Gaussian Process Emulators for Cardiac Digital Twins

Richard Wilkinson, Chris Lanyon

School of Mathematical Sciences
University of Nottingham

Cardiac Digital Twin summer school
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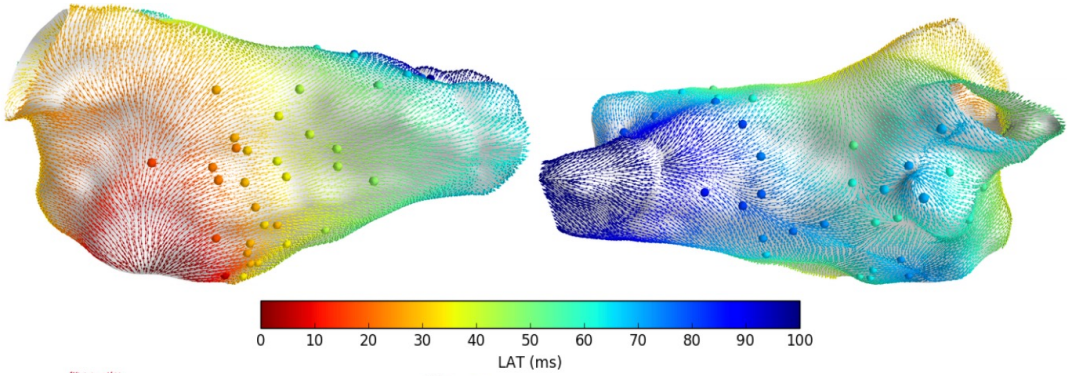
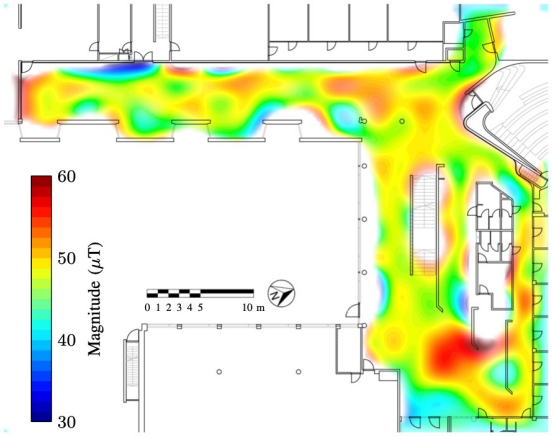
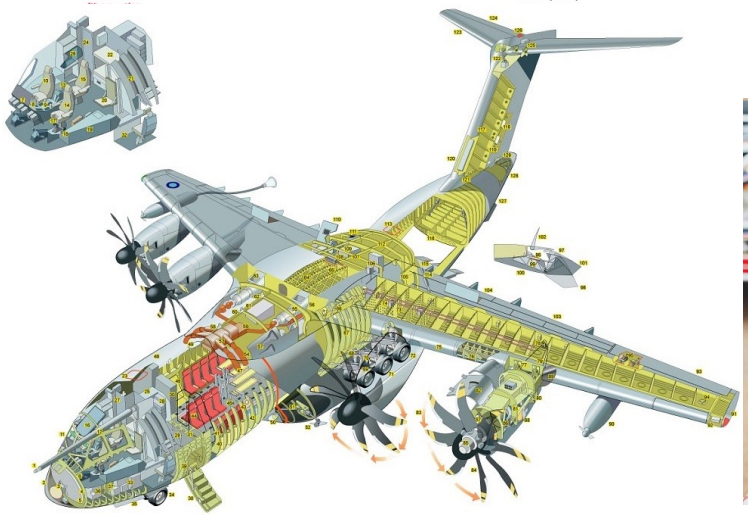
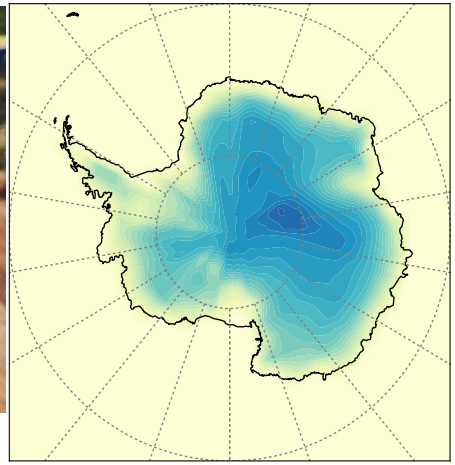
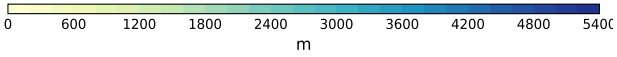
Recent Gaussian process applications











Computer models

Some notation

Scientists often build complex models that simulate some phenomenon:

- x - inputs to the simulator
- $f(x)$ - outputs of the simulator

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- Calibrated prediction

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Sacks, Welch, Mitchell, Wynn 1984

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- All inference must be done using a finite ensemble of model runs

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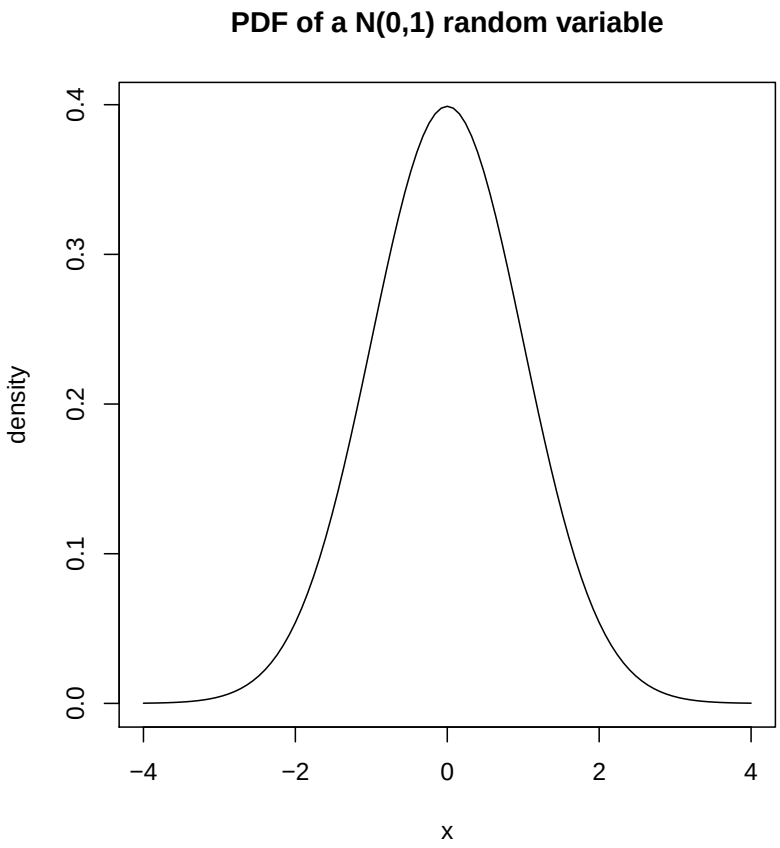
Gaussian processes (GPs) are the most widely used choice of emulator
People also use polynomial chaos, neural networks, other ML/stats regession tools (eg linear regression, random forests), ...

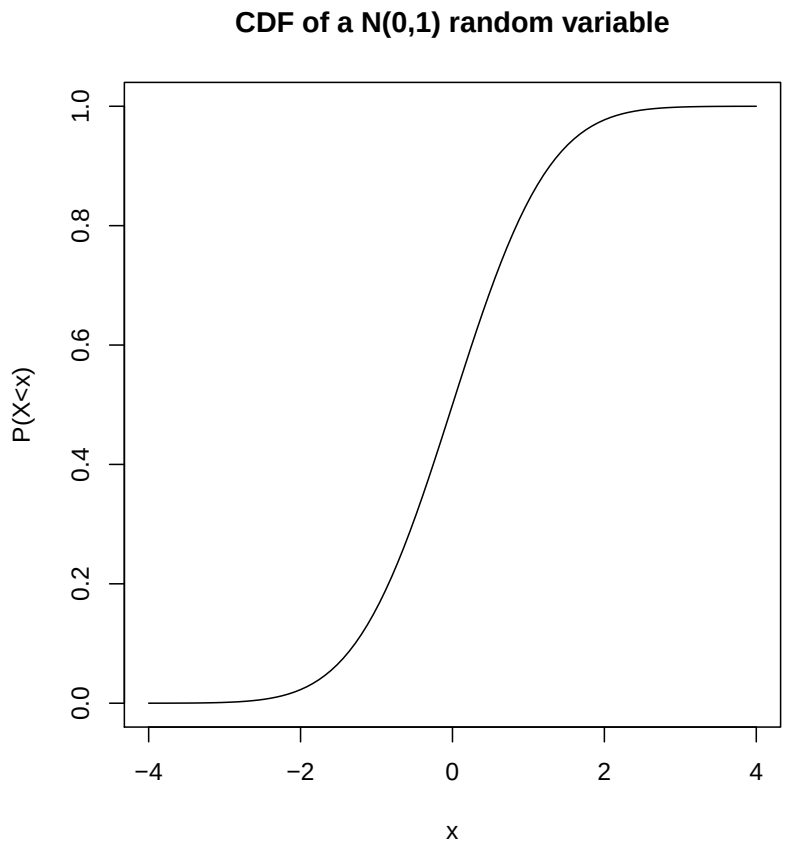
Introduction

- Gaussian process basics
- Difficulties of working with GPs
- Example

You can download a copy of these slides from
`https://github.com/cwlanyon/CardiacDTWorkshop`

Univariate Gaussian distributions





$$Y \sim N(\mu, \sigma^2)$$

PDF: $$f_Y(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right)$$

Univariate Gaussians

The normal/Gaussian distribution occurs naturally and is convenient mathematically

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- If Y and Z are jointly normally distributed and are uncorrelated, then they are independent
- Square-loss functions lead to procedures that have a Gaussian probabilistic interpretation
  eg mimizing $\sum(y_i - f_\beta(x_i))^2$

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$$Y = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \qquad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 \\ \rho_{21}\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

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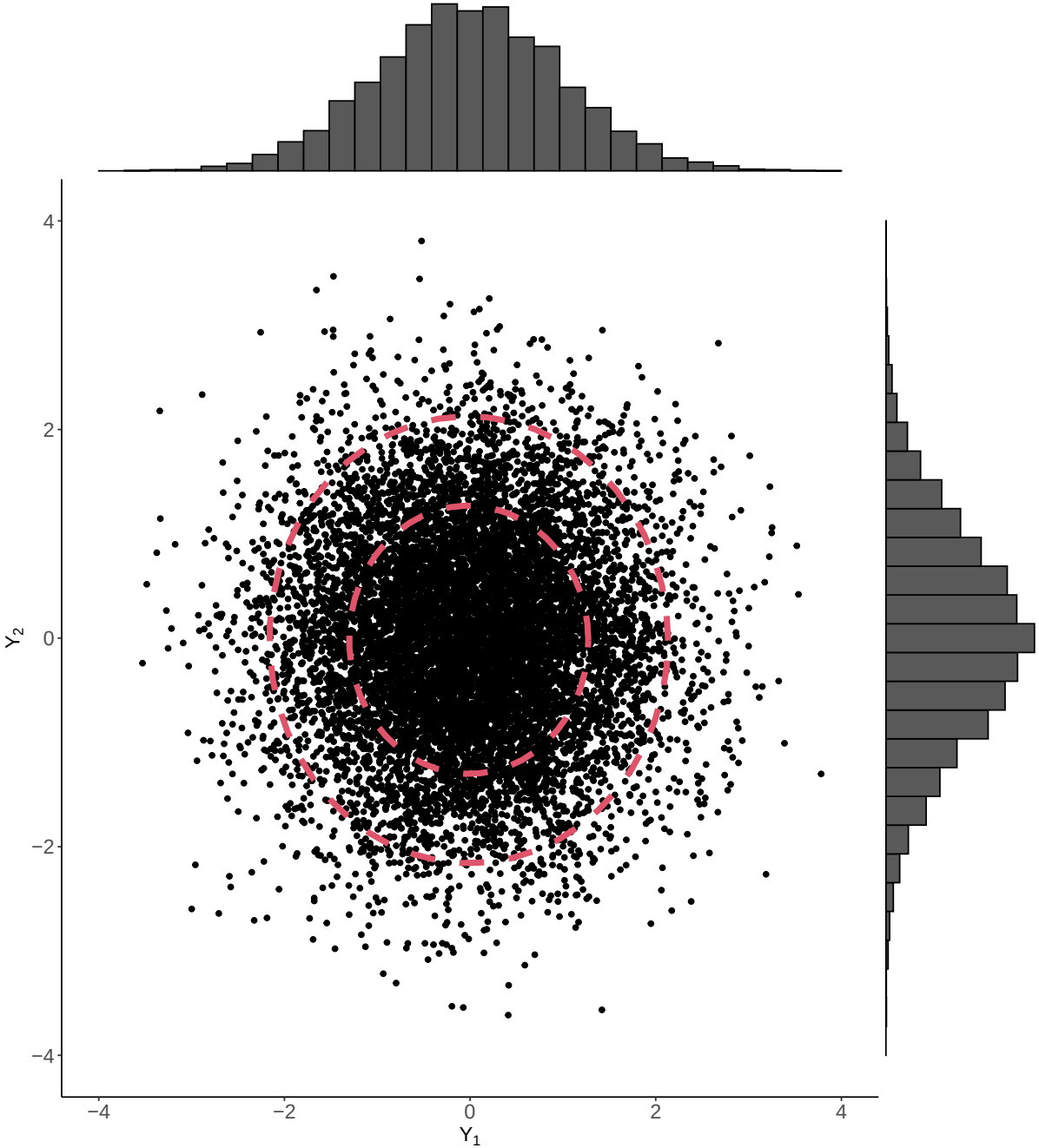
$$\text{pdf:} \quad f(y \mid \mu, \Sigma) = |\Sigma|^{-\frac{1}{2}}(2\pi)^{-\frac{d}{2}} \exp\left(-\frac{1}{2}(y-\mu)^\top \Sigma^{-1}(y-\mu)\right)$$



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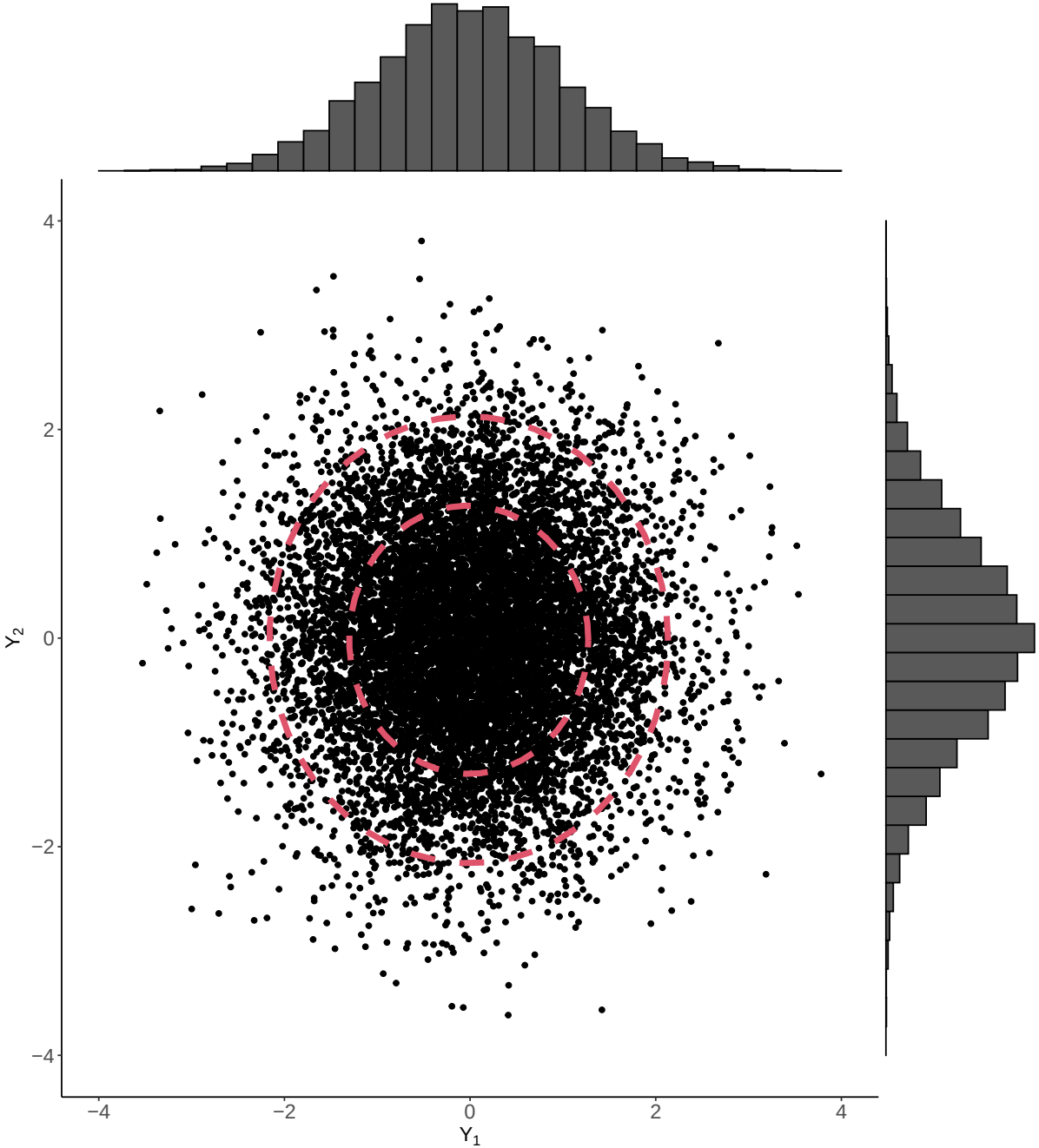

