

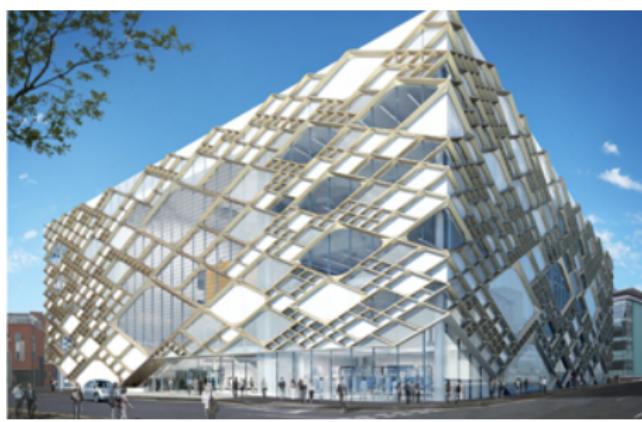
# An introduction to Gaussian Processes

Richard Wilkinson

School of Mathematical Sciences  
University of Nottingham

GP summer school  
September 2021

# Sheffield



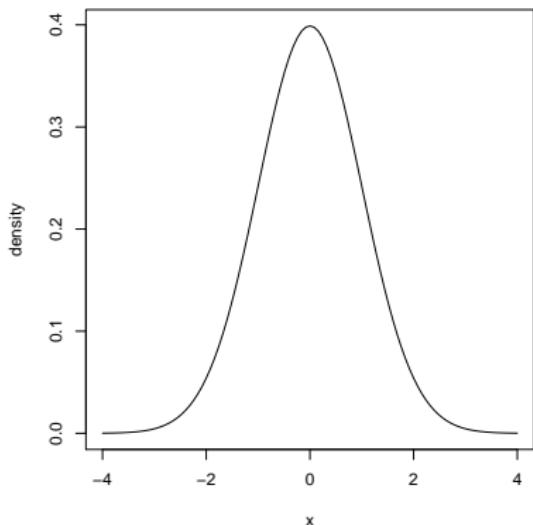
# Introduction

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

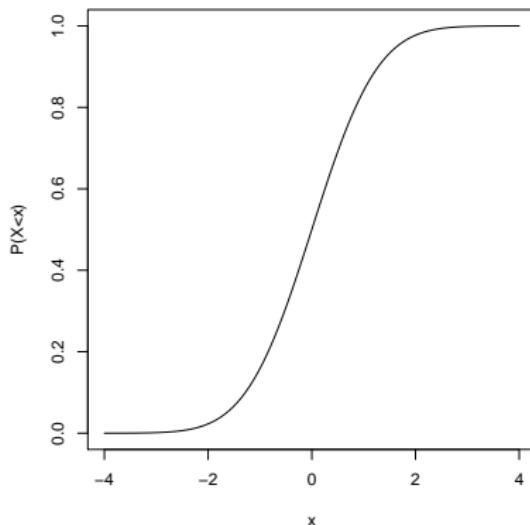
You can download a copy of these slides from [www.gpss.cc](http://www.gpss.cc)

# Univariate Gaussian distributions

PDF of a  $N(0,1)$  random variable



CDF of a  $N(0,1)$  random variable



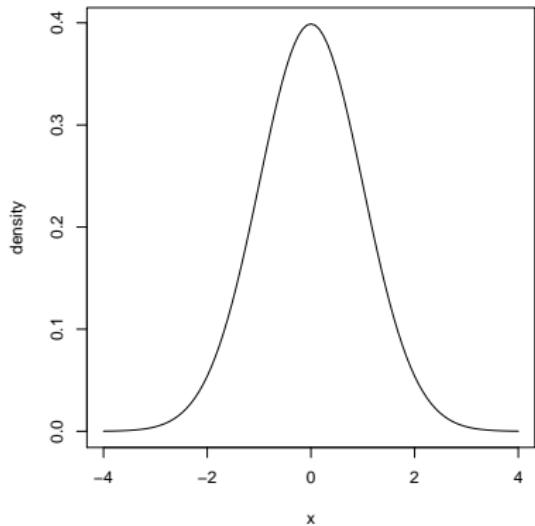
$$Y \sim N(\mu, \sigma^2)$$

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

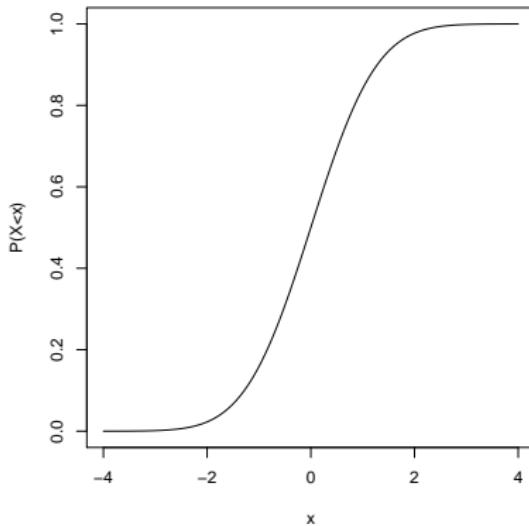
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If  $Z \sim N(0, 1)$  then  $Y = \mu + \sigma Z \sim N(\mu, \sigma^2)$

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- Infinite divisibility
- 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 Fit model  $f_\beta(x)$  to data  $y$  by minimizing  $\sum(y_i - f_\beta(x_i))^2$  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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**Bivariate Gaussian: d=2**

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

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$$\text{Var}(Y_i) = \sigma_i^2 \quad \text{Cov}(Y_i, Y_j) = \rho_{ij}\sigma_i\sigma_j \quad \text{Cor}(Y_i, Y_j) = \rho_{12} \text{ for } i \neq j$$

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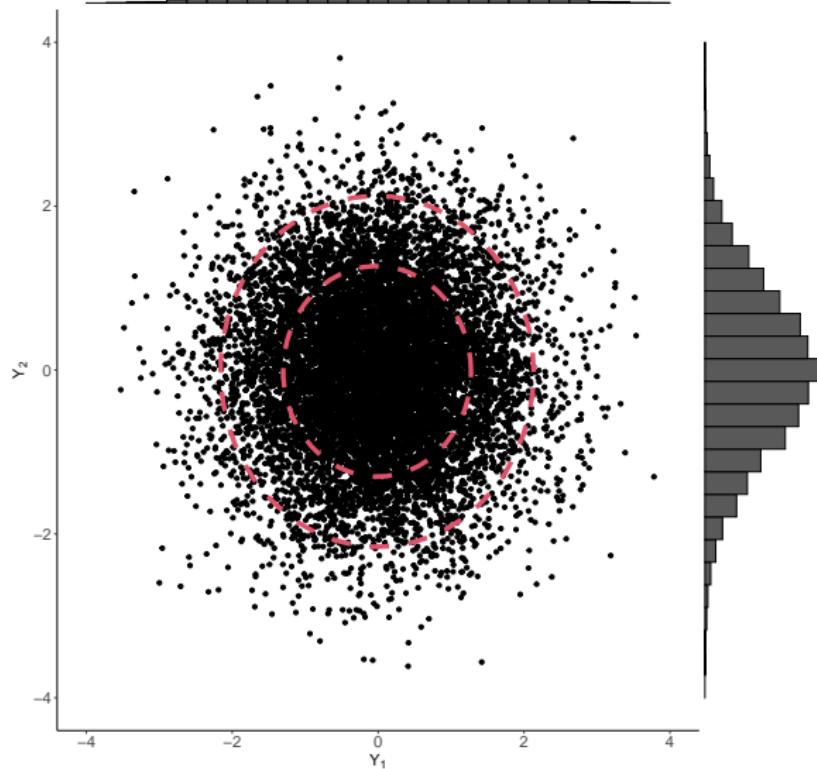
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pdf:  $f(y | \mu, \Sigma) = |\Sigma|^{-\frac{1}{2}}(2\pi)^{-\frac{d}{2}} \exp\left(-\frac{1}{2}(y - \mu)^\top \Sigma^{-1}(y - \mu)\right)$

