An introduction to Gaussian Processes

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University of Nottingham

GP summer school
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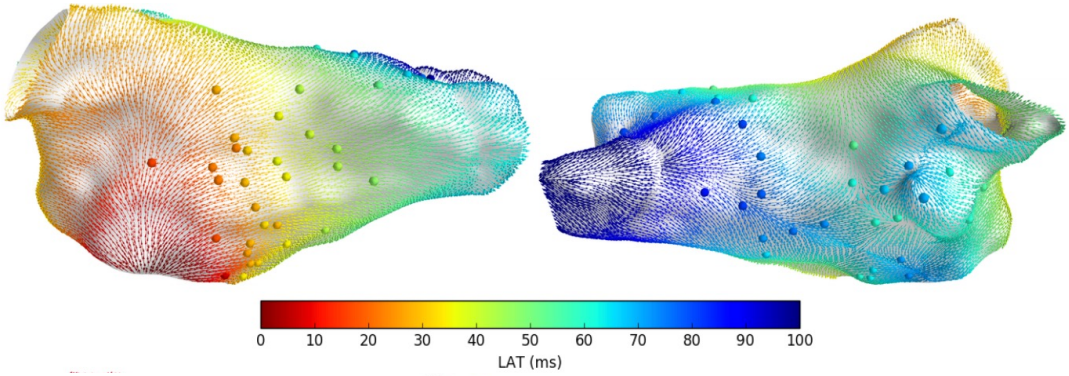
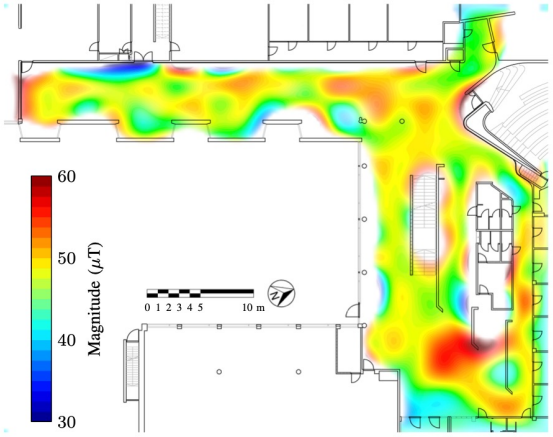
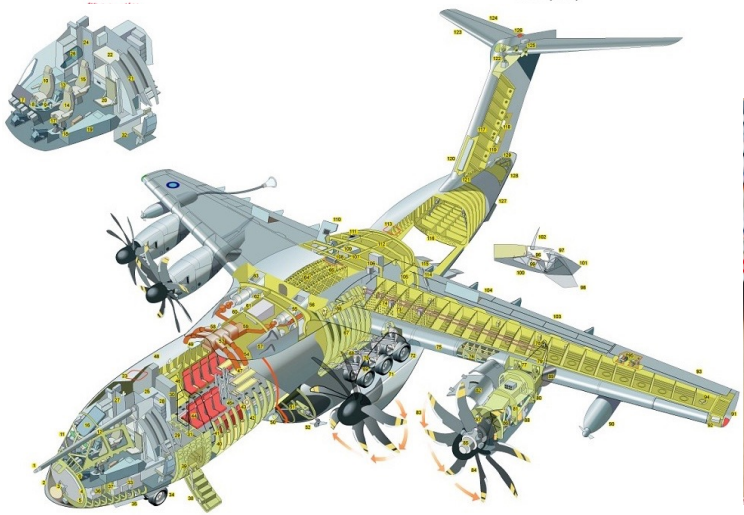
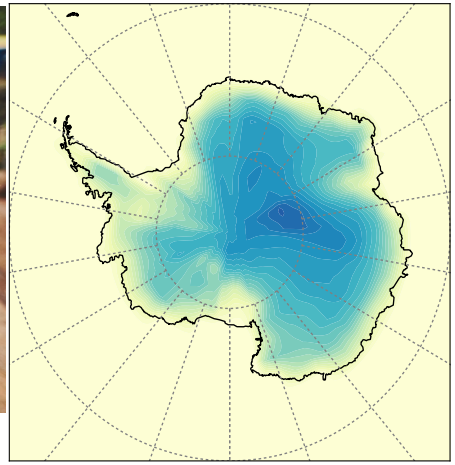
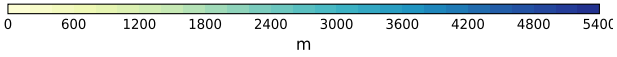
Recent GP Applications









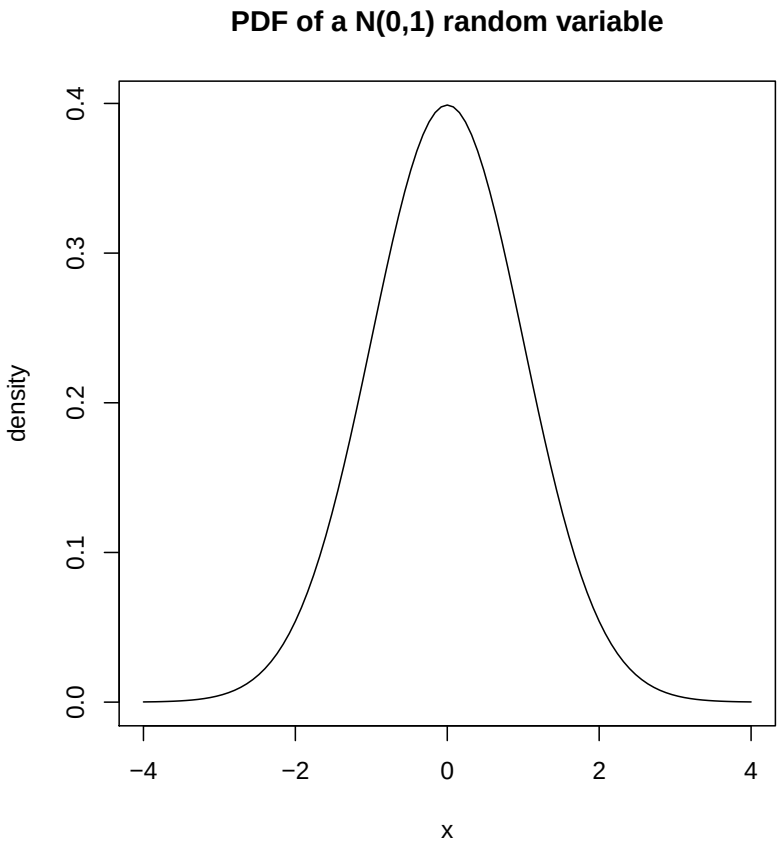


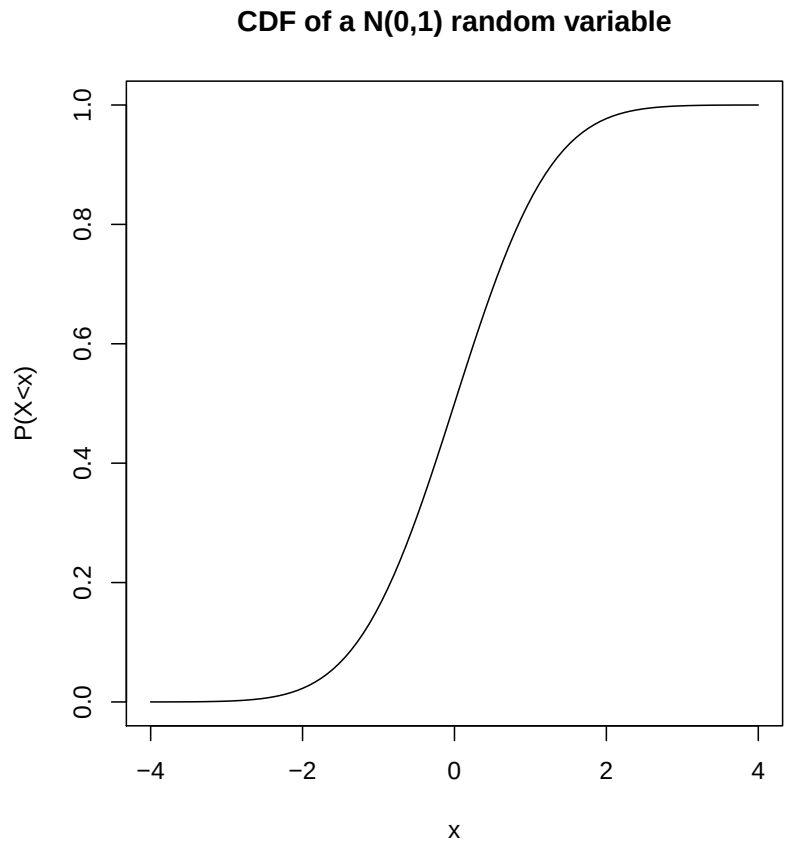
Introduction

- (Multivariate) Gaussian distributions
- Definition of Gaussian processes
- Motivations and derivations
- Difficulties

You can download a copy of these slides from `www.gpss.cc`

Univariate Gaussian distributions





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

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

CDF: $F_Y(y) = \mathbb{P}(Y \leq y)$ not known in closed form

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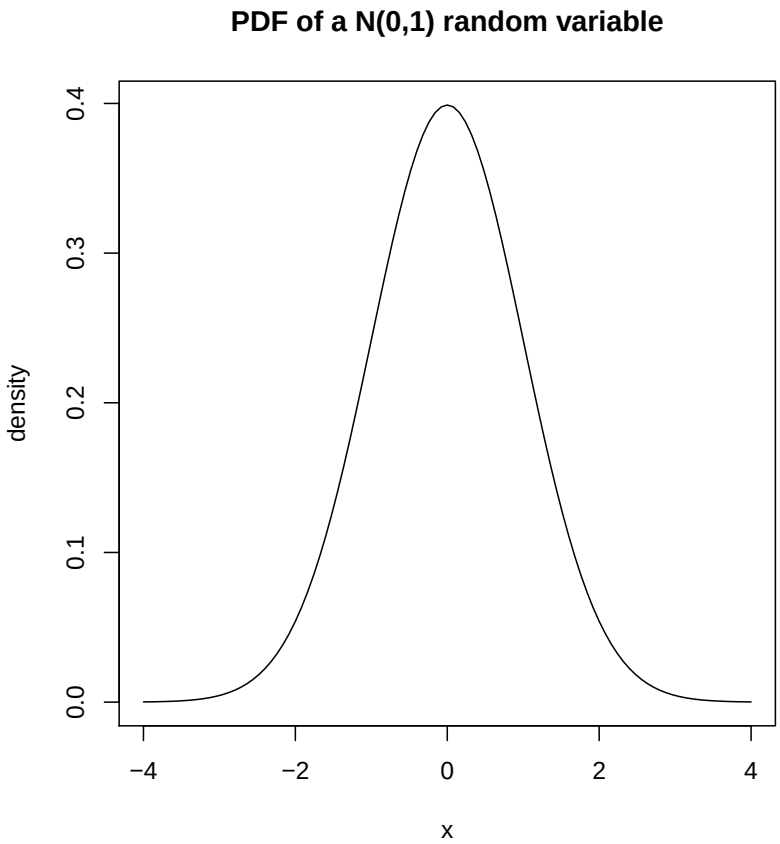

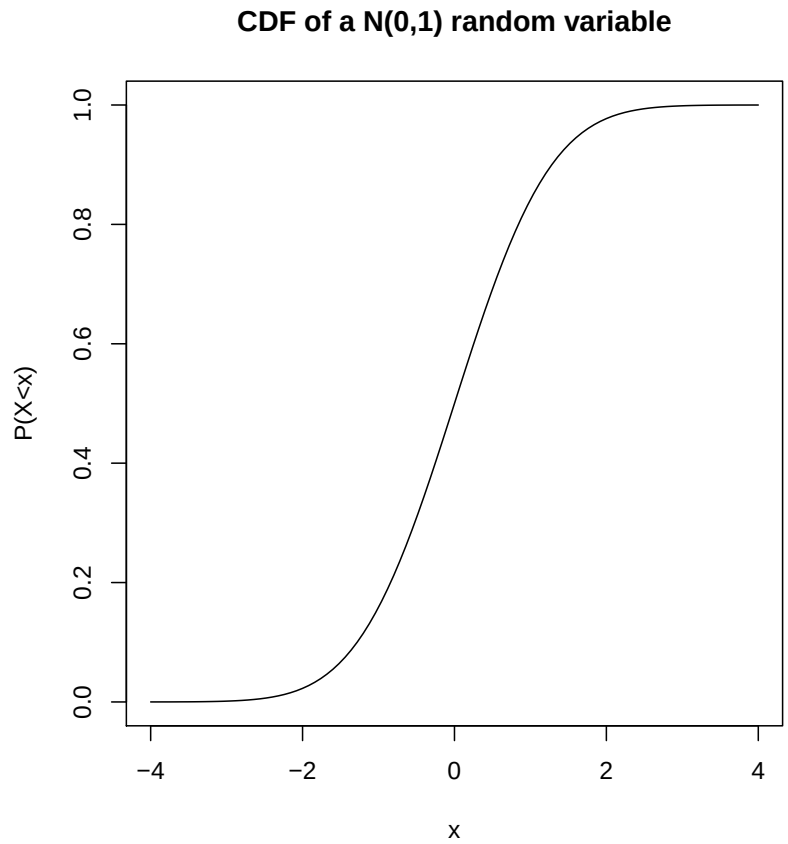

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If $Z \sim N(0,1)$ then $Y = \mu + \sigma Z \sim N(\mu, \sigma^2)$

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The normal/Gaussian distribution occurs naturally and is convenient mathematically

[1] max. ent. principle: the distribution with the largest entropy should be used as a least-informative default

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- Square-loss functions lead to procedures that have a Gaussian probabilistic interpretation
  eg Fit model $f_\beta(x)$ to data y by mimizing $\sum(y_i - f_\beta(x_i))^2$ is equivalent to maximum likelihood estimation under the assumption that $y = f_\beta(x) + \epsilon$ where $\epsilon \sim N(0, \sigma^2)$.

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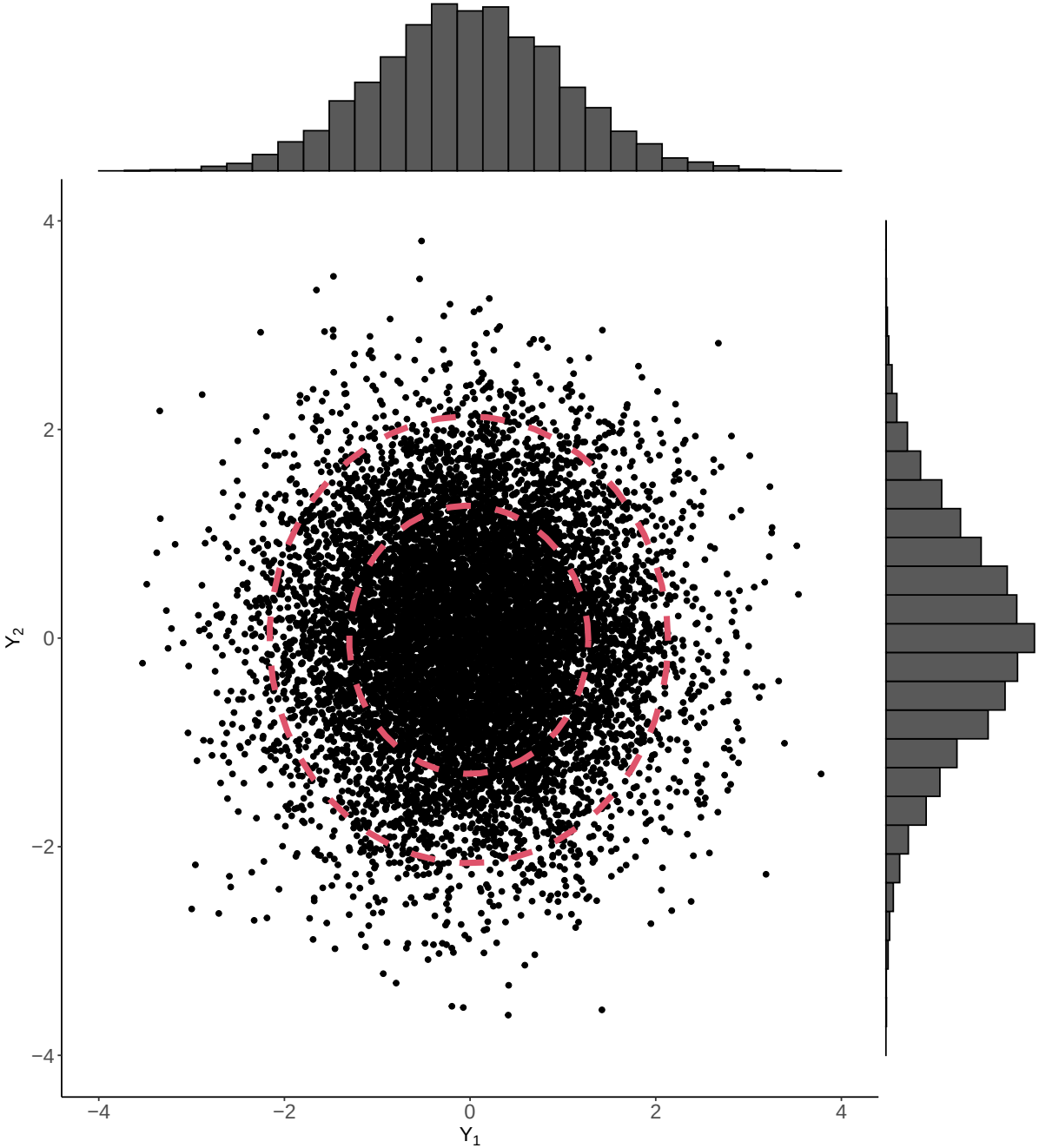
$$\text{pdf:} \quad f(y \mid \mu, \Sigma) = |\Sigma|^{-\frac{1}{2}}(2\pi)^{-\frac{d}{2}} \exp\left(-\frac{1}{2}(y-\mu)^\top \Sigma^{-1}(y-\mu)\right)$$



