Gaussian Processes for Regression

COMP9418 — Advanced Topics in Statistical Machine Learning

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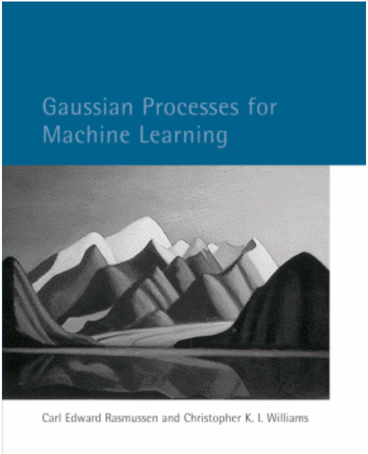
Acknowledgements



Carl Edward Rasmussen and Christopher K. I. Williams

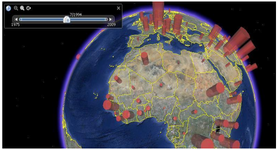
All chapters available online along with software and datasets:
http://www.gaussianprocess.org/gpml

Aims

This lecture will allow you to understand Gaussian processes as priors over functions and apply them to regression problems. Following it you should be to:

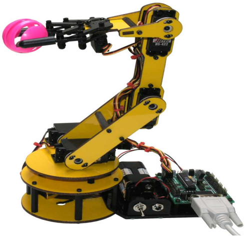
- Understand and apply Bayesian approaches to linear regression.
- Understand and apply Bayesian linear-in-the-parameters models to non-linear regression problems.
- Understand the connection between Bayesian regression with non-linear feature spaces and Gaussian process regression.
- Derive and apply the function-space view of Gaussian process regression.
- Carry out model selection in Gaussian process regression models.

Some Applications of Gaussian Process (GP) Models (1)

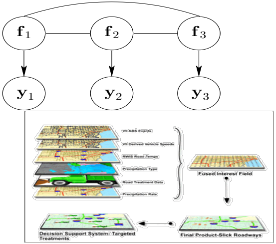


Spatio-temporal modelling

Classification

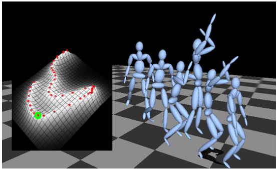


Robot inverse dynamics



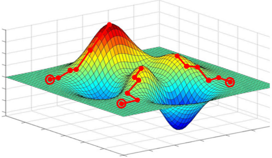
Data fusion / multi-task learning

Some Applications of GP Models (2)

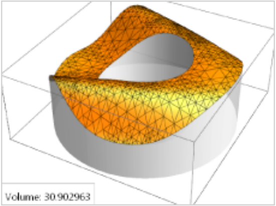


Style-based inverse kinematics

Preference learning



Bayesian optimisation

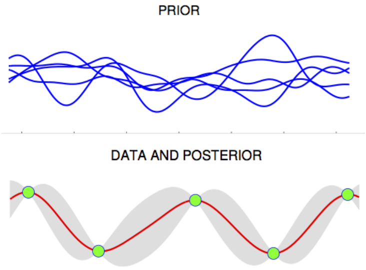


Bayesian quadrature

How can We ‘Solve’ All these Problems with the Humble Gaussian Distribution?

Key components of GP models:

- Non-parametric prior
- Bayesian
- Kernels (covariance functions)



Bayesian non-linear regression

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- Prediction (posterior inference)
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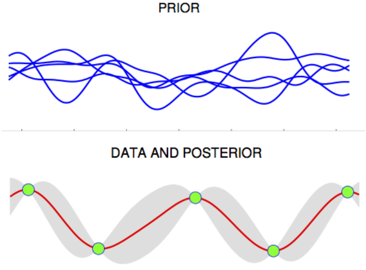

