An introduction to Gaussian Processes

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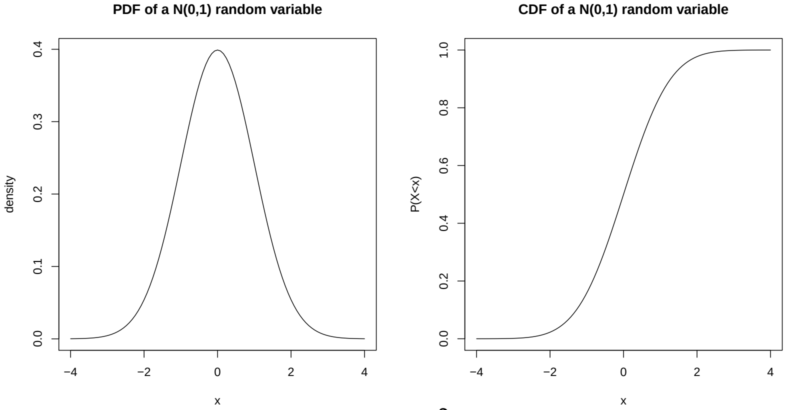
GP summer school
September 2019

Introduction

Univariate Gaussian distributions



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

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

CDF: $F_X(x) = \mathbb{P}(X \leq x)$ not known in closed form

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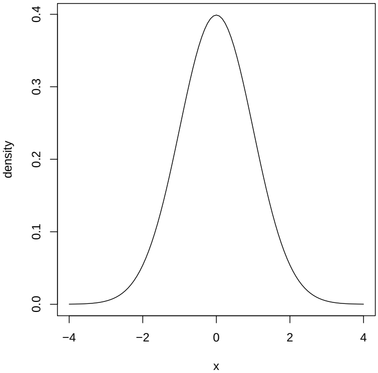
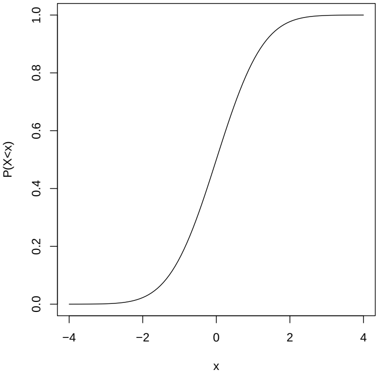

PDF of a N(0,1) random variable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If $Z \sim N(0,1)$ then $X = \mu + \sigma Z \sim N(\mu, \sigma^2)$

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- If normally distributed rvs X and Y 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 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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Write

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Bivariate Gaussian: d=2

$$X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \qquad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 \\ \rho_{21}\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

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$$\mathbb{V}\mathrm{ar}(X_i) = \sigma_i^2 \quad \mathbb{C}\mathrm{ov}(X_i, X_j) = \rho_{ij}\sigma_i\sigma_j \quad \mathrm{Cor}(X_i, X_j) = \rho_{12} \text{ for } i \neq j$$