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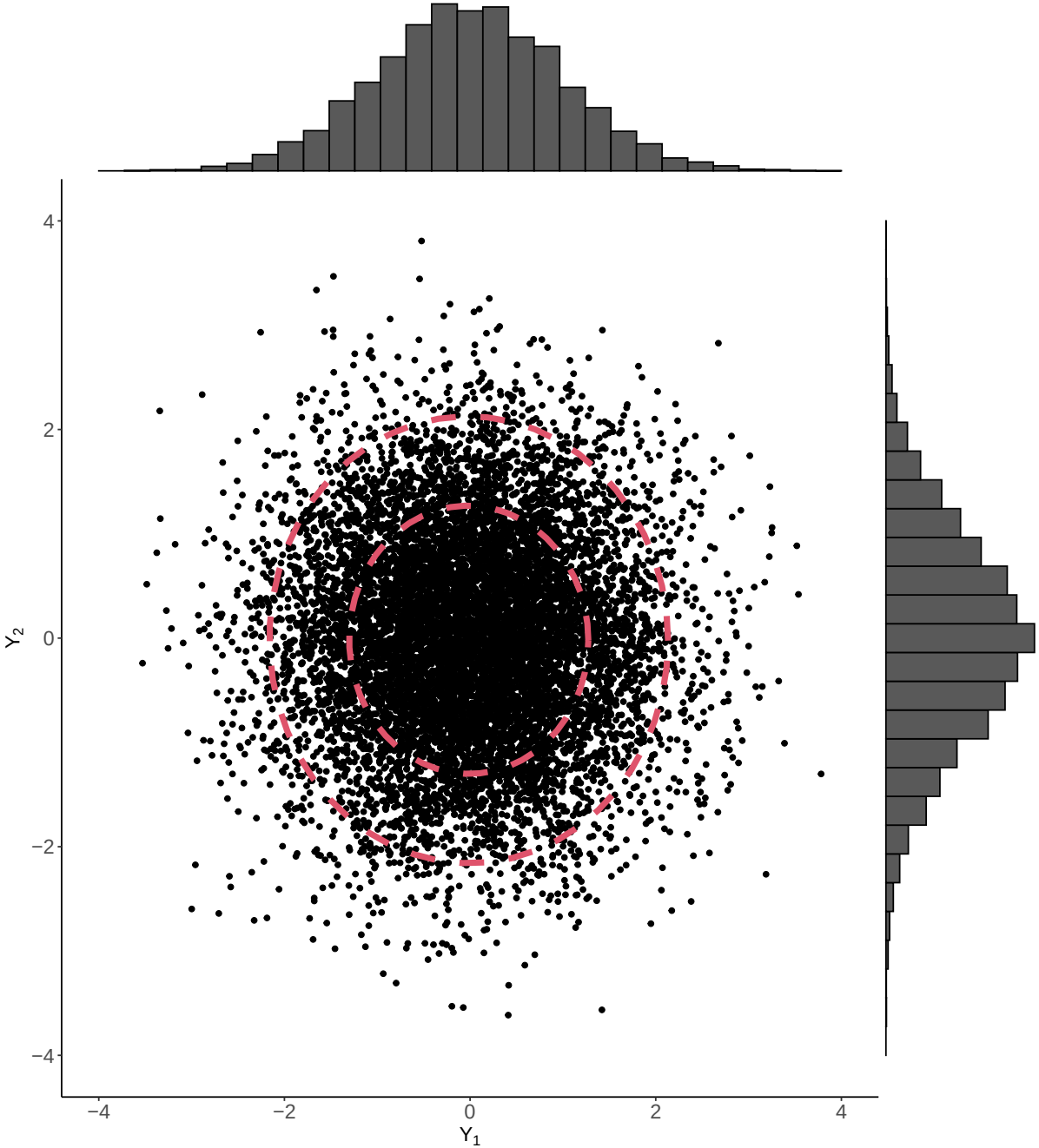

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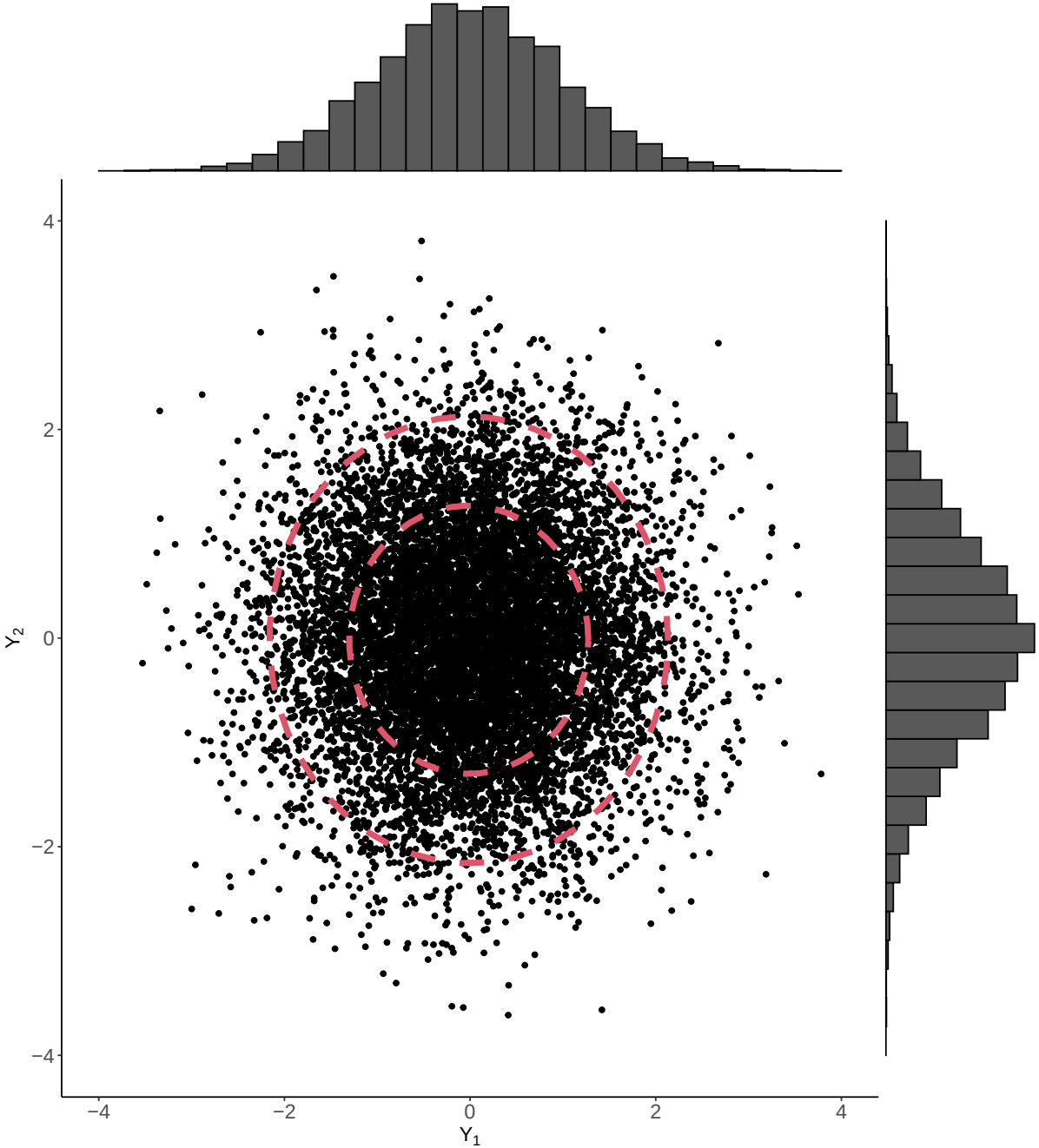
hence Y_1
independent of Y_2



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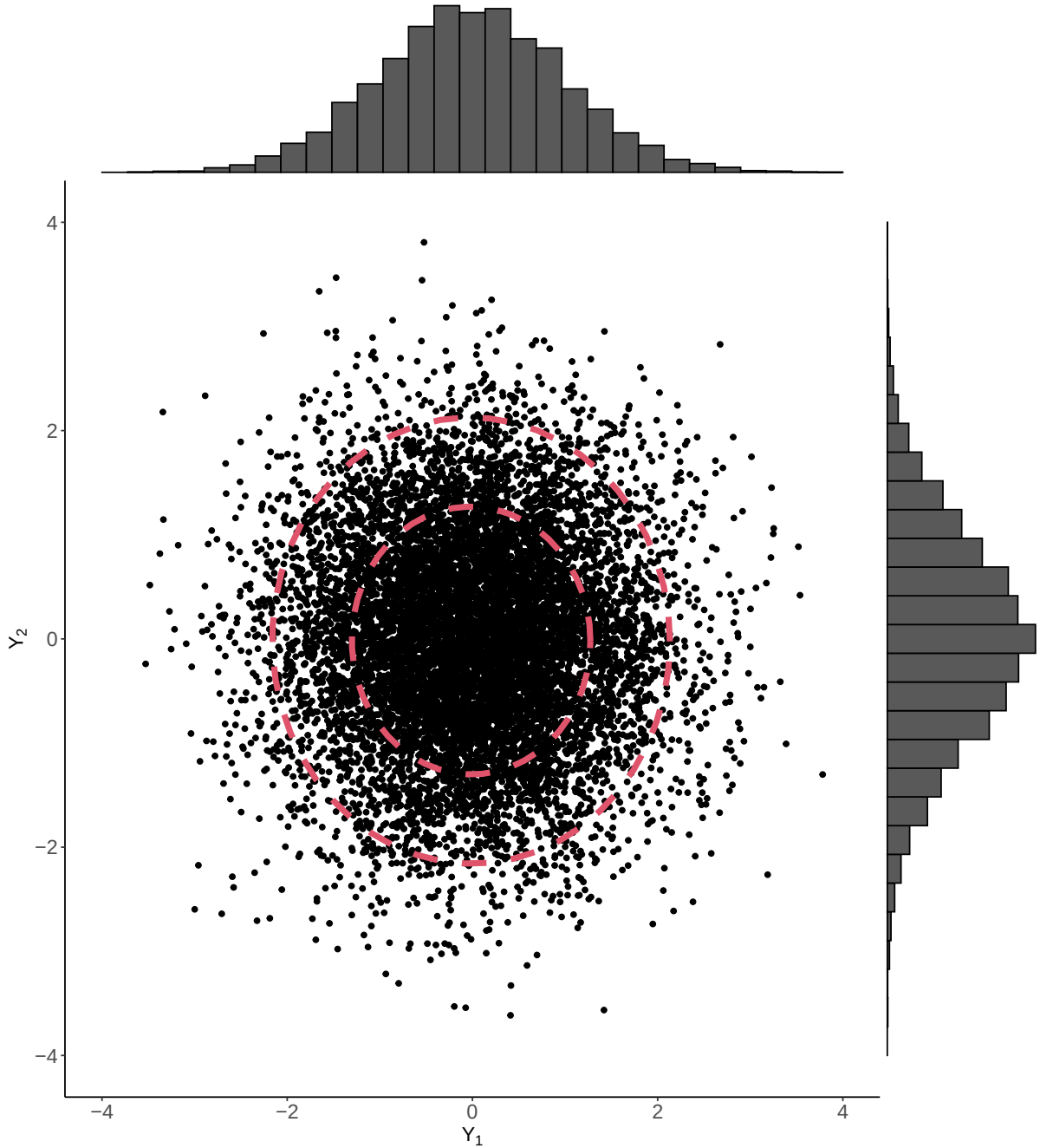

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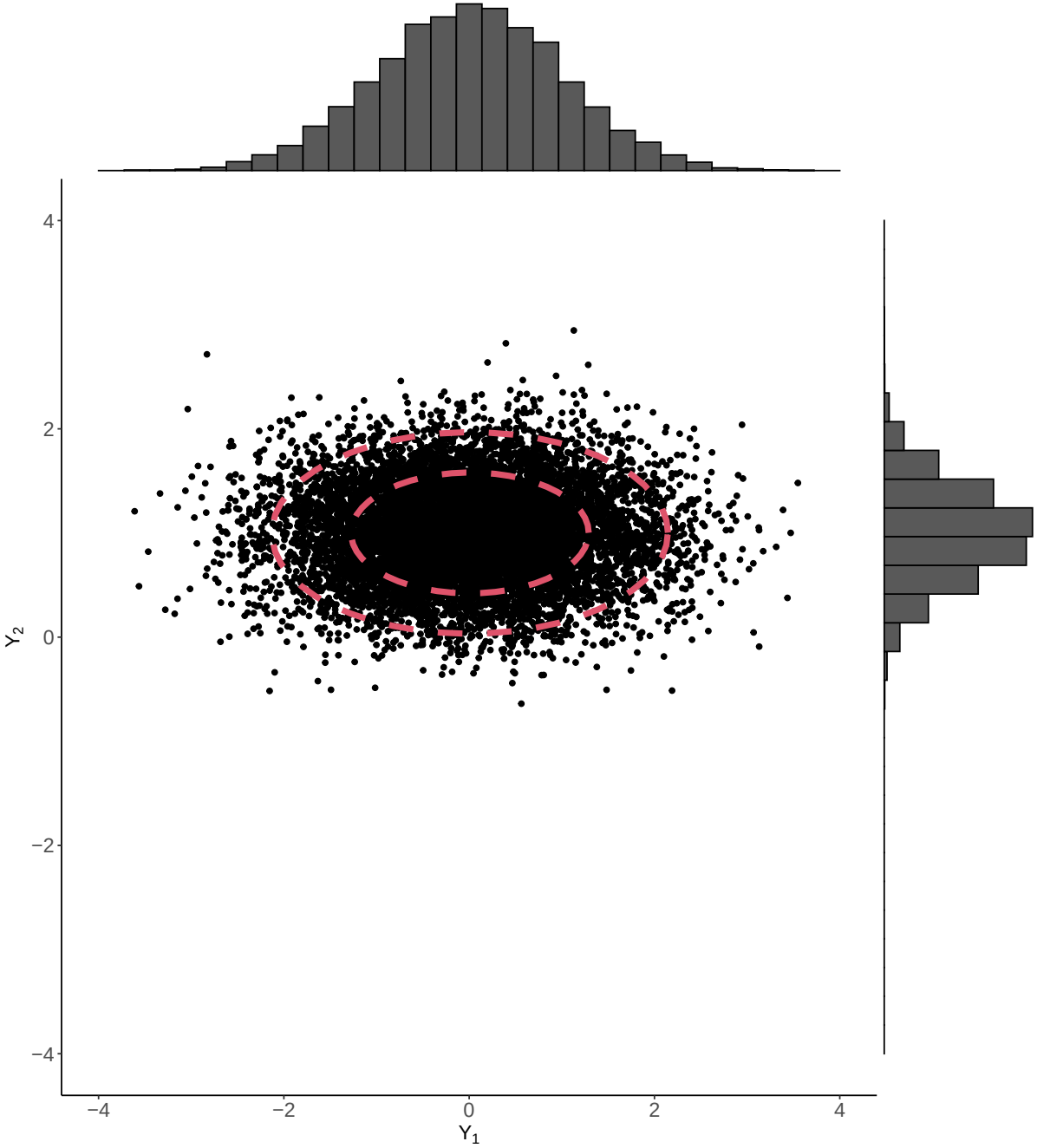
Conditional distributions:

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

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



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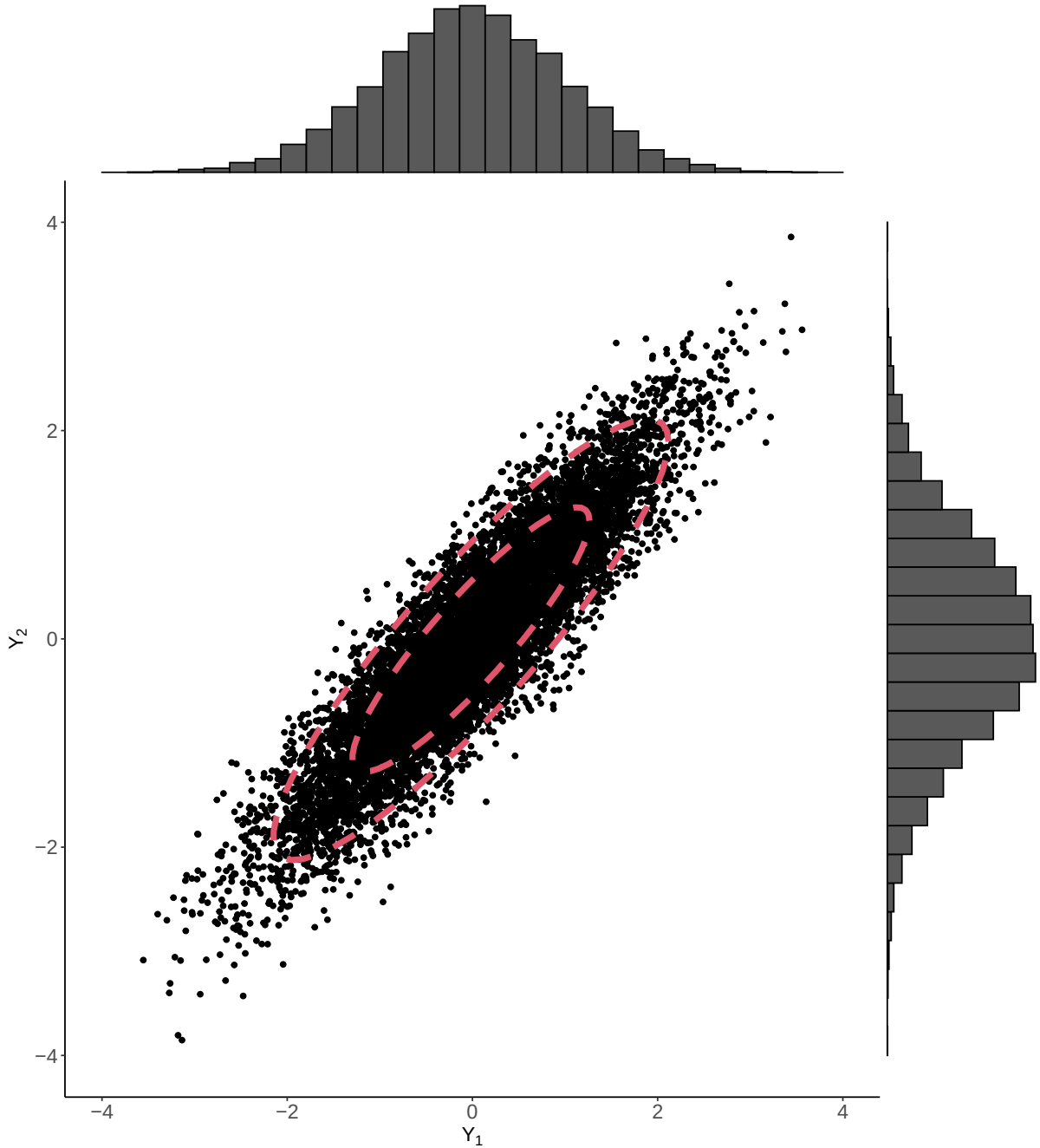
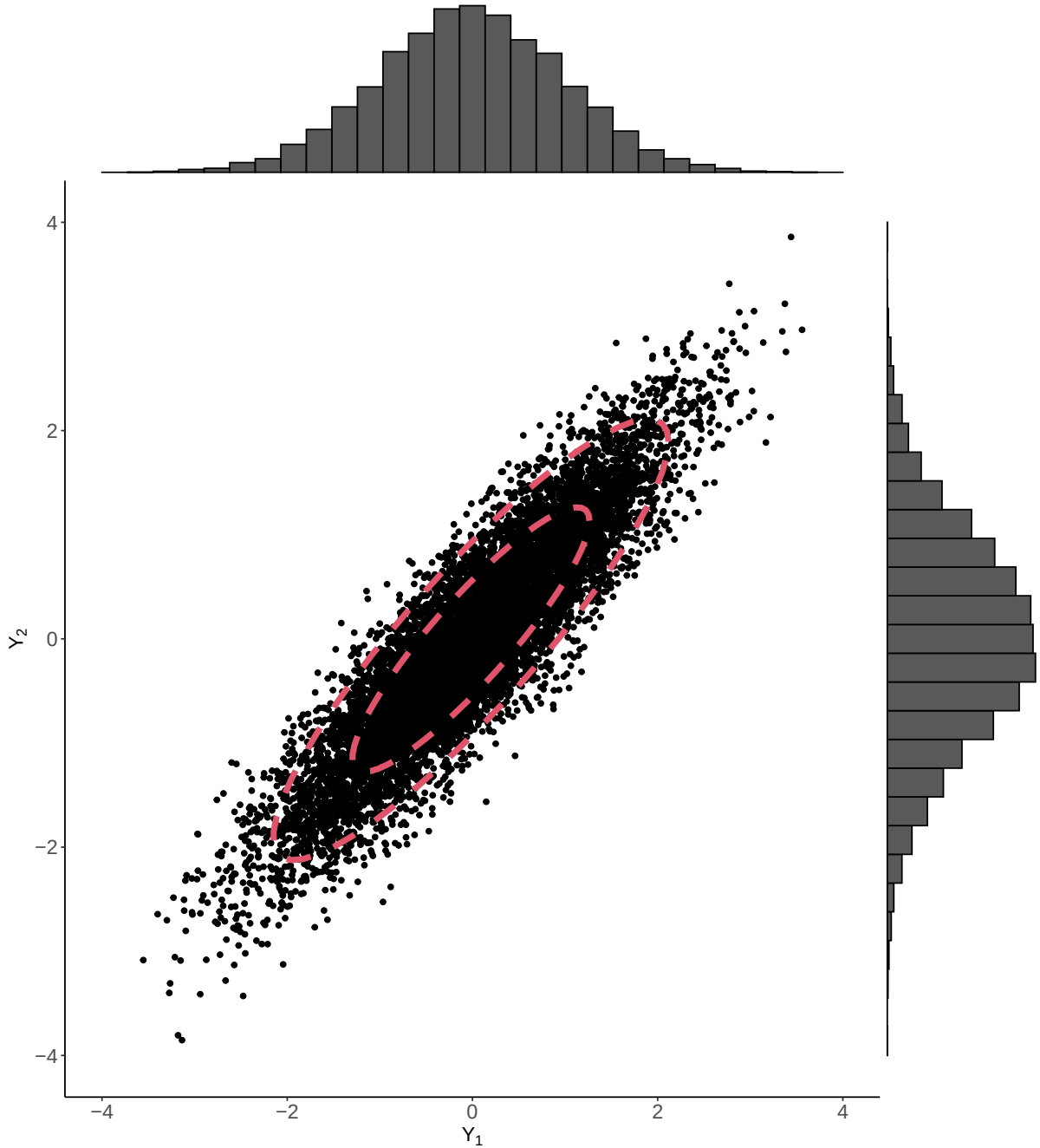


$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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



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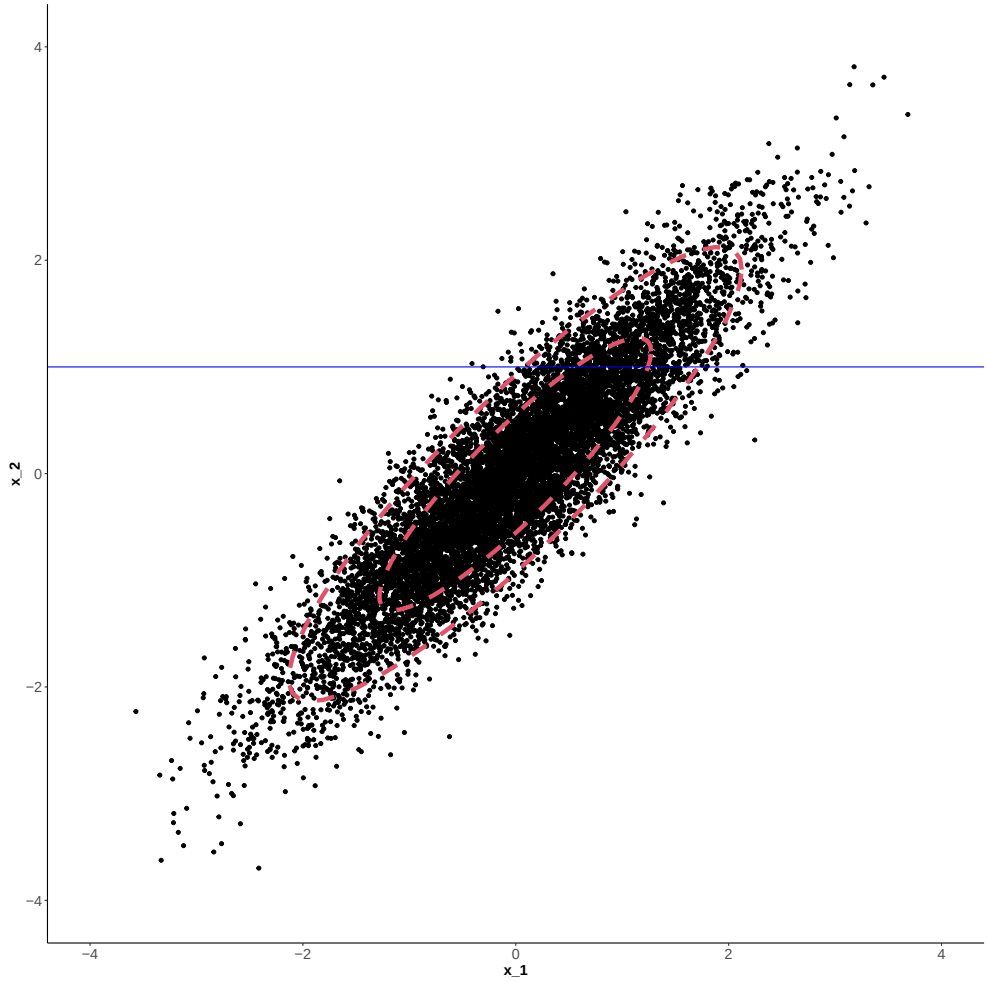
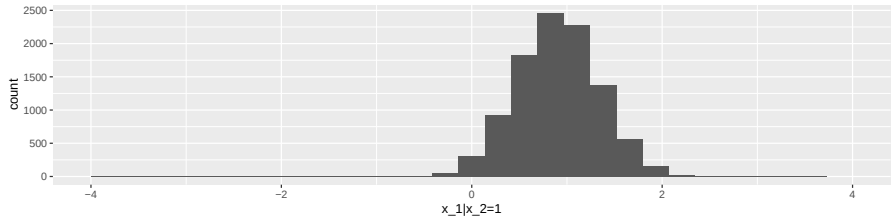
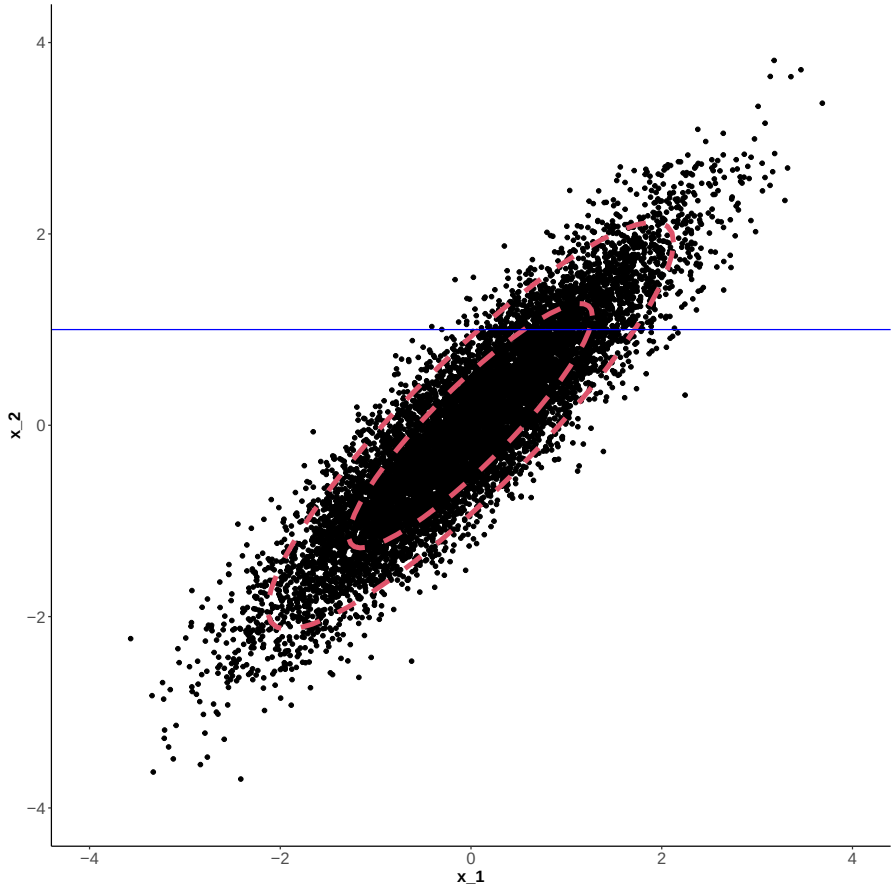


$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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