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

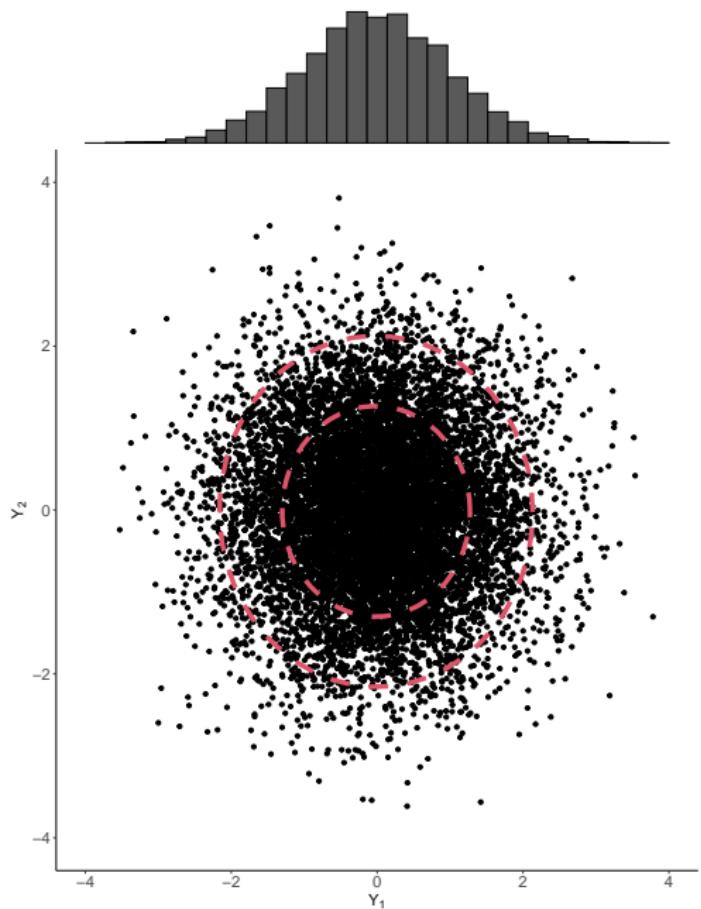
$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

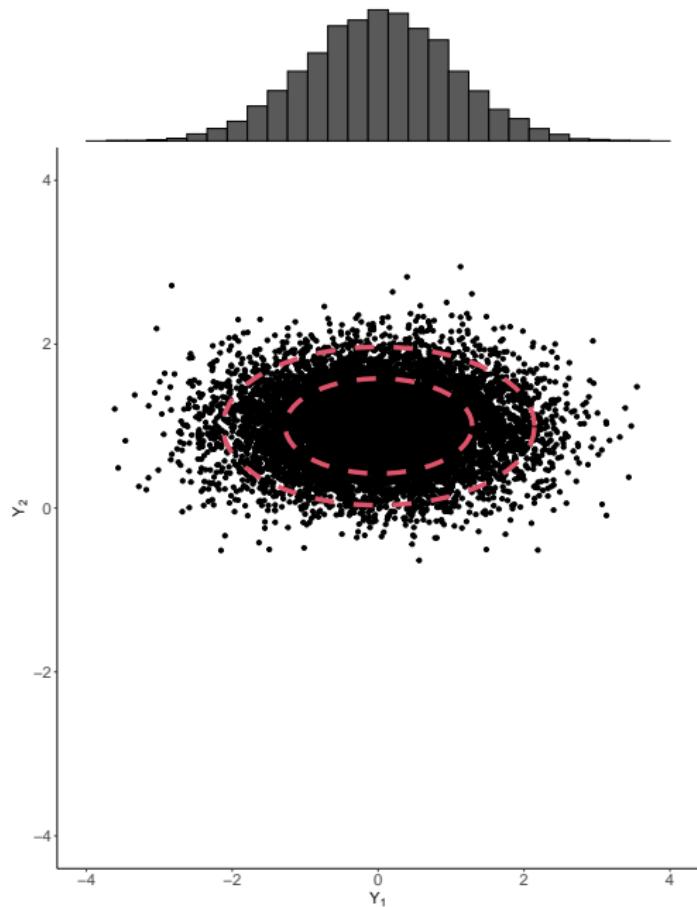


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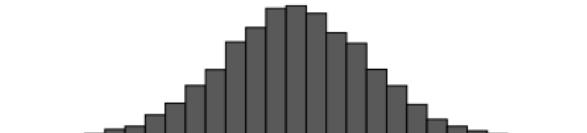
So  
 $\text{Cor}(Y_1, Y_2) = 0$   
hence  $Y_1$   
independent of  $Y_2$