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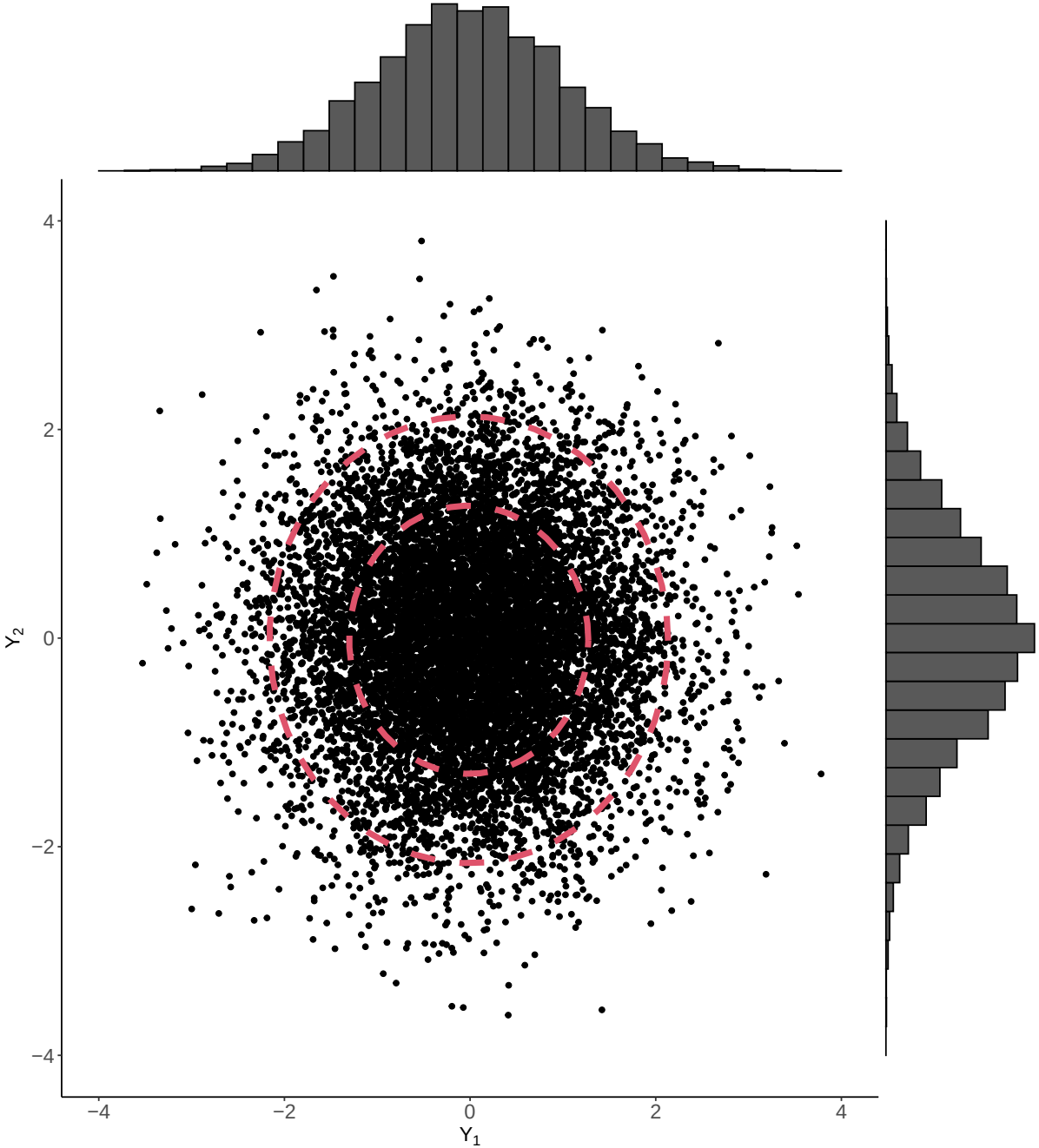
hence Y_1
independent of Y_2



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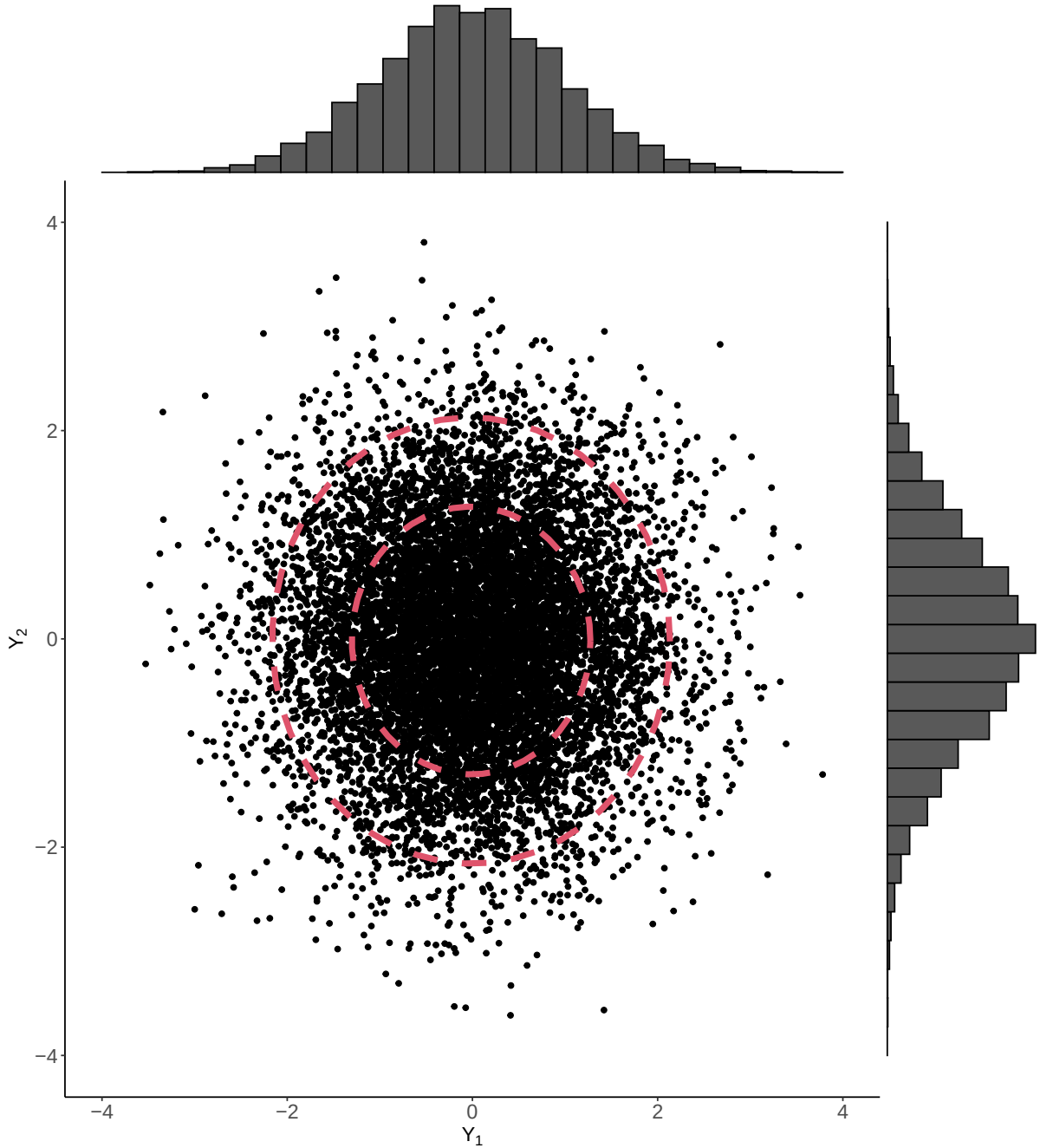

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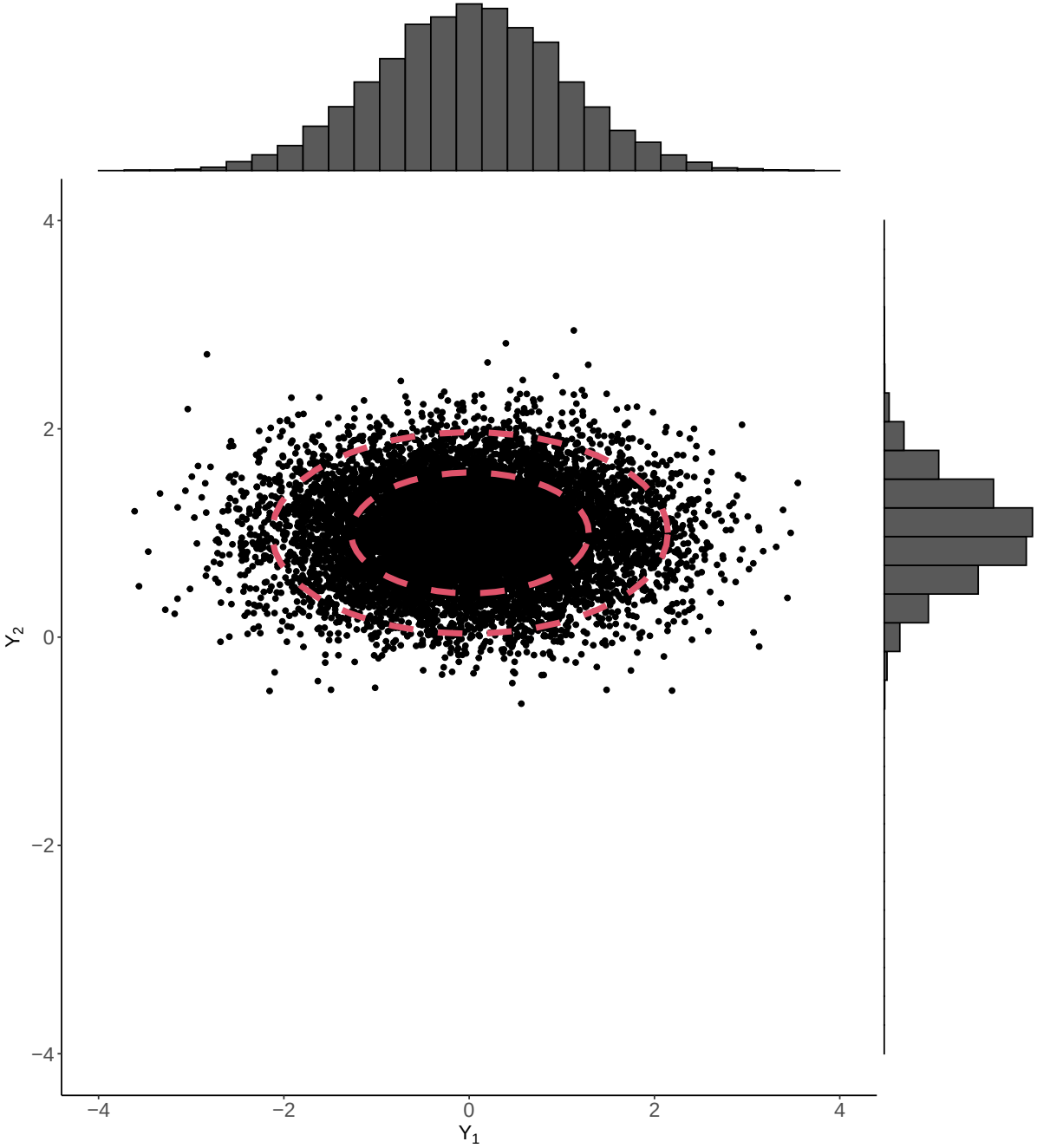
Conditional distributions:

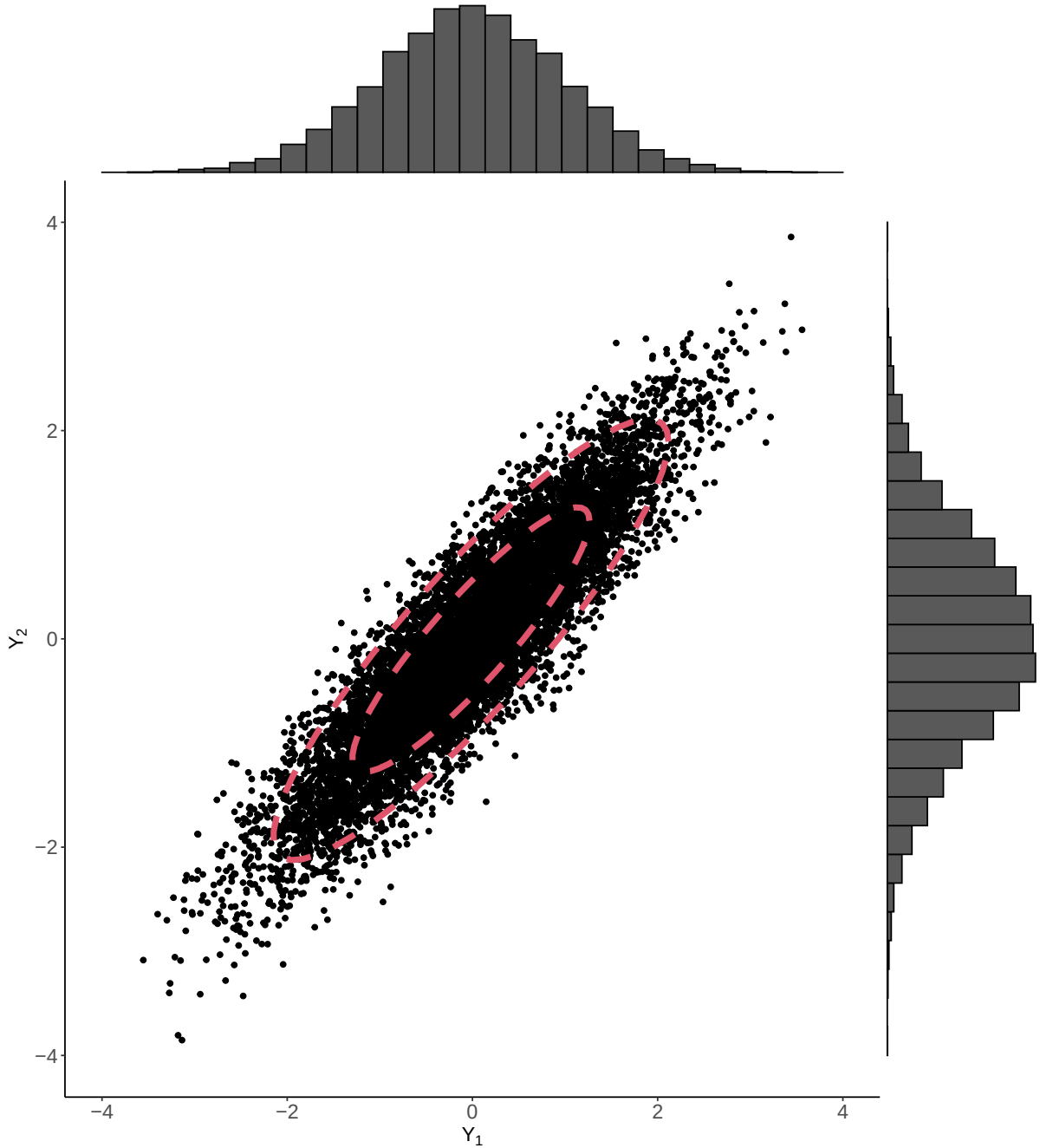
$$Y_1 | Y_2 \sim N(0, 1)$$

$$Y_2 | Y_1 \sim N(0, 1)$$



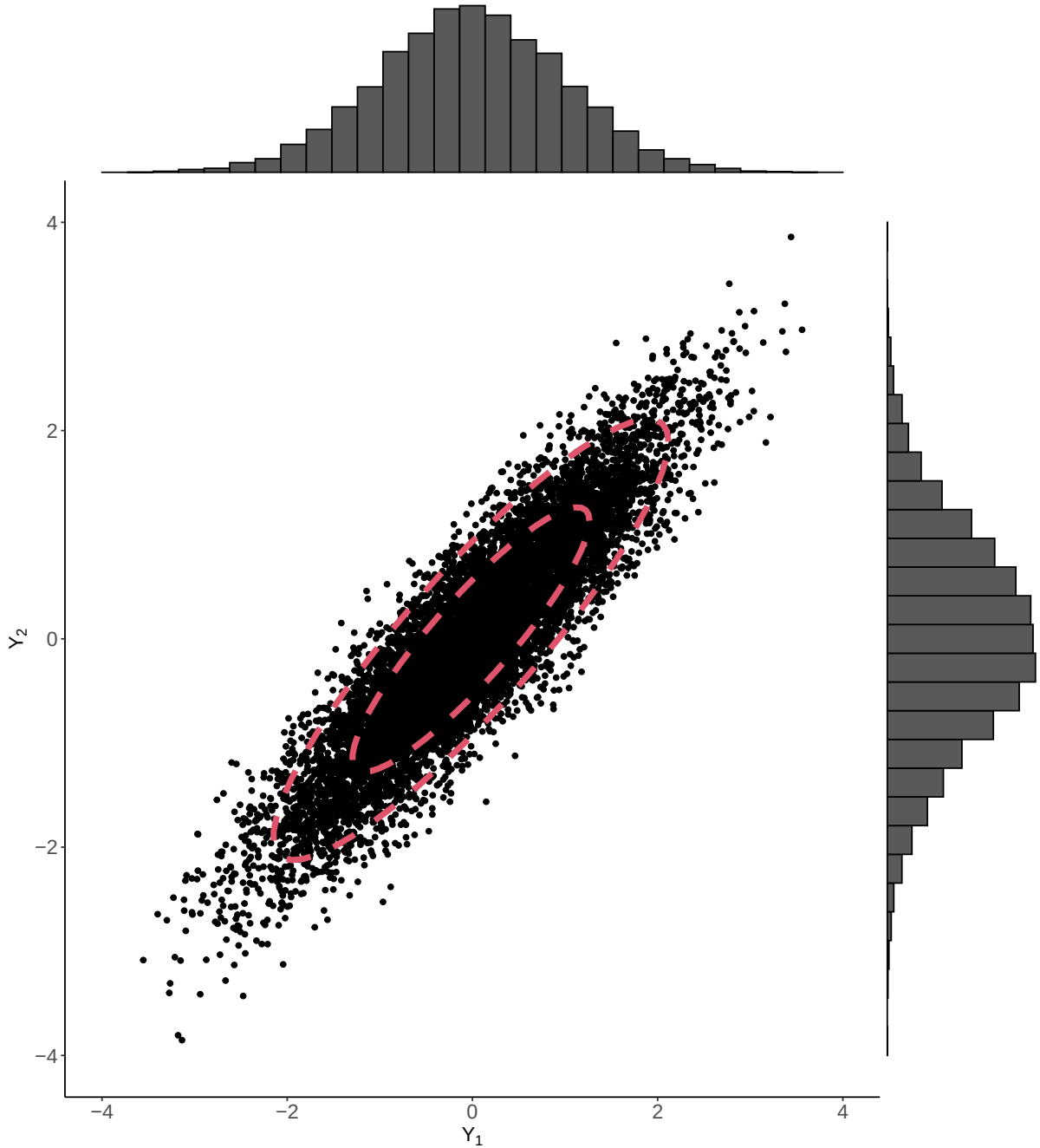
$$\mu = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}$$