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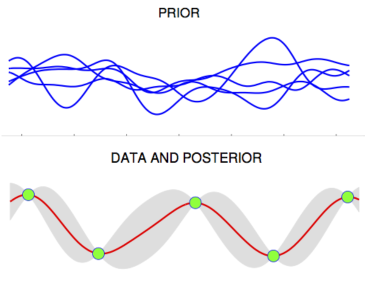


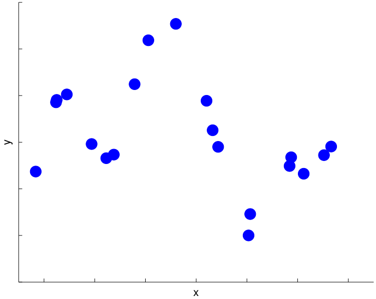
Bayesian non-linear regression

Challenges

- Intractability for non-Gaussian likelihoods
  - E.g. a sigmoid likelihood for classification
- High computational cost (in time and memory) with # datapoints

The Prediction Problem

Learn mapping $\mathbf{x} \rightarrow f(\mathbf{x})$ from observations $\{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^{N}$.



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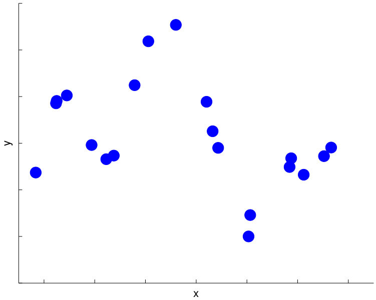

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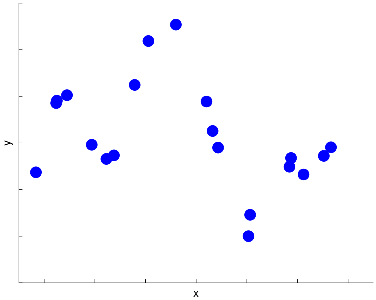

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- $f(\mathbf{x}) = \sum_j w_j x_j$

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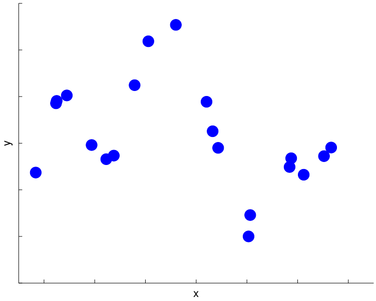

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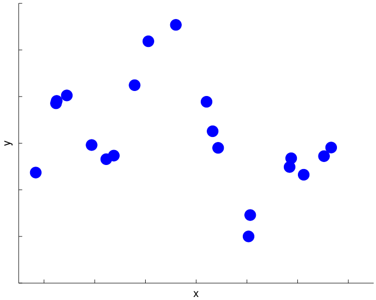

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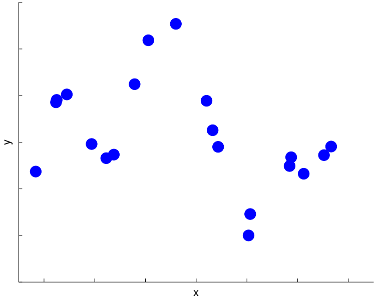

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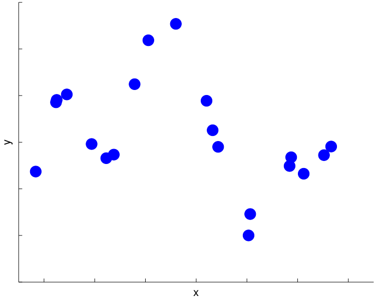

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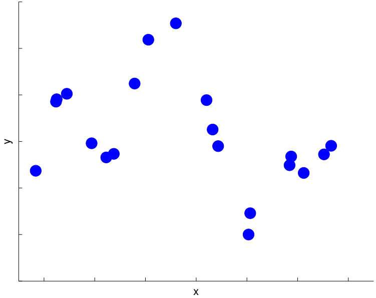