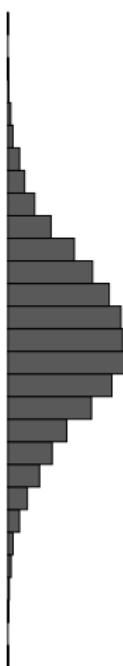


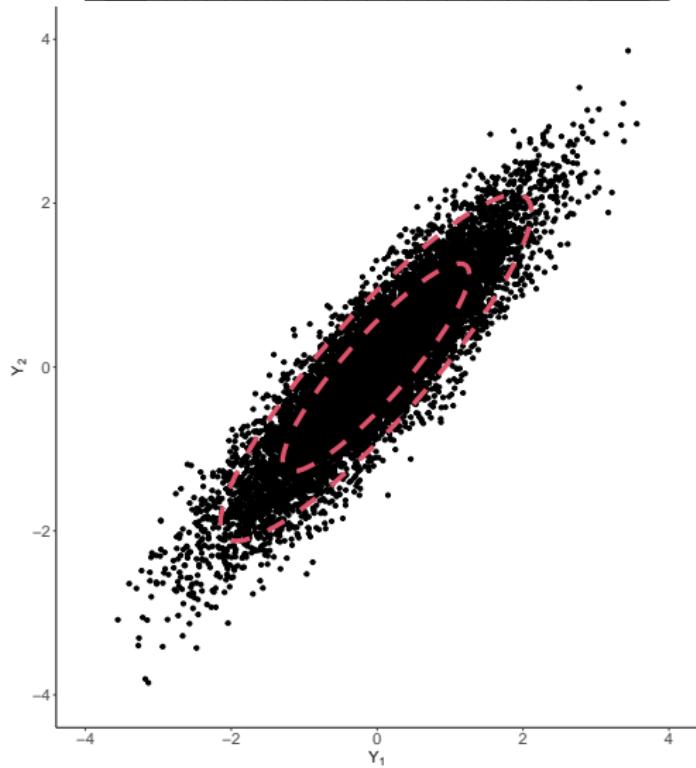


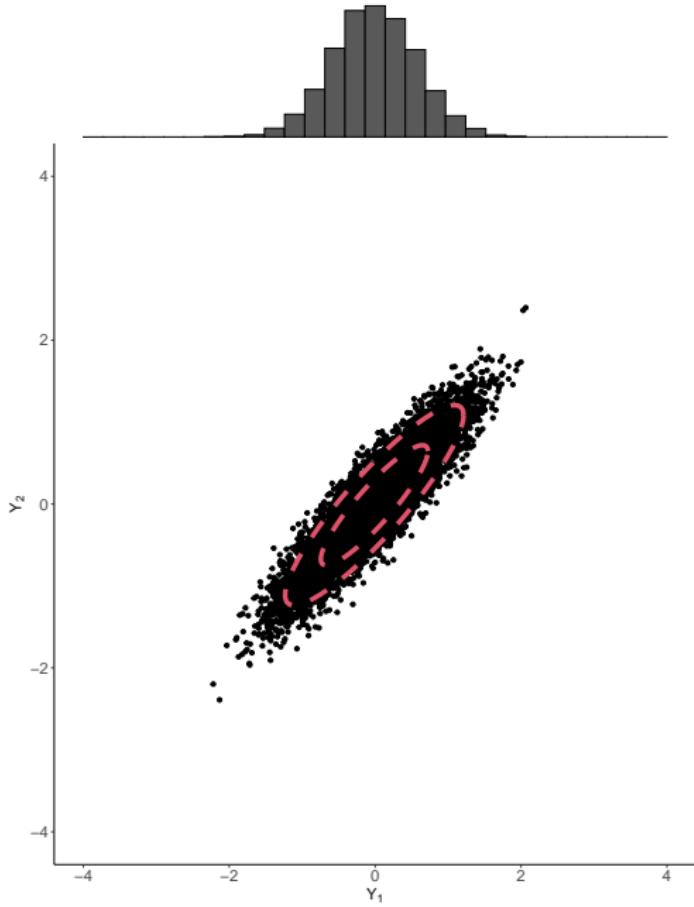
$$\mu = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

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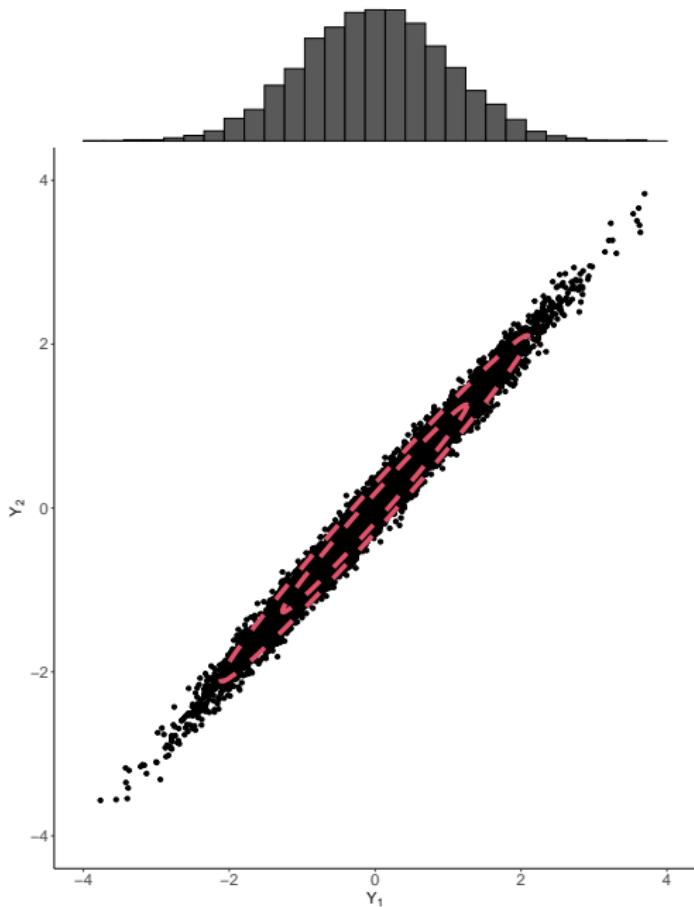

$$\Sigma = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$





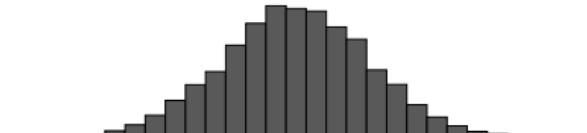
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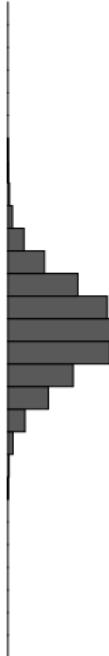
$$\Sigma = \frac{1}{3} \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$

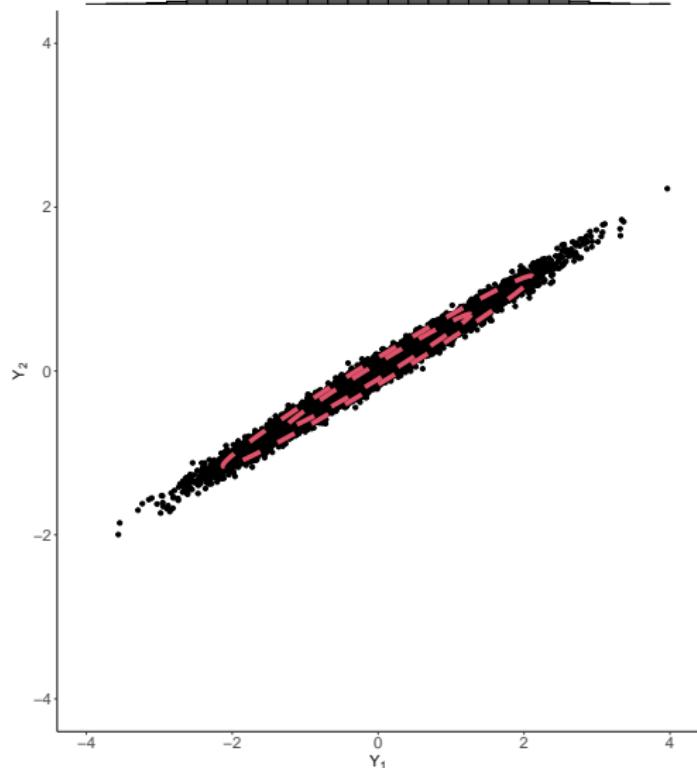


$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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


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


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

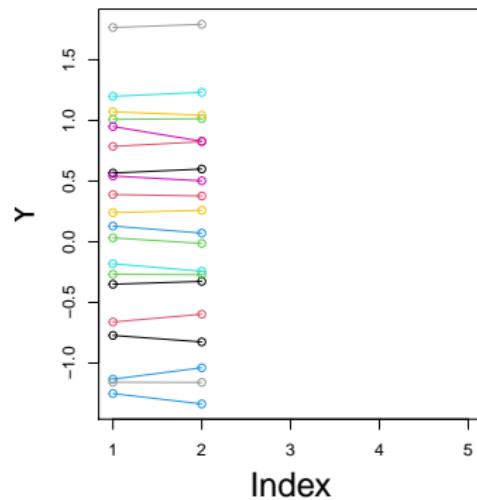
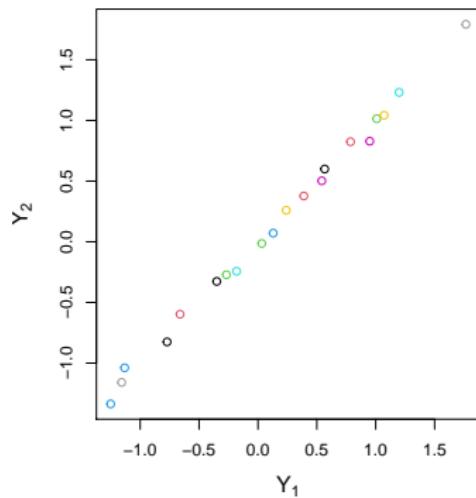