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





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

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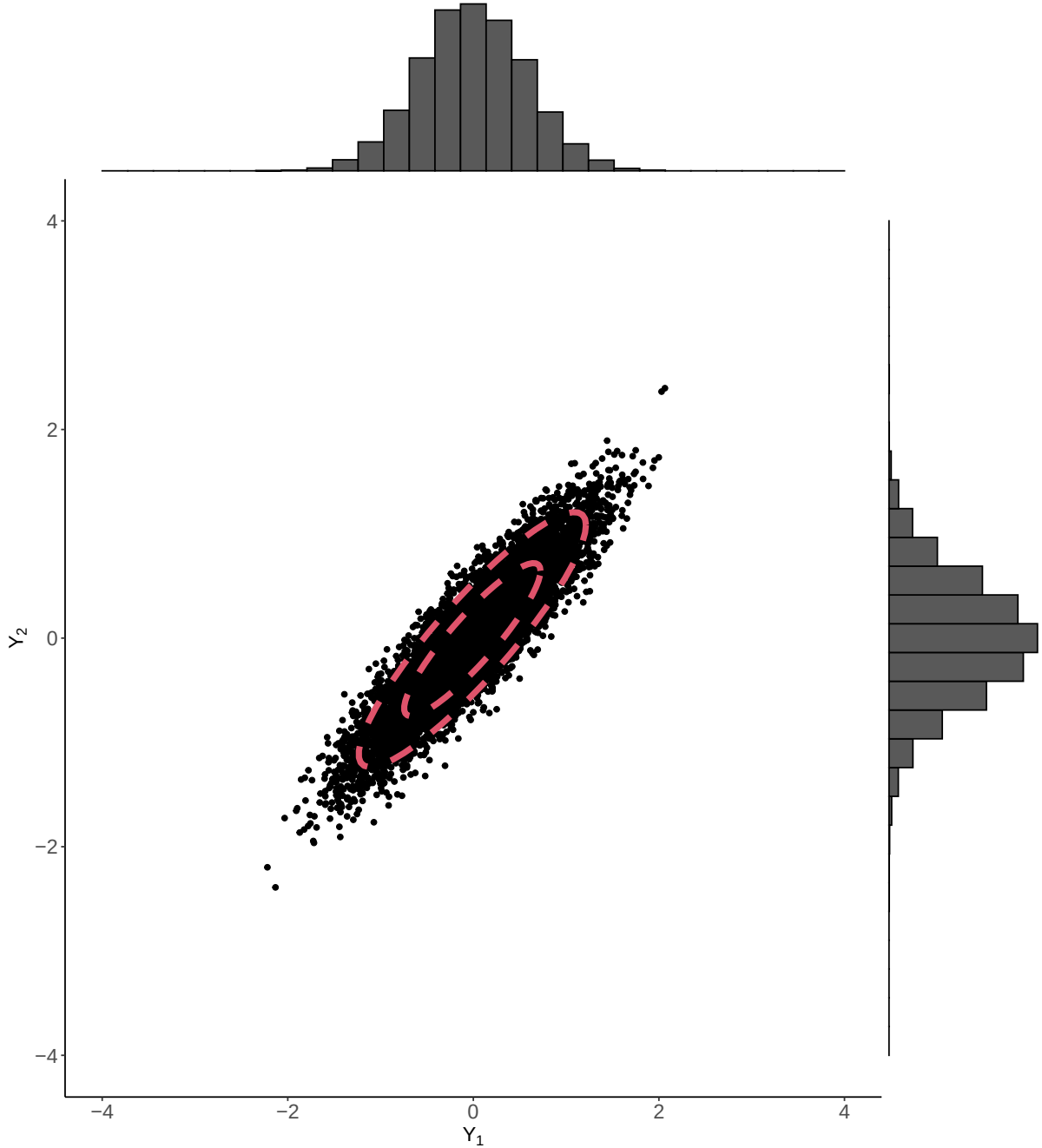
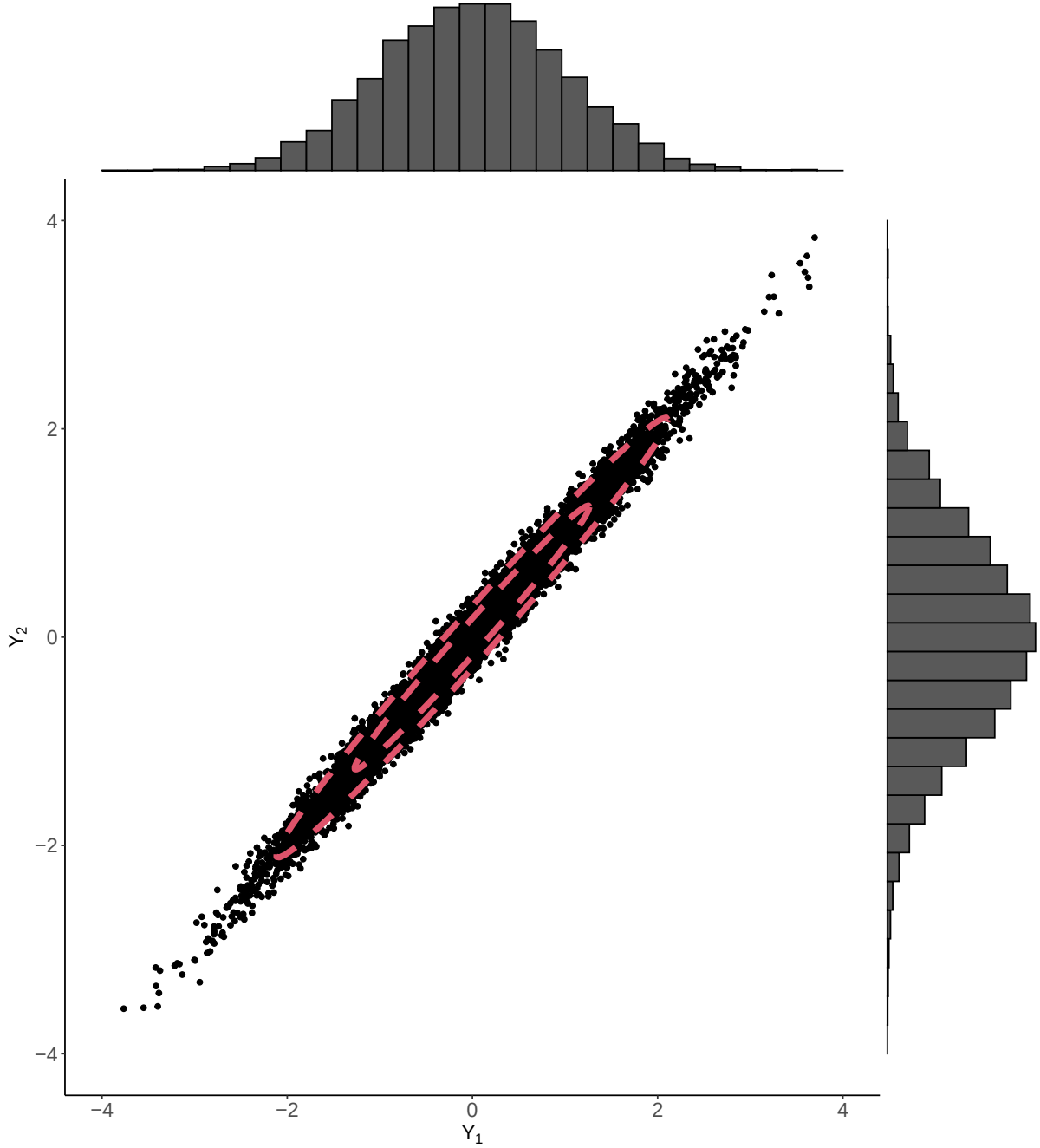
$$Y_1 | Y_2 = 1 \sim N(0.9, 0.19)$$



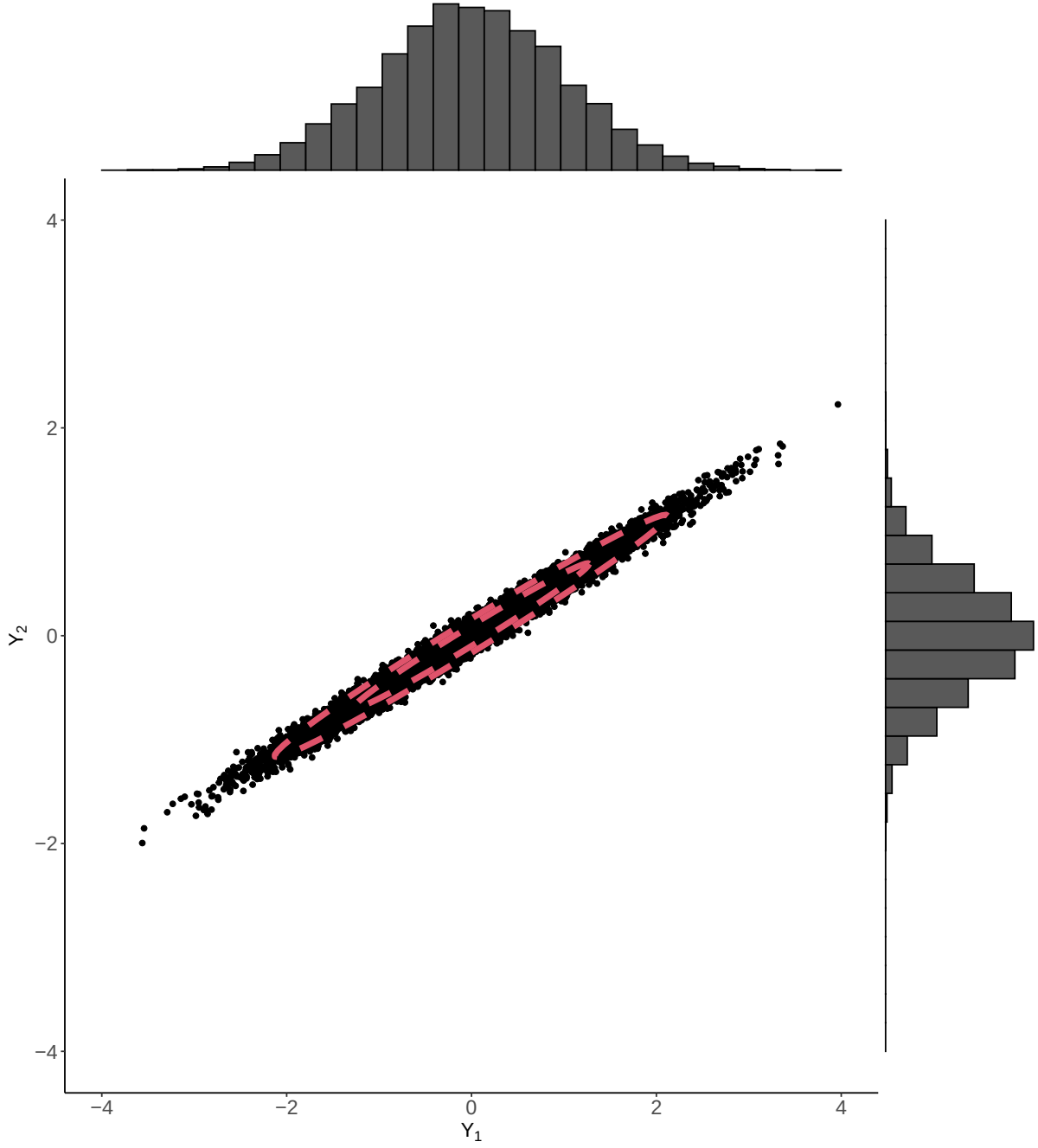
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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



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

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



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

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

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

More pictures

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

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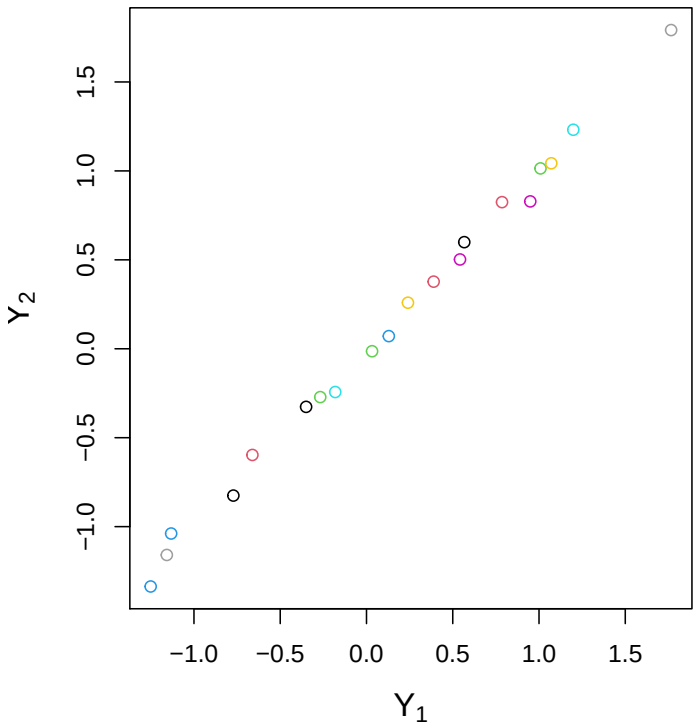
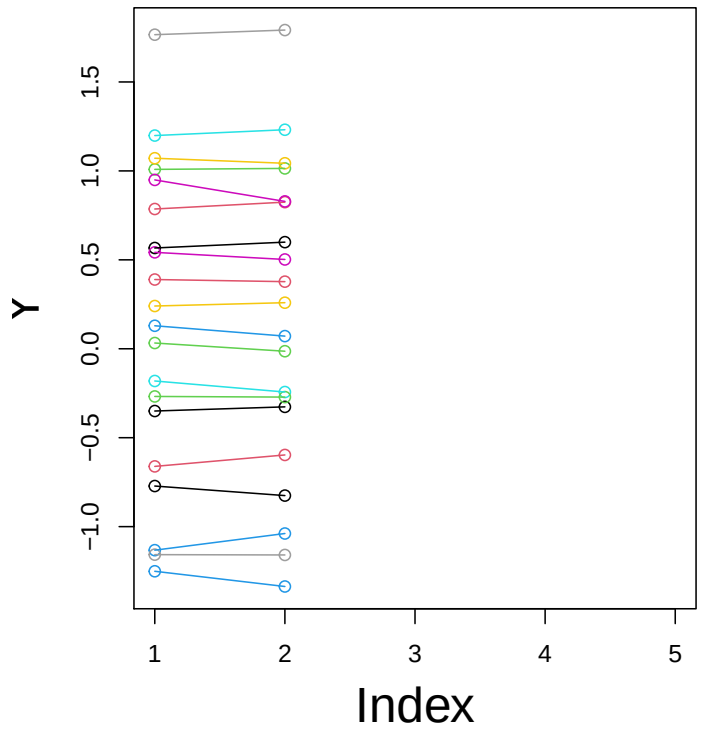
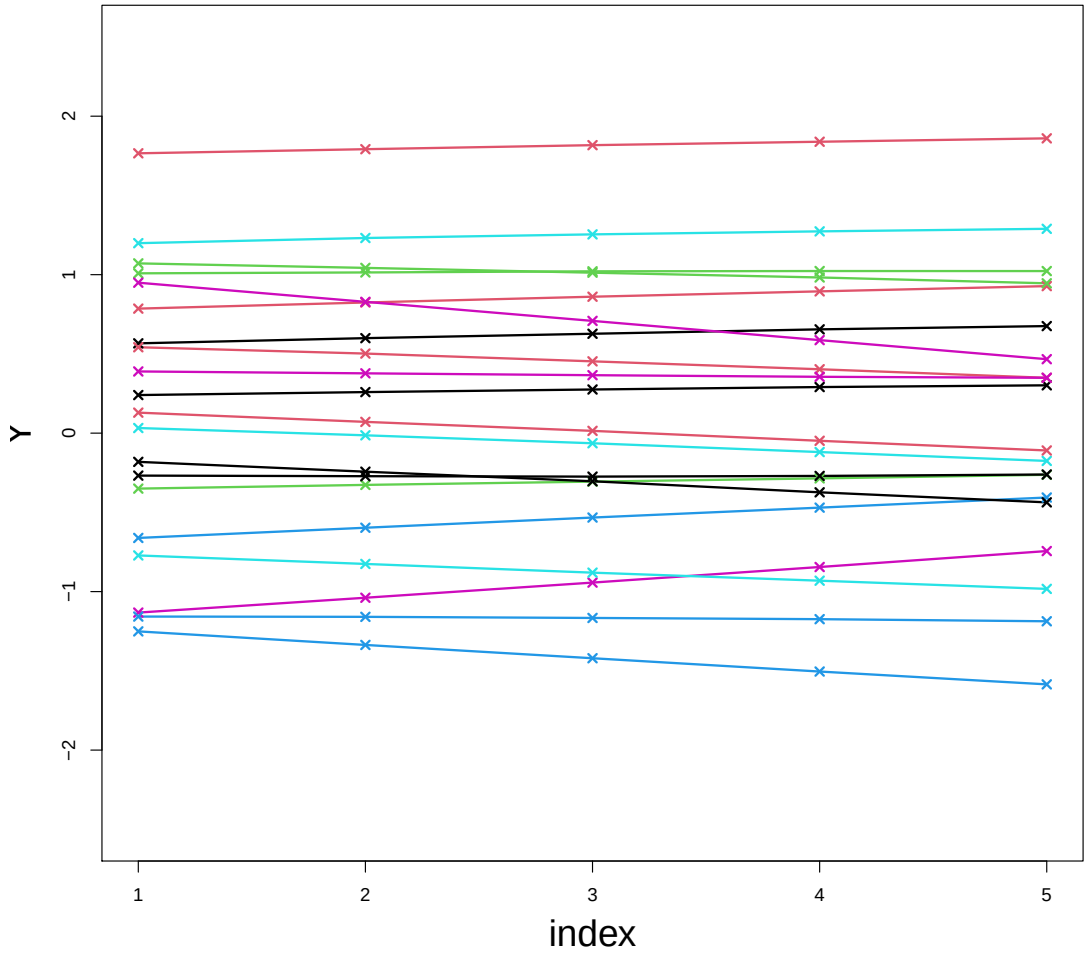
So for 2d instead of we have





Consider $d = 5$ with

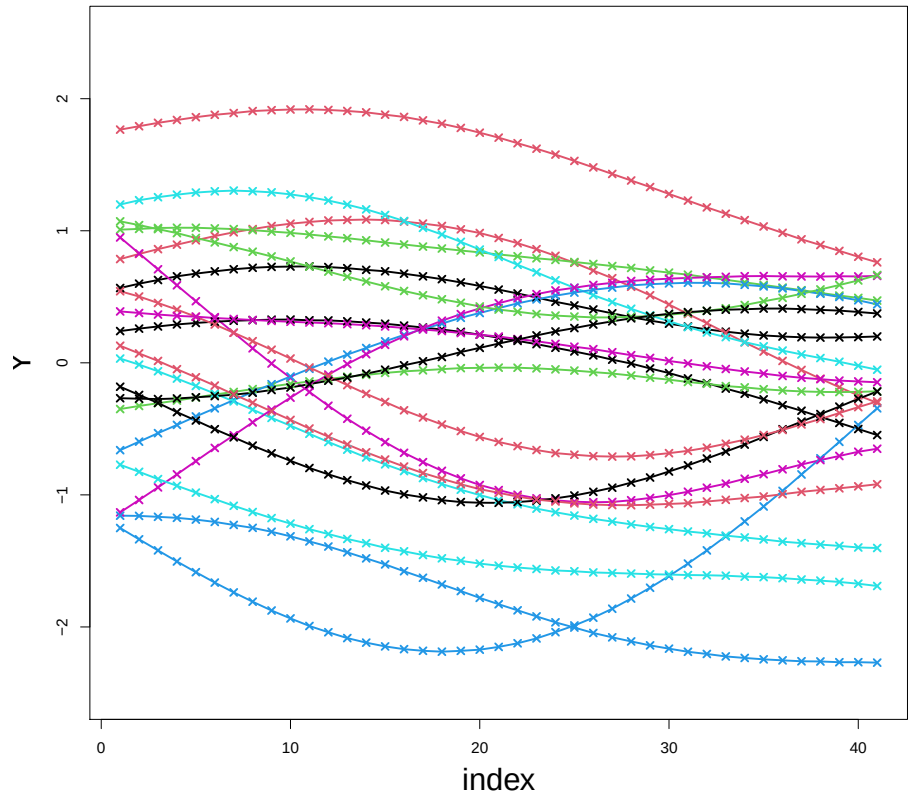
$$\mu = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.99 & 0.98 & 0.97 & 0.96 \\ 0.99 & 1 & 0.99 & 0.98 & 0.97 \\ 0.98 & 0.99 & 1 & 0.99 & 0.98 \\ 0.97 & 0.98 & 0.99 & 1 & 0.99 \\ 0.96 & 0.97 & 0.98 & 0.99 & 1 \end{pmatrix}$$



Each line is one sample.

