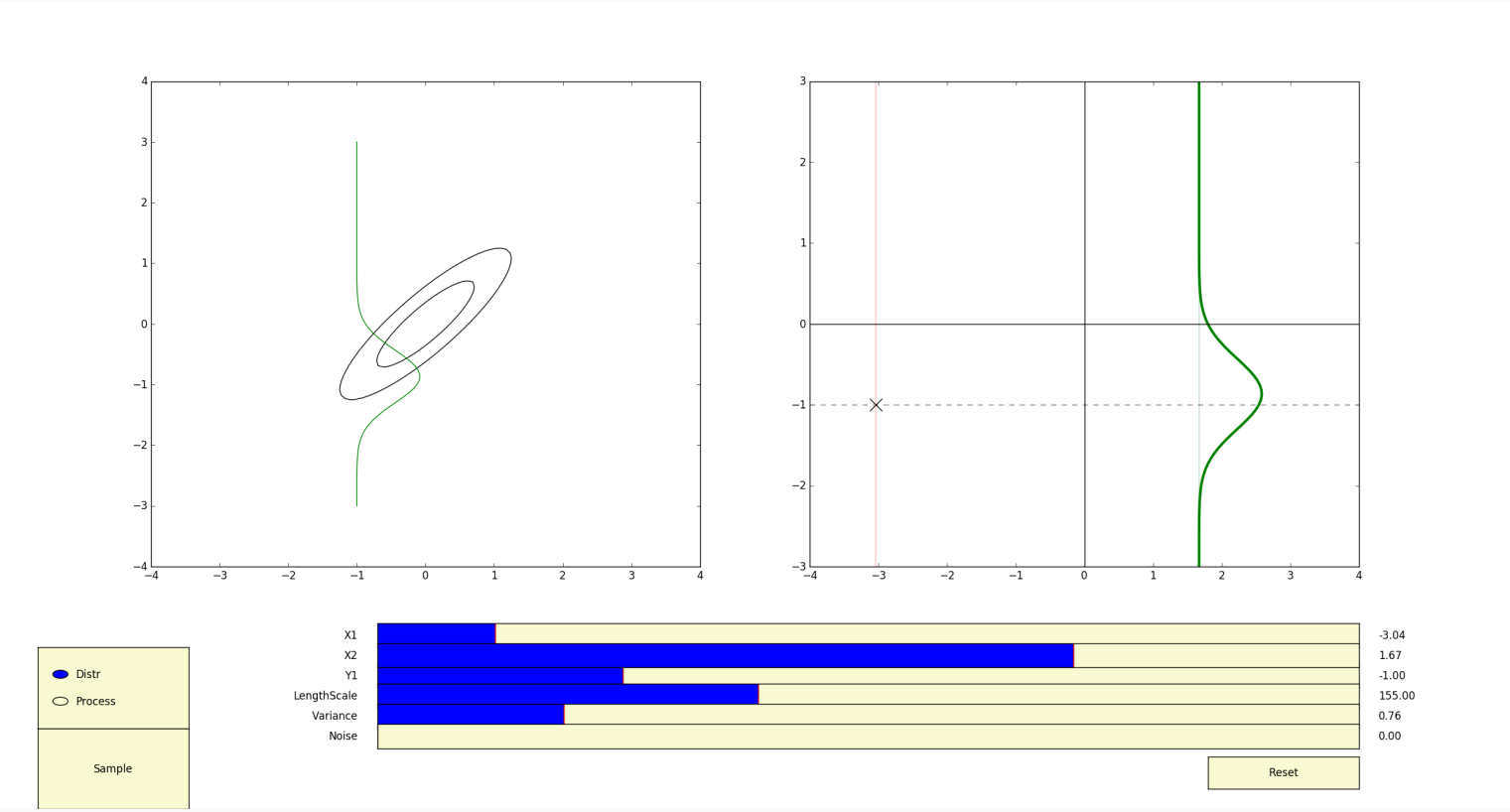
Gaussian Processes: Samples



Gaussian Processes: Samples



Demo


Distr
Process
Sample
X1
X2
Y1
LengthScale
Variance
Noise
-3.04
1.67
-1.00
155.00
0.76
0.00
Reset