$$Cor(Y_1, Y_2) = \\ 0.54 / \sqrt(0.3) = \\ 0.99$$

## More pictures

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

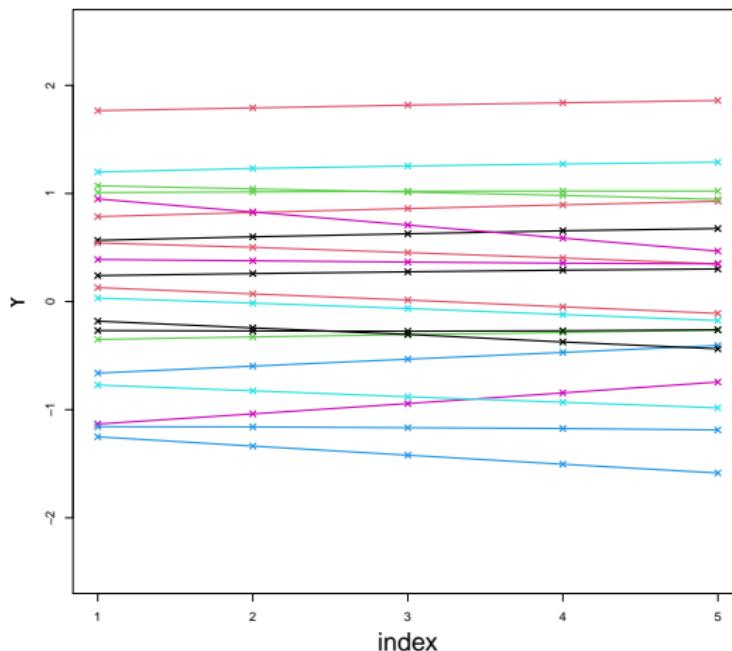
## More pictures

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



Consider  $d = 5$  with

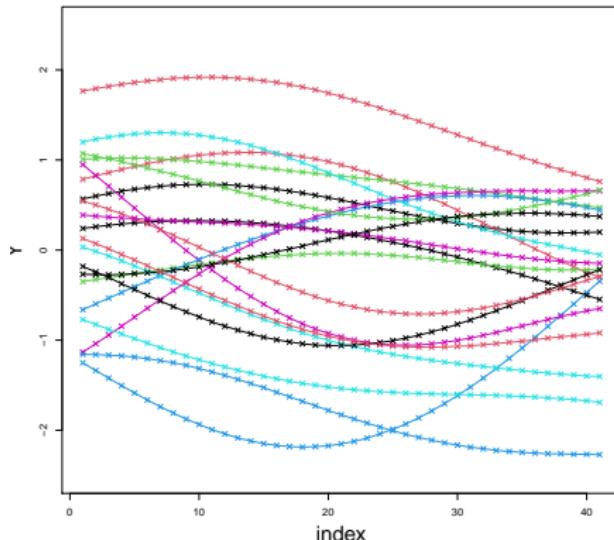
$$\mu = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \Sigma = \begin{pmatrix} 1 & 0.99 & 0.98 & 0.97 & 0.96 \\ 0.99 & 1 & 0.99 & 0.98 & 0.97 \\ 0.98 & 0.99 & 1 & 0.99 & 0.98 \\ 0.97 & 0.98 & 0.99 & 1 & 0.99 \\ 0.96 & 0.97 & 0.98 & 0.99 & 1 \end{pmatrix}$$



Each line is one sample.

$$d = 50$$

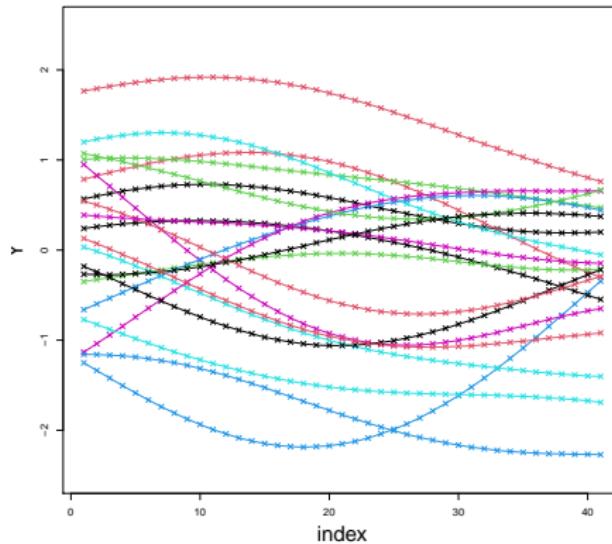
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We can think of Gaussian processes as an infinite dimensional distribution over functions - all we need to do is change the indexing

## Gaussian processes

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

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Thankfully, to understand the law of  $y$  we only need consider the finite dimensional distributions (FDDs), i.e., for all  $x_1, \dots, x_n$  and for all  $n \in \mathbb{N}$

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

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

where

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

$$\text{Cov}(y(x), y(x')) = k(x, x')$$

## Specifying the mean function

We are free to choose the mean  $\mathbb{E}(y(x))$  and covariance  $\text{Cov}(y(x), y(x'))$  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  $m(x) = \text{const}$  for all  $x$ , or  
 $m(x) = \beta^\top x$

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

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

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If  $\text{Cov}(y(x), y(x')) = k(\|x - x'\|)$  the covariance function is said to be **isotropic**.

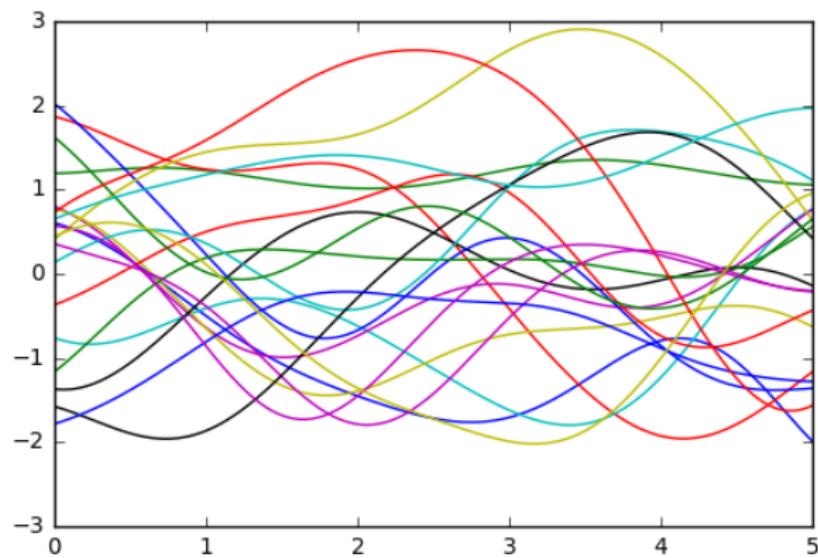
The covariance function determines the *nature* of the GP.