$d = 50$

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



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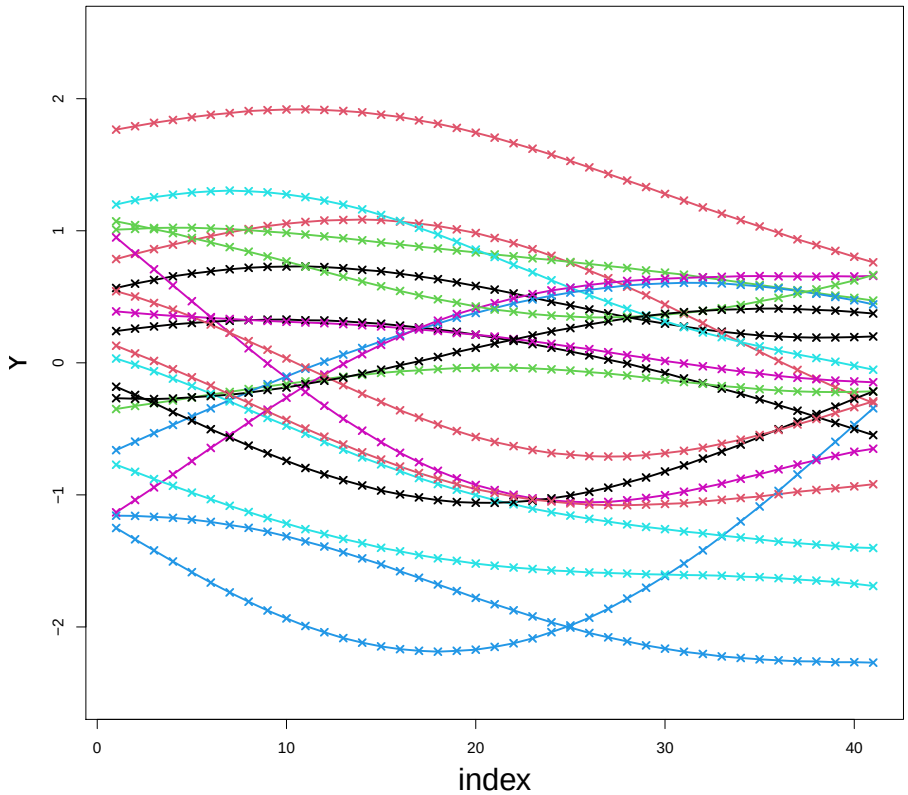

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We can think of Gaussian processes as an infinite dimensional distribution over functions - all we need to do is change the indexing

Gaussian processes

A stochastic process is a collection of random variables indexed by some variable $x \in \mathcal{X}$

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

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Thankfully, the law of y is uniquely determined by the finite dimensional distributions (FDDs), i.e., for all $x_1, \ldots, x_n$ and for all $n \in \mathbb{N}$

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A **Gaussian process** is a stochastic process with Gaussian FDDs, i.e.,

$$(y(x_1), \ldots, y(x_n)) \sim N_n(\mu, \Sigma)$$

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Usually $y(x) \in \mathbb{R}$ and $\mathcal{X} \subset \mathbb{R}^n$ - think of y as a function of x.
If $|\mathcal{X}| = \infty$, y is an infinite dimensional process, e.g., $|\mathcal{X}| = [0, 1]$
Thankfully, the law of y is uniquely determined by the finite dimensional distributions (FDDs), i.e., for all $x_1, \ldots, x_n$ and for all $n \in \mathbb{N}$

$$\mathbb{P}(y(x_1) \leq c_1, \ldots, y(x_n) \leq c_n)$$

A **Gaussian process** is a stochastic process with Gaussian FDDs, i.e.,

$$(y(x_1), \ldots, y(x_n)) \sim N_n(\mu, \Sigma)$$

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

Mean and covariance function

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

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

where

$$\mathbb{E}(y(x)) = m(x)$$
$$\mathbb{C}\text{ov}(y(x), y(x')) = k(x, x')$$

Specifying the mean function

We are free to choose the mean $\mathbb{E}(y(x))$ and covariance $\mathbb{C}\text{ov}(y(x), y(x'))$ 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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If $\mathbb{C}\text{ov}(y(x), y(x')) = k(||x - x'||)$ the covariance function is said to be isotropic.

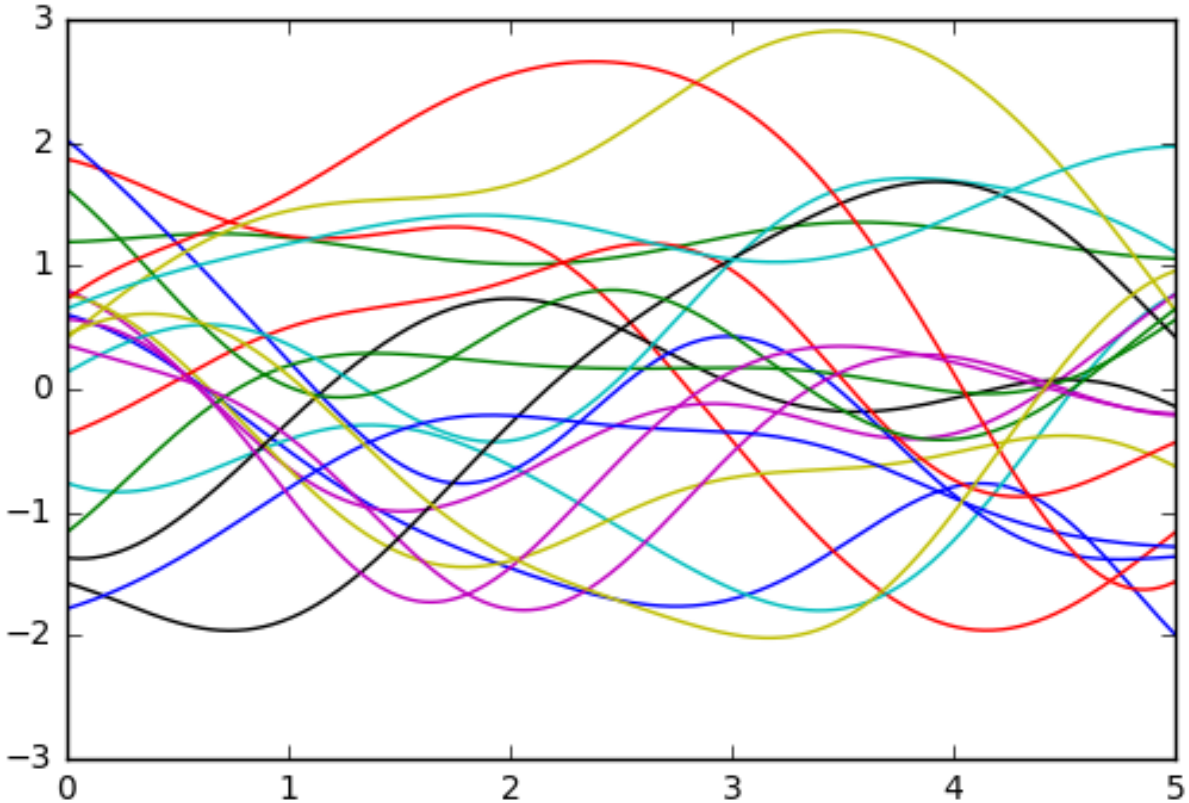
The covariance function determines the *nature* of the GP.

- k determines the hypothesis space/space of functions

Examples

RBF/Squared-exponential/exponentiated quadratic

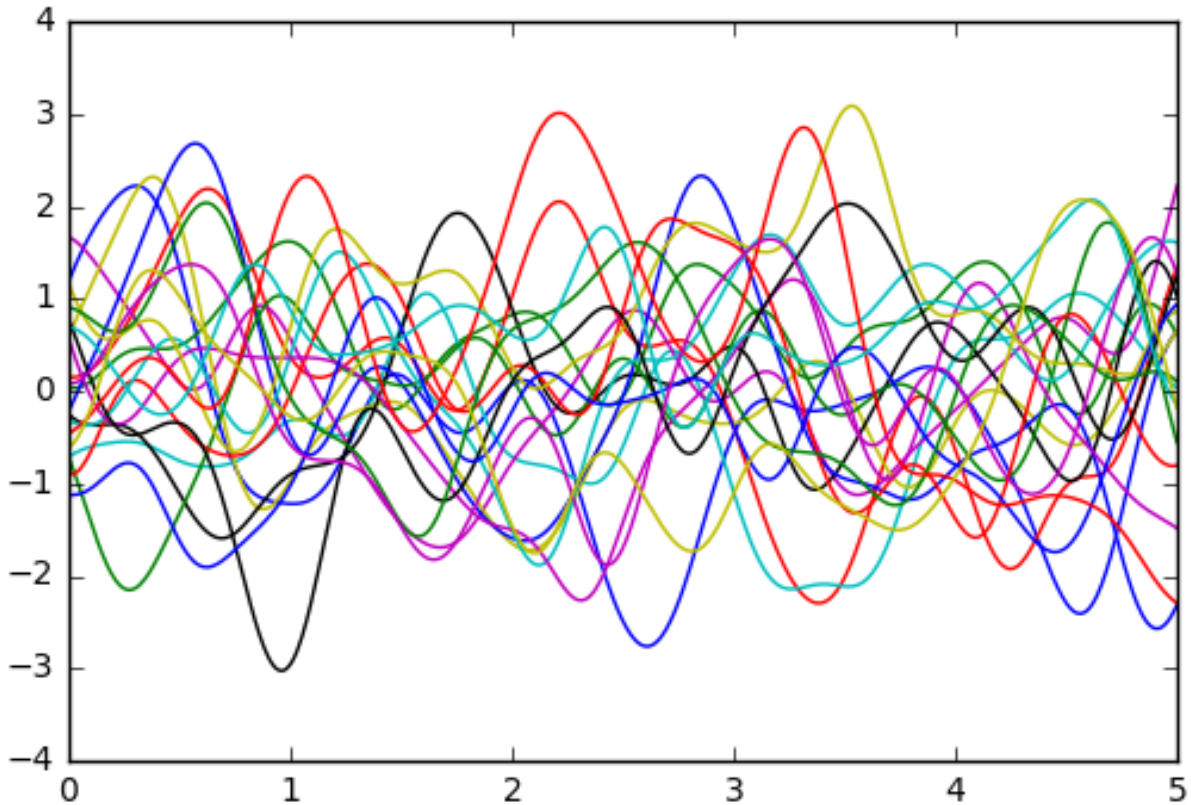
$$k(x, x') = \exp\left(-\frac{1}{2}(x - x')^2\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

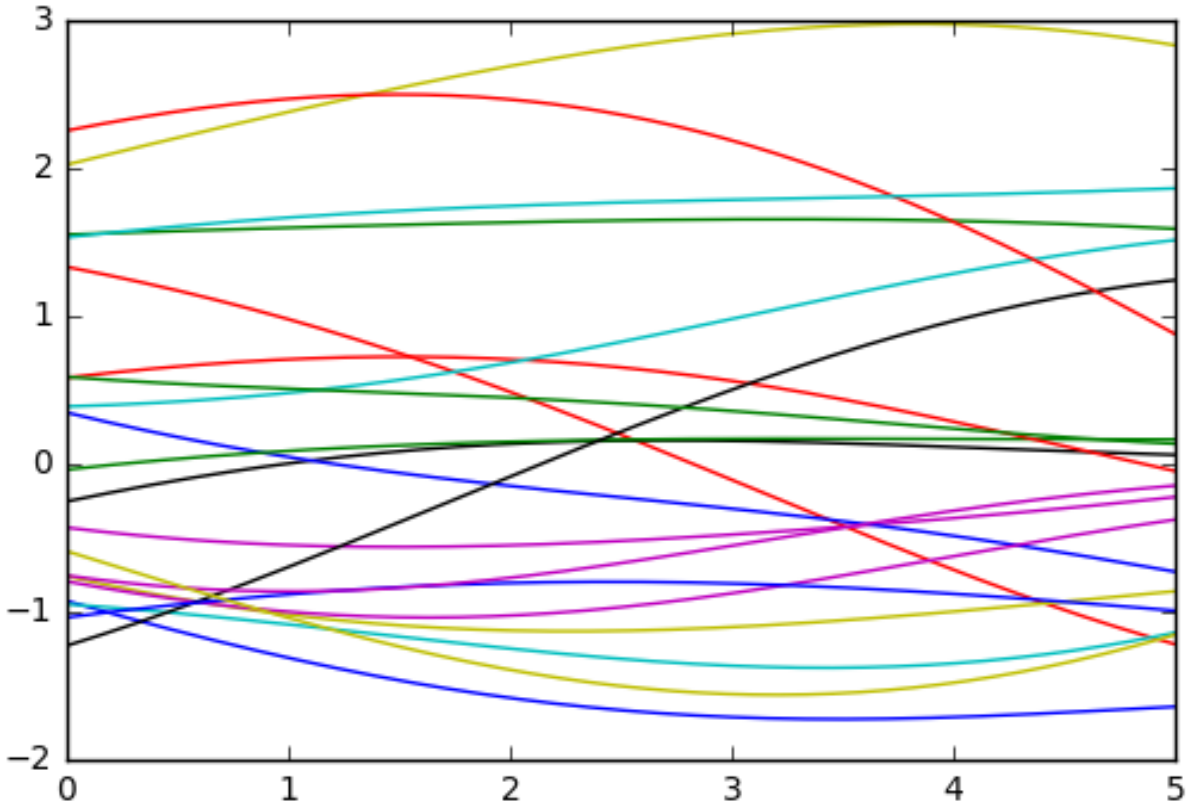
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{0.25^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

