An introduction to Gaussian Processes

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GP summer school
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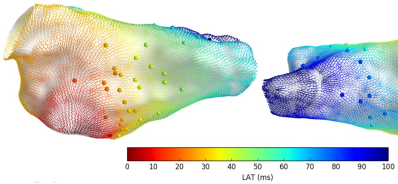
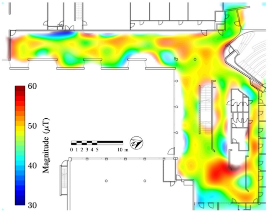
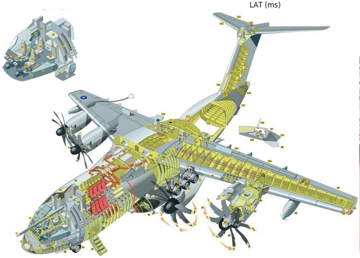
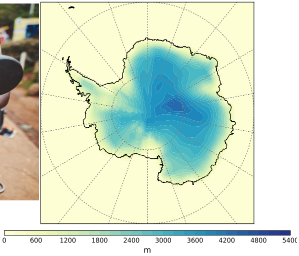
Recent GP Applications







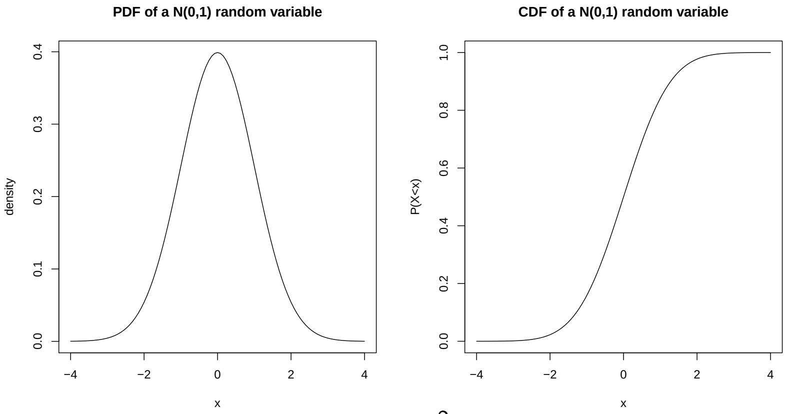


Introduction

- (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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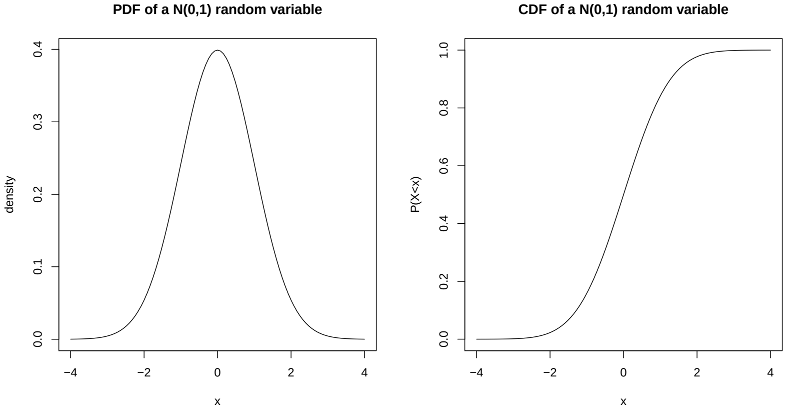

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If $Z \sim N(0,1)$ then $Y = \mu + \sigma Z \sim N(\mu, \sigma^2)$

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- 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 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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- **covariance matrix** $\Sigma \in \mathbb{R}^{d \times d}$.

Write

$$Y \sim N_d(\mu, \Sigma)$$

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Bivariate Gaussian: d=2

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

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$$\mathbb{V}\text{ar}(Y_i) = \sigma_i^2 \quad \mathbb{C}\text{ov}(Y_1, Y_2) = \rho_{12}\sigma_1\sigma_2 \quad \text{Cor}(Y_1, Y_2) = \rho_{12}$$