- $k$  determines the hypothesis space/space of functions

## Examples

RBF/Squared-exponential/exponentiated quadratic

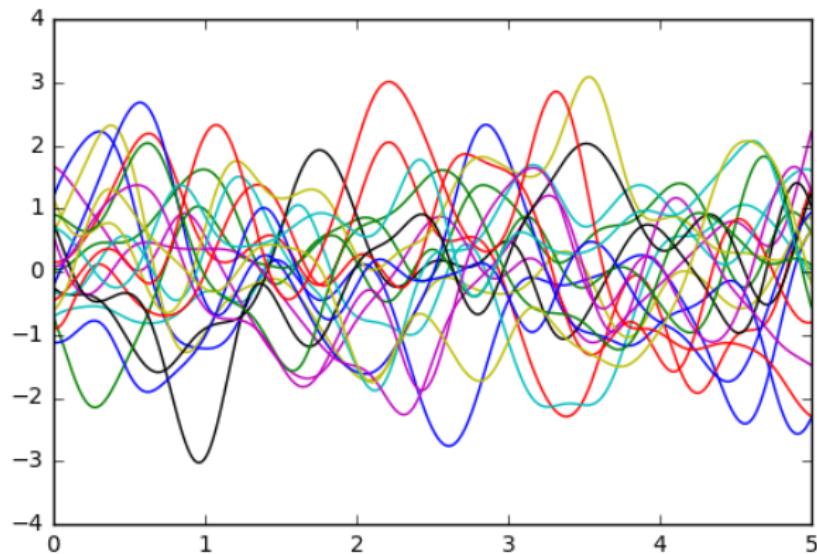
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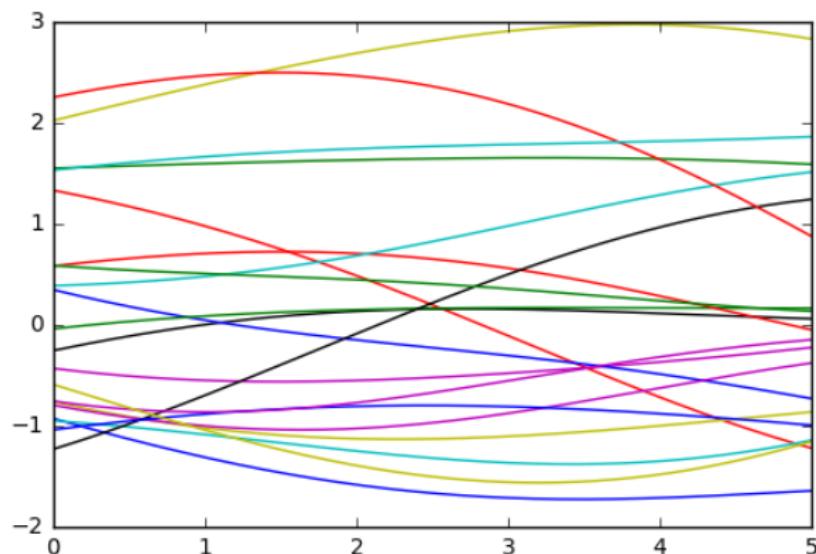
$$k(x, x') = \exp\left(-\frac{1}{2} \frac{(x - x')^2}{0.25^2}\right)$$



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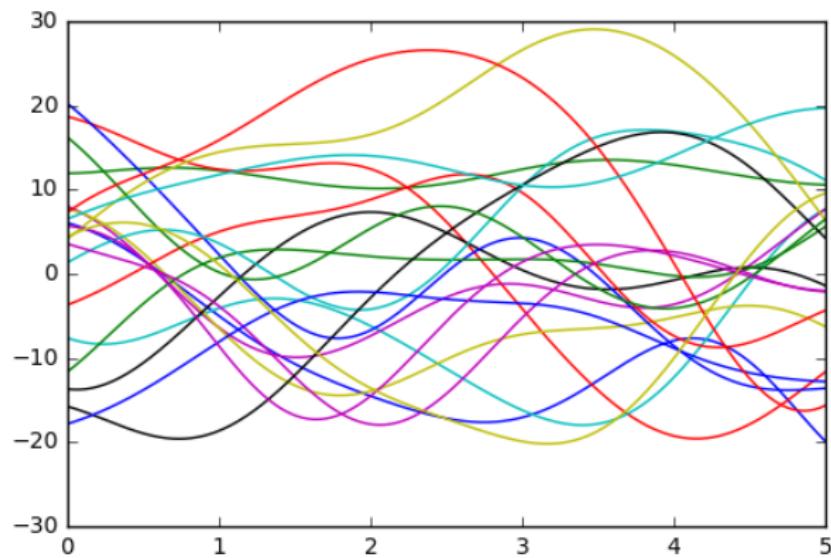
$$k(x, x') = \exp\left(-\frac{1}{2} \frac{(x - x')^2}{4^2}\right)$$



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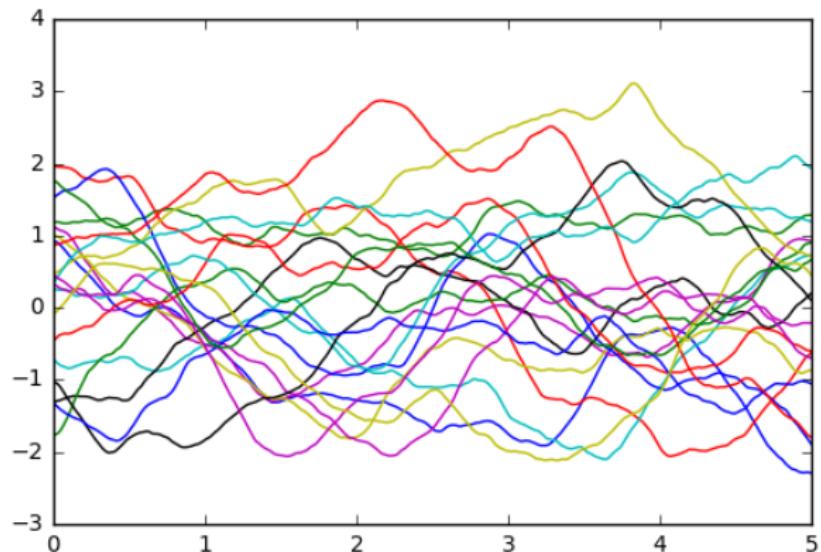
$$k(x, x') = \textcolor{red}{100} \exp\left(-\frac{1}{2}(x - x')^2\right)$$



## Examples

Matern 3/2

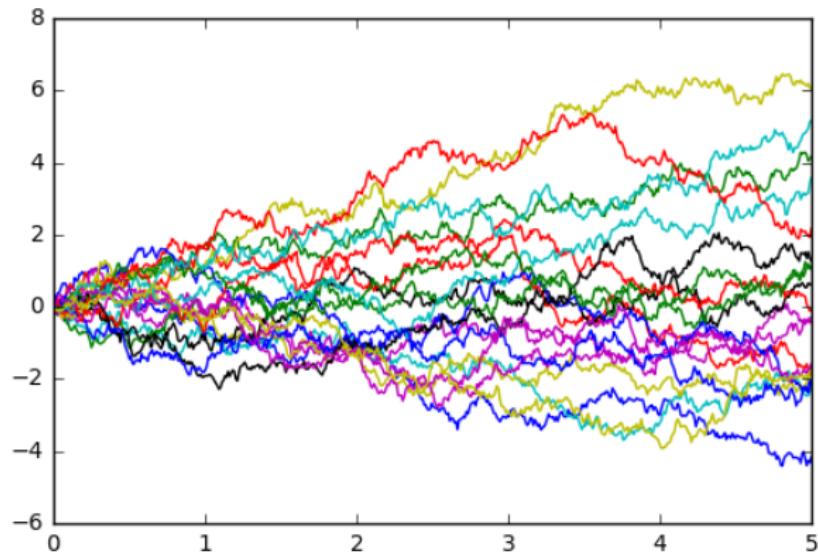
$$k(x, x') \sim (1 + |x - x'|) \exp(-|x - x'|)$$