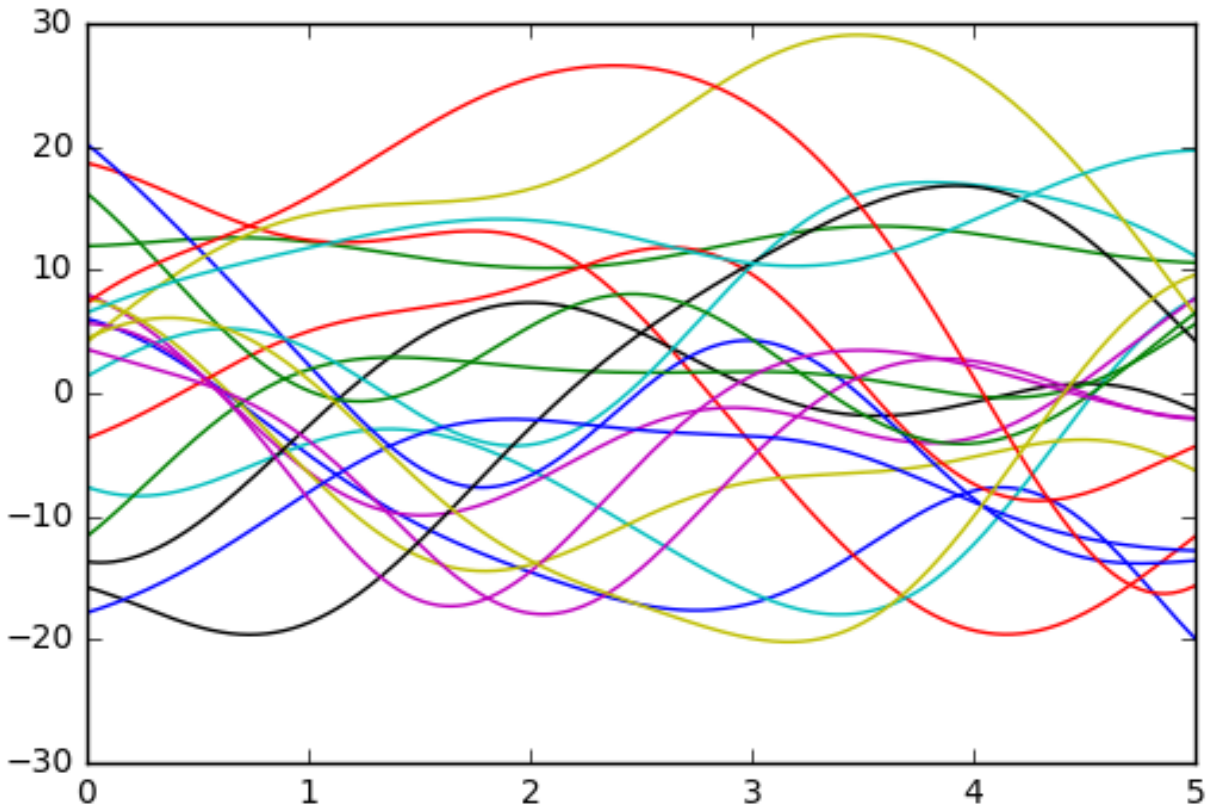
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{4^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

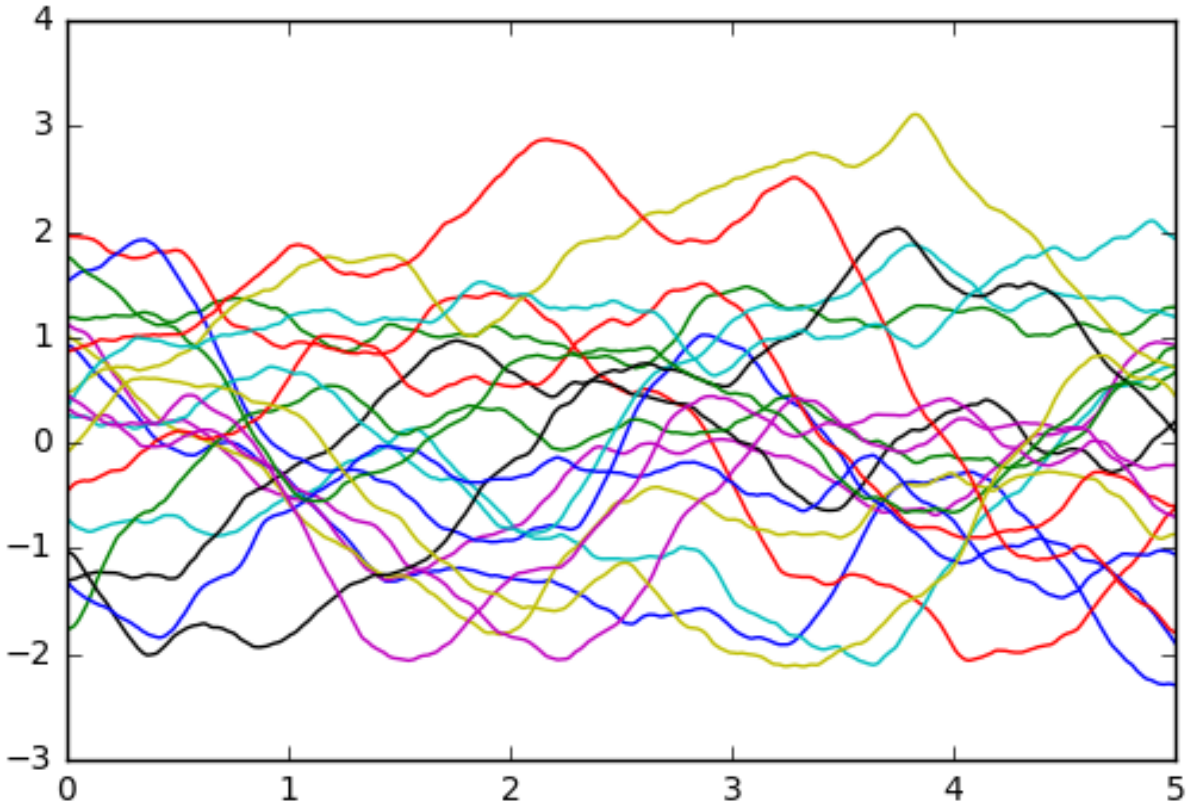
$$k(x, x') = 100 \exp\left(-\frac{1}{2}(x - x')^2\right)$$



Examples

Matern 3/2

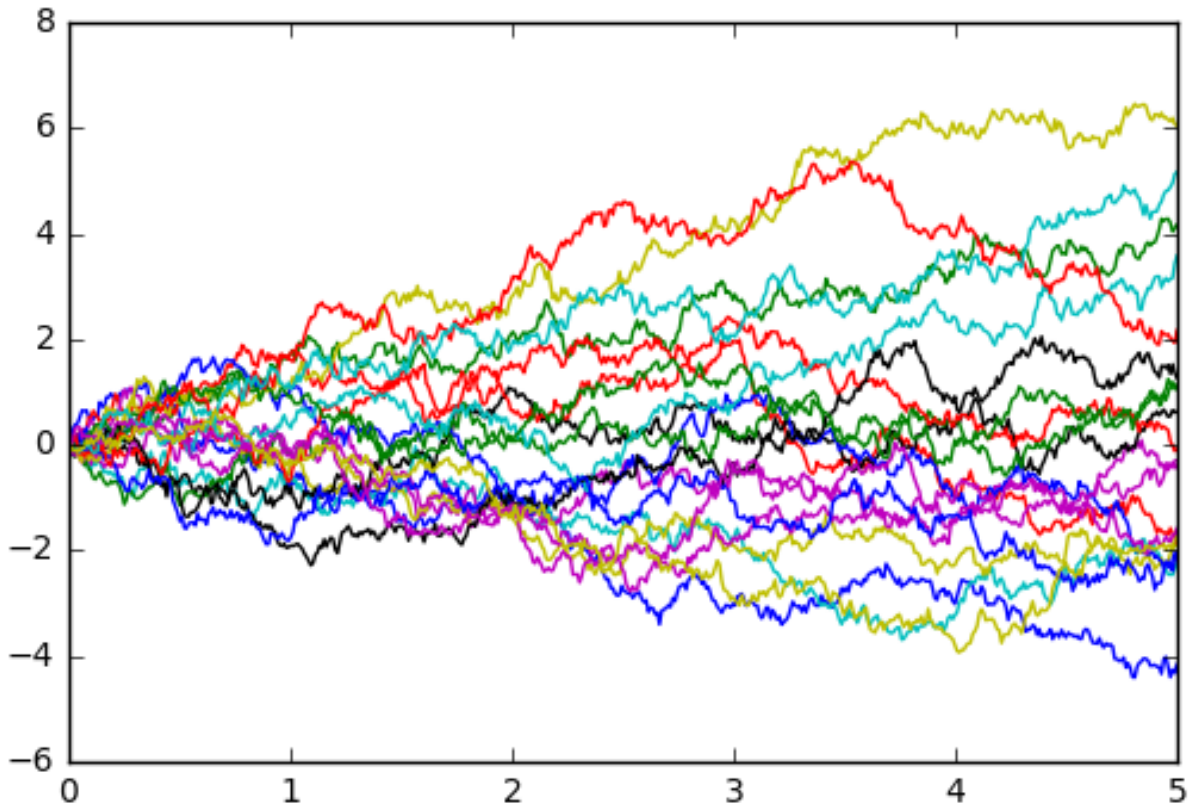
$$k(x, x') \sim (1 + |x - x'|) \exp\left(-|x - x'|\right)$$



Examples

Brownian motion

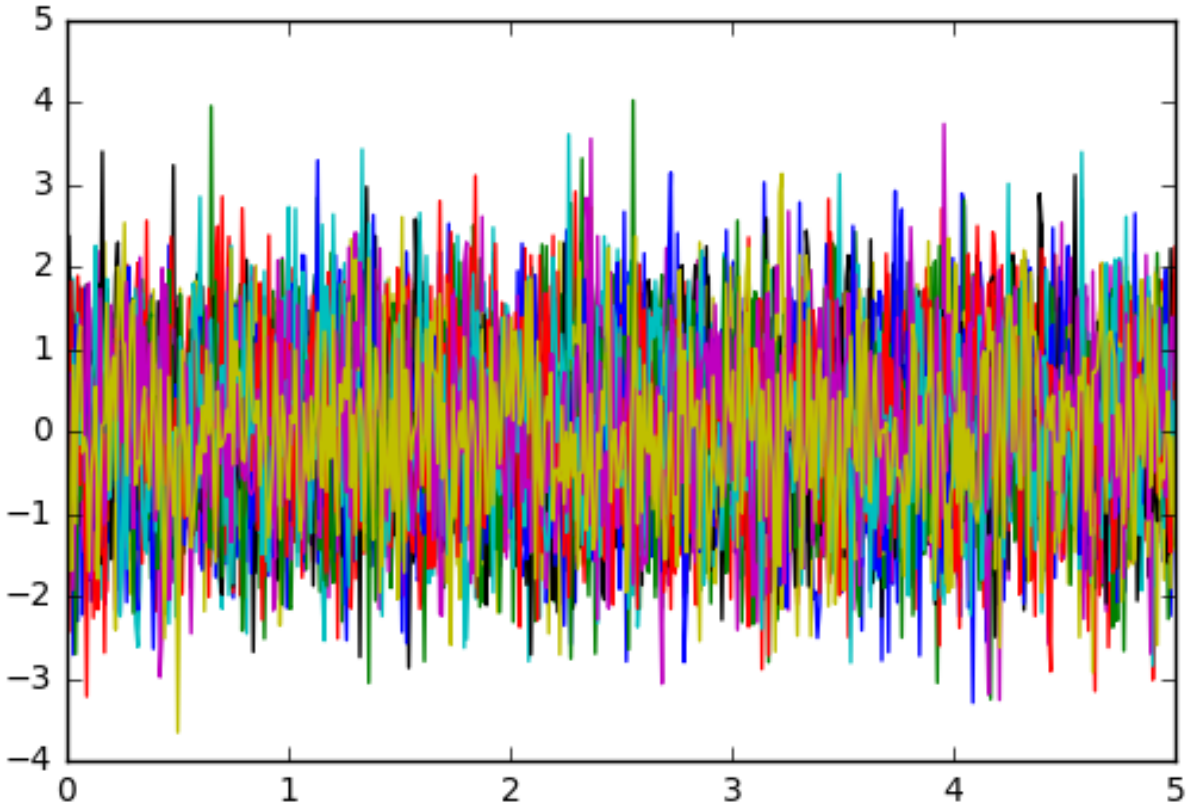
$$k(x, x') = \min(x, x')$$



Examples

White noise

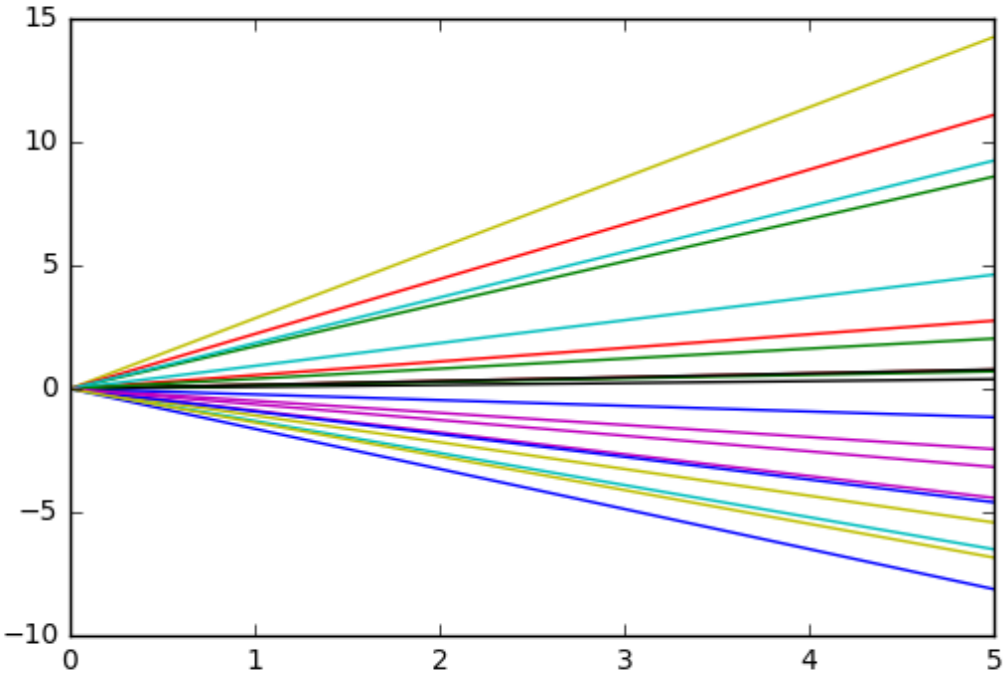
$$k(x, x') = \begin{cases} 1 \text{ if } x = x' \\ 0 \text{ otherwise} \end{cases}$$



Examples

A final example:

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



What is happening?

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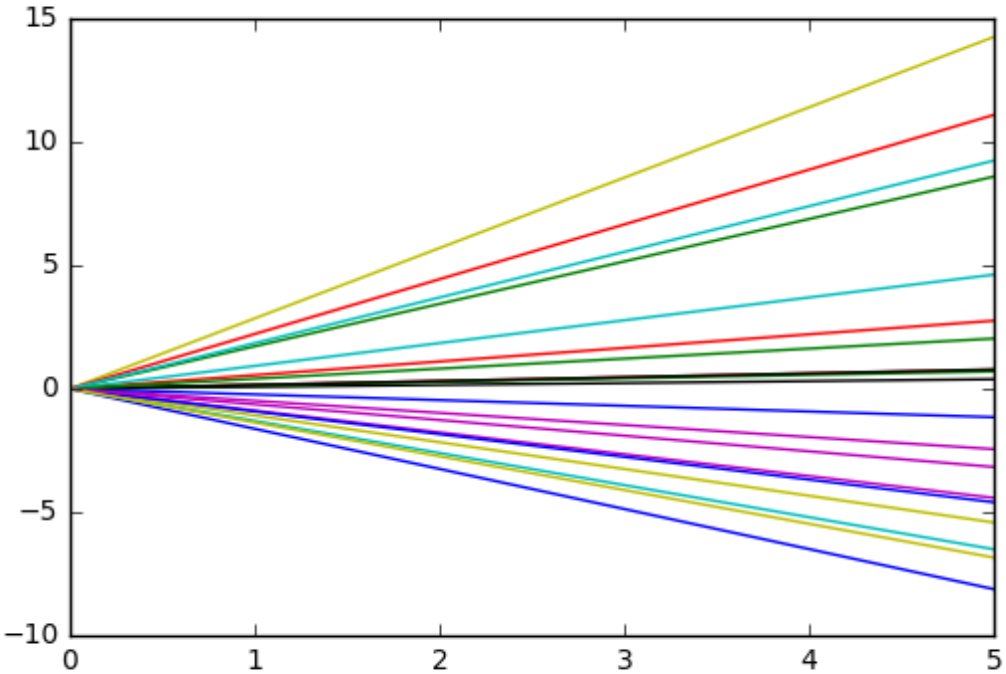

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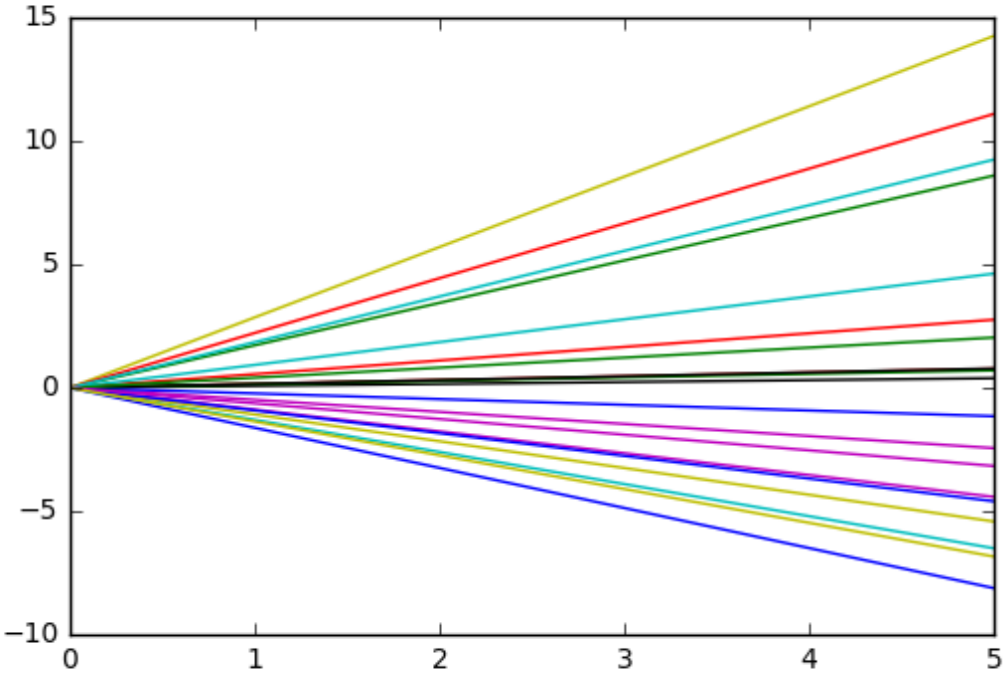

What is happening?