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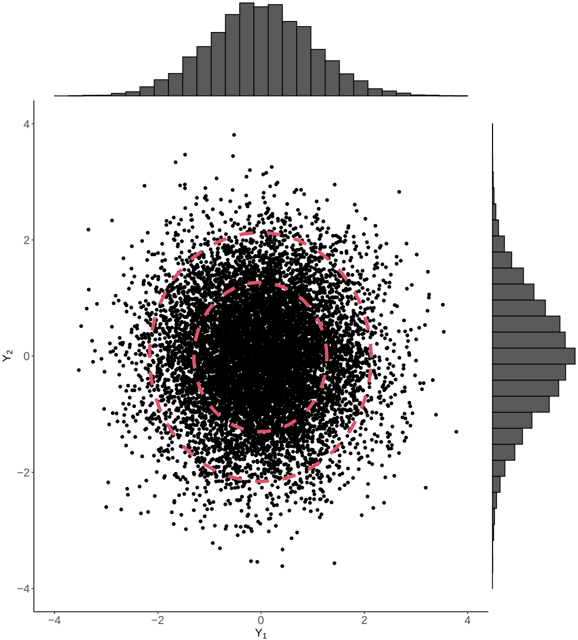
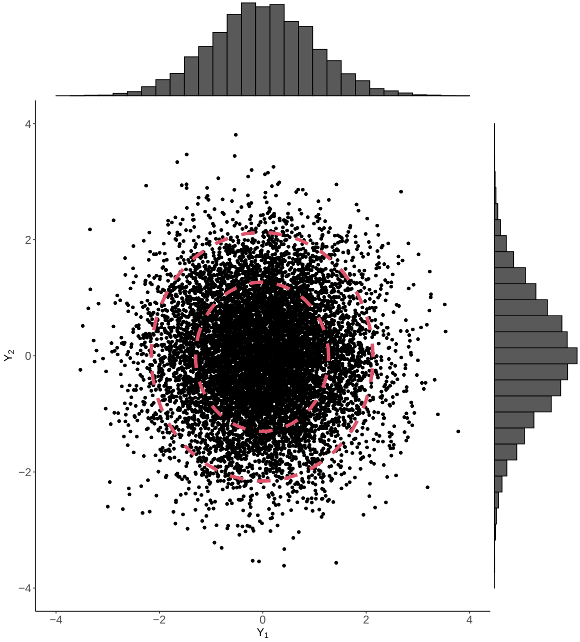
$$\text{pdf:} \quad f(y \mid \mu, \Sigma) = |\Sigma|^{-\frac{1}{2}}(2\pi)^{-\frac{d}{2}} \exp\left(-\frac{1}{2}(y-\mu)^\top \Sigma^{-1}(y-\mu)\right)$$



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

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



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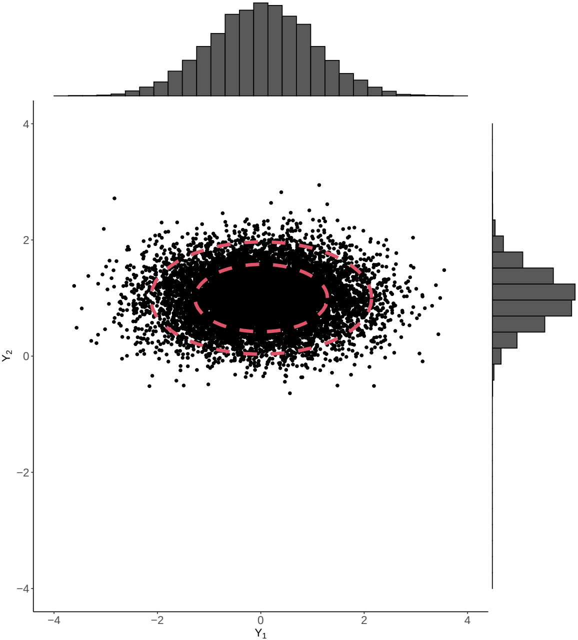
$Cor(Y_1, Y_2) = 0$
hence Y_1
independent of Y_2