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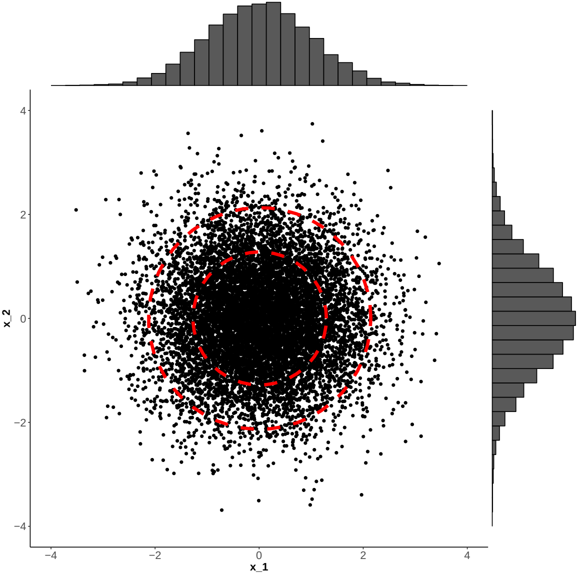
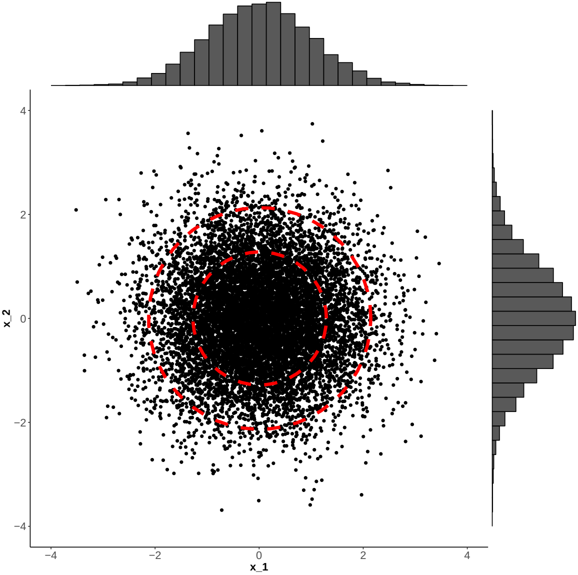
$$\text{pdf:} \quad f(x \mid \mu, \Sigma) = |\Sigma|^{-\frac{1}{2}}(2\pi)^{-\frac{d}{2}} \exp\left(-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right)$$



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

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



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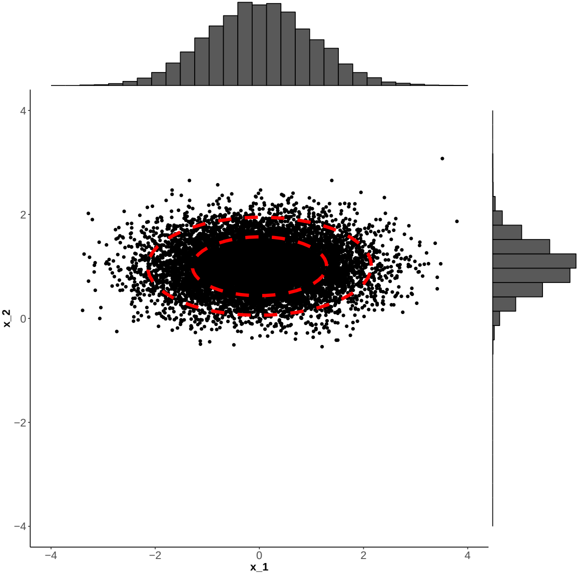
So
$Cor(X_1, X_2) = 0$
hence X_1
independent of X_2



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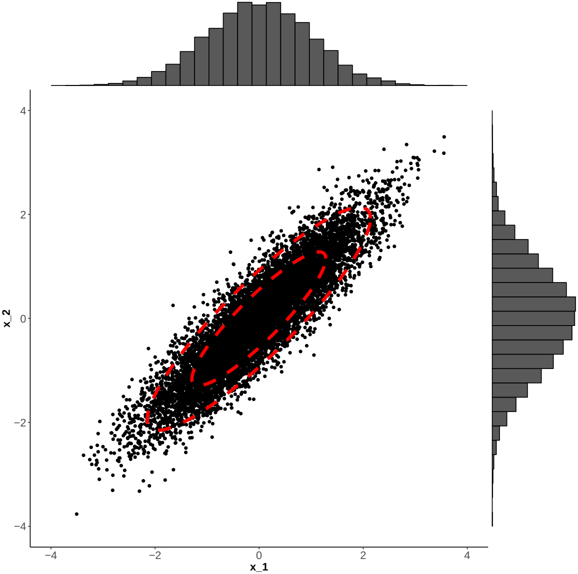
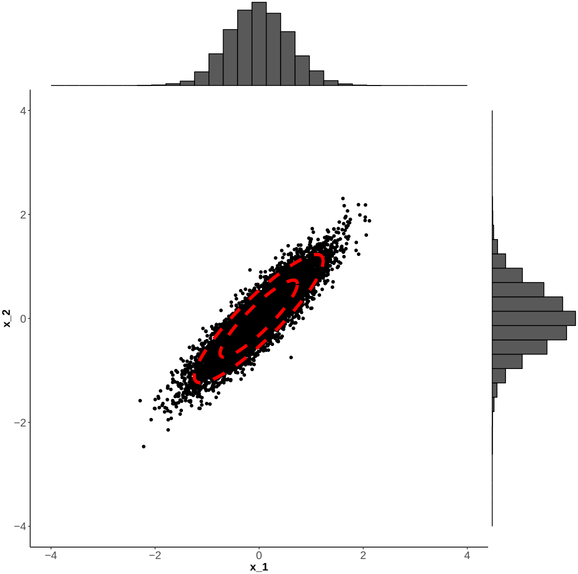