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

Choosing kernels and hyperparameters

GP properties are inherited primarily from the covariance function k.

- Continuity
- Differentiability
- Variance and length-scale

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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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$$Y \sim N_d(\mu, \Sigma) \text{ if and only if } AY \sim N_p(A\mu, A\Sigma A^\top)$$

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for all $A \in \mathbb{R}^{p \times d}$.
So sums of Gaussians are Gaussian, and marginal distributions of multivariate Gaussians are still Gaussian.

Property 2: Conditional distributions are still Gaussian

Suppose

$$Y = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \sim N_2(\mu, \Sigma)$$

where

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

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$$Y_2 \mid Y_1 = y_1 \sim N\left(\mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(y_1 - \mu_1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}\right)$$

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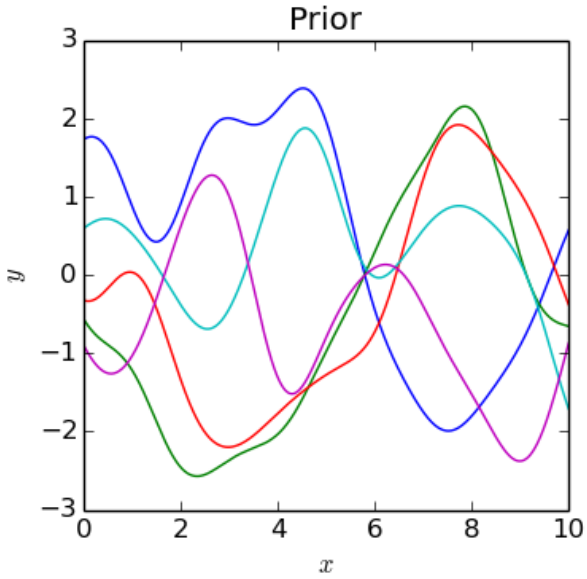
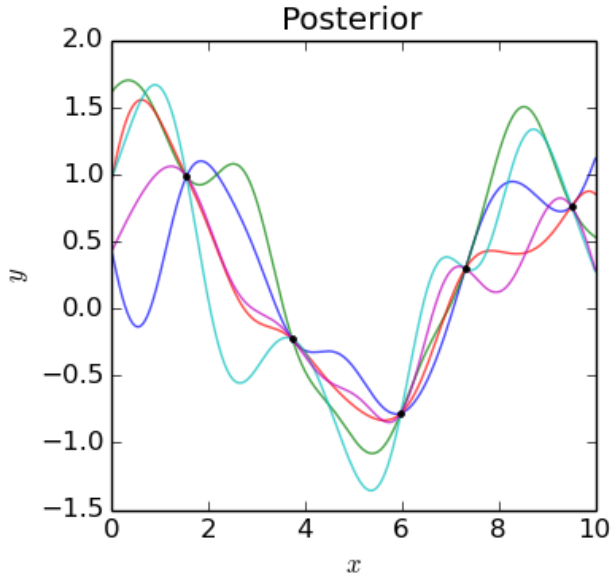
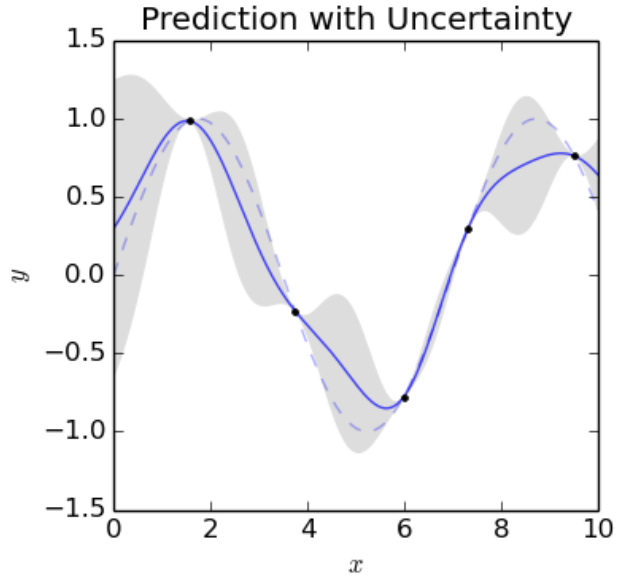
- f is still a GP even though we've observed its value at a number of locations.







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- 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

Conditional updates of Gaussian processes - revisited

Suppose f is a Gaussian process, then

$$f(x_1), \ldots, f(x_n), f(x) \sim N_{n+1}(0, \Sigma)$$

where

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Conditional updates of Gaussian processes - revisited

Suppose f is a Gaussian process, then

$$f(x_1), \ldots, f(x_n), f(x) \sim N_{n+1}(0, \Sigma)$$

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Conditional updates of Gaussian processes - revisited

Then

$$f(x)|f(x_1),\ldots,f(x_n) \sim N(\bar{m}(x),\bar{k}(x))$$

where

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

with

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

More generally, if

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

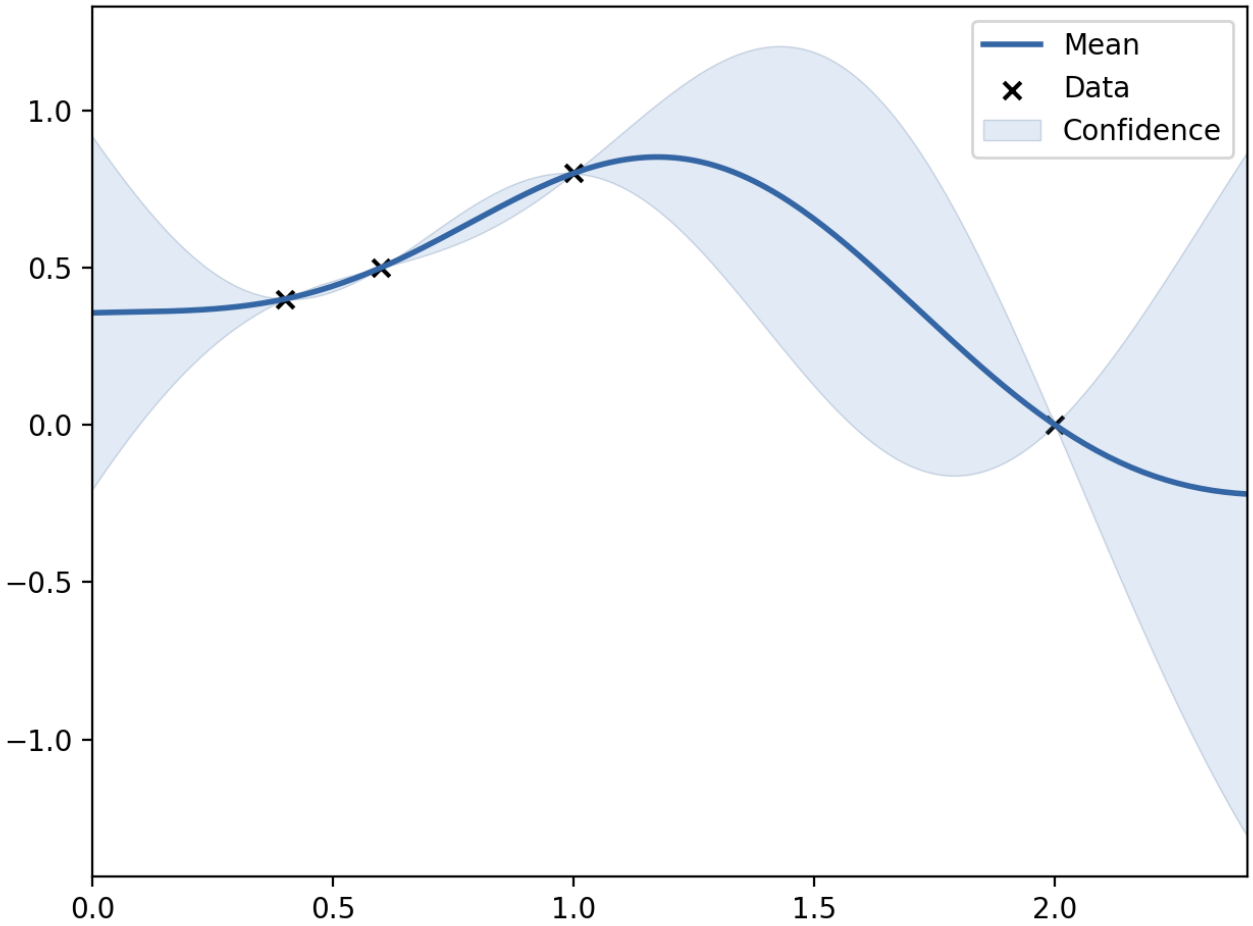
then

$$f(\cdot)|f(x_1), \ldots, f(x_n) \sim GP(\bar{m}(\cdot), \bar{k}(\cdot, \cdot))$$

with

$$\begin{aligned} \bar{m}(x) &= m(x) + k_X(x)^\top K_{XX}^{-1}\mathbf{f} \\ \bar{k}(x, x') &= k(x, x') - k_X(x)^\top K_{XX}^{-1} k_X(x') \end{aligned}$$

No noise/*nugget* - Interpolation



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

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

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Then

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

where

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

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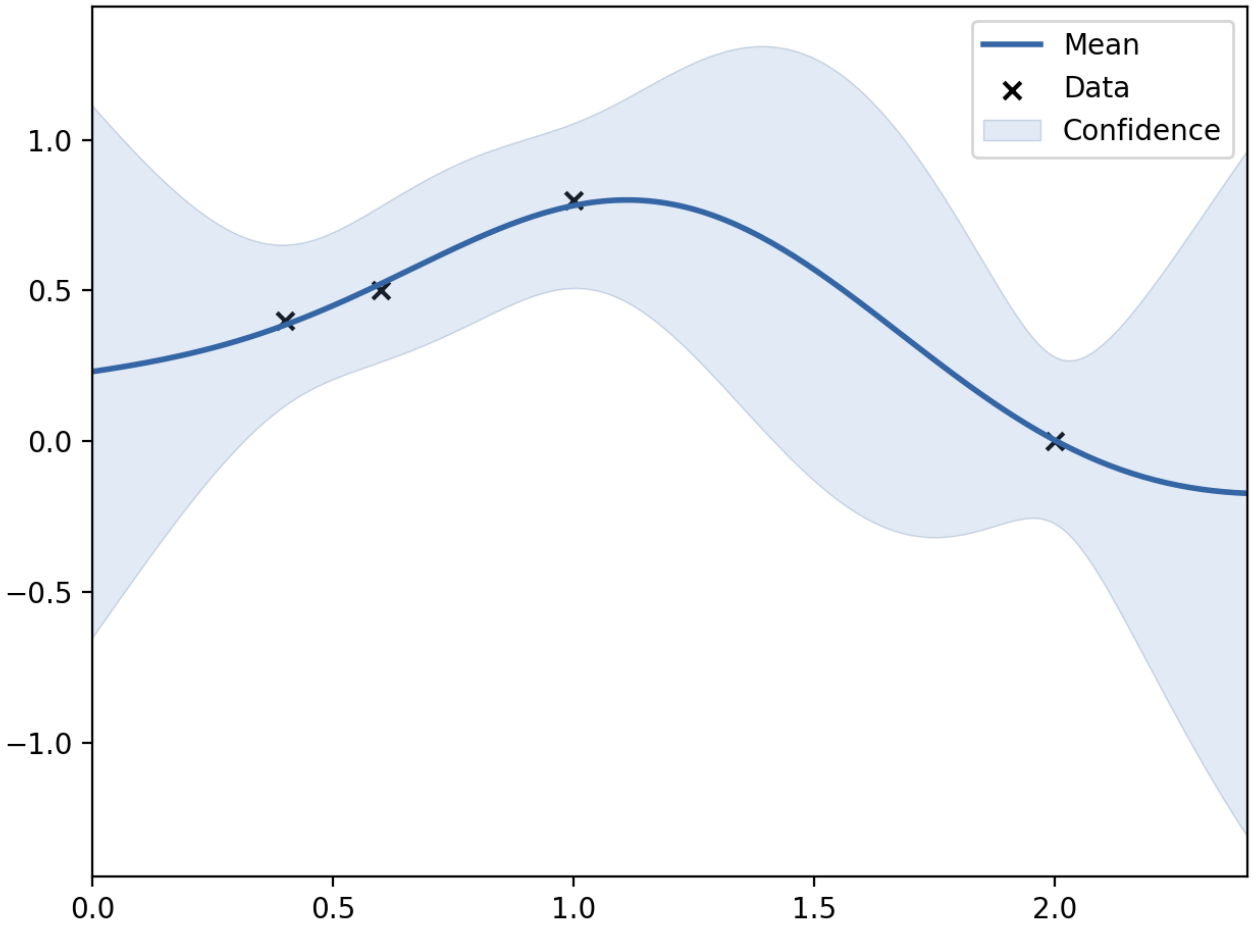
Nugget standard deviation $\sigma = 0.1$



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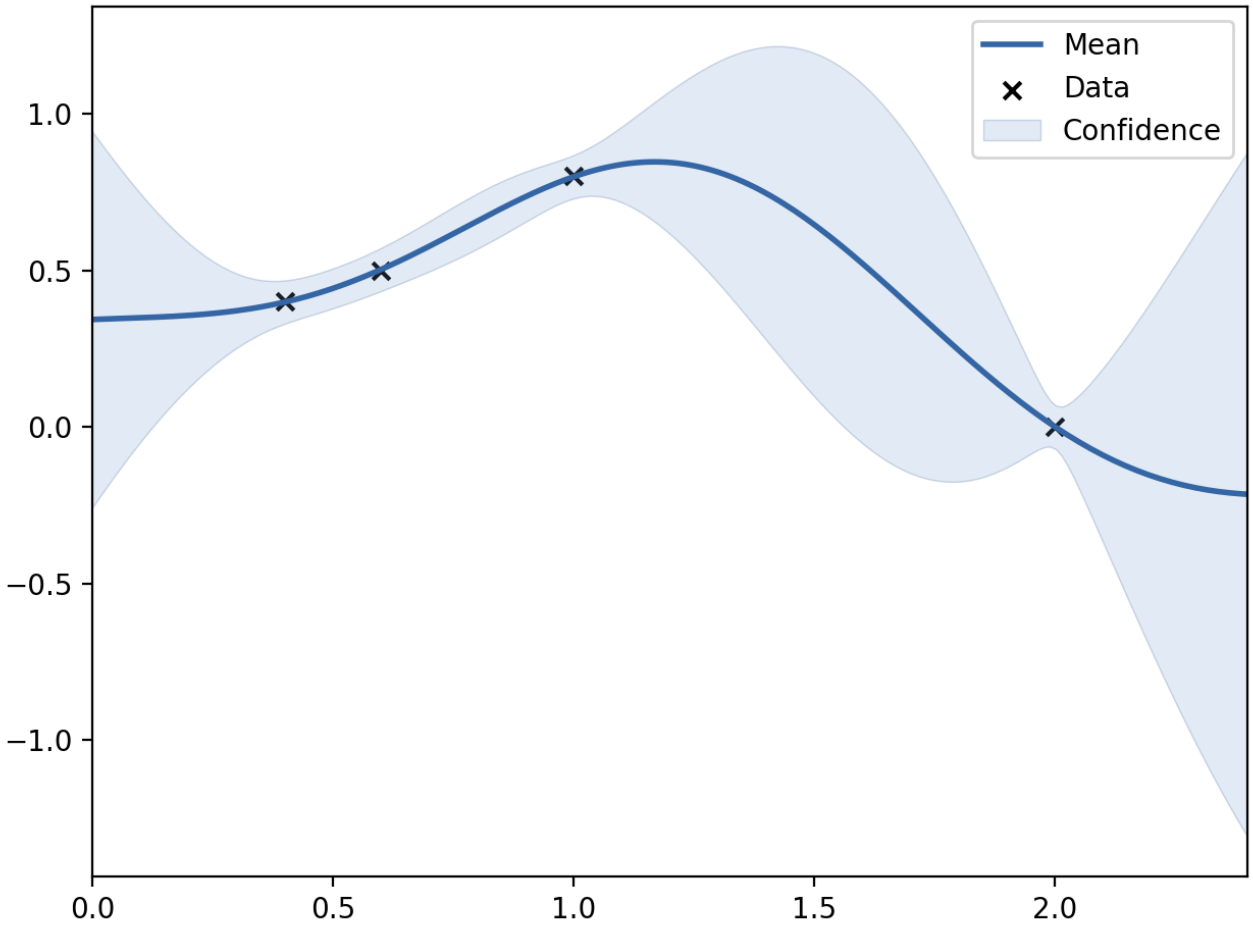
$$\bar{k}(x) = k(x,x) - k_X(x)^\top (K_{XX}^{-1} + \sigma^2 I) k_X(x)$$

Nugget standard deviation $\sigma = 0.025$



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- If mean is a linear combination of known regressor functions,

$$m(x) = \beta^\top h(x) \text{ for known } h(x)$$

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and we give σ^2 an inverse gamma prior (including $\pi(\sigma^2) \propto 1/\sigma^2$) then $y|D, \sigma^2 \sim GP$ and

$$y|D \sim \text{t-process}$$

with $n - p$ degrees of freedom.
In practice, for reasonable n, this is indistinguishable from a GP.