Gaussian Process: Posterior

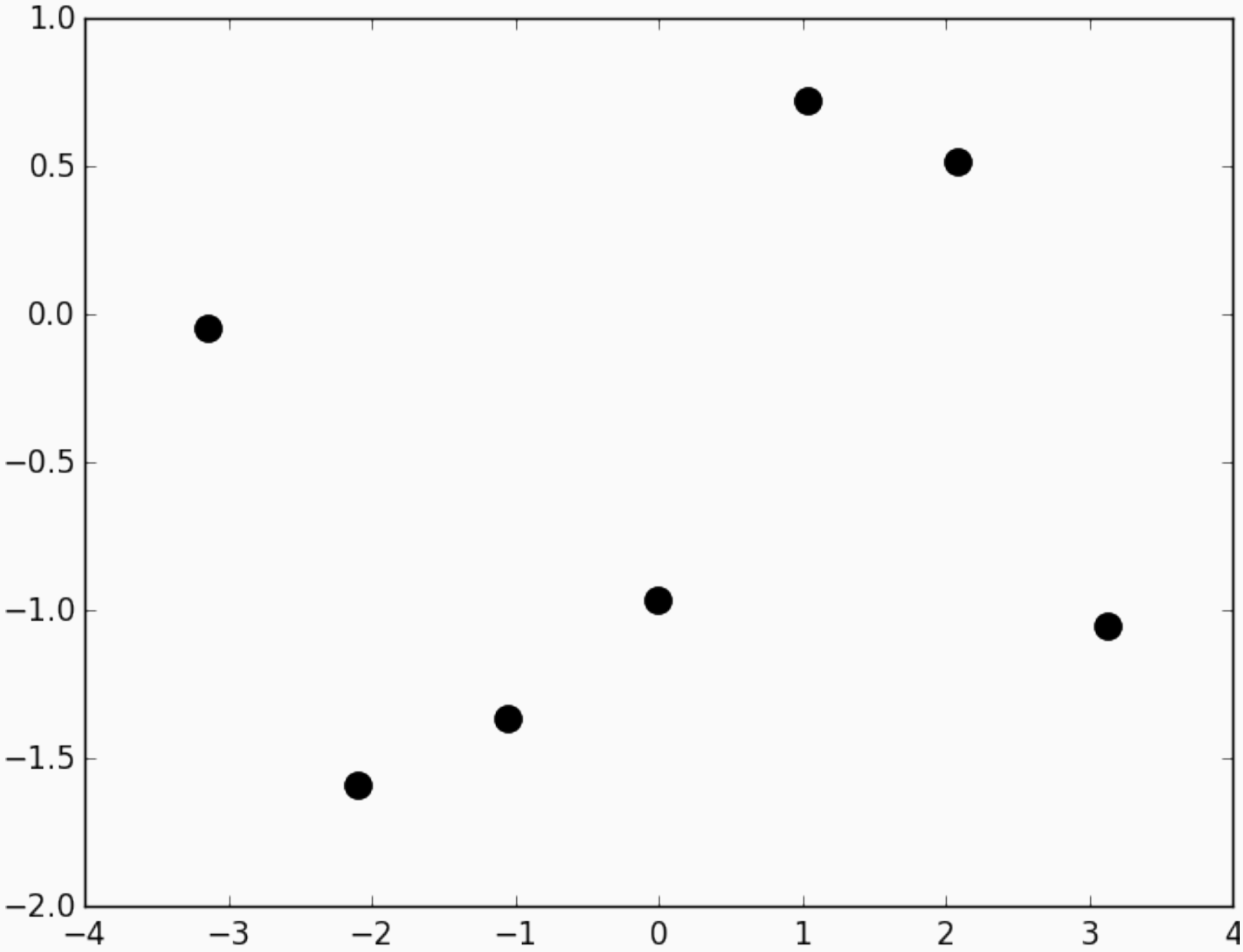
- All instantiations are jointly Gaussian