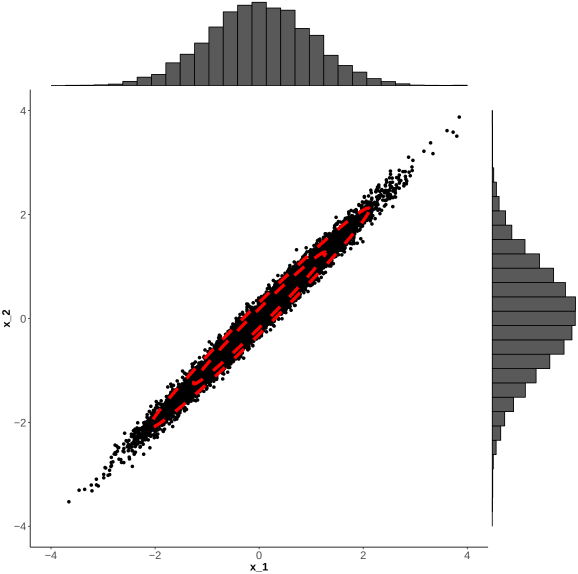
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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



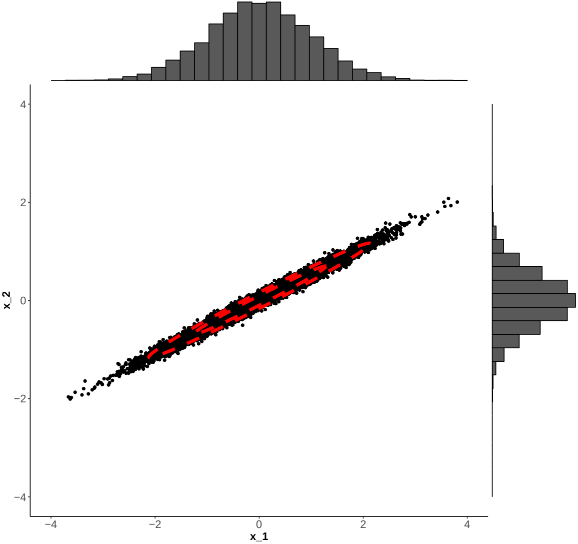
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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



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

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



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

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

$Cor(X_1, X_2) =$
$0.54/\sqrt(0.3) =$
0.99

More pictures

Consider $d = 5$ with

$$\Sigma = \begin{pmatrix} 1 & 0.9 & 0.8 & 0.7 & 0.6 \\ 0.9 & 1 & 0.9 & 0.8 & 0.7 \\ 0.8 & 0.9 & 1 & 0.9 & 0.8 \\ 0.7 & 0.8 & 0.9 & 1 & 0.9 \\ 0.6 & 0.7 & 0.8 & 0.9 & 1 \end{pmatrix}$$

It's hard to visualise in dimensions > 3, so let's stack points next to each other.