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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

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

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Note this is exactly the GP conditional mean we derived before.

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

- 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., $\phi(x) = (1\ x\ x^2)$

It doesn't change the expressions other than the inner product

$$k(x', x) = x'^{\top} x$$

is replaced by

$$k(x', x) = \phi(x')^{\top} \phi(x)$$

Including features II

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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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The same idea works with much larger feature vectors, sometimes even when $\phi(\mathbf{x}) \in \mathbb{R}^\infty$

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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[2]

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

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Example: If $\mathcal{X} = \mathbb{R}$, $c_0 = -\log N$, $c_N = \log N$, $c_{i+1} - c_i = 2\frac{\log N}{N}$ and

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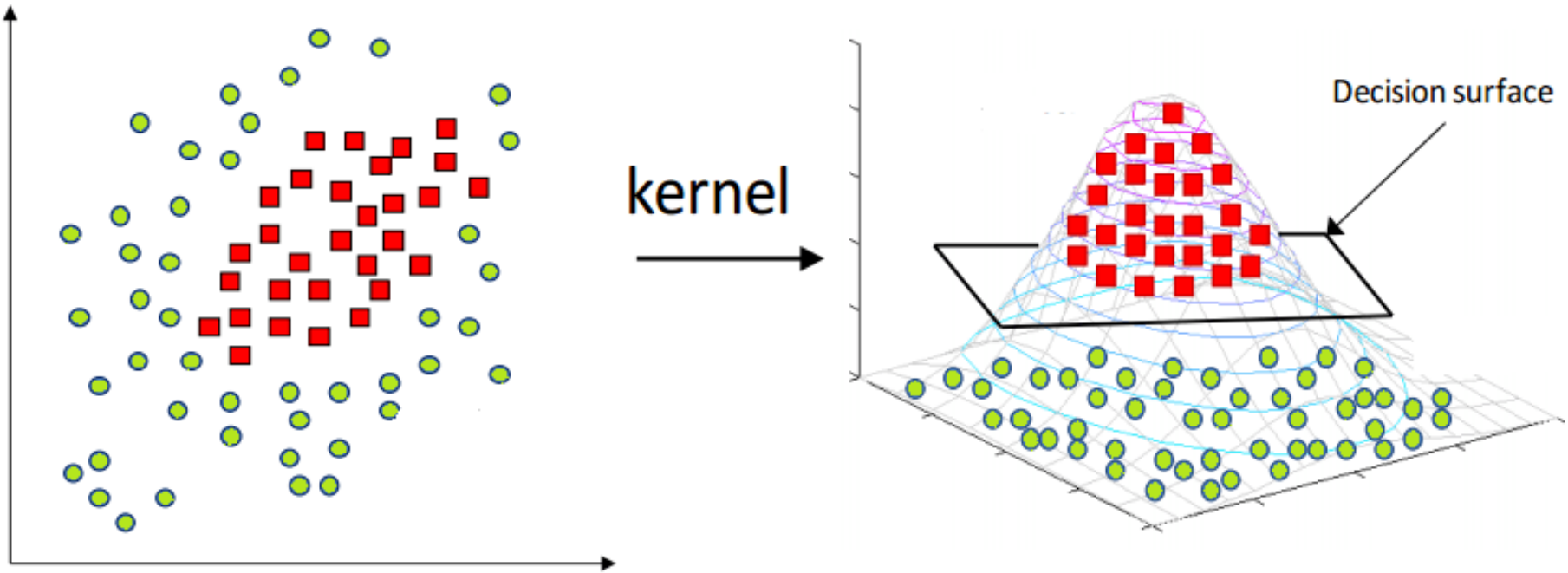
We can use an infinite dimensional feature vector $\phi(x)$, and because linear regression can be done solely in terms of inner-products (inverting a $n \times n$ matrix in the dual form) we never need evaluate the feature vector, only the kernel.

Kernel trick:

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



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We can show that

$$\bar{m}(x) = \arg \min_{f \in \mathcal{H}_k} L(f)$$

where $\bar{m}(x)$ is the same as the posterior mean when we assume $y_i = f(x_i) + N(0, \sigma^2)$ and $f(\cdot) \sim GP(0, k(\cdot, \cdot))$

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We can show that

$$\bar{m}(x) = \arg \min_{f \in \mathcal{H}_k} L(f)$$

where $\bar{m}(x)$ is the same as the posterior mean when we assume
$y_i = f(x_i) + N(0, \sigma^2)$ and $f(\cdot) \sim GP(0, k(\cdot, \cdot))$
Note that $\bar{m}(\cdot) \in \mathcal{H}_k$ (samples from a GP live in a slightly larger RKHS)

TL;DR

Functions live in function spaces (vector spaces with inner products). There are lots of different function spaces: the GP kernel implicitly determines which particular (RKHS) space we work with - our hypothesis space.

- Generally, we don't think too hard about this space/features, we just choose a kernel and validate our choice.

[3] and can be dense in some sets of continuous bounded functions

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Functions live in function spaces (vector spaces with inner products). There are lots of different function spaces: the GP kernel implicitly determines which particular (RKHS) space we work with - our hypothesis space.

- Generally, we don't think too hard about this space/features, we just choose a kernel and validate our choice.

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 an element close to the true functional form than any class of models that contains only a finite number of features.

This is the motivation for non-parametric methods.

[3] and can be dense in some sets of continuous bounded functions

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?

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

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

i.e., exactly the Gaussian process update for the posterior mean.
So GPs are in some sense second-order optimal.

Kriging

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

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)) \\
&= \mathbf{w}^\top K_{XX}\mathbf{w} + k(0) - 2\mathbf{w}^\top \mathbf{k}_X(x)
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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.

Why use GPs? Answer 4: Uncertainty estimates

We often think of our prediction as consisting of two parts

- point estimate
- uncertainty in that estimate

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Warning: the uncertainty estimates from a GP can be flawed. Note that given data $D = \{X, y\}$

$$\mathbb{V}\text{ar}(f(x)|X, y) = k(x, x) - k_X(x)K_{XX}^{-1}k_X(x)$$

The posterior variance of $f(x)$ does not directly depend upon y!

Variance estimates are particularly sensitive to the hyper-parameter estimates.

Difficulties of using GPs

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- We pick a covariance function from a small set, based usually on differentiability considerations.
- Possibly try a few (plus combinations of a few) covariance functions, and attempt to make a good choice using some sort of empirical evaluation.
- Covariance functions often contain hyper-parameters. E.g
  - RBF kernel

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

  Estimate these using your favourite statistical procedure (maximum likelihood, cross-validation, Bayes, expert judgement etc)

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Gelman *et al.* 2017, Bachoc 2020

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E.g. consider a zero mean GP on $[0, 1]$ with covariance function

$$k(x, x') = \sigma^2 \exp(-\kappa^2 |x - x|)$$

We can consistently estimate $\sigma^2\kappa$, but not σ^2 or κ, even as $n \to \infty$.

Problems with hyper-parameter optimization

As well as problems of identifiability, the likelihood surface that is being maximized is often flat and multi-modal, and thus the optimizer can sometimes fail to converge, or gets stuck in local-maxima.

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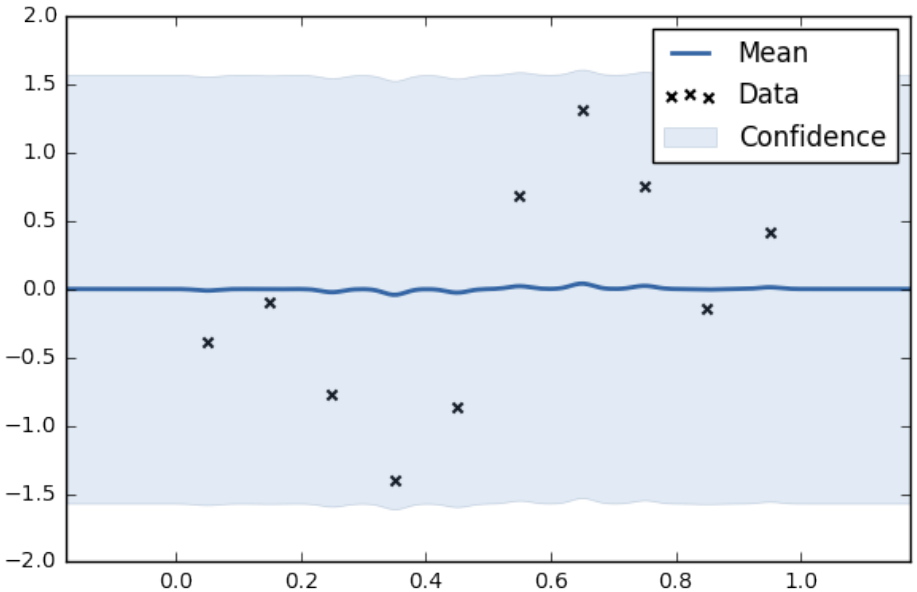
In practice, it is not uncommon to optimize hyper parameters and find solutions such as



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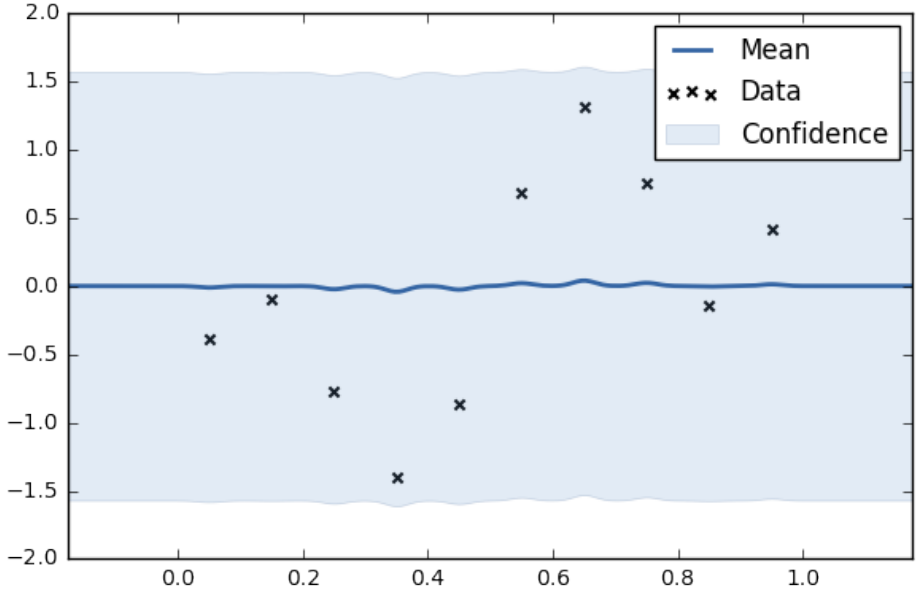

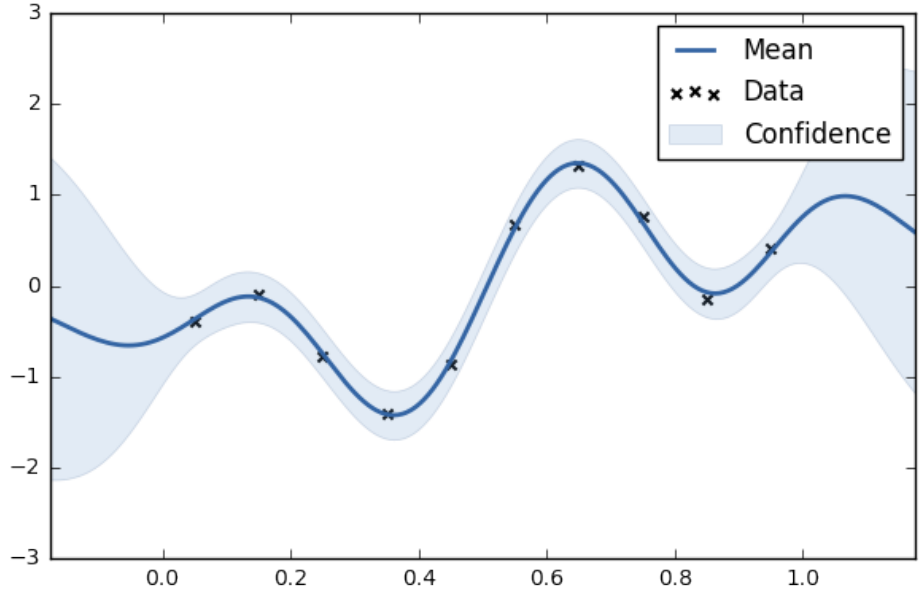

We often work around these problems by running the optimizer multiple times from random start points, using prior distributions, constraining or fixing hyper-parameters, or adding white noise.

Computational cost

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Suppose

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Then GP regression is equivalent to linear regression with covariates $\phi(x)$

- Dual form for regression coefficients costs $O(n^3)$, but primal solution only costs $O(m^3)$

In practice we may use a basis expansion with $m << n$ such that

$$k(x, x') \approx \sum_{i=1}^{m} \phi_i(x)\phi_i(x')$$

Choice of basis

There are many choices of basis. Two examples:

- **Mercer basis**: Consider the map

$$T_k(f)(\cdot) = \int_{\mathcal{X}} k(x, \cdot) f(x) \mathrm{d}x$$

Consider the eigenfunctions of this map, i.e., $\phi : \mathcal{X} \mapsto \mathbb{R}$ s.t. $T_k(\phi)(\cdot) = \lambda\phi(\cdot)$. Then Mercer's theorem says that

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$$f(x) = \sum_{i=1}^{\infty} Z_i \sqrt{\lambda_i} \phi_i(x) \quad \text{where } Z_i \overset{iid}{\sim} N(0, 1)$$

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We can approximate the process (& reduce cost to $O(m^3)$) by truncating the sum

$$f(x) = \sum_{i=1}^{m} Z_i \sqrt{\lambda_i} \phi_i(x)$$

The Mercer/KL basis minimizes the mean square truncation error.

Choice of basis

There are many choices of basis. Two examples:

- **Random Fourier features**:
  Bochner's theorem says that a stationary kernel can be represented as a Fourier transform of a distribution

$$k(x - x') = \int \exp(iw^\top (x - x'))p(w)dw = \mathbb{E}_{w\sim p} \exp(iw^\top (x - x'))$$
$$\approx \frac{1}{m} \sum (\cos(w_i^\top x),\ \sin(w_i^\top x)) \begin{pmatrix} \cos(w_i^\top x) \\ \sin(w_i^\top x) \end{pmatrix} \text{ if } w_i \sim p(\cdot)$$

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  by using Euler's identity and discarding the imaginary part
  Using the primal form for linear regression again reduces the complexity to $O(m^3)$.

  Recent work by Rudi and Rosasco (2017) shows that using $m = \sqrt{n}\log(n)$ features achieve similar performance to using the full kernel.

Conclusions

- GPs are now ubiquitous in statistics/ML.
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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.