$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$



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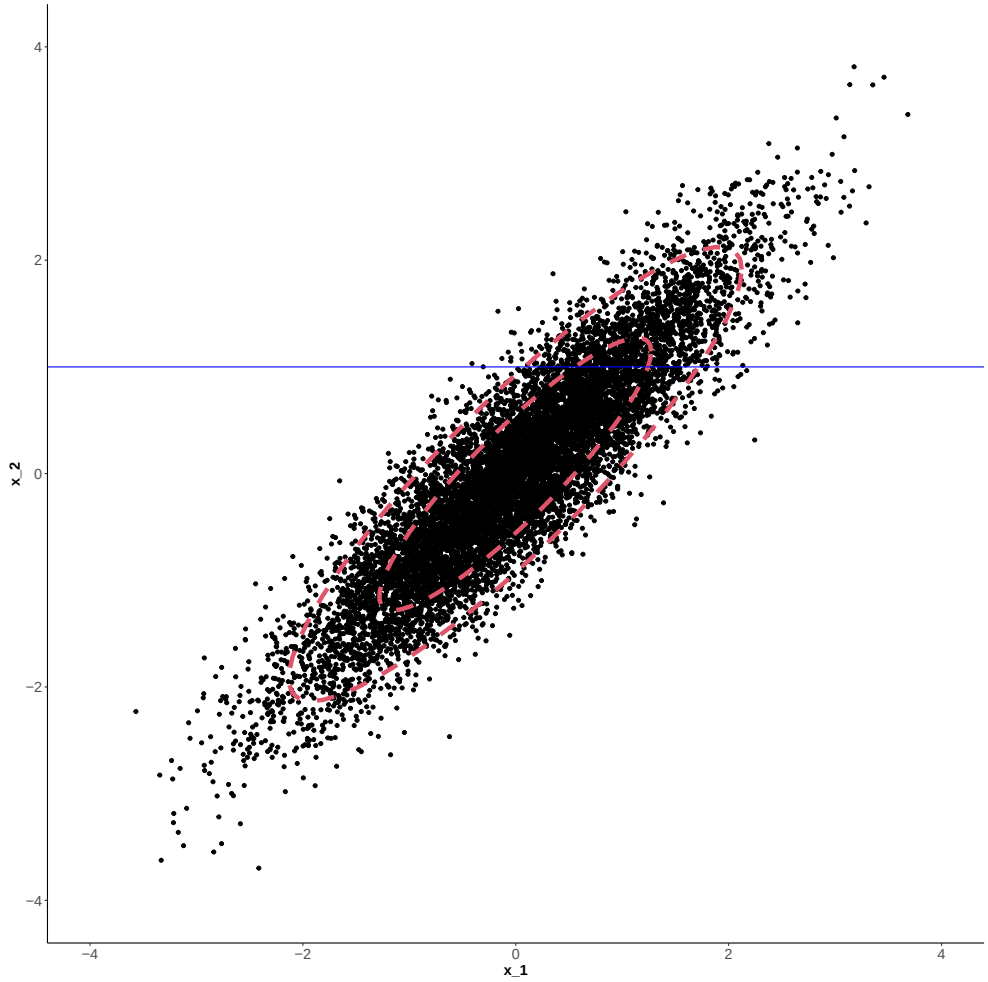

$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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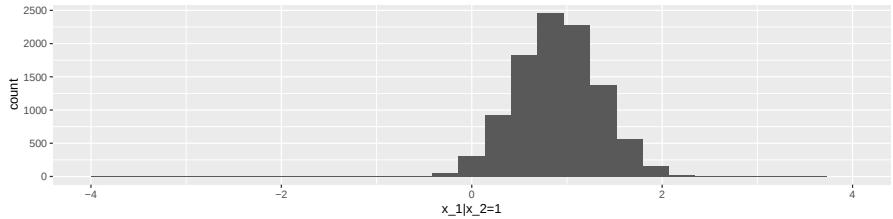
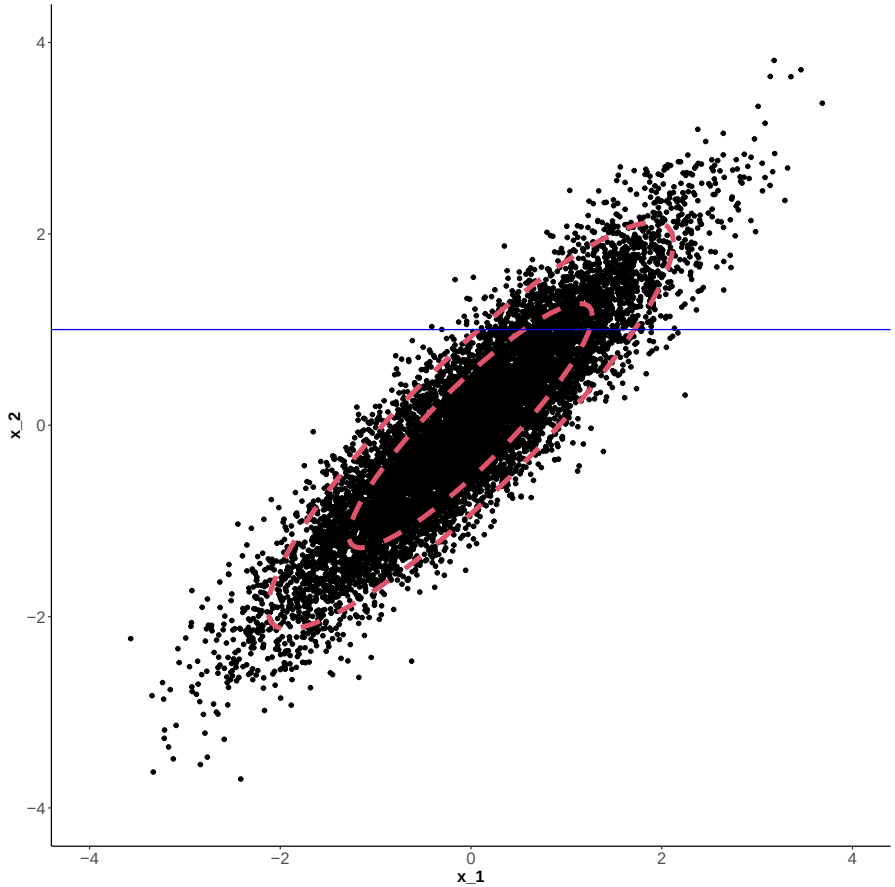
What is the conditional distribution of $Y_1 | Y_2 = 1$?

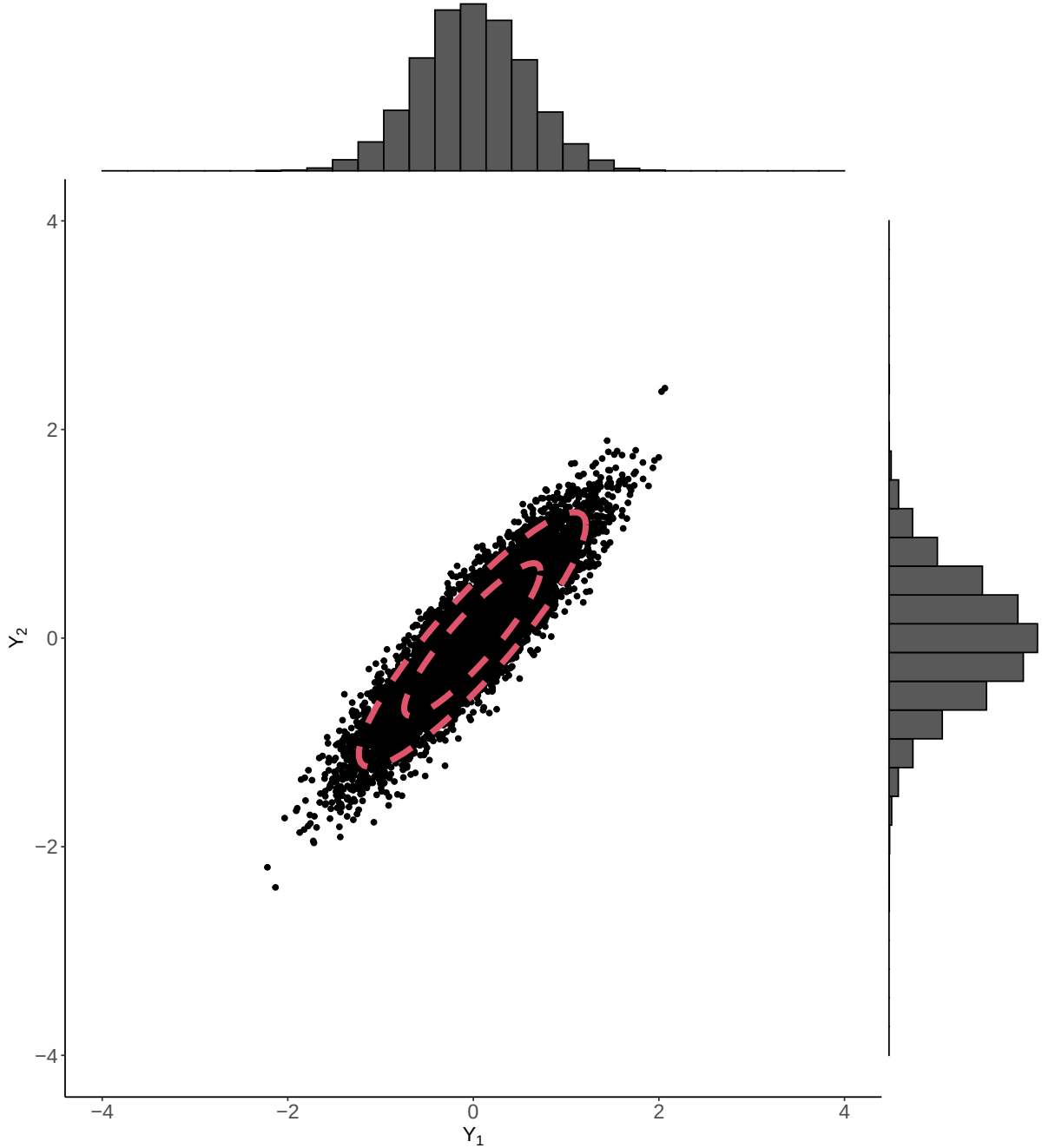




$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

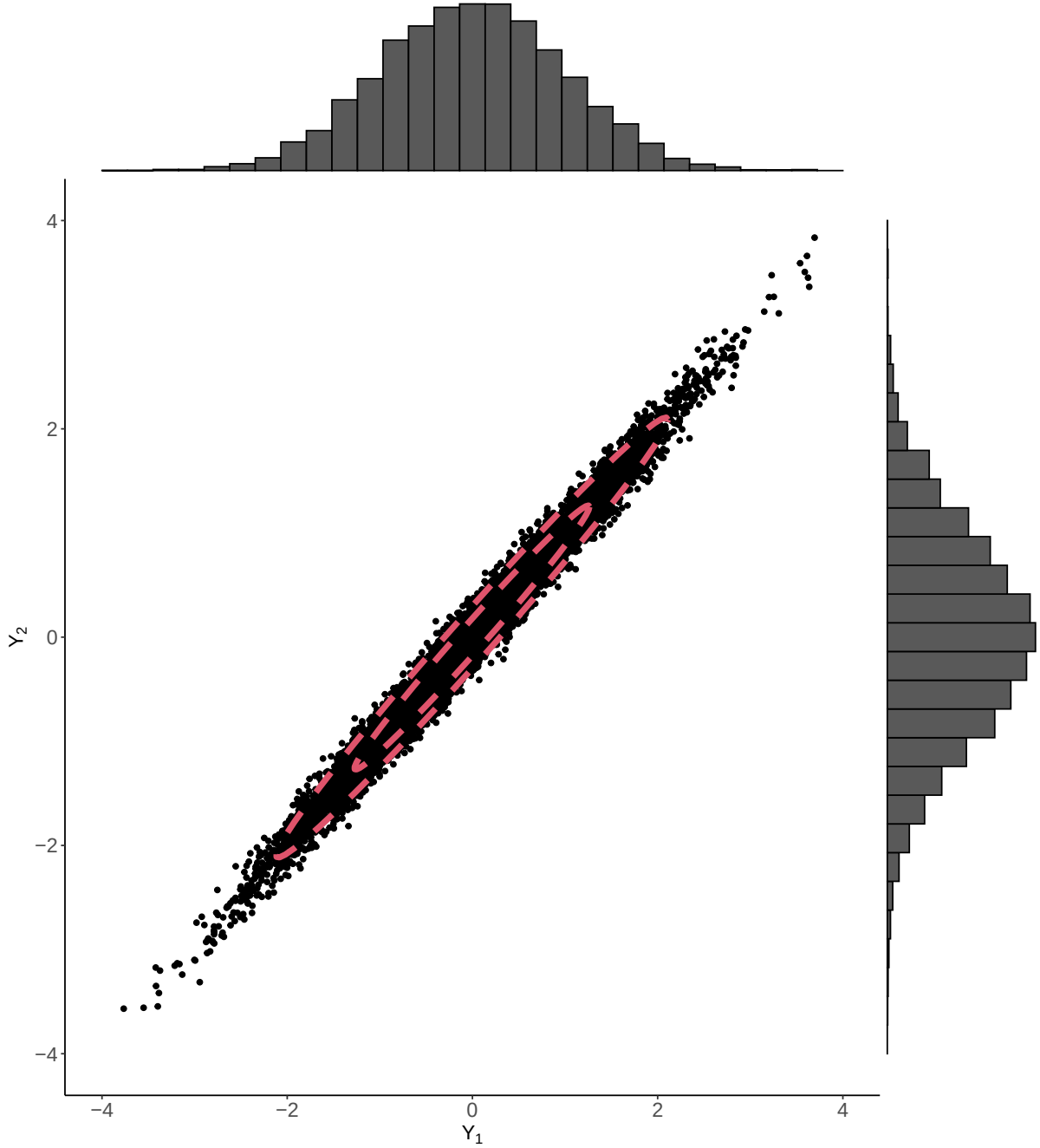
$$\Sigma = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$

$$Y_1 | Y_2 = 1 \sim N(0.9, 0.19)$$



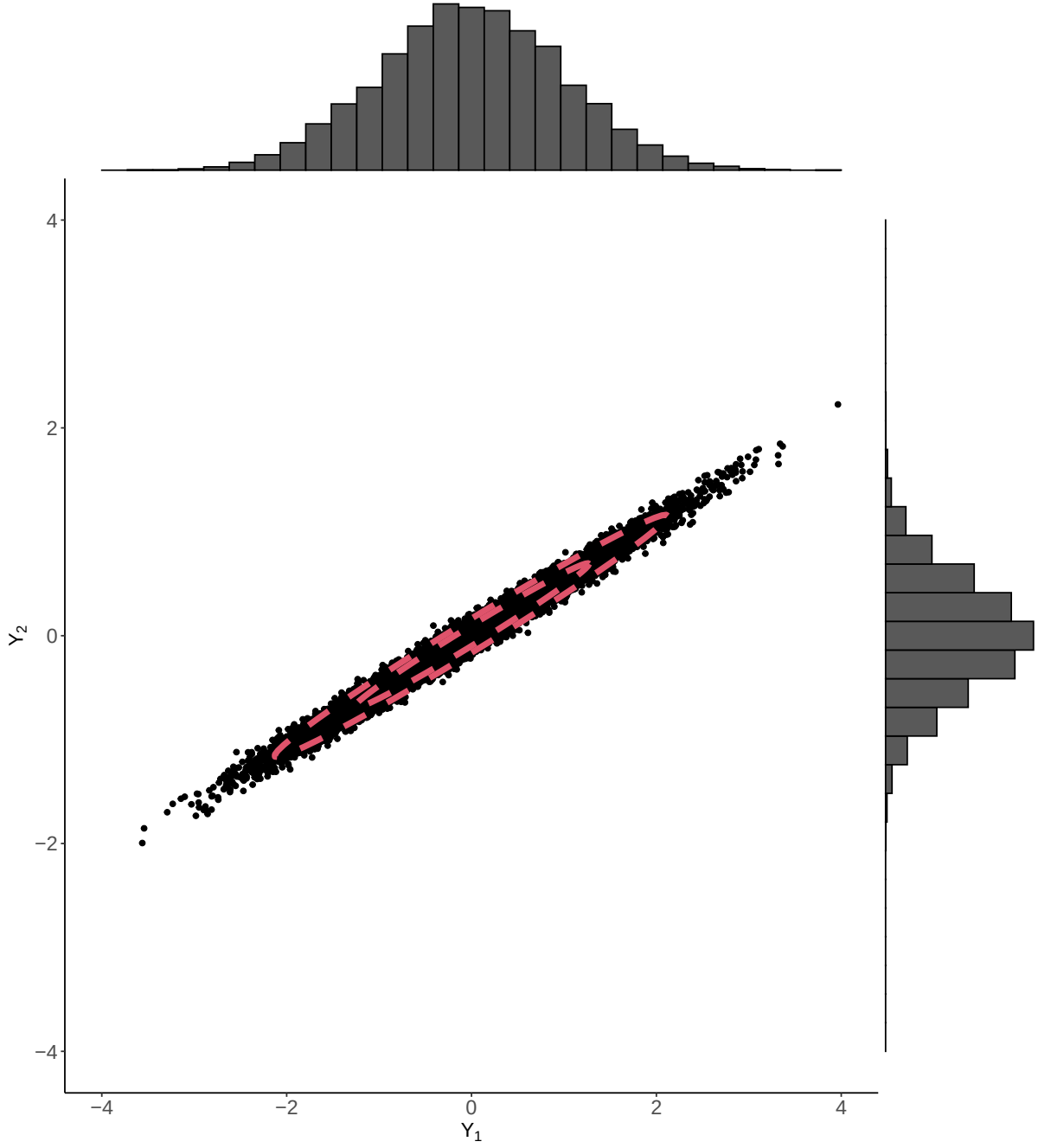
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Sigma = \frac{1}{3} \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$



$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0.99 \\ 0.99 & 1 \end{pmatrix}$$



$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0.54 \\ 0.54 & 0.3 \end{pmatrix}$$

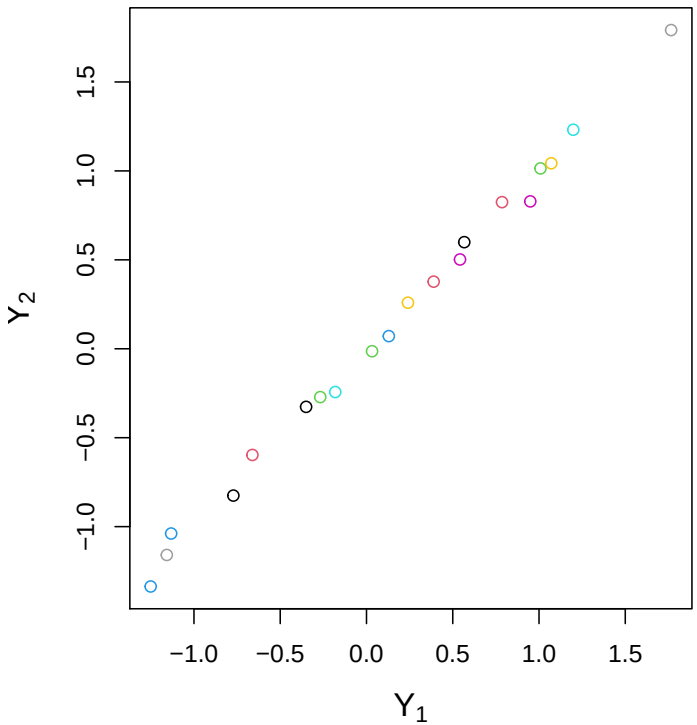
$Cor(Y_1, Y_2) = 0.54/\sqrt{(0.3)} = 0.99$

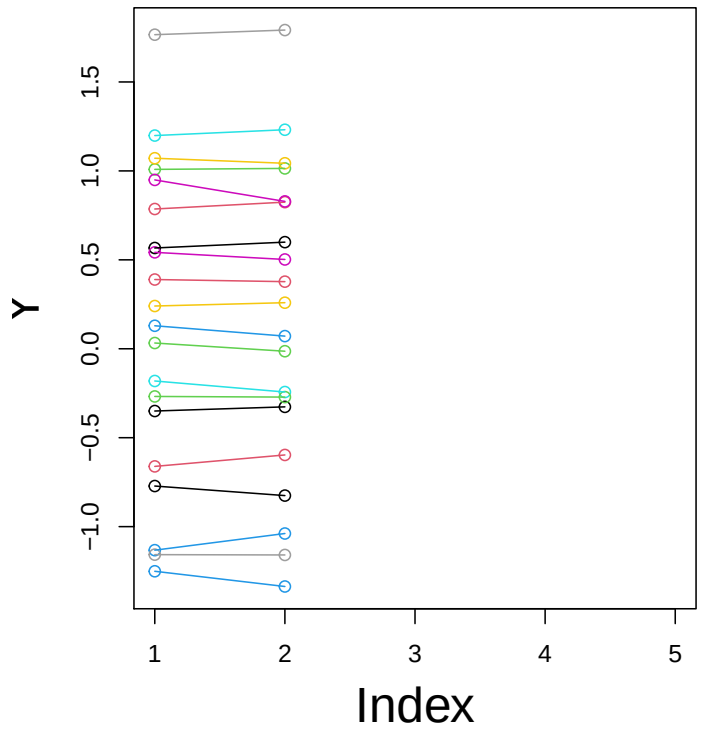
More pictures

Hard to visualise in dimensions > 2, so stack points next to each other.