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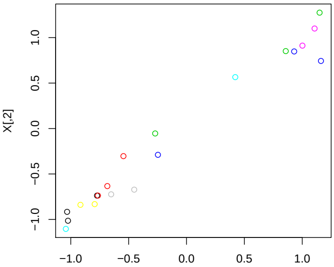
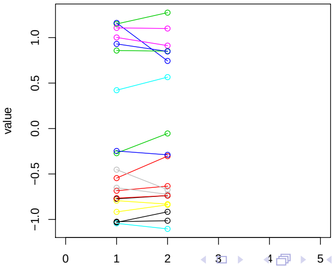
So for 2d instead of



we have



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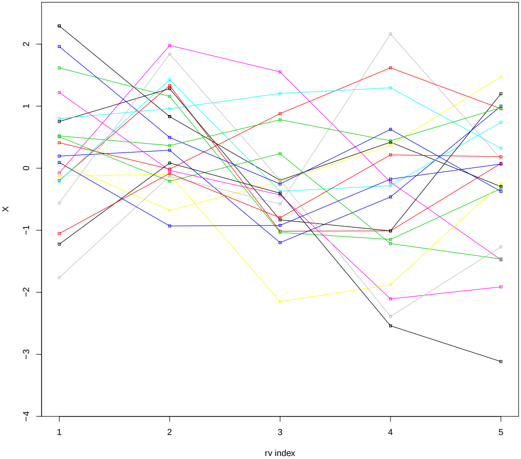

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THIS WAS CONFUSING. HAVING X as a rv here and then as an index in a few slides caused confusion. Also, people were thinking X_1 and X_2 were different covaariates, as in linear regression. Think about changing this.

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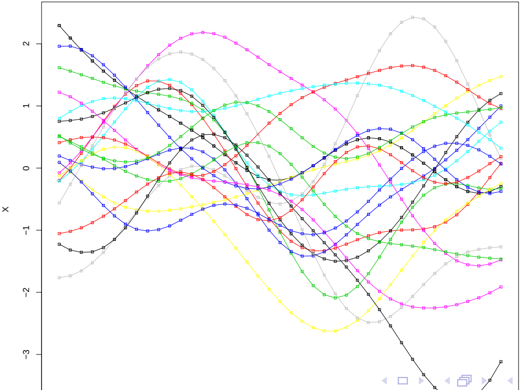

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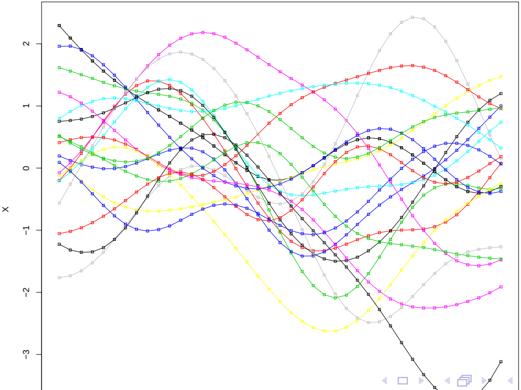

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Thankfully we only need consider the finite dimensional distributions (FDDs), i.e., for all $x_1, \ldots, x_n$ and for all $n \in \mathbb{N}$

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Conversely, any matrix Σ which is positive semi-definite is a valid covariance matrix:

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- Gives one way of generating multivariate Gaussians.

Property 2: Conditional distributions are still Gaussian

Suppose

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where

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\pi(x_2|x_1) &= \frac{\pi(x_1, x_2)}{\pi(x_1)} \propto \pi(x_1, x_2) \\
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&= \exp(-\frac{1}{2}\left[\left(\left(\begin{array}{c} x_1 \\ x_2 \end{array}\right) - \left(\begin{array}{c} \mu_1 \\ \mu_2 \end{array}\right)\right)^\top \left(\begin{array}{cc} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{array}\right) \cdots\right]
\end{aligned}$$

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Conditional updates of Gaussian processes

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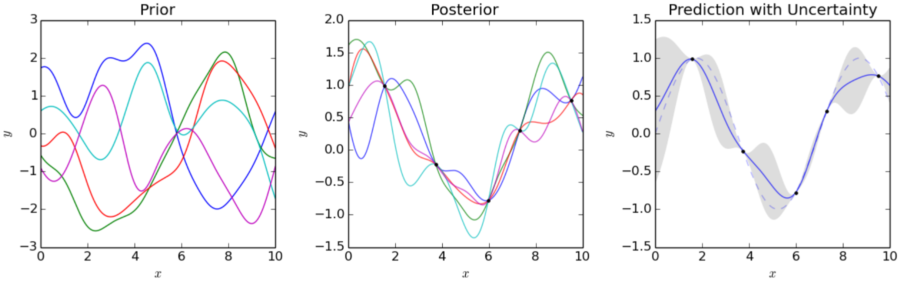
Note that we still believe f is a GP even though we've observed its value at a number of locations.