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

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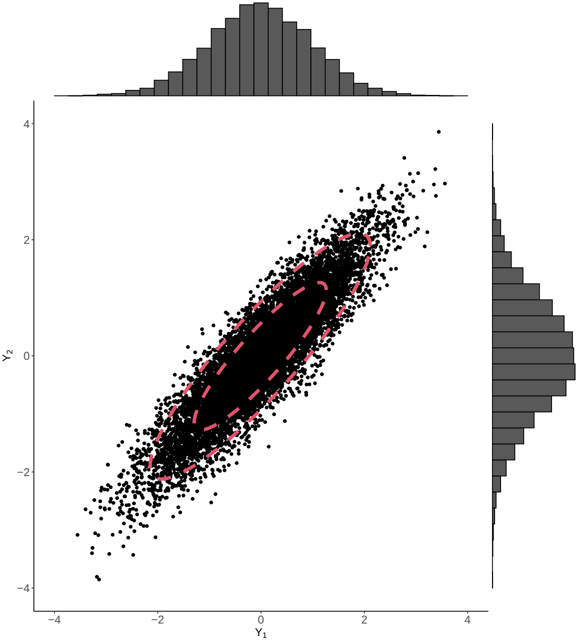
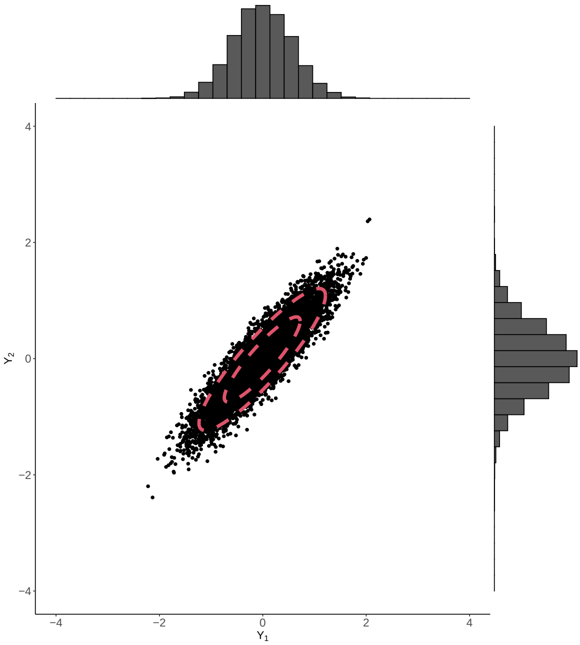


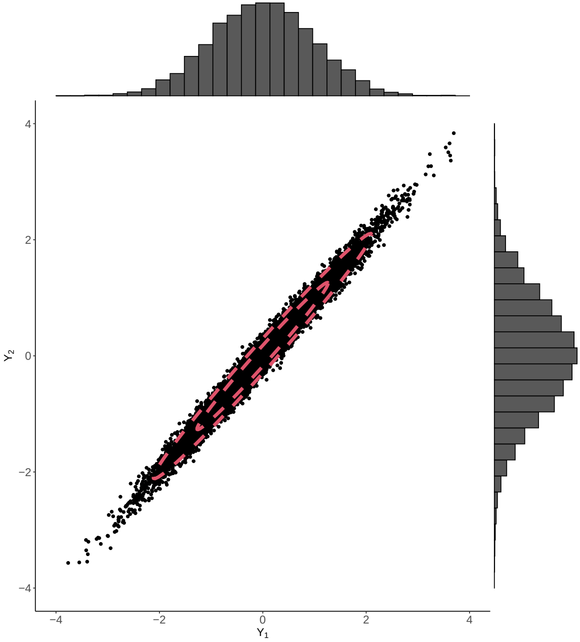
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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



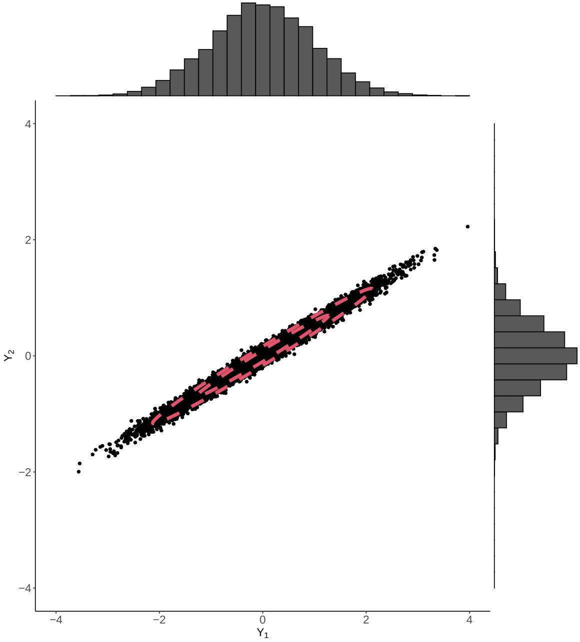
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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