More pictures

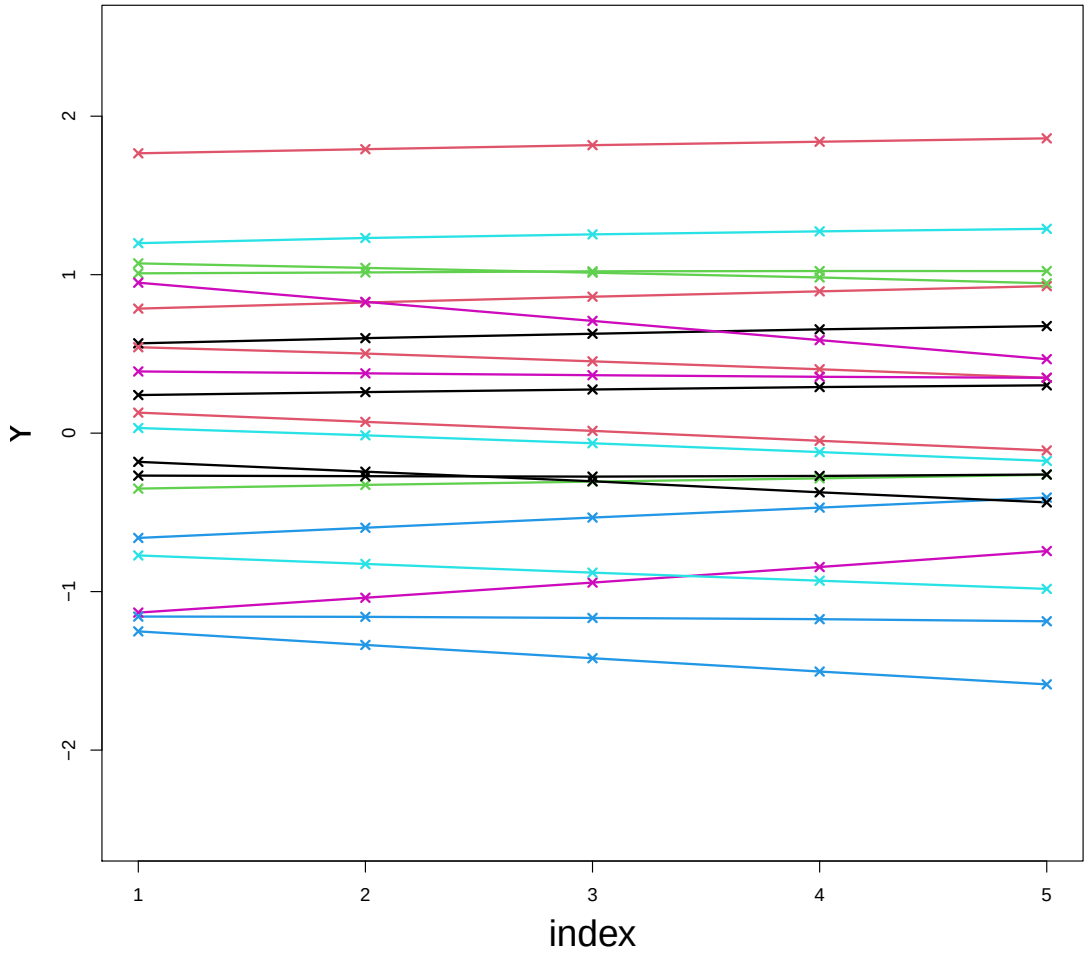
Hard to visualise in dimensions > 2, so stack points next to each other.
So for 2d instead of we have





Consider $d = 5$ with

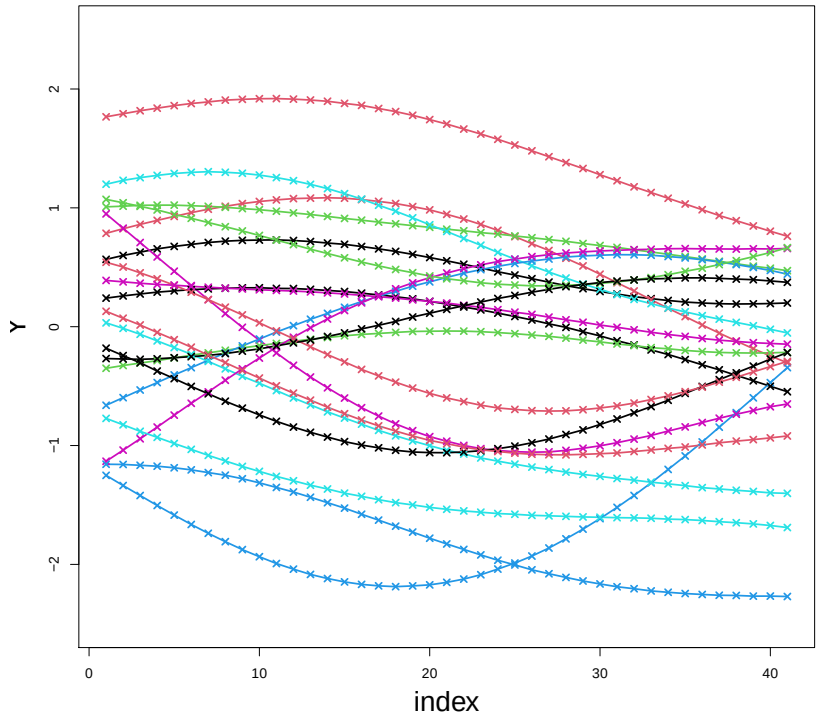
$$\mu = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.99 & 0.98 & 0.97 & 0.96 \\ 0.99 & 1 & 0.99 & 0.98 & 0.97 \\ 0.98 & 0.99 & 1 & 0.99 & 0.98 \\ 0.97 & 0.98 & 0.99 & 1 & 0.99 \\ 0.96 & 0.97 & 0.98 & 0.99 & 1 \end{pmatrix}$$



Each line is one sample.

$d = 50$

$$\mu = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.99 & 0.98 & 0.97 & 0.96 & \dots \\ 0.99 & 1 & 0.99 & 0.98 & 0.97 & \dots \\ 0.98 & 0.99 & 1 & 0.99 & 0.98 & \dots \\ 0.97 & 0.98 & 0.99 & 1 & 0.99 & \dots \\ 0.96 & 0.97 & 0.98 & 0.99 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$



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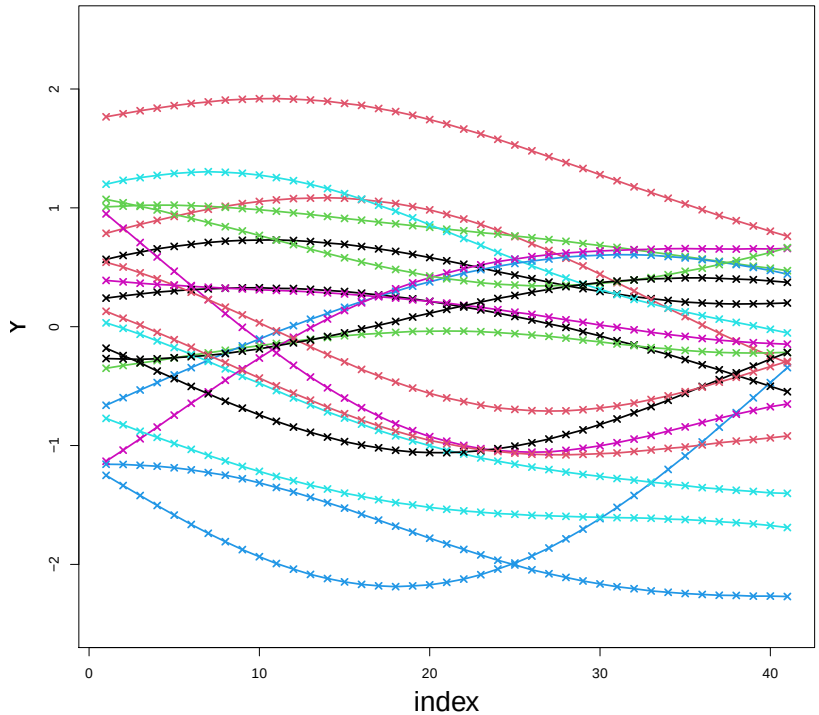

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We can think of Gaussian processes as an infinite dimensional distribution over functions - all we need to do is change the indexing

- We can let the index be x and let x take values in $\mathbb{R}$.

Gaussian processes

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$$y = \{y(x) : x \in \mathcal{X}\}$$

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Usually $y(x) \in \mathbb{R}$ and $\mathcal{X} \subset \mathbb{R}^n$

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Write $y(\cdot) \sim GP$ to denote that we model the *function* y as a GP.

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To fully specify the law of a Gaussian *distribution* we only need the mean and variance.

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$$\mathbb{E}(y(x)) = m(x)$$
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In GP software, these are often the only choices we need to make.

Specifying the mean function

We are free to choose the mean $m(x) = \mathbb{E}(y(x))$ and covariance $k(x, x') = \mathbb{C}\text{ov}(y(x), y(x'))$ functions however we like (e.g. trial and error), subject to some 'rules':

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- We can use any mean function we want:

$$m(x) = \mathbb{E}(y(x))$$

  Most popular choices are $m(x) = 0$ or $m(x) = const$ for all x, or $m(x) = \beta^\top x$

Covariance functions

We usually use a covariance function that is a function of the indexes/locations

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- Given locations $x_1, \ldots, x_n$, the $n \times n$ Gram matrix K with $K_{ij} = k(x_i, x_j)$

$$\begin{pmatrix} k(x_1, x_1) & k(x_1, x_2) & \ldots & k(x_1, x_n) \\ \vdots & & & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \ldots & k(x_n, x_n) \end{pmatrix}$$

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  must be a positive semi-definite matrix (ie a covariance matrix).
- This can be problematic...
  - Difficult to create semi-definite functions $k(x, x')$

We often assume k is a function of only the distance between locations

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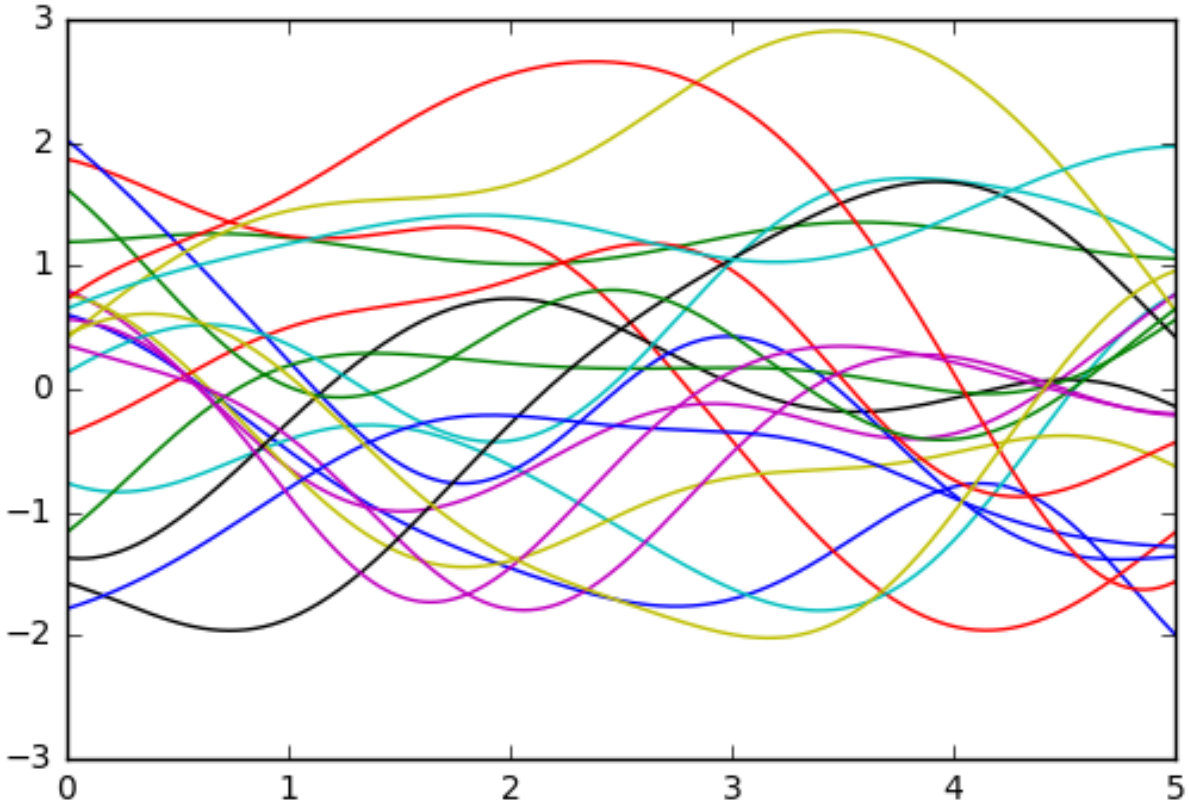
- k determines the hypothesis space/space of functions

We usually build k by selecting from a small candidate set of functions (that contain free parameters), and modifying them according to some rules.

Examples

RBF/Squared-exponential/exponentiated quadratic

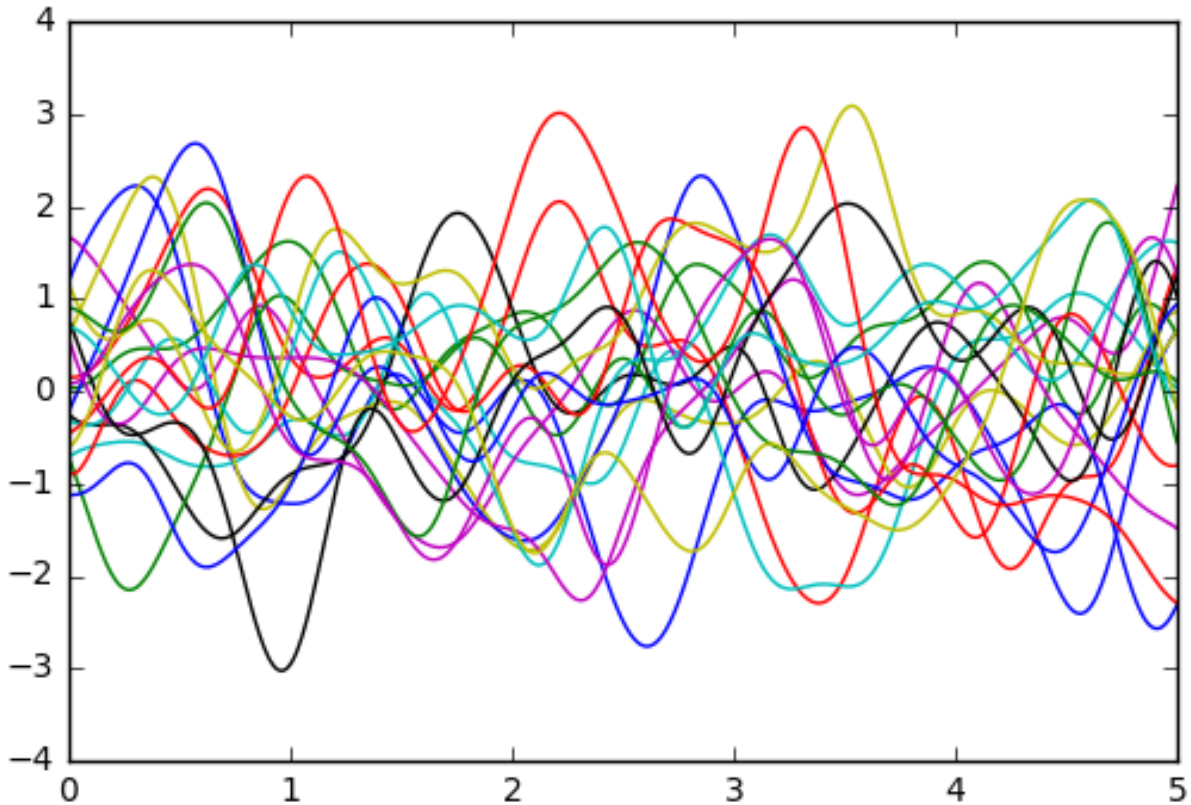
$$k(x, x') = \exp\left(-\frac{1}{2}(x - x')^2\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

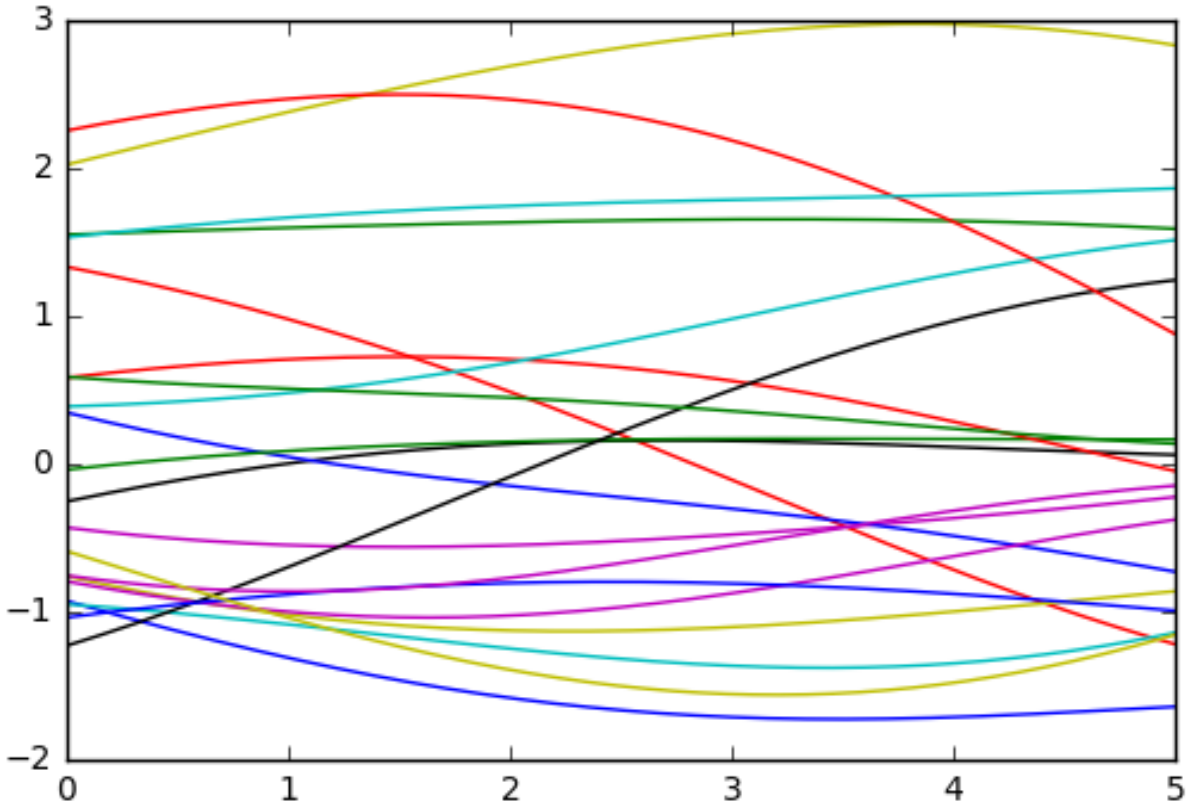
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{0.25^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