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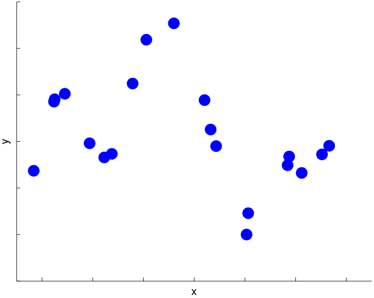

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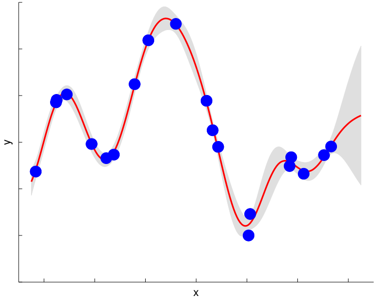

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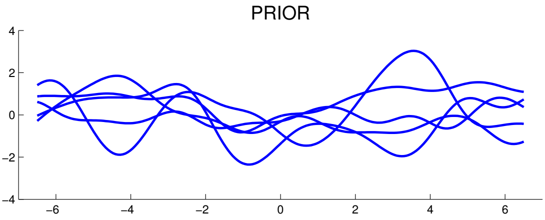
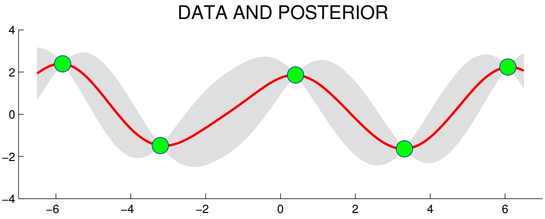
We can address these issues in a principled way with Gaussian process models

Demo





- Smooth functions
- Closeness in input space $\rightarrow$ closeness in output space

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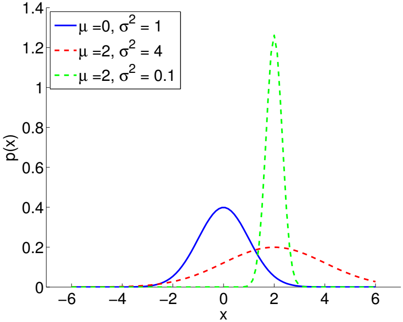
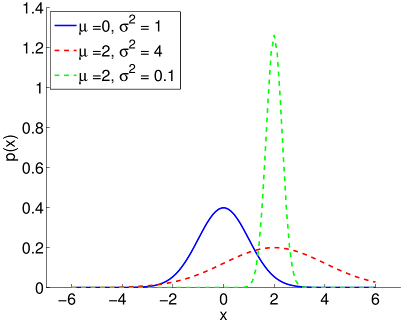
- Many standard regression models are special cases of GPs
- GP models also applicable to non-regression settings

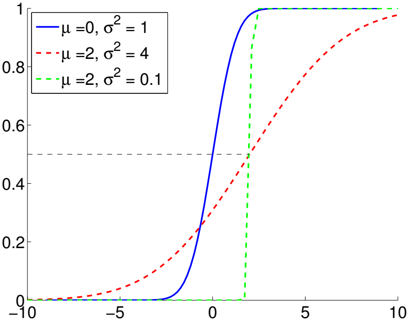
Outline

1. The Gaussian Distribution Revisited
2. Standard Bayesian Linear Regression
3. Bayesian Regression with Non-linear Feature Spaces
4. Gaussian Processes for Regression
   - Function-space View
   - Predictions
   - Model Selection
   - Other Covariance Functions