## Examples

Brownian motion

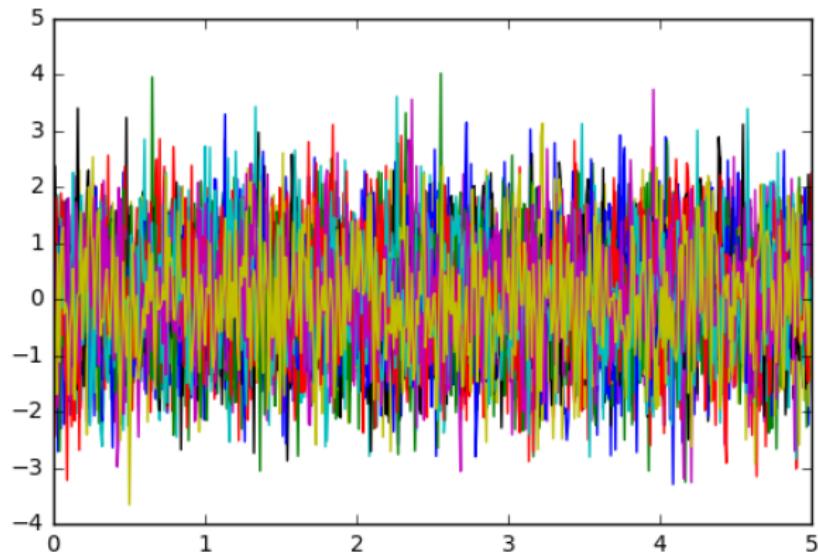
$$k(x, x') = \min(x, x')$$



## Examples

White noise

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



## Examples

The GP inherits its properties primarily from the covariance function  $k$ .

- Smoothness
- Differentiability
- Variance

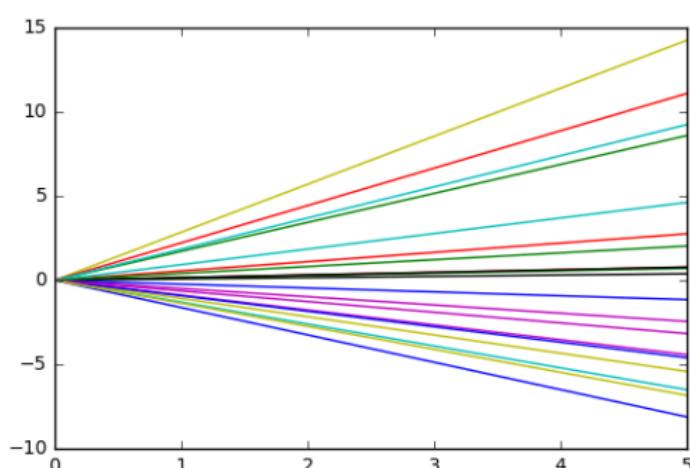
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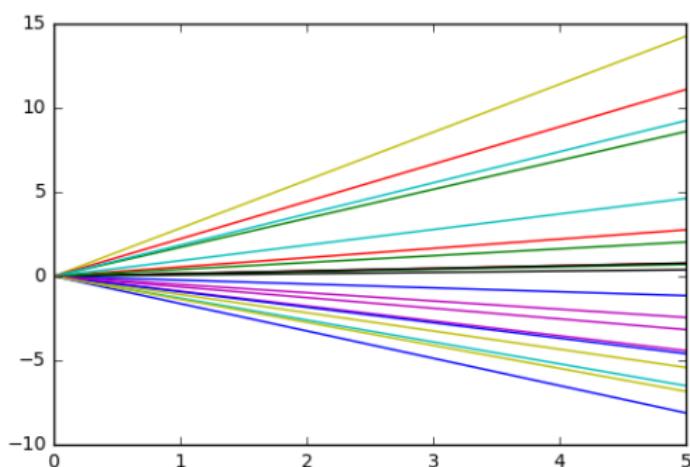
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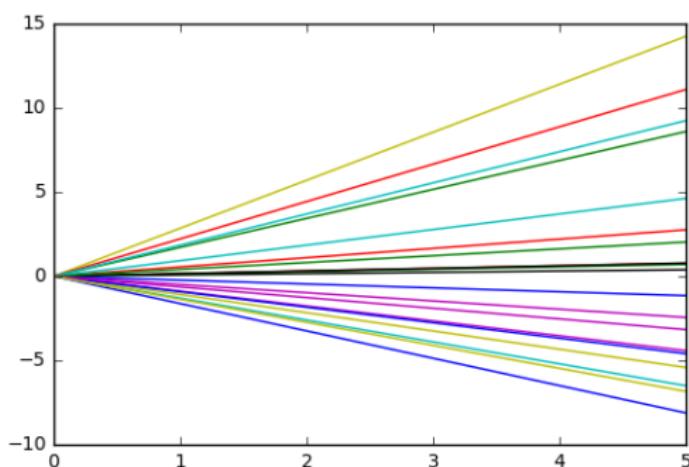
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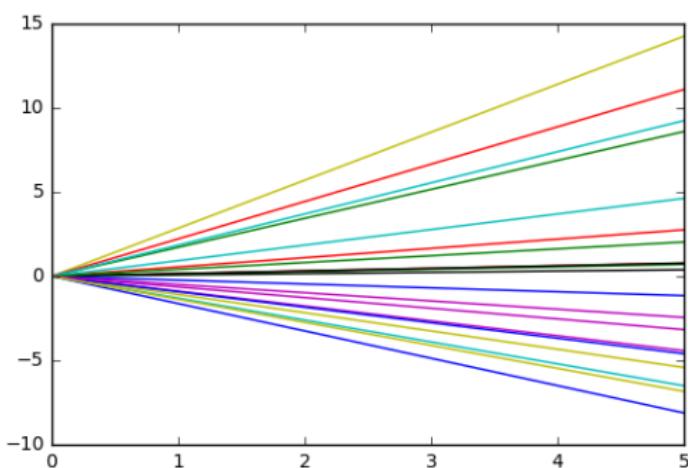
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So  $y(\cdot) \sim GP(0, k(x, x'))$  with  
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Conversely, any matrix  $\Sigma$  which is positive semi-definite is a valid covariance matrix:

If  $Z \sim N_d(0_d, I_d)$  then  $Y = \mu + \Sigma^{\frac{1}{2}}Z \sim N_d(\mu, \Sigma)$ .

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- Gives one way of generating multivariate Gaussians.