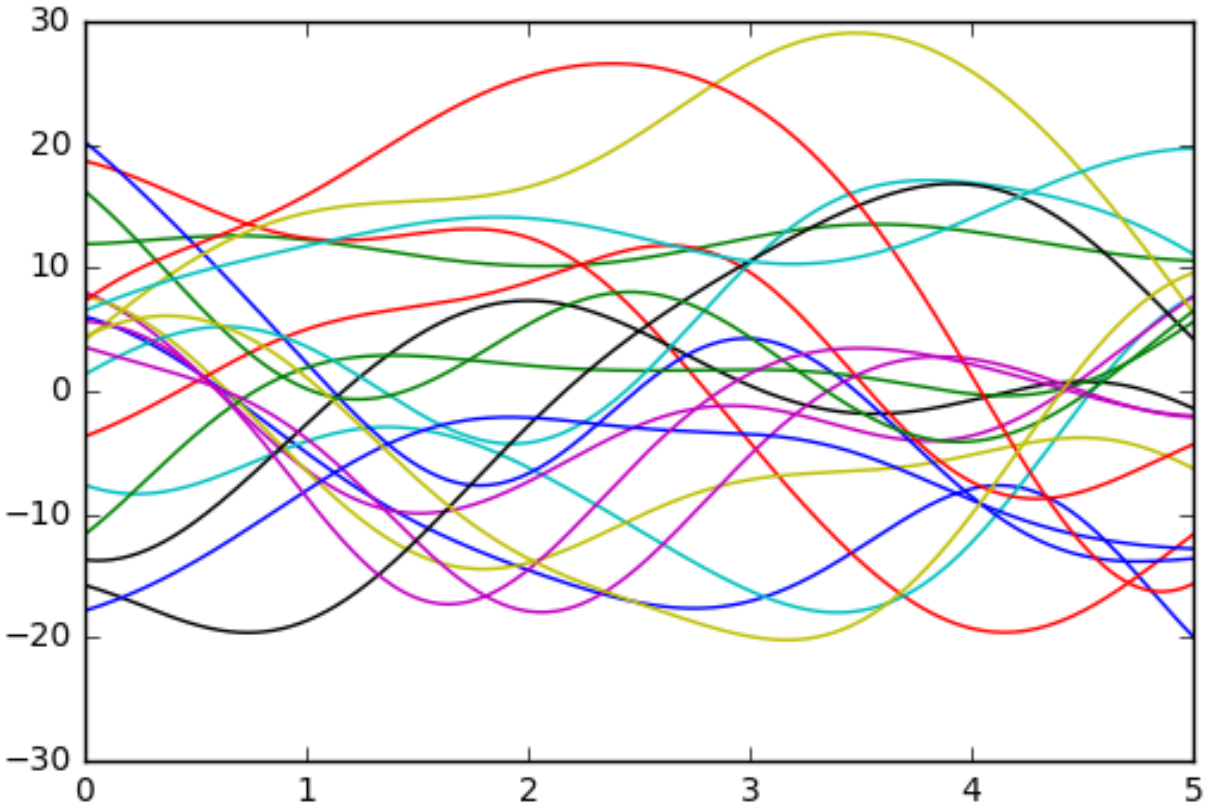
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{4^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

$$k(x, x') = 100 \exp\left(-\frac{1}{2}(x - x')^2\right)$$



In general $k(x, x') = \sigma^2 \exp\left(-\frac{1}{2}\frac{(x - x')^2}{\lambda^2}\right)$

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Matérn Covariance functions

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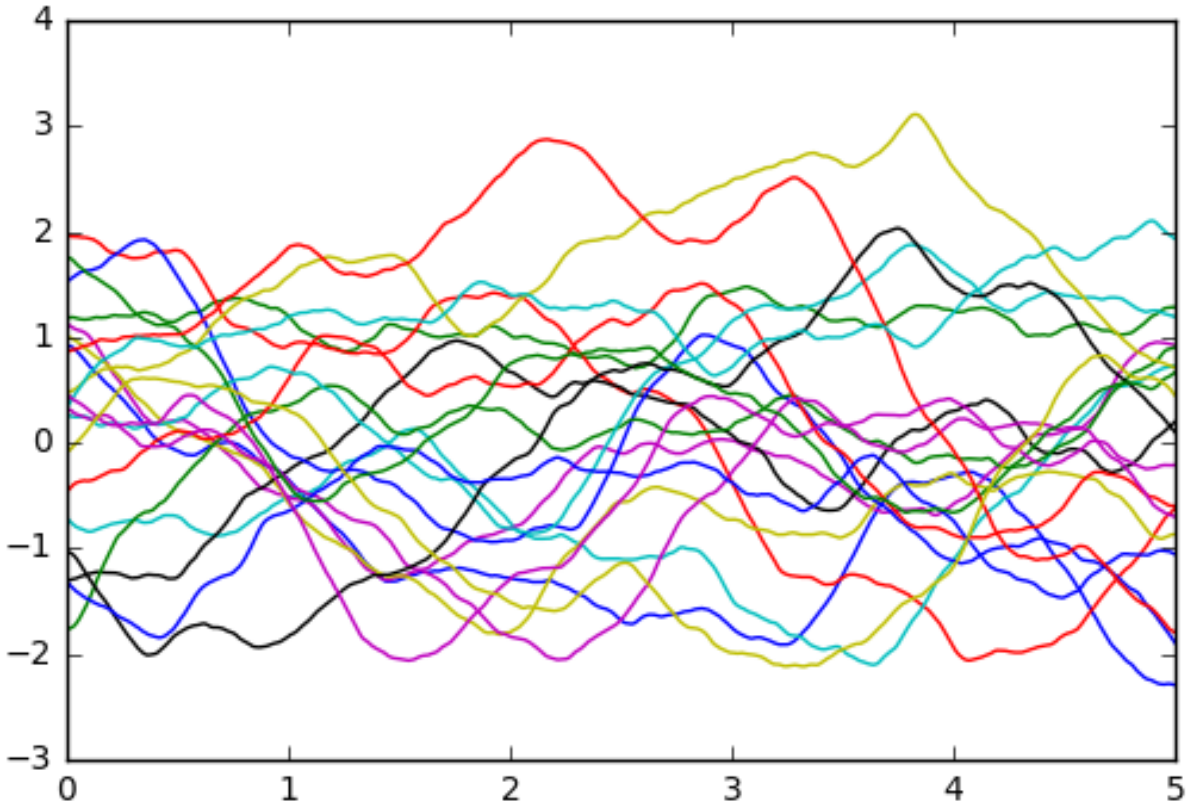
- $\nu = 5/2$: $k(x, x') = \sigma^2 \left(1 + \frac{\sqrt{5}|x-x'|}{\lambda} + \frac{5|x-x'|^2}{3\lambda^2}\right) \exp\left(-\frac{\sqrt{5}|x-x'|}{\lambda}\right)$ gives functions that are twice differentiable

Examples

Matern 3/2

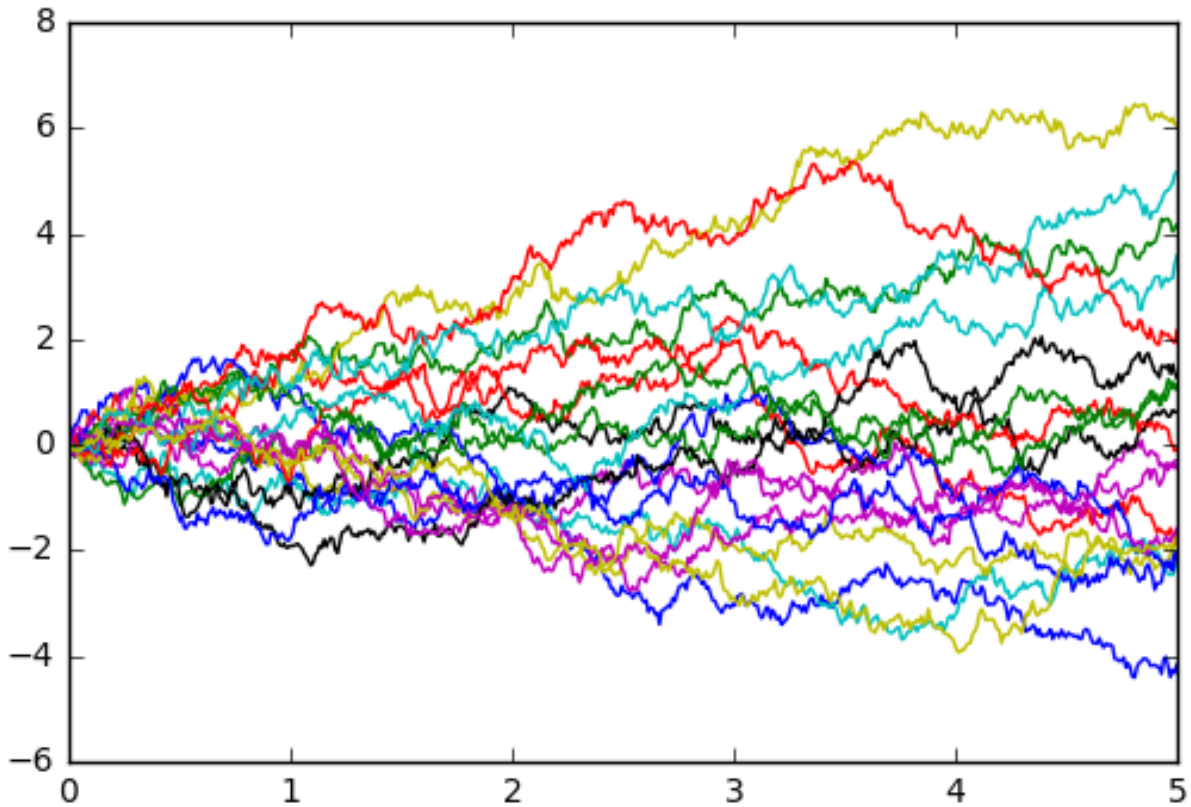
$$k(x, x') \sim (1 + |x - x'|) \exp\left(-|x - x'|\right)$$



Examples

Brownian motion

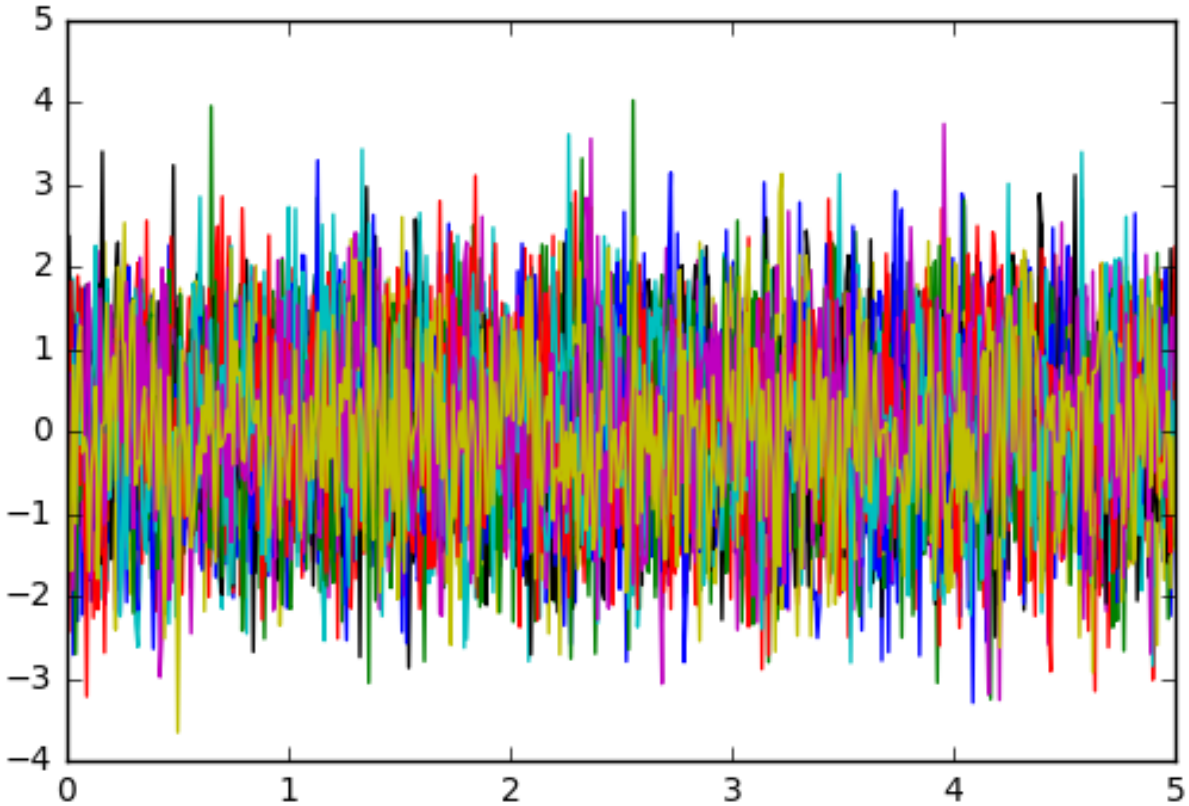
$$k(x, x') = \min(x, x')$$



Examples

White noise

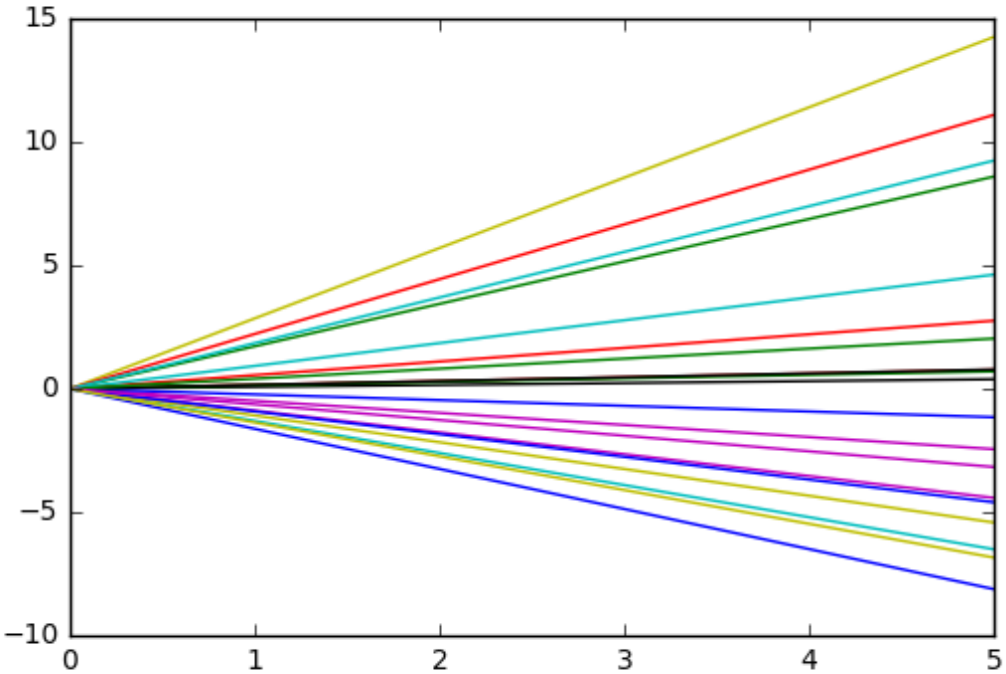
$$k(x, x') = \begin{cases} 1 \text{ if } x = x' \\ 0 \text{ otherwise} \end{cases}$$



Examples

A final example:

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



What is happening?

Examples

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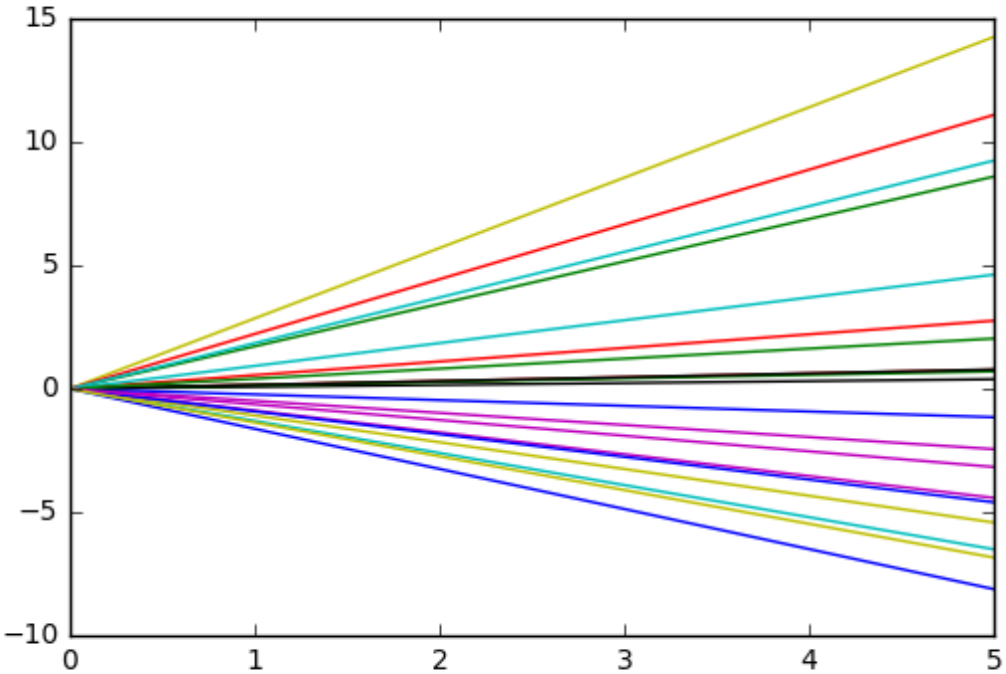

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Suppose $y(x) = cx$ where $c \sim N(0, 1)$.