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

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



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

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

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

More pictures

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

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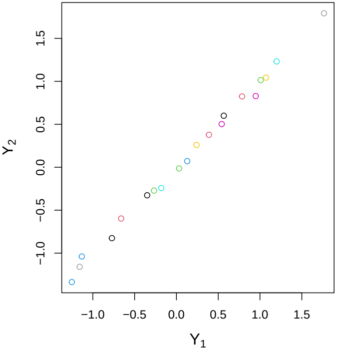
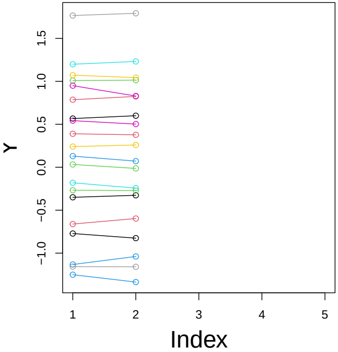
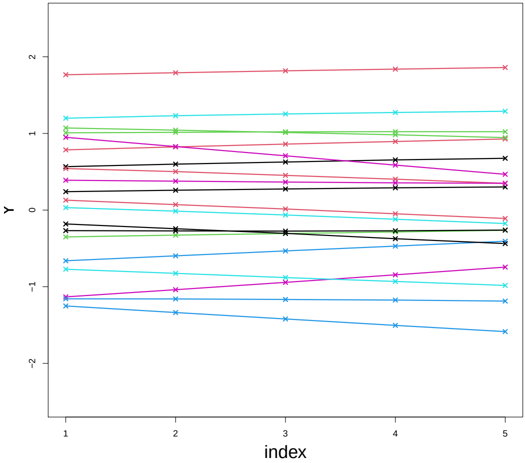
Hard to visualise in dimensions > 2, so stack points next to each other. So for 2d instead of  we have 

Consider $d = 5$ with

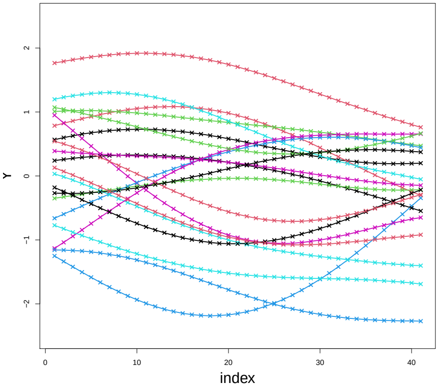
$$\mu = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.99 & 0.98 & 0.97 & 0.96 \\ 0.99 & 1 & 0.99 & 0.98 & 0.97 \\ 0.98 & 0.99 & 1 & 0.99 & 0.98 \\ 0.97 & 0.98 & 0.99 & 1 & 0.99 \\ 0.96 & 0.97 & 0.98 & 0.99 & 1 \end{pmatrix}$$



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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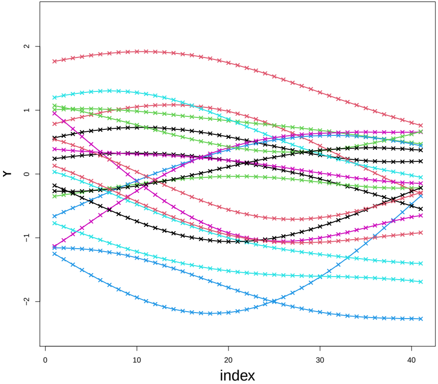

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We can think of Gaussian processes as an infinite dimensional distribution over functions - all we need to do is change the indexing

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 $x_1, \ldots, x_n$ and for all $n \in \mathbb{N}$

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

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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

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

Specifying the mean function

We are free to choose the mean $\mathbb{E}(y(x))$ and covariance $\mathbb{C}\mathrm{ov}(y(x), y(x'))$ 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 $m(x) = \beta^\top x$

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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.