Prior

Posterior

Prediction with Uncertainty

Why use GPs? Answer 1

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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

Determining the mean and covariance function

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

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

  and $\beta \sim N(\cdot, \cdot)$ is given a normal prior (including $\pi(\beta) \propto 1$), then $f|D, \beta \sim GP$ and

  $$f|D \sim GP$$

  with slightly modified mean and variance formulas.

Covariance functions

- We usually use a covariance function that is a function of distance between the locations

$$k(x, x') = \mathbb{C}\text{ov}(f(x), f(x')),$$

  which has to be positive semi-definite, i.e., lead to valid covariance matrices.

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  - This can be problematic (see Nicolas' talk)

- If

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

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

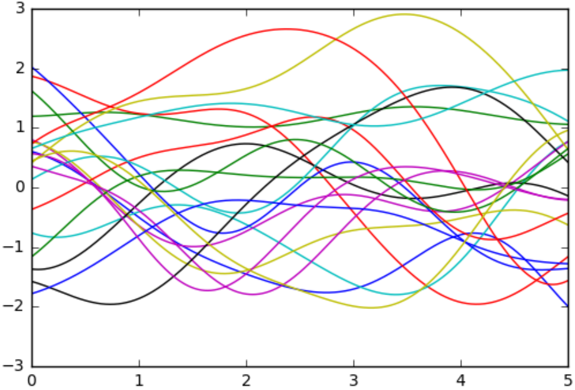
  $$f|D \sim \text{t-process}$$

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

Examples

RBF/Squared-exponential/exponentiated quadratic

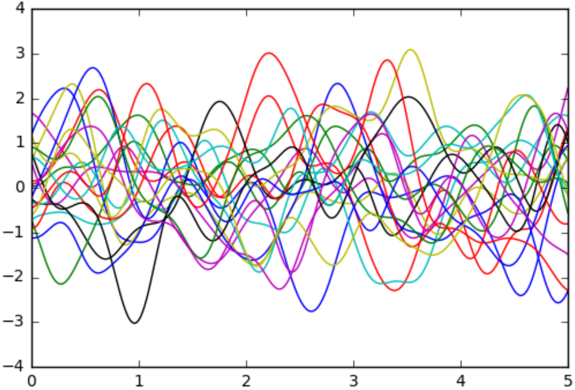
$$k(x, x') = \exp\left(-\frac{1}{2}(x - x')^2\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

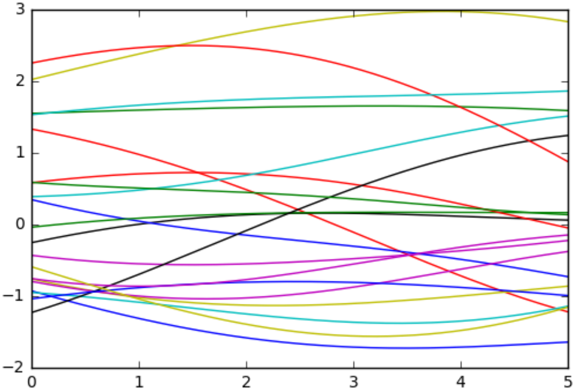
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{0.25^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