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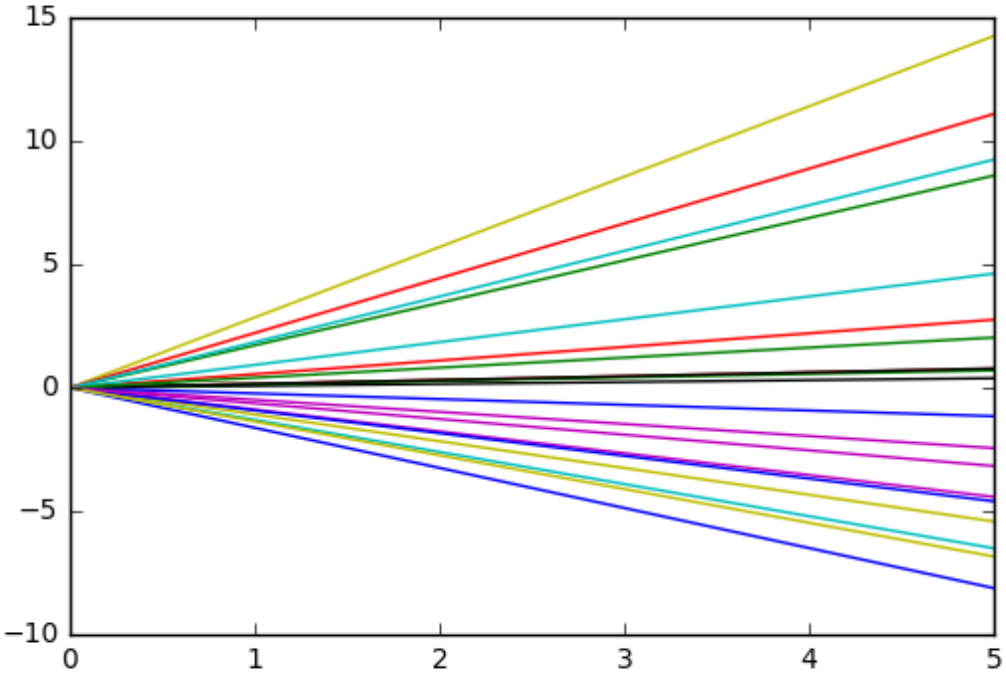

What is happening?

Suppose $y(x) = cx$ where $c \sim N(0, 1)$.

Then
$$\begin{aligned}\mathbb{C}\text{ov}(y(x), y(x')) &= \mathbb{C}\text{ov}(cx, cx') = x\mathbb{C}\text{ov}(c, c)x' \\ &= xx'\end{aligned}$$

So $y(\cdot) \sim GP(0, k(x, x'))$ with $k(x, x') = xx'$

Rules for combining covariance functions

Let k_1 and k_2 be valid covariance functions. Then

- $k_1 + k_2$ is a valid covariance function (even if k_1 and k_2 take different inputs).
- $k_1 k_2$ is a valid covariance function (also true if different inputs).
- For any function g, $k_1(g(x), g(x'))$ is a valid covariance function as is $g(x)k_1(x, x')g(x')$

Using these rules we can combine our standard set of positive definite covariance functions to create a richer family of covariance functions.

Choosing kernels and hyperparameters

GP properties are inherited primarily from the covariance function k.

- Continuity
- Differentiability
- Variance and length-scale

[2] f is mean square cts at x if for all sequences $x_k \to x$ we have $\mathbb{E}(f(x_k) - f(x))^2 \to 0$

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  - $f(x) \sim GP$ is (mean square[2]) continuous at x^* ifF $k(x, x')$ and $m(x)$ are continuous at $x = x' = x^*$
  - For stationary kernels, only require continuity at $k(0)$
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  - how much f varies between samples
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Typically choose the family of kernels by

- measures of fit (marginal likelihood, Bayes factors, ...)
- predictive skill (held-out data, cross-validation, ...)

Choose hyperparameters by maximum likelihood, Bayes, etc.

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Conditional updates of Gaussian processes

If f is a Gaussian process $f(\cdot) \sim GP(m(\cdot), k(\cdot, \cdot))$, then

$$f(x_1), \ldots, f(x_n), f(x) \sim N_{n+1}(\mu, \Sigma)$$

where

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where

$$\mu = \begin{pmatrix} m(x_1) \\ \vdots \\ m(x_n) \\ \hline m(x) \end{pmatrix} = \begin{pmatrix} | \\ m_X \\ | \\ \hline m(x) \end{pmatrix}$$

and

$$\Sigma = \left(\begin{array}{ccc|c} k(x_1,x_1) & \ldots & k(x_1,x_n) & k(x_1,x) \\ \vdots & & \vdots & \vdots \\ k(x_n,x_1) & \ldots & k(x_n,x_n) & k(x_n,x) \\ \hline k(x,x_1) & \ldots & k(x,x_n) & k(x,x) \end{array}\right) = \left(\begin{array}{c|c} K_{XX} & k_X(x) \\ \hline k_X(x)^\top & k(x,x) \end{array}\right)$$

where $X = \{x_1, \ldots, x_n\}$, $[K_{XX}]_{ij} = k(x_i, x_j)$ is the Gram/kernel matrix,

Conditional updates of Gaussian processes

Then

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$$\bar{m}(x) = m(x) + k_X(x)^\top K_{XX}{}^{-1}(\mathbf{f} - m_X)$$
$$\bar{k}(x) = k(x,x) - k_X(x)^\top K_{XX}{}^{-1} k_X(x)$$

where

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The prior mean and covariance functions m and k, are replaced by the posterior mean and covariance functions $\bar{m}$ and $\bar{k}$,

Summary: Conditional updates of Gaussian processes

If f is a Gaussian process,

$$f(\cdot) \sim GP(m(\cdot), k(\cdot, \cdot))$$

then if we observe f at $x_1, \ldots, x_n$, then

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where $\bar{m}$ and $\bar{k}$ are the *posterior* mean and covariance functions on the previous slide.

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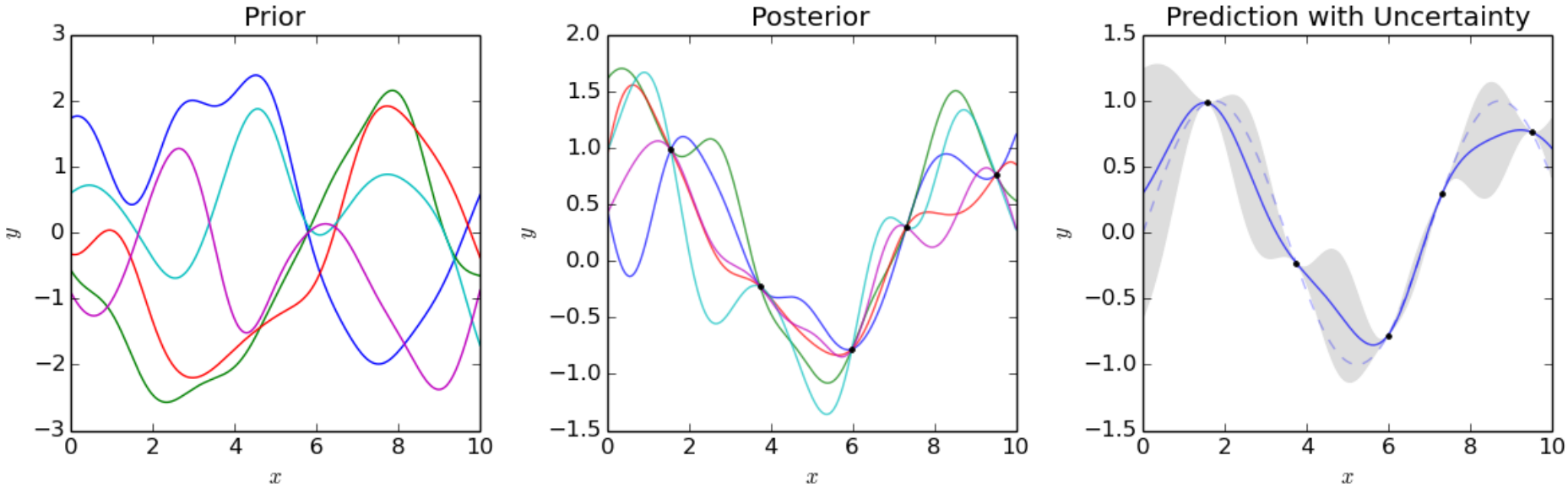
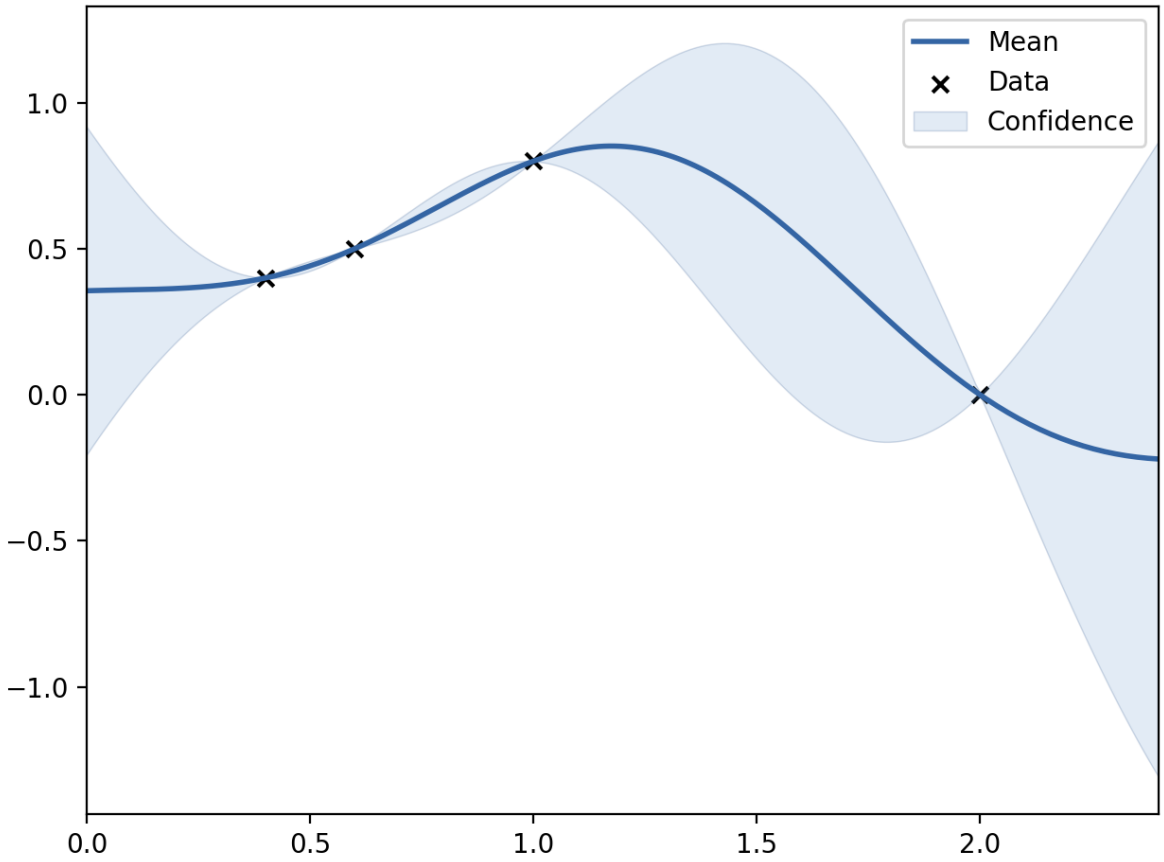
- f is still a GP even though we've observed its value at a number of locations.



No noise/*nugget* - Interpolation



Solid line $\quad \bar{m}(x) = m(x) + k_X(x)^\top K_{XX}^{-1}(\mathbf{f} - m_X)$

Shaded region $\quad \bar{m}(x) \pm 1.96\sqrt{\bar{k}(x)}$

$$\bar{k}(x) = k(x,x) - k_X(x)^\top K_{XX}^{-1} k_X(x)$$

Noisy observations/with nugget - Regression

In practice, we don't usually observe $f(x)$ directly. If we observe

$$y_i = f(x_i) + N(0, \sigma^2)$$

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where

$$\Sigma = \left(\begin{array}{ccc|c} & & & k(x_1, x) \\ & K_{XX} + \sigma^2 I & & k(x_2, x) \\ & & & \vdots \\ & & & k(x_n, x) \\ \hline k(x, x_1) & k(x, x_2) & \ldots \; k(x, x_n) & k(x, x) \end{array}\right)$$

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$$y_1, \ldots, y_n, f(x) \sim N_{n+1}(0, \Sigma)$$

where

$$\Sigma = \left(\begin{array}{ccccc|c} & & & & & k(x_1, x) \\ & & K_{XX} + \sigma^2 I & & & k(x_2, x) \\ & & & & & \vdots \\ & & & & & k(x_n, x) \\ \hline k(x, x_1) & & k(x, x_2) & \ldots & k(x, x_n) & k(x, x) \end{array}\right)$$

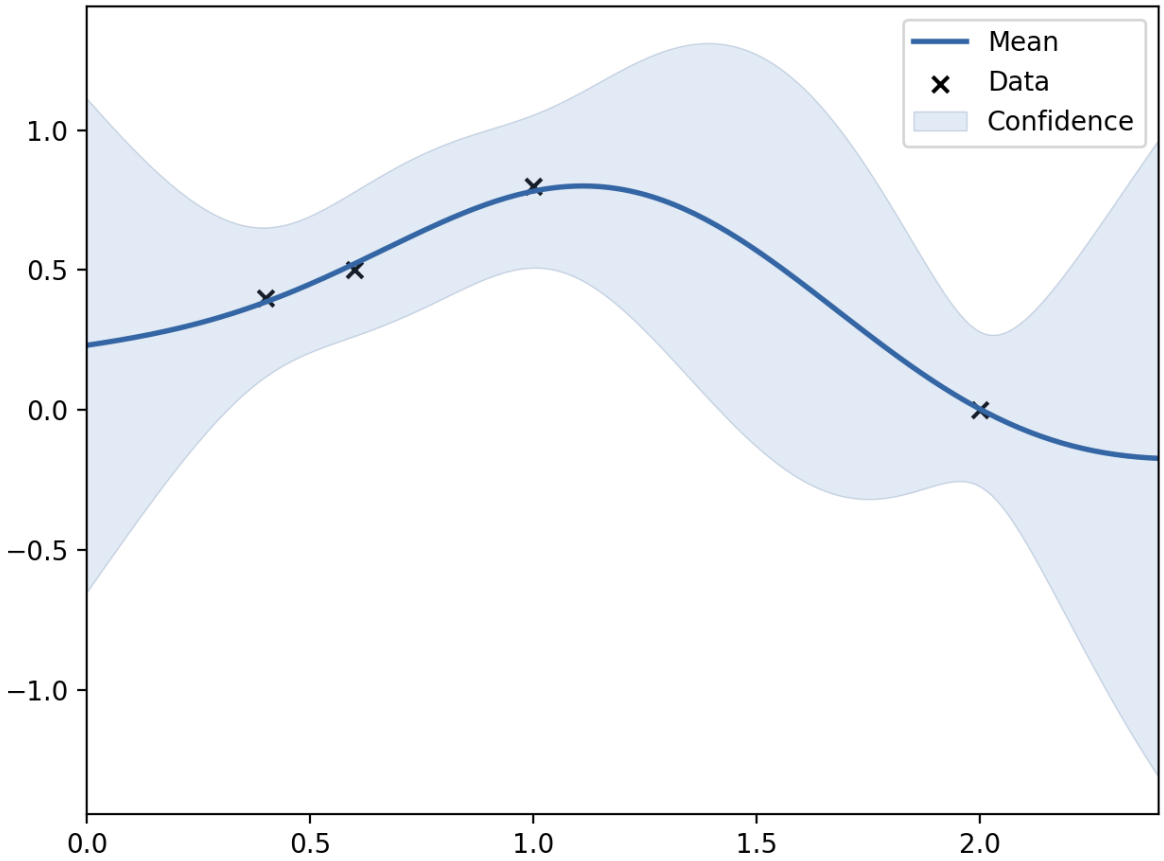
Then

$$f(x) \mid y_1, \ldots, y_n \sim N(\bar{m}(x), \bar{k}(x))$$

where

$$\bar{m}(x) = m(x) + k_X(x)^\top (K_{XX} + \sigma^2 I)^{-1} (\mathbf{y} - m_X)$$
$$\bar{k}(x) = k(x, x) - k_X(x)^\top (K_{XX} + \sigma^2 I)^{-1} k_X(x)$$

Nugget standard deviation $\sigma = 0.1$



Solid line $\quad \bar{m}(x) = m(x) + k_X(x)^\top K_{XX}^{-1}(\mathbf{y} - m_X)$

Shaded region $\quad \bar{m}(x) \pm 1.96\sqrt{\bar{k}(x)}$

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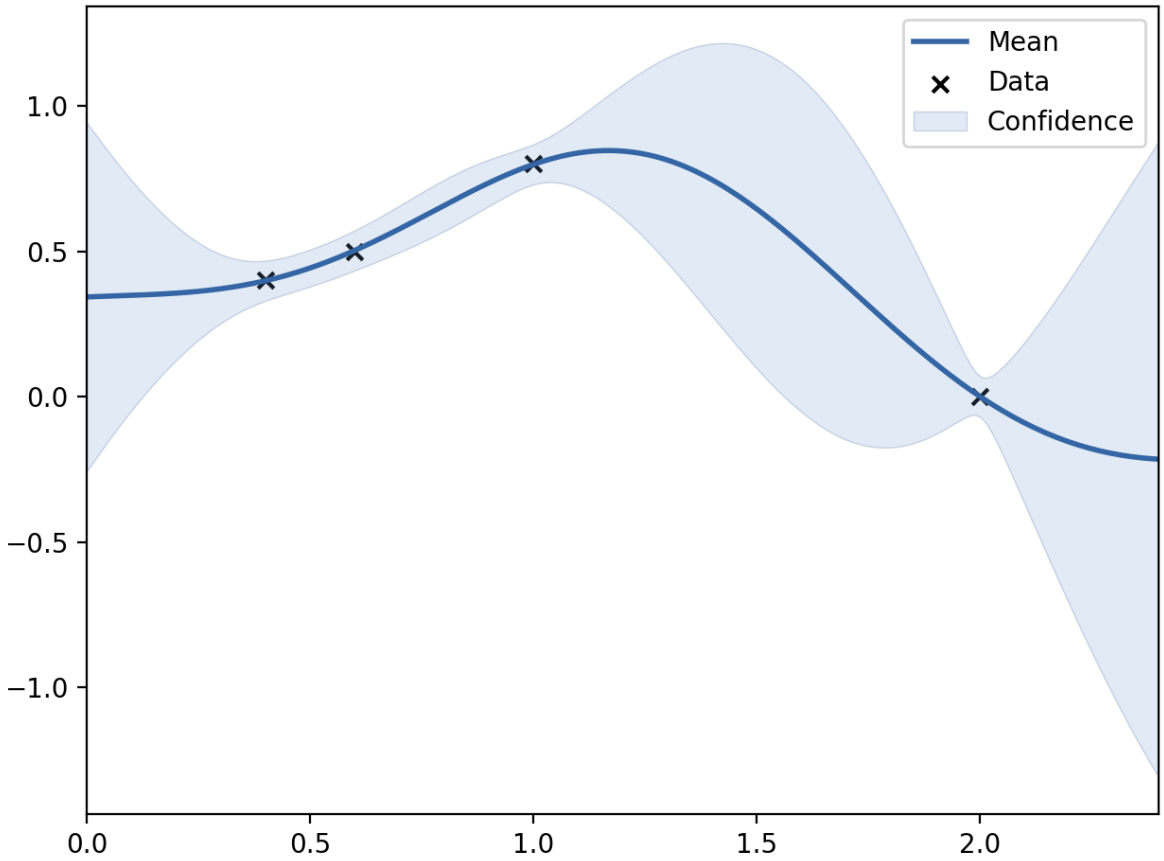
Nugget standard deviation $\sigma = 0.025$



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$$f_1(\cdot), f_2(\cdot) \sim GP \quad \text{then} \quad (f_1 + f_2)(\cdot) \sim GP$$

- Closed under any linear operator. If $f \sim GP(m(\cdot), k(\cdot,\cdot))$, then if $\mathcal{L}$ is a linear operator

$$\mathcal{L} \circ f \sim GP(\mathcal{L} \circ m, \mathcal{L}^2 \circ k)$$

e.g. $\frac{df}{dx}$, $\int f(x)dx$, Af are all GPs

Motivation for non-parametric models

Functions live in function spaces (vector spaces with inner products). There are lots of different function spaces: the GP kernel k implicitly determines a particular (RKHS) function/hypothesis space

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Although reality may not lie in the RKHS defined by k, this space is much richer than any parametric regression model[3],

- thus is more likely to contain a function close to the truth than any finite dimensional class of functions (eg linear models)

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3. Possibly try a few k (plus a few combinations), and use empirical evaluation to make a good choice.