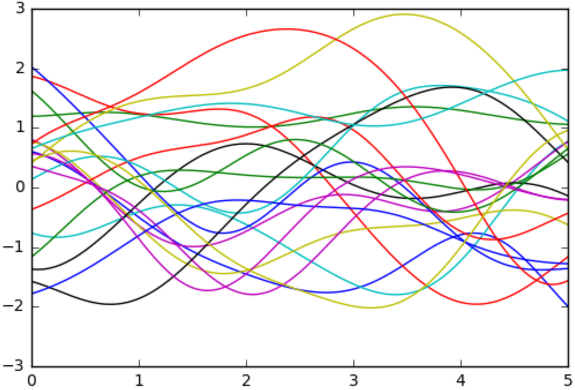
The covariance function determines the *nature* of the GP.

- k determines the hypothesis space/space of functions

Examples

RBF/Squared-exponential/exponentiated quadratic

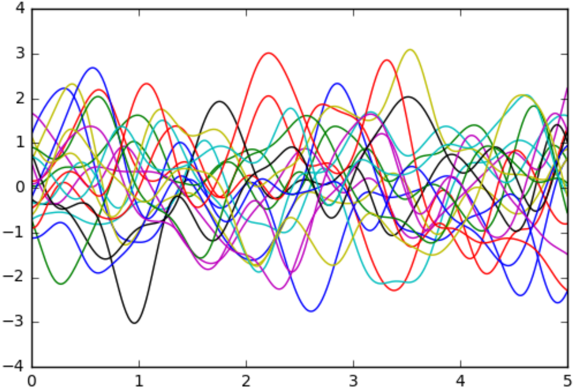
$$k(x, x') = \exp\left(-\frac{1}{2}(x - x')^2\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

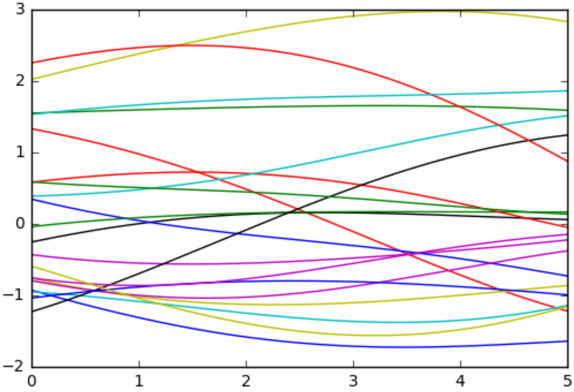
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{0.25^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

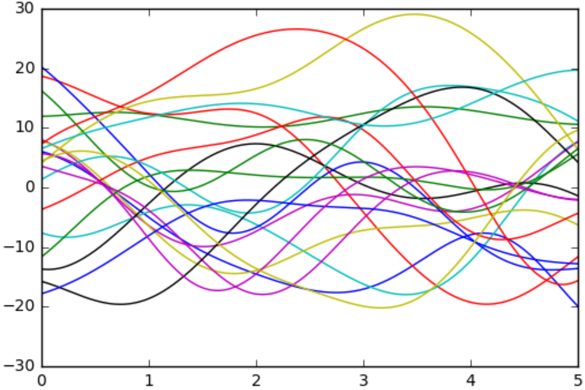
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{4^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

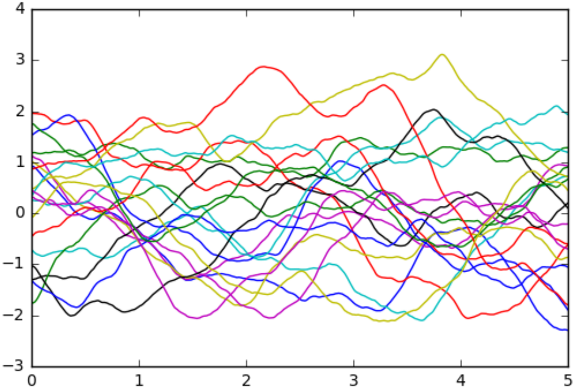
$$k(x, x') = 100 \exp\left(-\frac{1}{2}(x - x')^2\right)$$



Examples

Matern 3/2

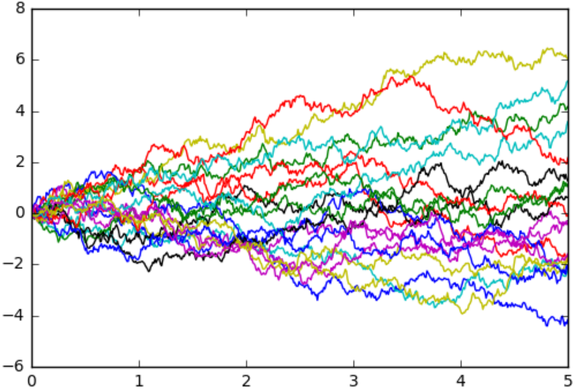
$$k(x, x') \sim (1 + |x - x'|) \exp\left(-|x - x'|\right)$$