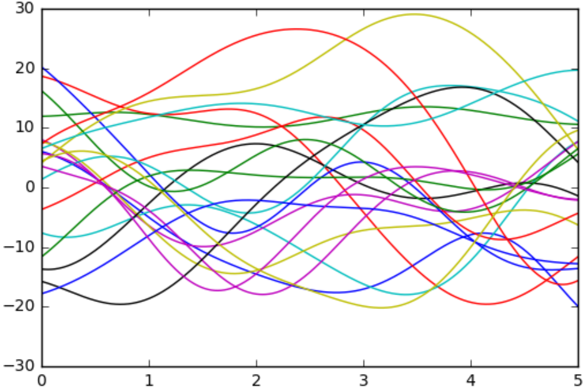
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{4^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

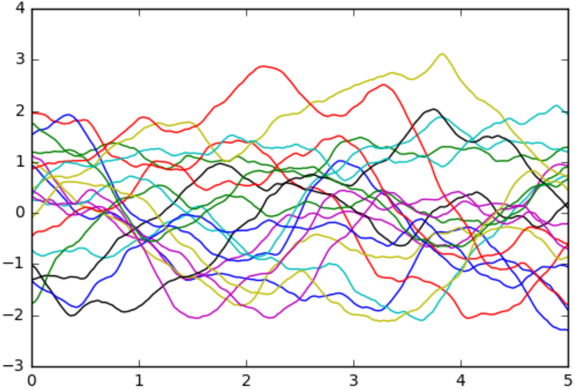
$$k(x, x') = 100 \exp\left(-\frac{1}{2}(x - x')^2\right)$$



Examples

Matern 3/2

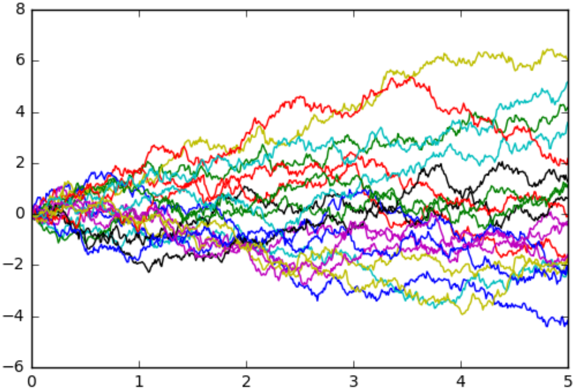
$$k(x, x') \sim (1 + |x - x'|) \exp\left(-|x - x'|\right)$$



Examples

Brownian motion

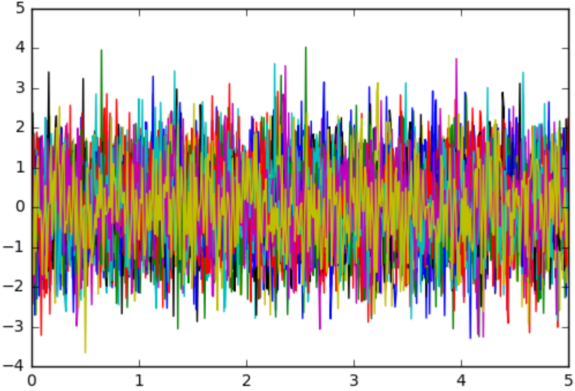
$$k(x, x') = \min(x, x')$$



Examples

White noise

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



Examples

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

- Smoothness
- Differentiability
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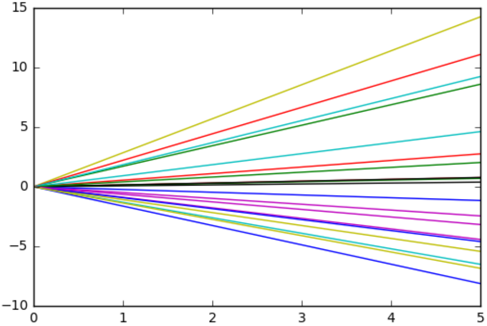
$$k(x, x') = x^\top x'$$



What is happening?

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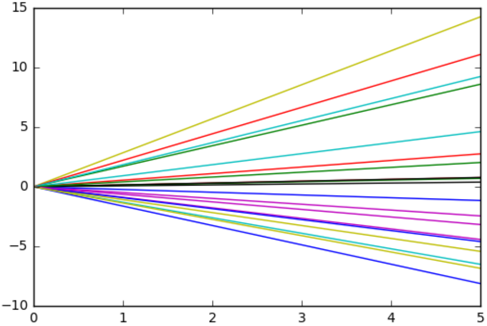

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Suppose $f(x) = cx$ where $c \sim N(0, 1)$.