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





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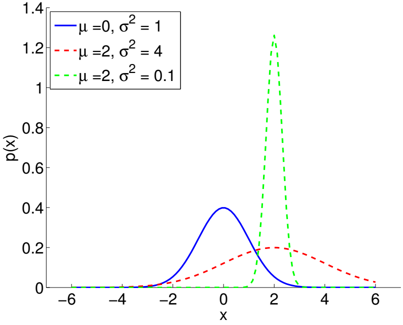
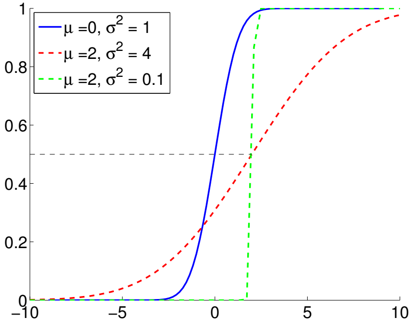
The Gaussian Distribution

1D Example





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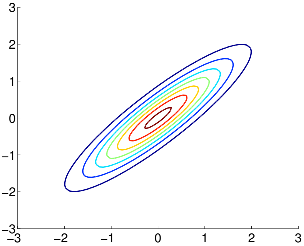
In general: $$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{|2\pi\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)$$

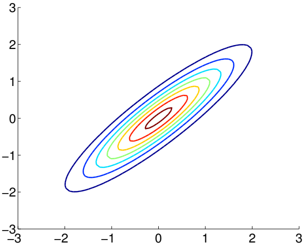


$$p(x_1, x_2) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Joint

The Gaussian Distribution

2D Example



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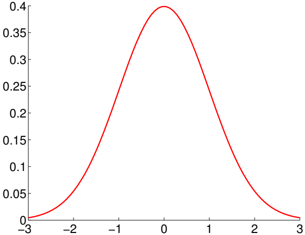
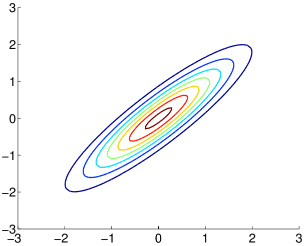


$p(x_1)$

Marginal



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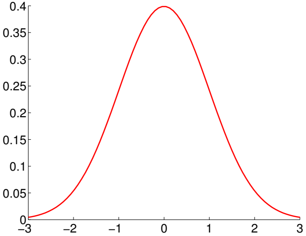

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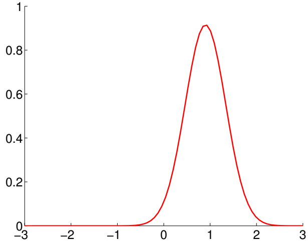
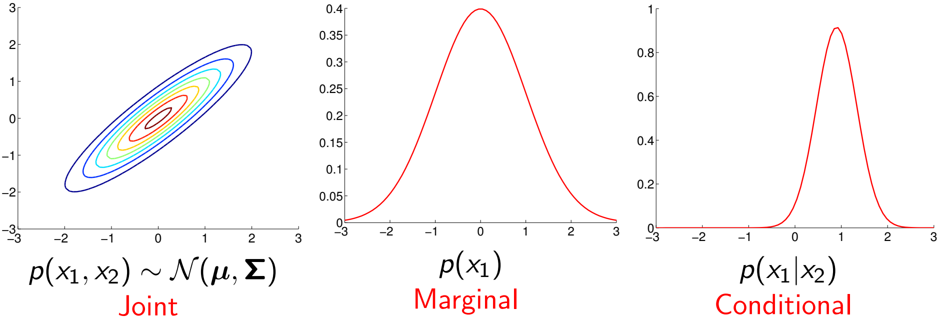


$p(x_1 | x_2)$

Conditional

The Gaussian Distribution
2D Example



The marginal and the conditional distributions are also Gaussians

Partitioned Gaussians

For general Gaussian random vectors $\mathbf{x}$, we can partition:

$$\mathbf{x} \stackrel{\text{def}}{=} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{12}^T & \boldsymbol{\Sigma}_{22} \end{bmatrix} \right),$$

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where $\boldsymbol{\mu}_{1|2} = \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)$,

and $\boldsymbol{\Sigma}_{1|2} = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T$