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likelihood = gpt.likelihoods.GaussianLikelihood()
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4. Optimize the hyper parameters;

```
optimizer = torch.optim.Adam(model.parameters(), lr=0.1)
mll = gpt.mlls.ExactMarginalLogLikelihood(likelihood, model)
for i in range(1000):
    output = model(X)
    loss = -mll(output, y)
    loss.backward()
    optimizer.step()
```

Software

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There are many other Python (and R, Julia., Matlab,...) GP packages

- GPy - easy to use, no longer supported, hard to modify
- GPerks - easy to use, but limited functionality and hard to modify
- GPflow - uses tensorflow and is similar to GPyTorch
- ...

Benefits of GPs: Uncertainty estimates

GP predictions consist of two parts:

- point estimate $m(x) = \mathbb{E}f(x)$
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- Something that assesses the uncertainty quantification:
  - Coverage: e.g., what % of predictions lie in the GP 90% credible interval?
- Predictive log-likelihood (or another proper score) - assesses both aspects (point and uncertainty) but hard to interpret - best for comparing different covariance functions.

Problems with hyper-parameter optimization

The likelihood surface that is maximized in hyper-parameter estimation is often flat and multi-modal,

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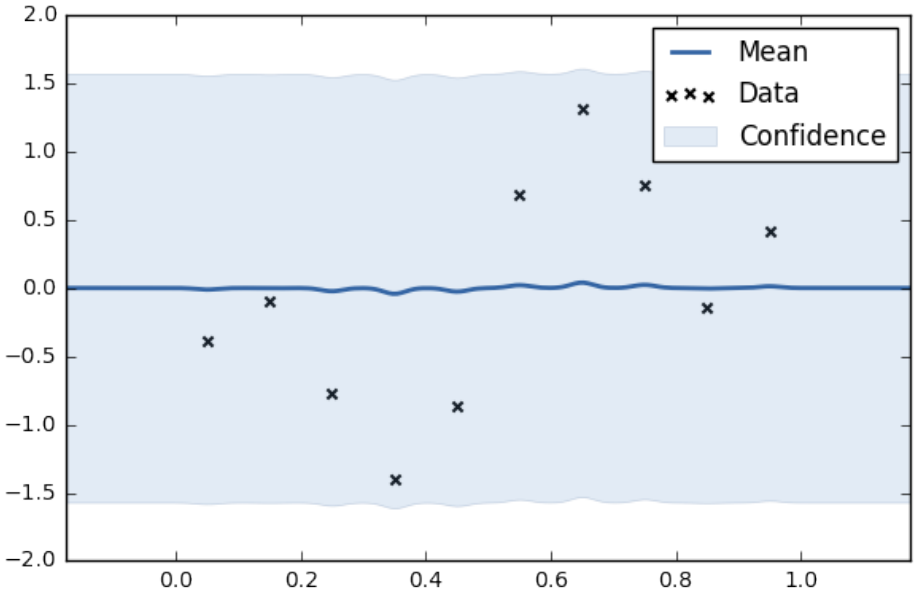

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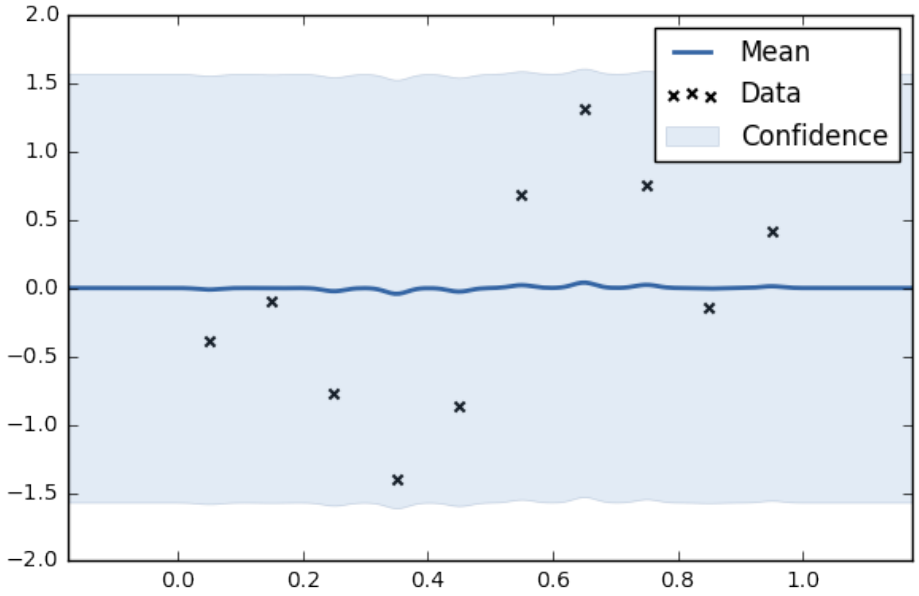

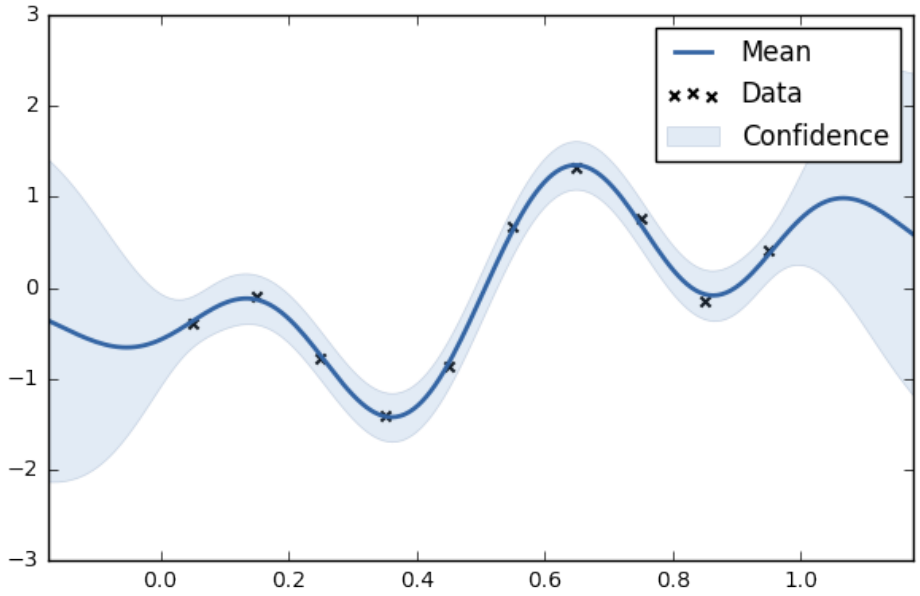

Work around these problems by running the optimizer multiple times from random start points, using prior distributions, constraining or fixing hyper-parameters, or adding white noise.

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It is possible now to do GP regression with $\sim 10^{6-7}$ data points.

- But GPs are primarily used in the low-data regime ($n \leq 10^4$), with neural networks a more popular choice if big datasets are available.

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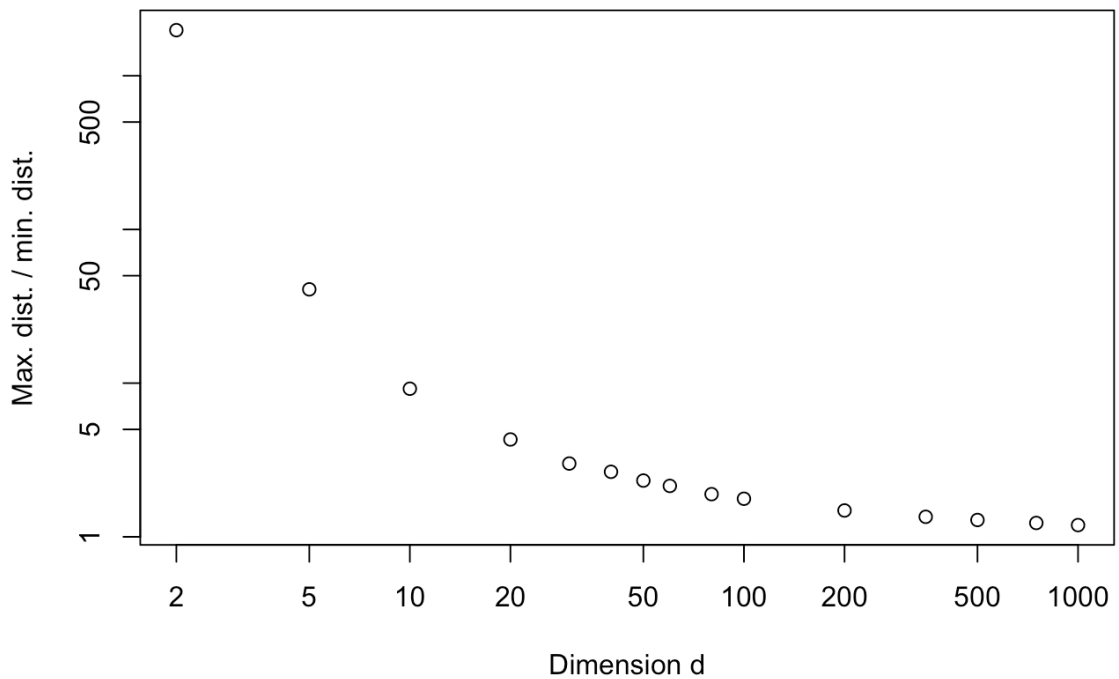

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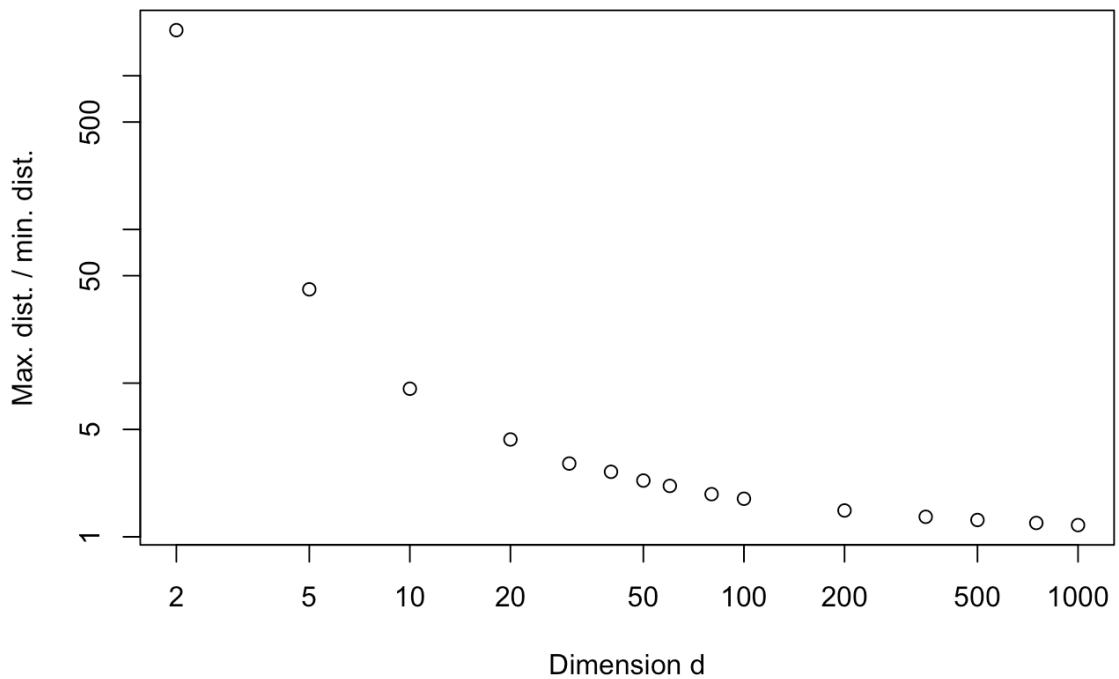


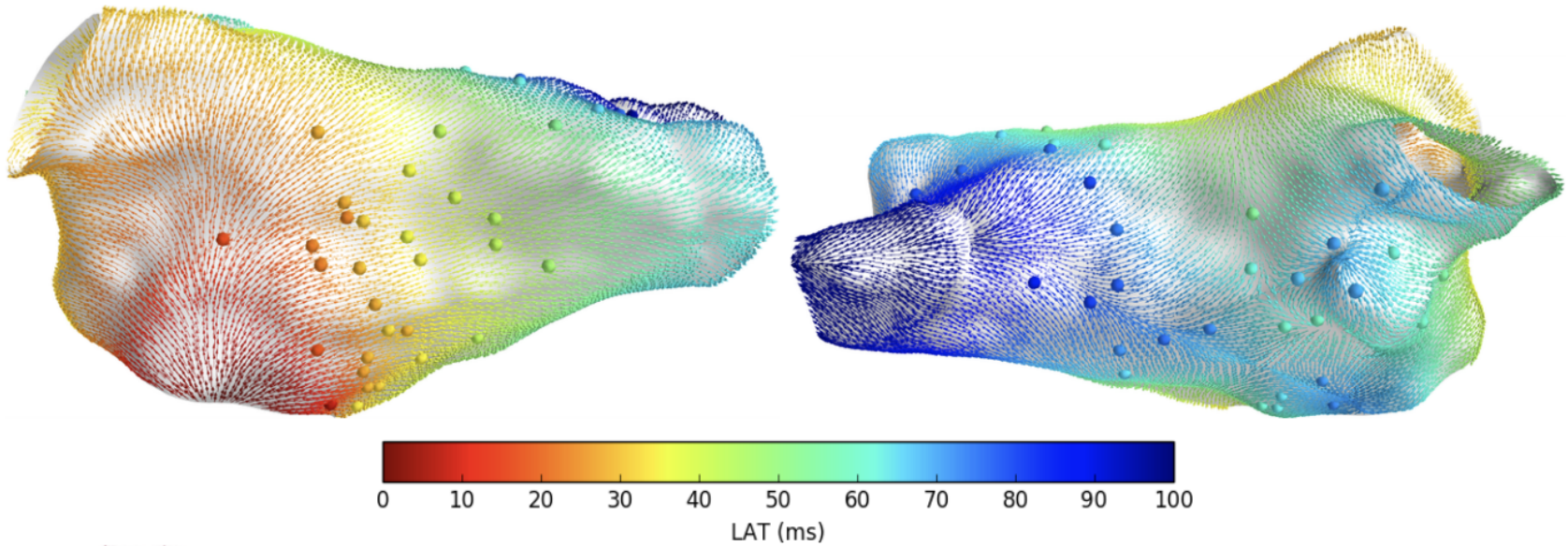
Can use dimension reductions to try to find informative low-dimensional manifolds: PCA, sensitivity analysis, random projection...

Example of GPs in Cardiac Digital Twins: Interpolating LATs

Coveney *et al.* 2019, 2020

We want to estimate activation times at all locations on the atria (the *LAT map*)

- Typically, only able to measure LAT a small number ($\sim$10) of locations on the atrium.