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

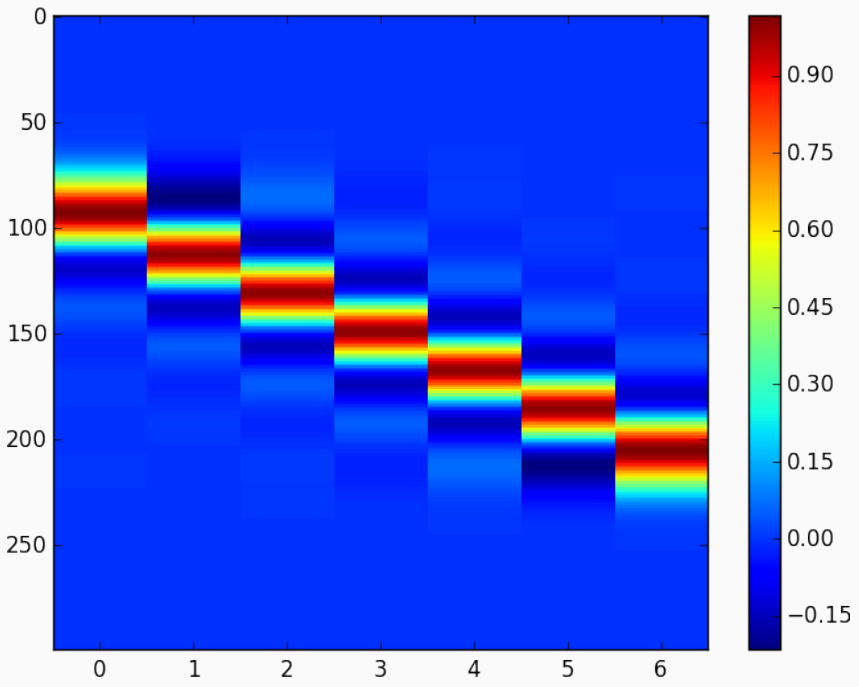
- Conditional Gaussian (same as always)

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

Gaussian Process: Posterior

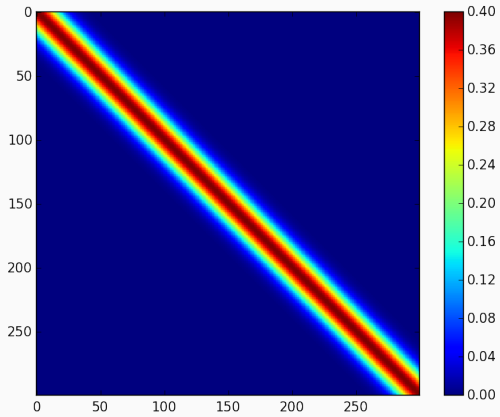


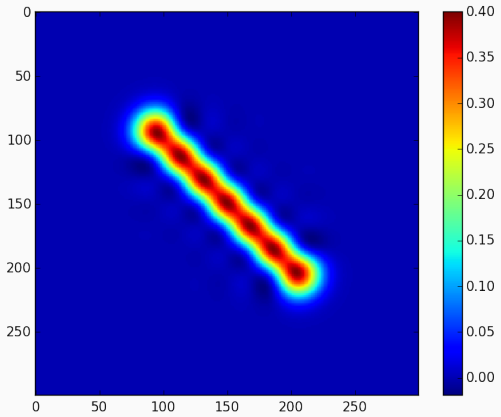
Does it make sense

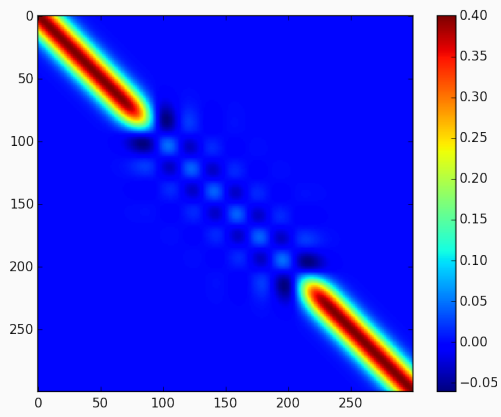


$$k(\mathbf{x}_*, \mathbf{X})^{\mathrm{T}} k(\mathbf{X}, \mathbf{X})^{-1} \mathbf{f}$$