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{|2\pi\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$

$\boldsymbol{\Sigma}$: is the covariance matrix

$\boldsymbol{\Sigma}^{-1}$: is the precision matrix

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- An entry $\boldsymbol{\Sigma}^{-1}_{ij} = 0$ indicates that the variables i and j are conditionally independent given all the other variables.
- An entry $\boldsymbol{\Sigma}_{ij} = 0$ indicates that the variables i and j are marginally independent given all the other variables.
- Marginalizing out a variable leaves $\boldsymbol{\Sigma}$ unchanged but changes $\boldsymbol{\Sigma}^{-1}$.
  - This is crucial when parameterizing a Gaussian process.

Gaussian Quiz

Data : $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^{N}$, $\mathbf{x} \in \mathbb{R}^D$, $y \in \mathbb{R}$

Input : $(\mathbf{X})_{D \times N}$, Targets: $(\mathbf{y})_{N \times 1}$

Goal : $\mathbf{x} \stackrel{f(\mathbf{x})}{\rightarrow} \mathbf{y}$

The Standard Linear Regression Model

Notation and Settings

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Input : $(\mathbf{X})_{D \times N}$, Targets: $(\mathbf{y})_{N \times 1}$

Goal : $\mathbf{x} \overset{f(\mathbf{x})}{\rightarrow} \mathbf{y}$

Model	$f(\mathbf{x}) = \sum_{j=1}^{D} w_j x_j$	$= \mathbf{w}^T \mathbf{x}$
Noise	$y = f(\mathbf{x}) + \eta$	with $\eta \sim \mathcal{N}(\eta \vert 0, \sigma^2)$
Likelihood	$y \vert f(\mathbf{x}) \sim \mathcal{N}(y \vert f(\mathbf{x}), \sigma^2)$	$= \mathcal{N}(y \vert \mathbf{w}^T \mathbf{x}, \sigma^2)$

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\text{Model} \quad & f(\mathbf{x}) = \textstyle\sum_{j=1}^{D} w_j x_j && = \mathbf{w}^T \mathbf{x} \\
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Thus, the data-likelihood is given by:

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We need do to inference on $\mathbf{w}$.

Consider a zero-mean Gaussian prior over the weights:

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- MAP solution (non-Bayesian): negative log prior as penalty term
- This penalized maximum likelihood is known as **ridge regression**
  - Consider $\mathbf{\Sigma}_w = \lambda\mathbf{I}$ Then :

$$\bar{\mathbf{w}} = (\mathbf{X}\mathbf{X}^T + \frac{1}{\lambda}\sigma^2\mathbf{I})^{-1}\mathbf{X}\mathbf{y}$$

We are interested in making predictions at a new test point $\mathbf{x}_*$

- In fact we obtain the predictive distribution by averaging over all possible parameter values (weighted by their posterior probabilities):

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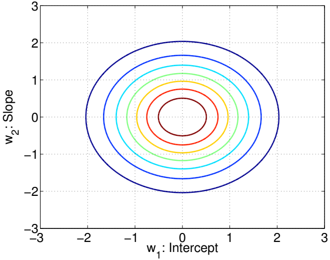
- Point predictions: Need to consider the expected loss (or **risk**):

$$y_{\text{opt}} = \underset{y_{\text{pred}}}{\text{argmin}} \int \mathcal{L}(f_*, y_{\text{pred}}) p(f_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) df_*$$

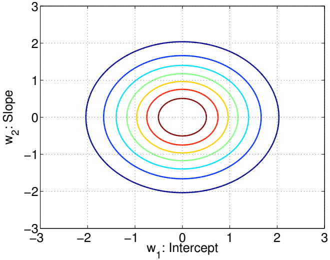
  - e.g. Square loss $\mathcal{L} = (y_{\text{pred}} - f_*)^2$
  - c.f. Empirical risk minimization (ERM)