Examples

Brownian motion

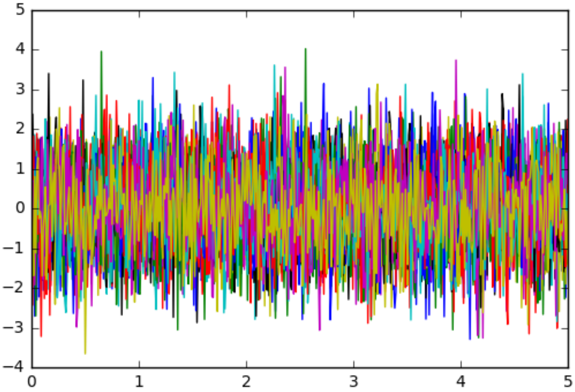
$$k(x, x') = \min(x, x')$$



Examples

White noise

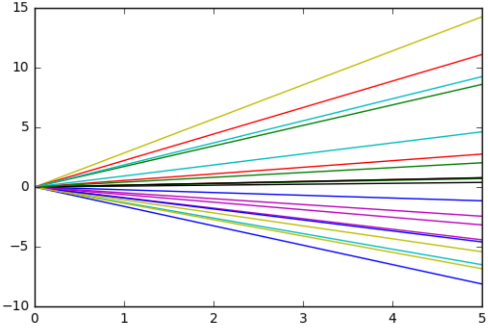
$$k(x, x') = \begin{cases} 1 \text{ if } x = x' \\ 0 \text{ otherwise} \end{cases}$$



Examples

A final example:

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



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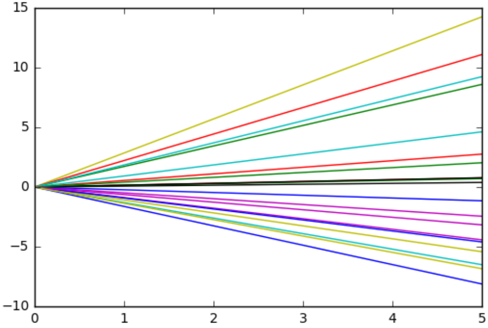

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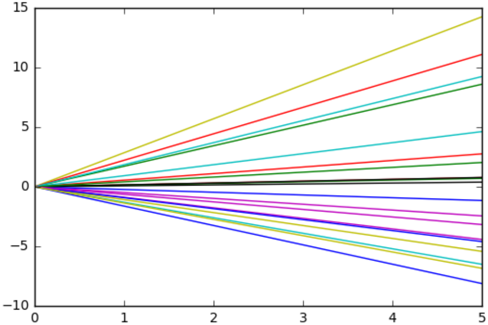

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Then
$$\mathbb{C}\text{ov}(y(x), y(x')) = \mathbb{C}\text{ov}(cx, cx') = x\mathbb{C}\text{ov}(c, c)x'$$
$$= xx'$$

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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  - For stationary kernels, require continuity at $k(0)$
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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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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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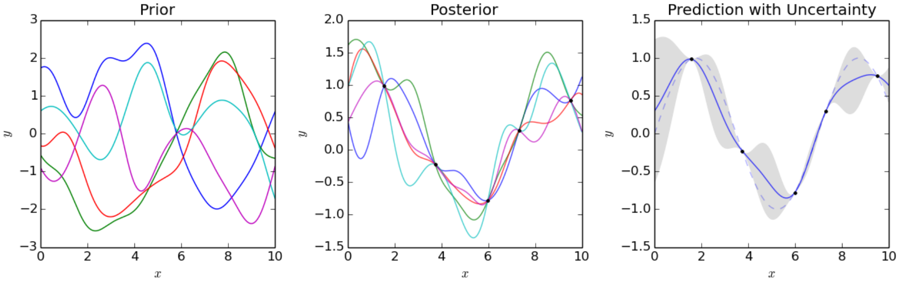
- f is still a GP even though we've observed its value at a number of locations.