Does it make sense

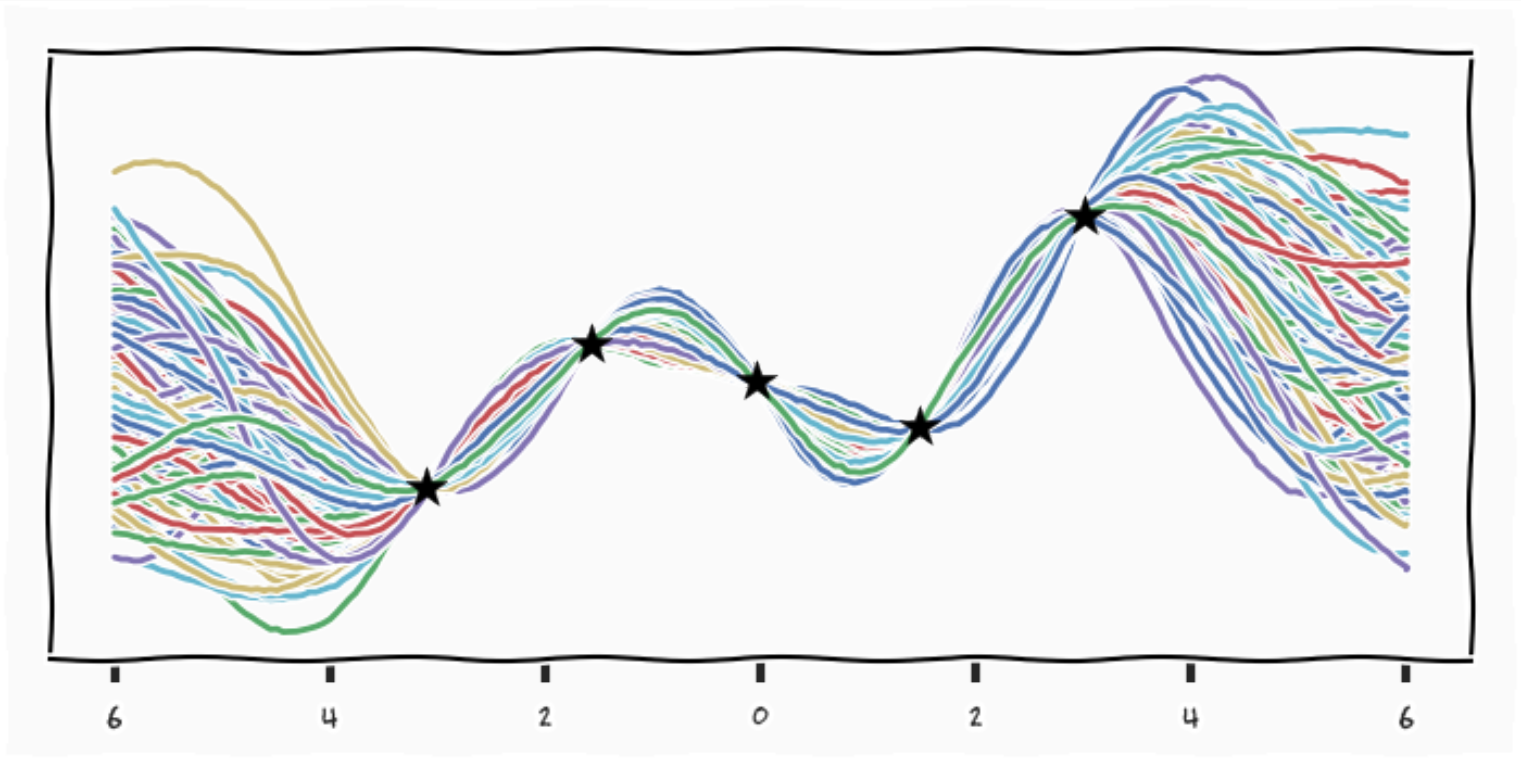




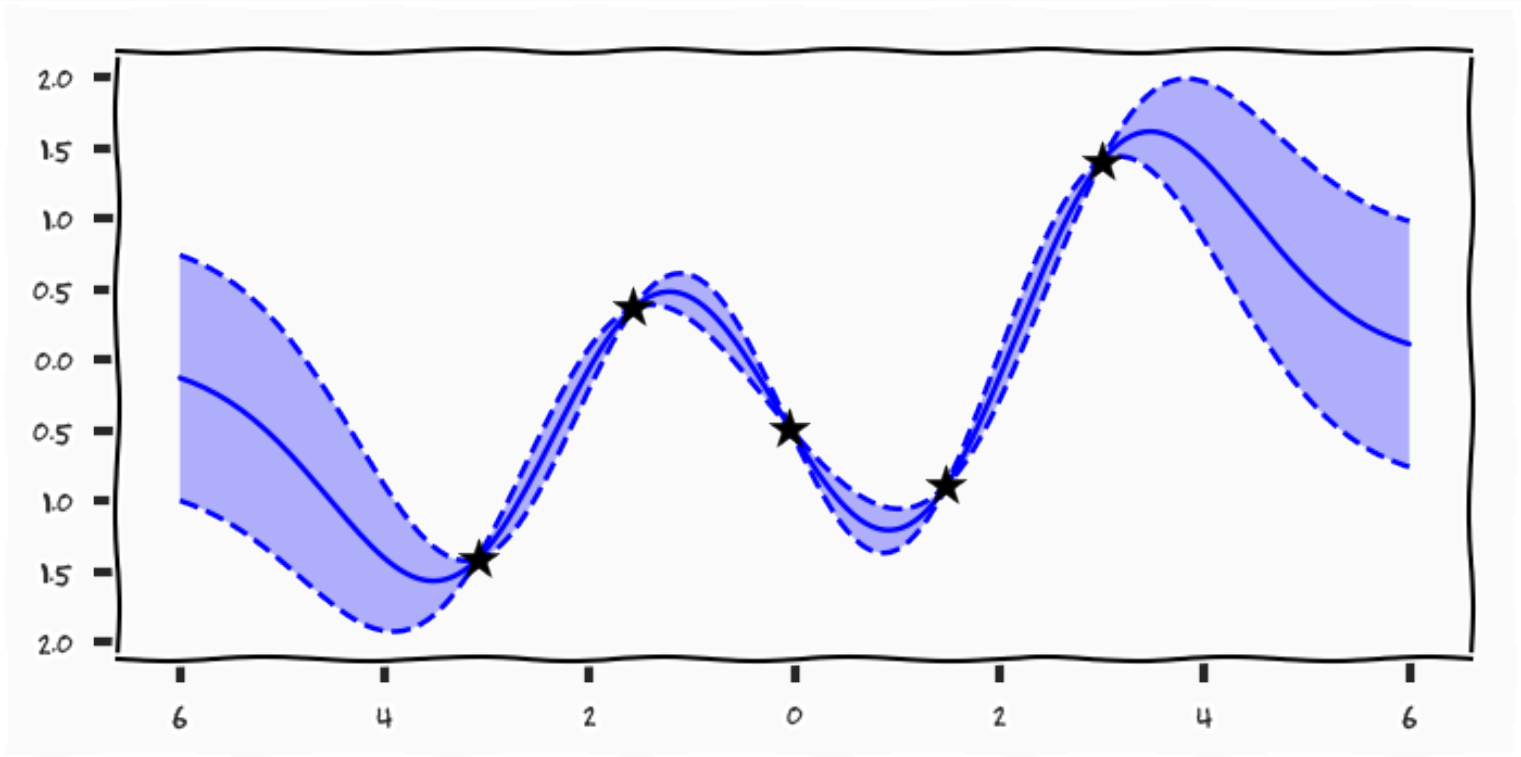


$$k(\mathbf{x}_*, \mathbf{x}_*) - k(\mathbf{x}_*, \mathbf{X})^{\mathrm{T}} k(\mathbf{X}, \mathbf{X})^{-1} k(\mathbf{X}, \mathbf{x}_*)$$