## Property 2: Conditional distributions are still Gaussian

Suppose

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

where

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

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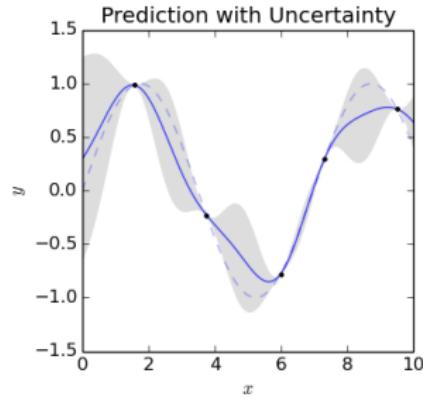
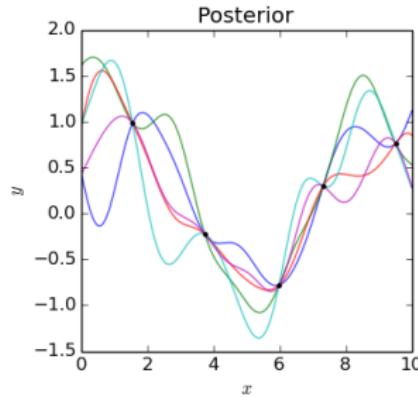
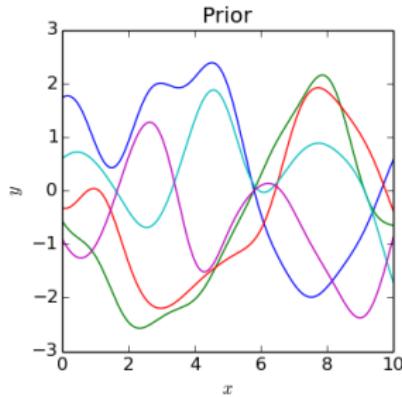
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Note that we still believe  $f$  is a GP even though we've observed its value at a number of locations.



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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

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Suppose  $f$  is a Gaussian process, then

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

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with

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More generally, if

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

then

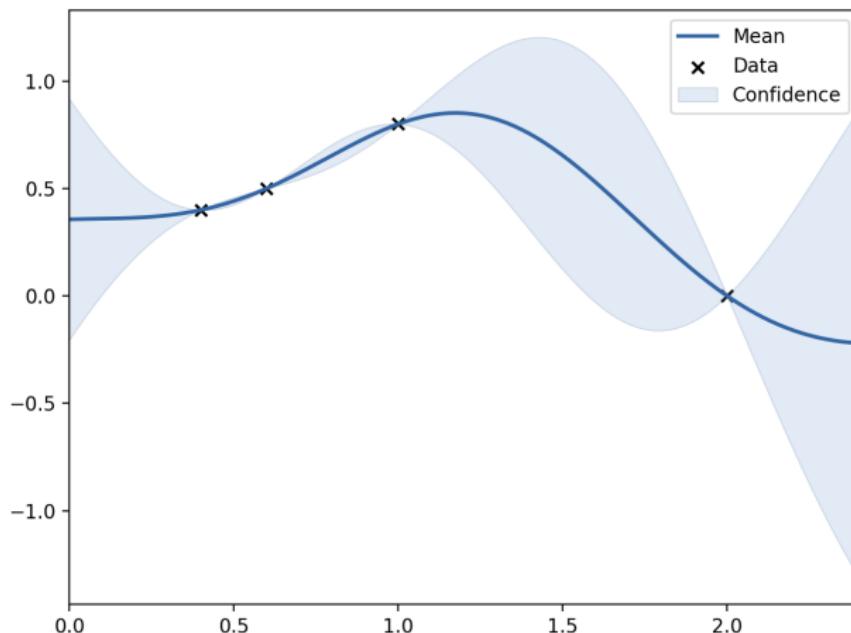
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with

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

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

## No noise/nugget - Interpolation



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

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

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

## Noisy observations/with nugget - Regression

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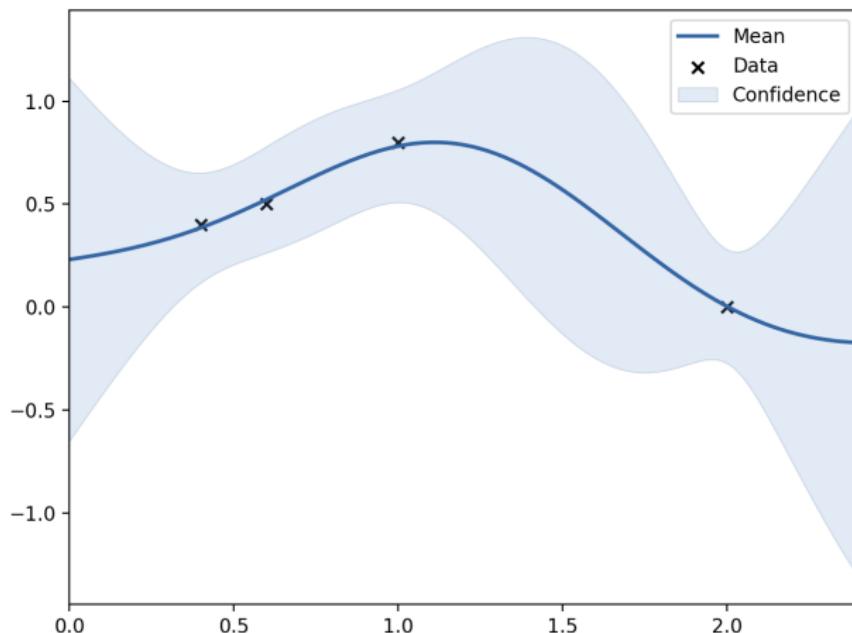
$$f(x) \mid y_1, \dots, y_n \sim N(\bar{m}(x), \bar{k}(x))$$

where

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

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

## Nugget standard deviation $\sigma = 0.1$

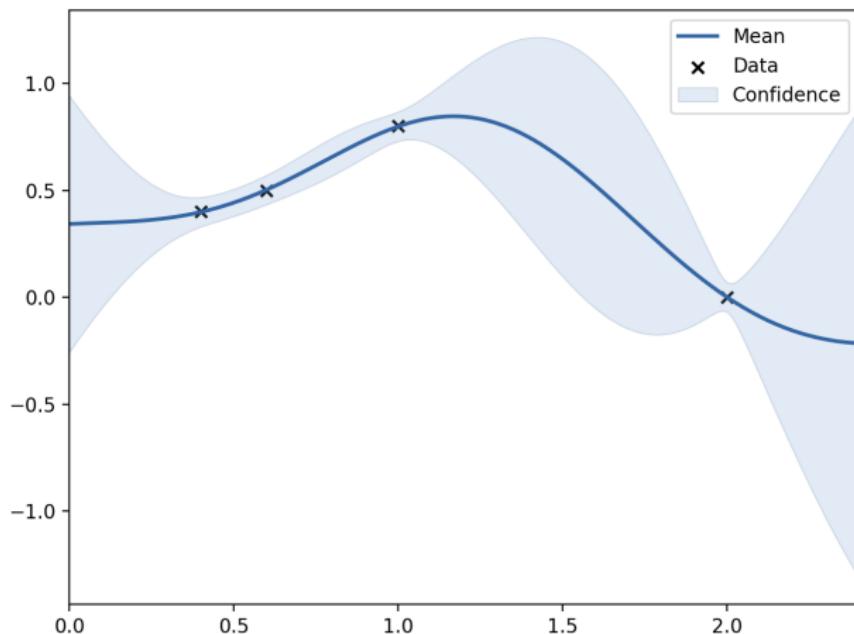


Solid line  $\bar{m}(x) = k_X(x)^\top K_{XX}^{-1} \mathbf{y}$

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

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

## Nugget standard deviation $\sigma = 0.025$



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

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

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- If

$$k(x, x') = \sigma^2 c(x, x')$$

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

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

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.

- $k$  determines the space of functions that sample paths live in.

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where  $X = \begin{pmatrix} x_1^\top \\ x_2^\top \\ \vdots \\ x_n^\top \end{pmatrix}$

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

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

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

— This is useful!

## Prediction

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

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

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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

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

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

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i.e., linear regression using all the linear and quadratic terms, and first order interactions.