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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

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

where

$$\Sigma = \left(\begin{array}{ccc|c} k(x_1, x_1) & \dots & k(x_1, x_n) & k(x_1, x) \\ \vdots & & \vdots & \vdots \\ k(x_n, x_1) & \dots & k(x_n, x_n) & k(x_n, x) \\ \hline k(x, x_1) & \dots & k(x, x_n) & k(x, x) \end{array}\right)$$

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

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

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

More generally, if

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

then

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with

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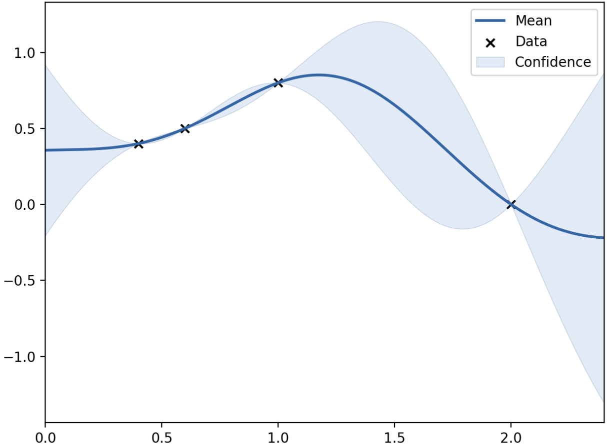
\bar{m}(x) &= m(x) + k_X(x)^\top K_{XX}^{-1}\mathbf{f} \\
\bar{k}(x,x') &= k(x,x') - k_X(x)^\top K_{XX}^{-1} k_X(x')
\end{aligned}$$

No noise/*nugget* - Interpolation



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

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

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Noisy observations/with nugget - Regression

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

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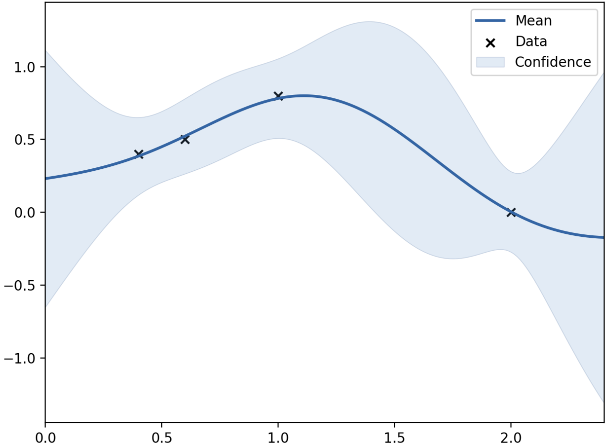
Nugget standard deviation $\sigma = 0.1$



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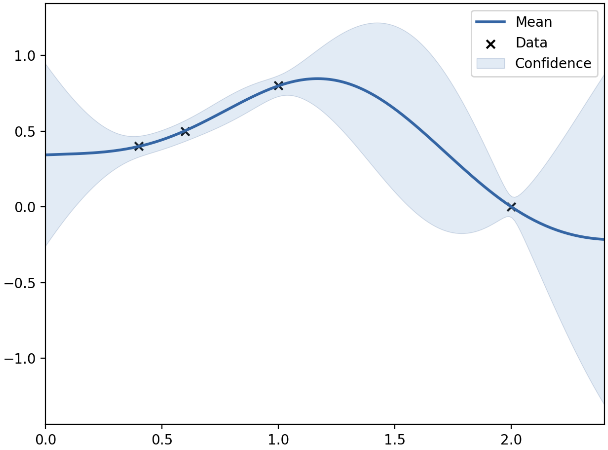
Nugget standard deviation $\sigma = 0.025$



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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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- 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 $y|D, \sigma^2 \sim GP$ and

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

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

Why use GPs? Answer 2: non-parametric/kernel regression

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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Suppose we're given data $\{(x_i, y_i)_{i=1}^n\}$ with $x_i \in \mathbb{R}^p, y_i \in \mathbb{R}$

$$\hat{\beta} = \arg\min_{\beta} ||y - X\beta||_2^2 + \sigma^2 ||\beta||_2^2 \quad \text{regularised least squares}$$