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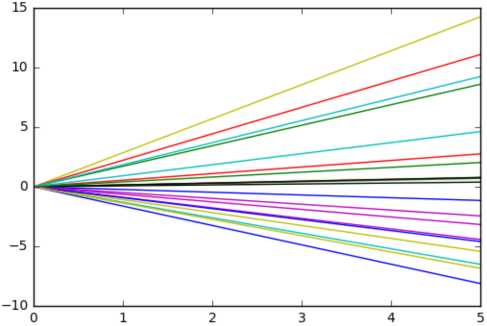

What is happening?
Suppose $f(x) = cx$ where $c \sim N(0, 1)$.
Then

$$\begin{aligned}\mathbb{C}\mathrm{ov}(f(x), f(x')) &= \mathbb{C}\mathrm{ov}(cx, cx') \\ &= x^\top \mathbb{C}\mathrm{ov}(c, c) x' \\ &= x^\top x'\end{aligned}$$

Conditional updates of Gaussian processes - revisited

ERROR: here covariance is Sigma, but on next slide I have Sigma + sigma2 I.
So suppose f is a Gaussian process, then

$$f(x_1), \dots, f(x_n), f(x) \sim N(0, \Sigma)$$

where

$$\Sigma = \begin{pmatrix} & & & & k(x_1, x) \\ & & K & & k(x_2, x) \\ & & & & \vdots \\ & & & & k(x_n, x) \\ k(x, x_1) & k(x, x_2) & \dots & k(x, x_n) & k(x, x) \end{pmatrix}$$

where $K_{ij} = k(x_i, x_j)$ is the Gram/kernel matrix.

Conditional updates of Gaussian processes - revisited

Then

$$f(x)|f(x_1),\dots,f(x_n) \sim N(m(x),c(x))$$

where

$$m(x) = k(x)(K+\sigma^2 I)^{-1} y$$

with

$$k(x) = \begin{pmatrix} k(x,x_1) & k(x,x_2) & \dots & k(x,x_n) \end{pmatrix} \in \mathbb{R}^{1\times n}$$

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

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But the dual form only uses inner products.

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

— This is useful!

Prediction

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

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

where $k(x') := (x'^{\top}x_1, \ldots, x'^{\top}x_n)$ and $K_{ij} := x_i^{\top}x_j$

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

$$m(x) = t(x)(K + \sigma^2 I)^{-1}y$$

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

- We know that we can replace x by a feature vector in linear regression, e.g., $\phi(x) = (1\ x\ x^2)$ etc.
  Then
  $$K_{ij} = \phi(x_i)^\top \phi(x_j) \qquad \text{etc}$$

- For some sets of features, the inner product is equivalent to evaluating a kernel function

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

where

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

is a semi-positive definite function.

NEEDS CLARIFICATION. ADD PICTURE OF FEATURES ETC. ADD THEORY AND TIGHTEN UP.

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  Example: If (modulo some detail)

  $$\phi(x) = (e^{-\frac{(x-c_1)^2}{2\lambda^2}}, \ldots, e^{-\frac{(x-c_N)^2}{2\lambda^2}})$$