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To evaluate  $k(\mathbf{x}, \mathbf{z})$  we didn't need to explicitly compute the feature vectors  $\phi(\mathbf{x}), \phi(\mathbf{z}) \in \mathbb{R}^6$

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

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 $k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$

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**Theorem:** A function

$$k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$$

is positive semi-definite (and thus a valid covariance function) if and only if we can write<sup>2</sup>

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

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WARNING: SOMETHING NOT QUITE RIGHT HERE.

**Example:** If  $\mathcal{X} = [0, 1]$ ,  $c_0 = 0$ ,  $c_1 = \frac{1}{N}$ ,  $c_2 = \frac{2}{N}, \dots, c_N = 1$  then (modulo some detail) if

$$\phi(x) \propto (e^{-\frac{(x-c_0)^2}{2\lambda^2}}, \dots, e^{-\frac{(x-c_N)^2}{2\lambda^2}})$$

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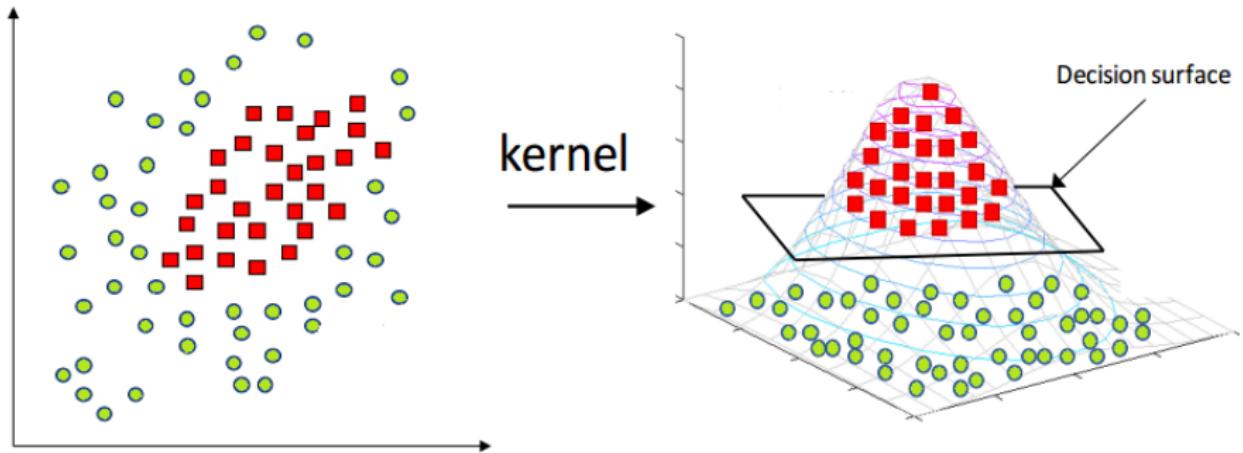
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We can use an infinite dimensional feature vector  $\phi(x)$ , and because linear regression can be done solely in terms of inner-products (inverting a  $n \times n$  matrix in the dual form) we never need evaluate the feature vector, only the kernel.

## Kernel trick:

lift  $x$  into feature space by replacing inner products  $x^T x'$  by  $k(x, x')$



## Kernel regression

Kernel regression and GP regression are closely related.

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ie functions of the form  $\sum_{i=1}^n \alpha_i k(x, x_i)$  with inner product

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

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.

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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<sup>3</sup>,

- 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.

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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

$$\mathbb{E}(X|Y) = \mathbb{E}(X) + \text{Cov}(X, Y)\text{Var}(Y)^{-1}(Y - \mathbb{E}(Y))$$

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

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One option is to find the best linear unbiased predictor (BLUP) of  $Y(x)$ .

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Consider the linear estimator

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

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

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

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

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and thus

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

as before.

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

## Why use GPs? Answer 4: Uncertainty estimates from emulators

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- point estimate
- uncertainty in that estimate

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It is important to check both aspects.

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

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

so that the posterior variance of  $f(x)$  does not depend upon  $y$ !

The 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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So the posterior can concentrate not on a point, but on some submanifold of parameter space, and the projection of the prior on this space continues to impact the posterior even as more and more data are collected.

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  $\sigma^2$  or  $\kappa$ , even as  $n \rightarrow \infty$ .

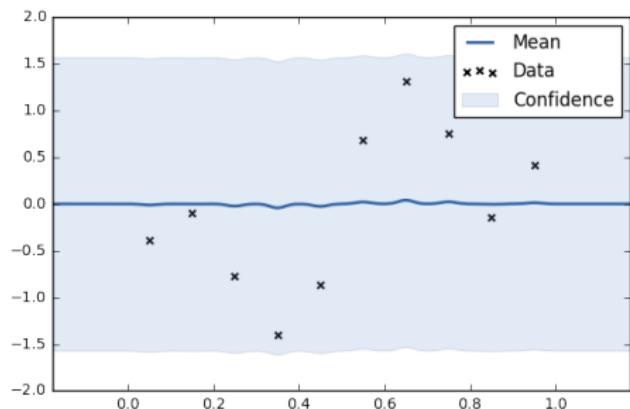
## Problems with hyper-parameter optimization

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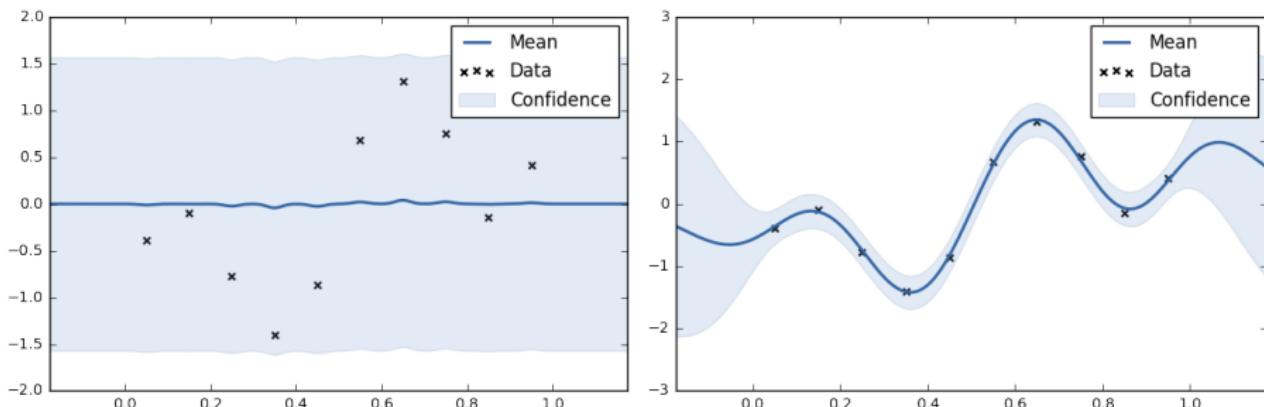
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We often work around these problems by running the optimizer multiple times from random start points, using prior distributions, constraining or fixing hyper-parameters, or adding white noise.

## Computational cost

One difficulty with GP is the computational cost of training them is  $O(n^3)$  (and  $O(n^2)$  memory)

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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  $m \ll n$  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

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

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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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. ↗ ↘ ↙

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- **Random Fourier features:**

Bochner's theorem says that a stationary kernel can be represented as a Fourier transform of a distribution

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

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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

- Once the good china, GPs are now ubiquitous in statistics/ML.
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  - ▶ Naturalness of the framework
  - ▶ Mathematical tractability
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Thank you for listening!

## References

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