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

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$$\begin{aligned}\hat{\beta} &= \arg\min_{\beta} ||y - X\beta||_2^2 + \sigma^2||\beta||_2^2 \quad \text{regularised least squares} \\ &= (X^\top X + \sigma^2 I)^{-1} X^\top y \quad \text{usual ridge regression estimator}\end{aligned}$$

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

Why use GPs? Answer 2: non-parametric/kernel regression

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

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

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

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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

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

is positive semi-definite (and thus a valid covariance function) if and only if we can write[1]

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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

$$\phi_N(x) = \frac{1}{\sqrt{N}}(e^{-\frac{(x-c_0)^2}{2\lambda^2}}, \dots, e^{-\frac{(x-c_N)^2}{2\lambda^2}})$$

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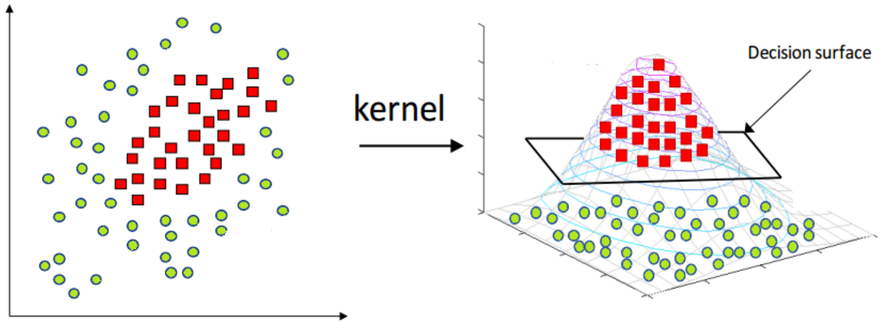
We can use an infinite dimensional feature vector $\phi(x)$, and because linear regression can be done solely in terms of inner-products (inverting a $n \times n$ matrix in the dual form) we never need evaluate the feature vector, only the kernel.

Kernel trick:

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



Kernel regression (see Kanagawa et al. 2019)

Kernel regression and GP regression are closely related.

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Consider the space of functions

$$\mathcal{H}_k = \overline{\text{span}}\{k(\cdot, x) : x \in \mathcal{X}\}$$

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

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$$L(f) = \sum_i (f(x_i) - y_i)^2 + \sigma^2 ||f||^2_{\mathcal{H}_k}$$

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

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.

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

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- 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 [2],

- 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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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

$$\mathbb{E}Y(x) = \mu \; \forall \; x$$
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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

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

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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

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

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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.

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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.

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Assuming a GP model for your data imposes a complex structure on the data.

The number of parameters in a GP is essentially infinite, and so they are not always identified even asymptotically.

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 σ^2 or κ, even as $n \to \infty$.

Problems with hyper-parameter optimization

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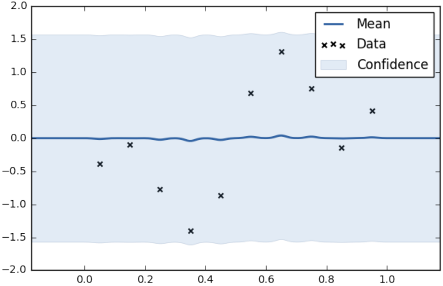

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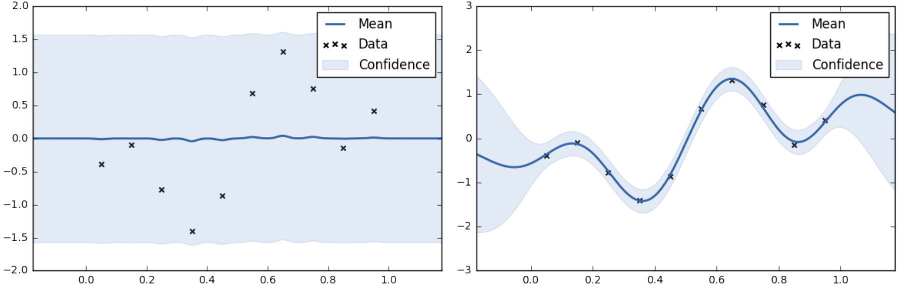

We often work around these problems by running the optimizer multiple times from random start points, using prior distributions, constraining or fixing hyper-parameters, or adding white noise.

Computational cost

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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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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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  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
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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.