  then as $N \to \infty$ then

  $$\phi(x)^\top \phi(x) = \exp\left(-\frac{(x-x')^2}{2\lambda^2}\right)$$

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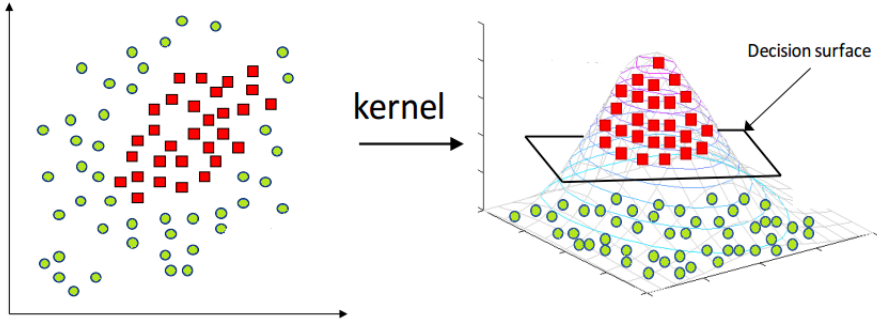
- We can use an infinite dimensional feature vector $\phi(x)$, and because linear regression can be done solely in terms of inner-products (inverting a $n \times n$ matrix in the dual form) we never need evaluate

Kernel trick:

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



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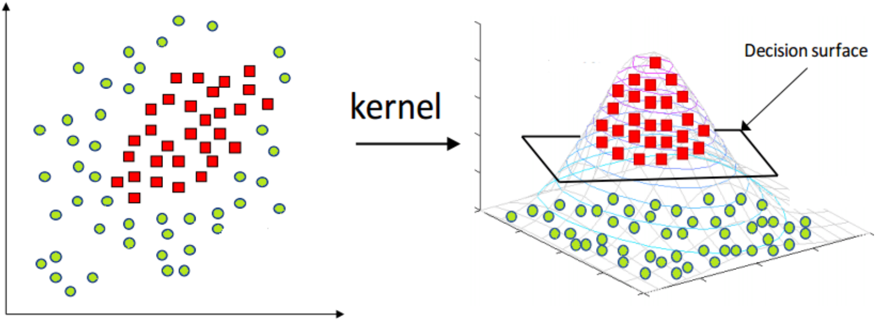

Kernel regression/non-parametric regression/GP regression all closely related:

$$\hat{y}' = m(x') = \sum_{i=1}^{n} \alpha_i k(x, x_i)$$

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$$f(x) = \sum_i c_i k(x, x_i)^1$$

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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 (and can be dense in some sets of continuous bounded functions), and is thus 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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Why use GPs? Answer 3: Naturalness of GP framework

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

[2]

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One answer might come from Bayes linear methods[2].
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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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.
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See also kernel Bayes and kriging/BLUP.

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Why use GPs? Answer 4: Uncertainty estimates from emulators

We often think of our prediction as consisting of two parts

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

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

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

The variance estimates are particularly sensitive to the hyper-parameter estimates.

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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 some standard procedure (maximum likelihood, cross-validation, Bayes etc)

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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 $n \to \infty$.

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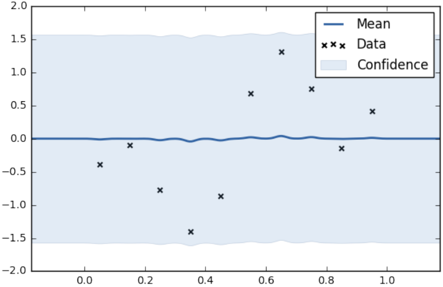

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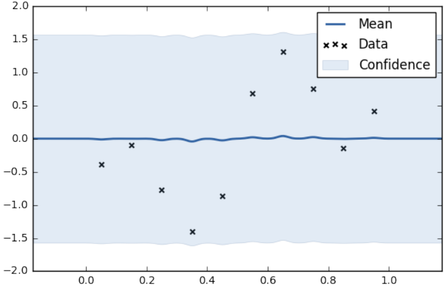

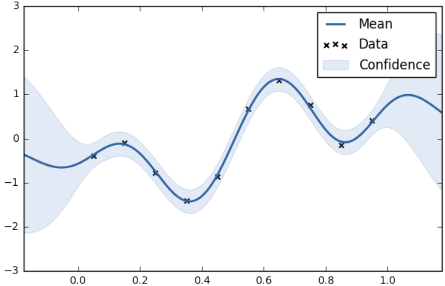

We often work around these problems by running the optimizer multiple times from random start points, using prior distributions, constraining or fixing hyper-parameters, or adding white noise.