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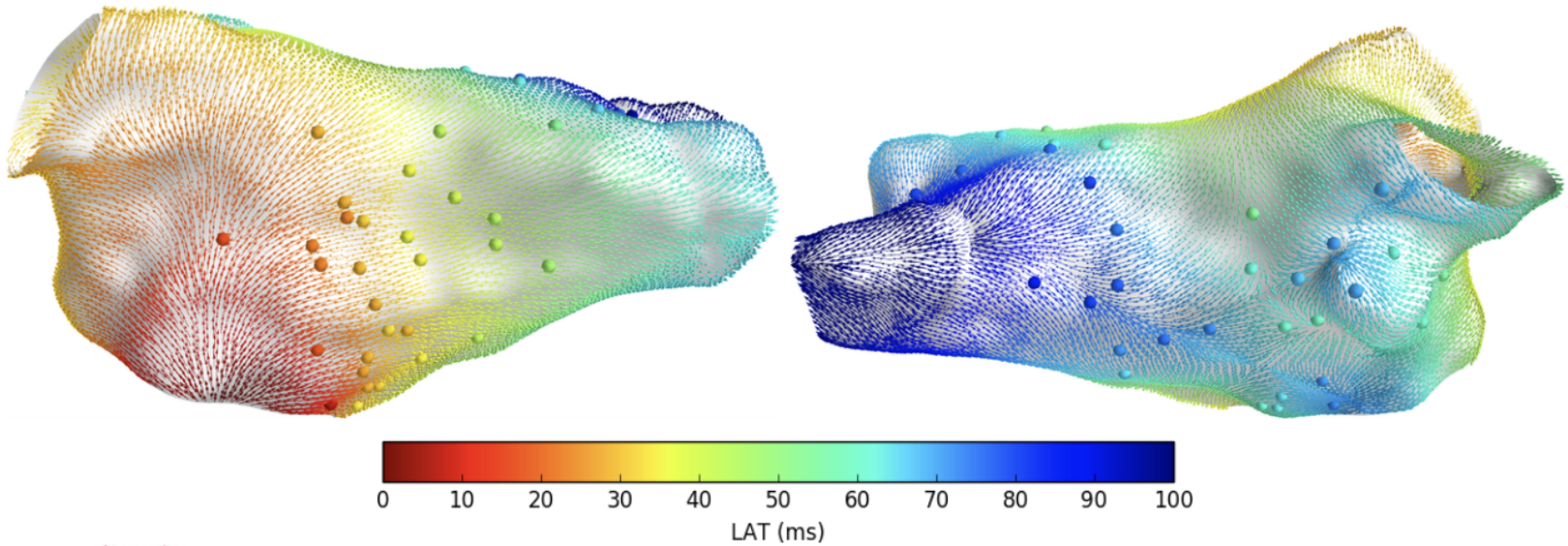


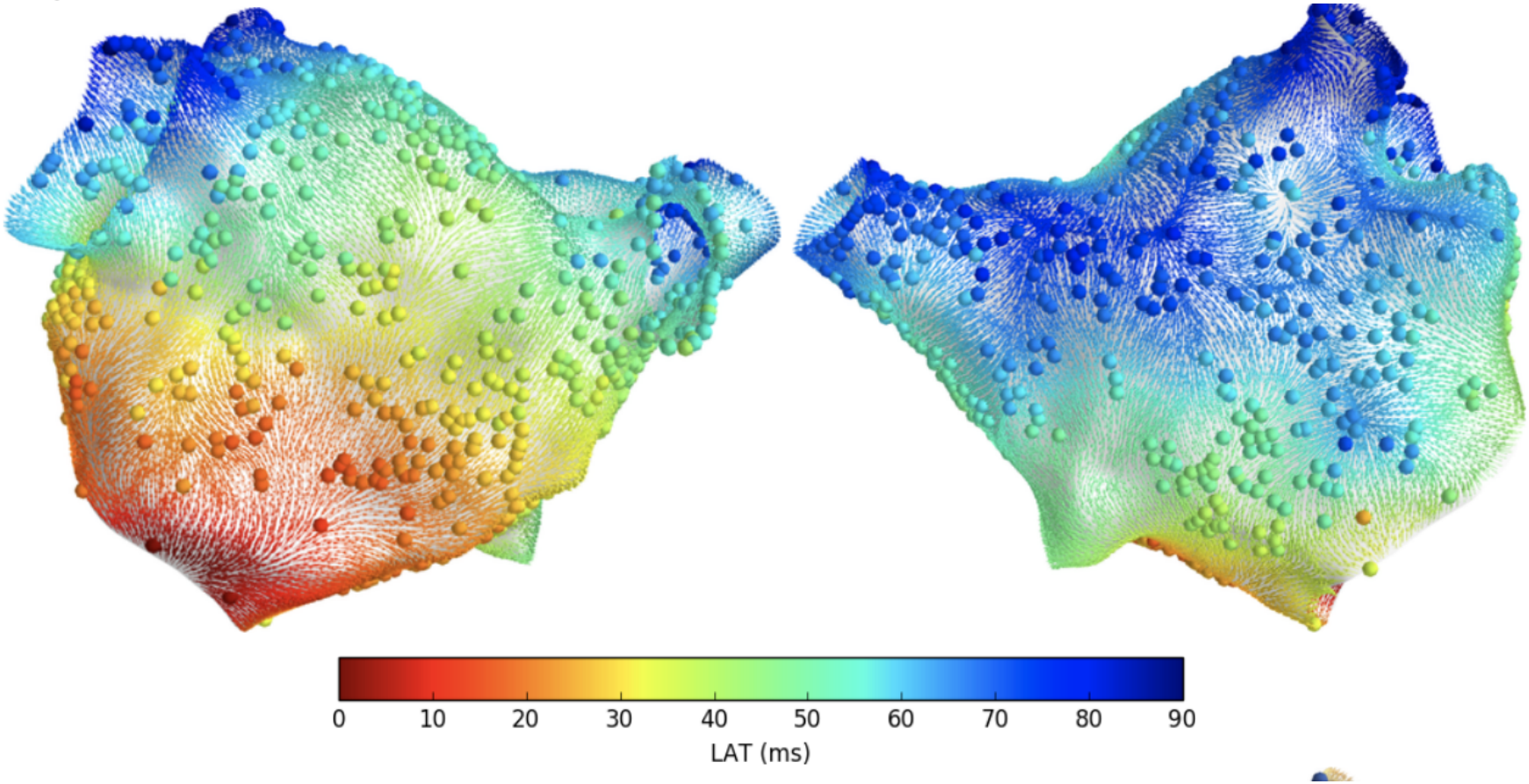
How can we interpolate to other locations and estimate conduction velocities?

$$LAT_{obs}(x) = \mathrm{LAT}_{true}(x) + \epsilon$$

Results

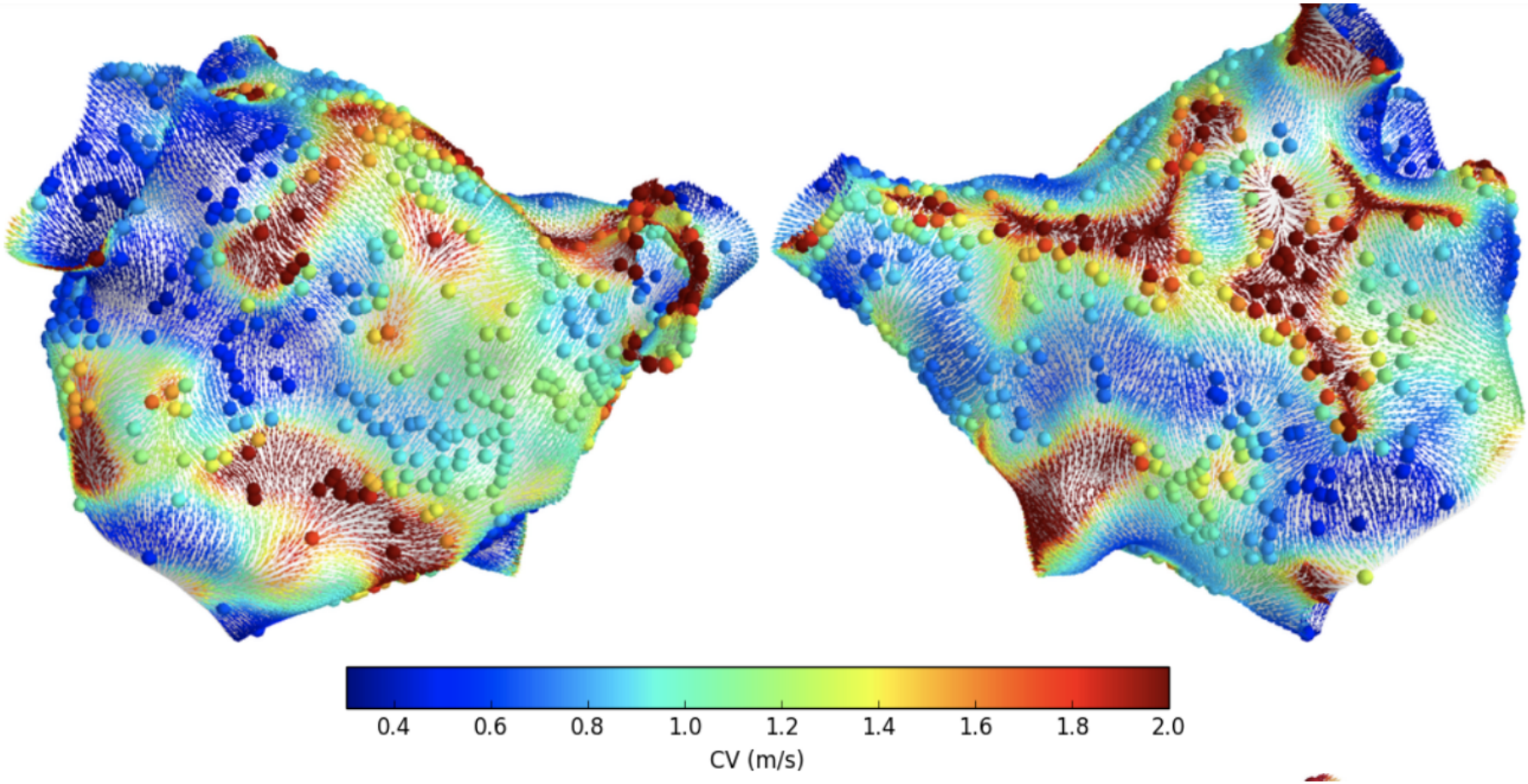
Coveney *et al.* 2019, 2020

Using a basis function approach we can model on the atrial manifold:



Results

Because GPs are differentiable, the approach easily gives conduction velocity:



Conclusions

- GPs are now ubiquitous in statistics/ML, and a key part of the cardiac digital twin pipeline.
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Thank you for listening!

References

- Rasmussen and Williams. *Gaussian processes for machine learning*. MIT press, 2006.
- Stein. *Interpolation of Spatial Data: Some Theory for Kriging*. Springer, 1999
- Kanagawa, Hennig, Sejdinovic, and Sriperumbudur. *Gaussian processes and kernel methods: A review on connections and equivalences.*. arXiv:1807.02582 2018.
- Many tutorial talks available at `gpss.cc`

Why use GPs? Answer 3: Naturalness of GP framework

Why use **Gaussian** processes as non-parametric models?

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If we only knew the expectation and variance of some random variables, X and Y, then how should we best do statistics?

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Why use **Gaussian** processes as non-parametric models?

If we only knew the expectation and variance of some random variables, X and Y, then how should we best do statistics?

It has been shown, using coherency arguments, or geometric arguments, or..., that the best second-order inference we can do is to update our beliefs about X given Y using

$$\mathbb{E}(X|Y) = \mathbb{E}(X) + \mathbb{C}\text{ov}(X, Y)\mathbb{V}\text{ar}(Y)^{-1}(Y - \mathbb{E}(Y))$$

i.e., exactly the Gaussian process update for the posterior mean.

So GPs are in some sense second-order optimal.

Kriging

Kriging

Suppose $Y(x)$ is a (second order stationary) stochastic process with

$$\mathbb{E}Y(x) = \mu \; \forall \; x$$
$$\mathbb{C}\text{ov}(Y(x), Y(x')) = k(x - x') \; \forall \; x, x'$$

NB we're not assuming Y has a Gaussian distribution.

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If someone tells you $\mathbf{y} = (Y(x_1), \ldots, Y(x_n))^\top$, how would you predict $Y(x)$?
One option is to find the best linear unbiased predictor (BLUP) of $Y(x)$.

Best Linear Unbiased Predictors (BLUP)

Consider the linear estimator

$$\hat{Y}(x) = c + \sum w_i Y(x_i) = c + \mathbf{w}^\top \mathbf{y}$$

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If we require $\hat{Y}(x)$ to be unbiased,

$$\begin{aligned} \mu &= \mathbb{E}\hat{Y}(x) \\ &= \mathbb{E}(c + \mathbf{w}^\top \mathbf{y}) \\ &= c + \mathbf{w}^\top \boldsymbol{\mu} \end{aligned}$$

where $\boldsymbol{\mu} = (\mu, \ldots, \mu)^\top$.

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Thus $c = \mu - \mathbf{w}^\top \boldsymbol{\mu}$ and we must have

$$\hat{Y}(x) = \mu + \mathbf{w}^\top (\mathbf{y} - \boldsymbol{\mu})$$

Best Linear Unbiased Predictors (BLUP) - II

The best linear unbiased predictor minimises the mean square error

$$
\begin{aligned}
MSE(\hat{Y}(x)) &= \mathbb{E}((\hat{Y}(x) - Y(x))^2) \\
&= \mathbb{E}\left((\mathbf{w}^\top(\mathbf{y} - \boldsymbol{\mu}) + (\mu - Y(x))^2\right) \\
&= \mathbf{w}^\top \mathbb{V}\mathrm{ar}(\mathbf{y})\mathbf{w} + \mathbb{V}\mathrm{ar}(Y(x)) - 2\mathbf{w}^\top \mathbb{C}\mathrm{ov}(\mathbf{y}, Y(x)) \\
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If we differentiate wrt w and set the gradient equal to zero, we find

$$0 = 2K_{XX}\mathbf{w} - 2\mathbf{k}_X(x)$$

Best Linear Unbiased Predictors (BLUP) - II

The best linear unbiased predictor minimises the mean square error

$$\begin{aligned} MSE(\hat{Y}(x)) &= \mathbb{E}((\hat{Y}(x) - Y(x))^2) \\ &= \mathbb{E}\left((\mathbf{w}^\top(\mathbf{y} - \boldsymbol{\mu}) + (\mu - Y(x))^2\right) \\ &= \mathbf{w}^\top \mathbb{V}\mathrm{ar}(\mathbf{y})\mathbf{w} + \mathbb{V}\mathrm{ar}(Y(x)) - 2\mathbf{w}^\top \mathbb{C}\mathrm{ov}(\mathbf{y}, Y(x)) \\ &= \mathbf{w}^\top K_{XX}\mathbf{w} + k(0) - 2\mathbf{w}^\top \mathbf{k}_X(x) \end{aligned}$$

If we differentiate wrt w and set the gradient equal to zero, we find

$$0 = 2K_{XX}\mathbf{w} - 2\mathbf{k}_X(x)$$

and thus

$$\hat{Y}(x) = \mu + \mathbf{k}_X(x)^\top K_{XX}^{-1}(\mathbf{y} - \mu)$$

as before.

So the Gaussian process posterior mean is optimal (i.e. is the BLUP) even if we don't assume Gaussianity.

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We can also view GPs as a non-parametric extension to linear regression.

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$$\text{as} \qquad (X^\top X + \sigma^2 I) X^\top = X^\top (XX^\top + \sigma^2 I)$$

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But the dual form only uses inner products between vectors in $\mathbb{R}^n$

$$XX^\top = \begin{pmatrix} x_1^\top \\ \vdots \\ x_n^\top \end{pmatrix} (x_1 \dots x_n) = \begin{pmatrix} x_1^\top x_1 & \dots & x_1^\top x_n \\ \vdots & & \\ x_n^\top x_1 & \dots & x_n^\top x_n \end{pmatrix}$$

$$= K_{XX} \text{ if } k(x, x') = x^\top x'$$

— This is useful!

Prediction

The best prediction of y at a new location x' is

$$\begin{aligned}\hat{y}' &= x'^{\top}\hat{\beta} \\ &= x'^{\top}X^{\top}(XX^{\top}+\sigma^2 I)^{-1}y \\ &= k_X(x')^{\top}(K_{XX}+\sigma^2 I)^{-1}y\end{aligned}$$

where $k_X(x')^{\top} := (x'^{\top}x_1, \ldots, x'^{\top}x_n)$ and $[K_{XX}]_{ij} := x_i^{\top}x_j$

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Note this is the GP conditional mean we derived before with $m(x) = 0$.

$$m(x) = k_X(x)^\top (K_{XX} + \sigma^2 I)^{-1} y$$

- linear regression and GP regression are equivalent when $k(x, x') = x^\top x'$.

Including features I

We can replace x by a feature vector in linear regression, e.g., $\phi(x) = (1\ x\ x^2)$

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Note $k(x', x) = \phi(x')^{\top} \phi(x)$ is a semi-definite function for any choice of $\phi(x)$.

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E.g., Consider $\mathcal{X} = \mathbb{R}^2$ and let

$$\phi : \mathbf{x} = (x_1, x_2) \mapsto (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2)^\top$$

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Then

$$\begin{aligned} k(\mathbf{x}, \mathbf{z}) &= \phi(x)^\top \phi(z) \\ &= (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2)(1, \sqrt{2}z_1, \sqrt{2}z_2, z_1^2, \sqrt{2}z_1z_2, z_2^2)^\top \\ &= (1 + (x_1, x_2)(z_1, z_2)^\top)^2 \\ &= (1 + \mathbf{x}^\top \mathbf{z})^2 \end{aligned}$$

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Theorem: A function

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is positive semi-definite (and thus a valid covariance function) if and only if we can write

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So GP regression with k can be thought of as linear regression with $\phi(x)$.

Example: If $\mathcal{X} = \mathbb{R}$, set $\phi_c(x) = e^{-\frac{(x-c_0)^2}{2\lambda^2}}$ and

$$\phi^N(x) = \frac{1}{\sqrt{N}}(\phi_{c_0}(x), \ldots, \phi_{c_N}(x))$$

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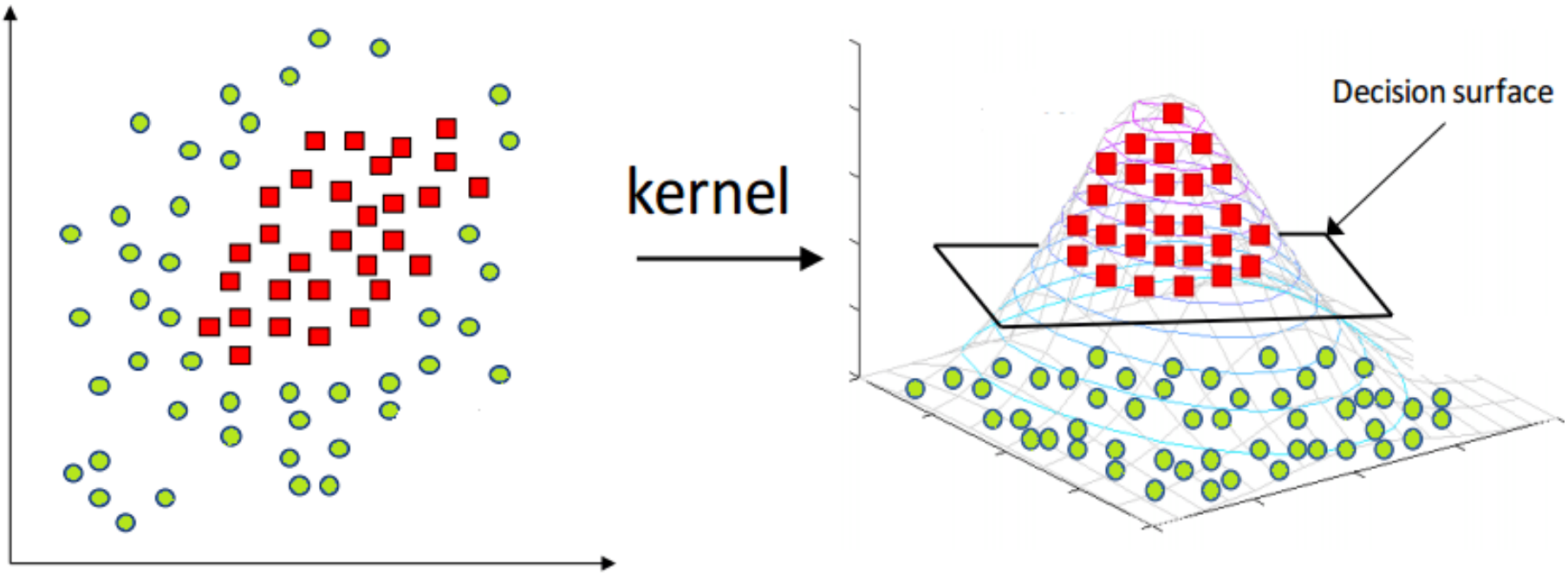
We can use an infinite dimensional feature vector $\phi(x)$, and because linear regression can be done solely in terms of inner-products (inverting a $n \times n$ matrix in the dual form) we never need evaluate the feature vector, only the kernel.

Kernel trick:

lift x into feature space by replacing inner products $x^\top x'$ by $k(x, x')$



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Note: $\bar{m}(\cdot) \in \mathcal{H}_k$ but samples from a GP live in a slightly larger RKHS.