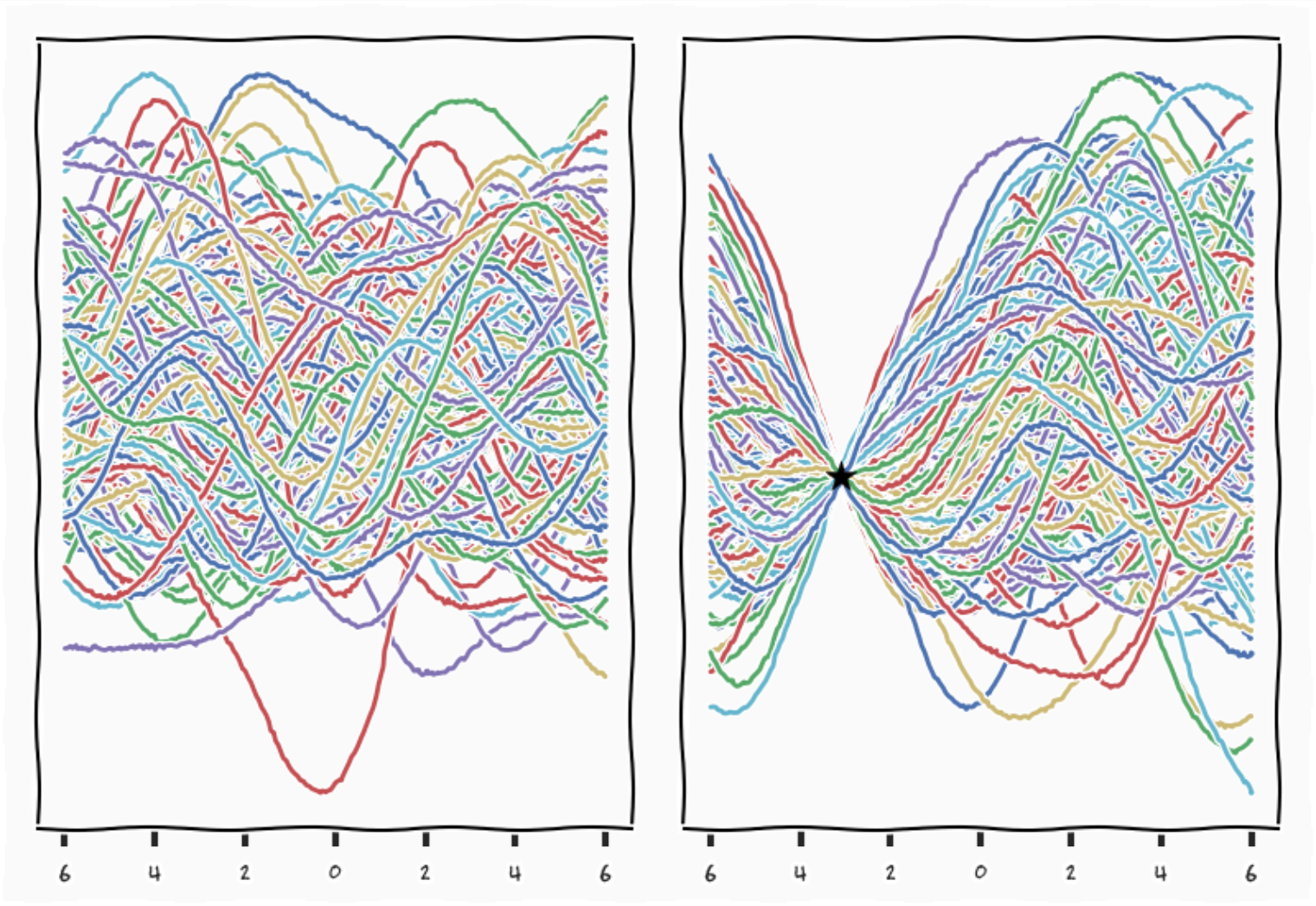
Gaussian Processes Posterior



Gaussian Processes Posterior



Gaussian Processes: Posterior Samples



Gaussian Processes: Noisy observations

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

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

- Add noise to observations

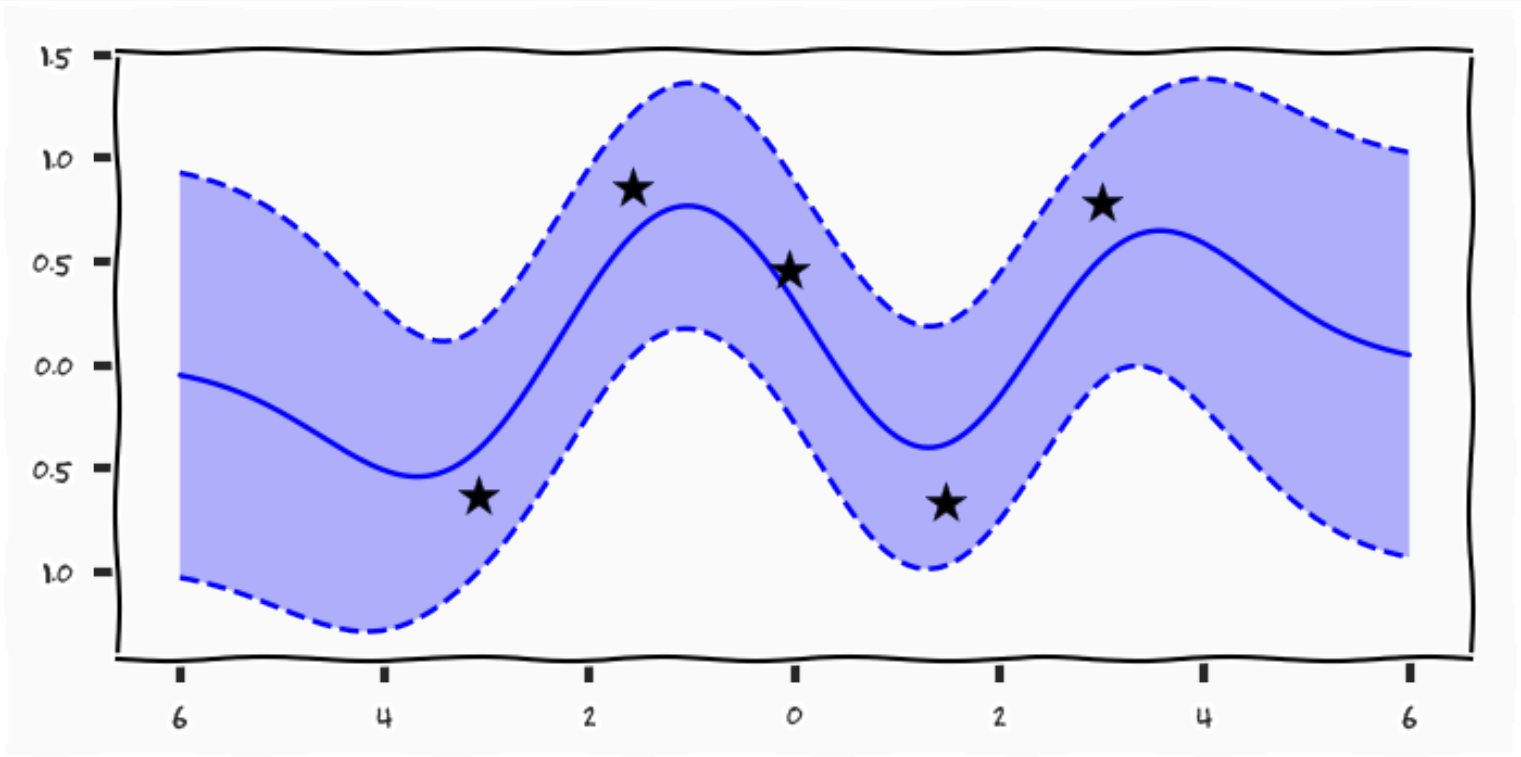
Gaussian Processes: Noisy observations

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

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

- Add noise to observations
- *Do you recognise the mean?*

Gaussian Processes



Summary

Summary

- Repeat of the machine learning proceedure
  - assumption + data + compute $\rightarrow$ updated assumption
  - don't worry it will become clear eventually
- Gaussian processes
  - infinite generalisation of Gaussian distribution
  - prior over the space of functions
  - contains all functions

Useful?

eof

References


Christopher M. Bishop.
Pattern Recognition and Machine Learning (Information Science and Statistics).
Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2006.