Bayesian Linear Regression Example



Prior Weights

Bayesian Linear Regression Example



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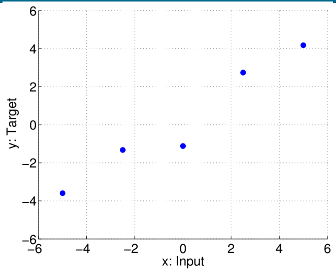

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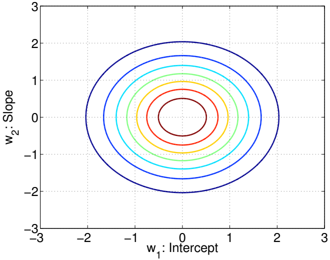

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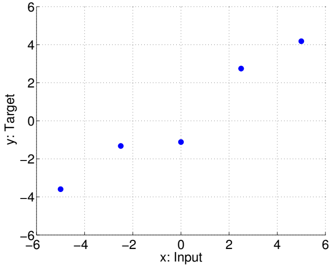

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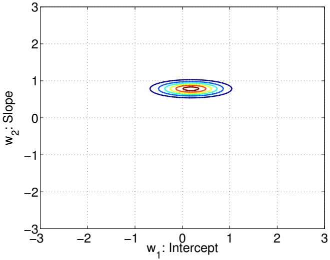

Likelihood

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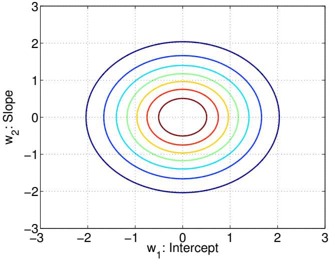

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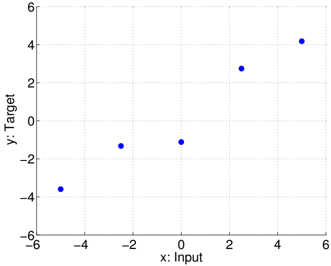

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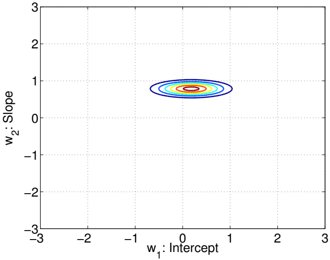

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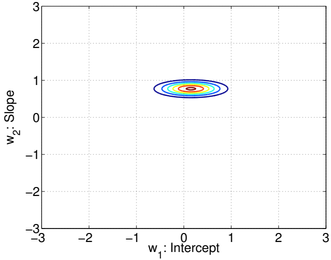
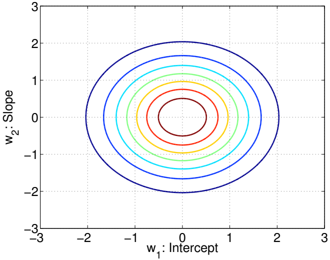


Posterior Weights

Bayesian Linear Regression Example



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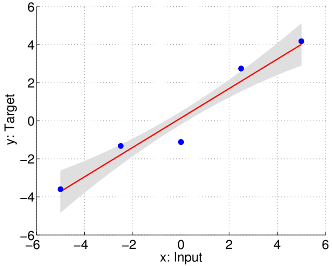
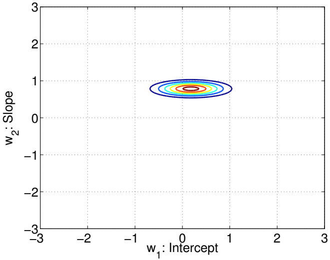


Predictive Distribution



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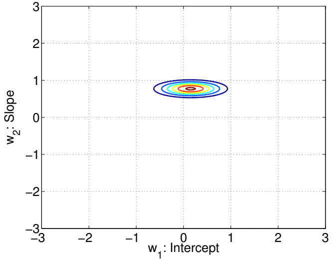

Posterior Weights

Non-linear Feature Spaces

- Consider the model $f(\mathbf{x}) = \sum_{i=1}^{D'} w_i \phi_i(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$
  - Each $\phi_i(\mathbf{x})$ is a (non-linear) feature on $\mathbf{x}$, e.g. $x_1, x_2, x_1^2, x_2^2, x_1 x_2 \ldots$
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- Note that in:

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- The mean and the covariance function for this stochastic process is given by:

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From a Prior over Weights to a Prior over Functions

- Consider the kinds of functions that can be generated from a set of basis functions with random weights.
- Then $f(\mathbf{x})$ at a particular point is a random variable:

$$f(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) \text{ with } \mathbf{w} \sim \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{\Sigma}_w)$$

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- A collection of these random variables indexed by $\mathbf{x}$: $f(\mathbf{x}^{(1)}), \ldots, f(\mathbf{x}^{(N)})$, define a stochastic process in a consistent way.
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Sample Functions from the Linear Model

1. Define $\phi_i(x) = \exp(-\frac{1}{2}(x - \mu_i)^2)$, for $i = 1, 2, 3$
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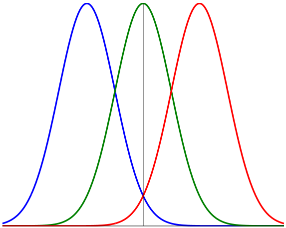

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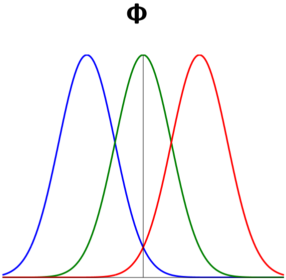

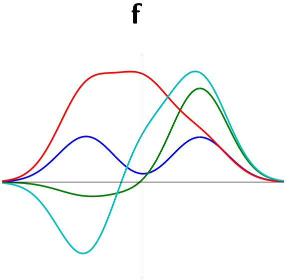

Function-space View

Gaussian Process (GP)

$f(\mathbf{x})$ is a Gaussian process if for any finite subset of points $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}$, the function values $f(\mathbf{x}^{(1)}), \ldots, f(\mathbf{x}^{(N)})$ follow a Gaussian distribution.

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- It specifies the covariance between pairs of random variables:

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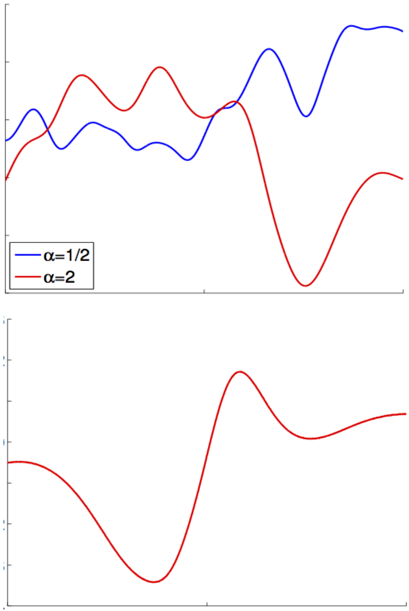
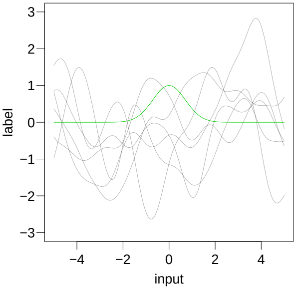
Samples from a Gaussian Process

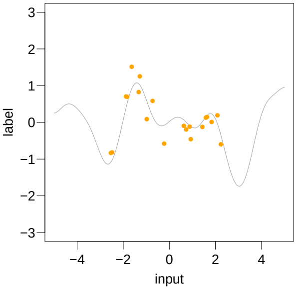


Computing with Infinite Vectors

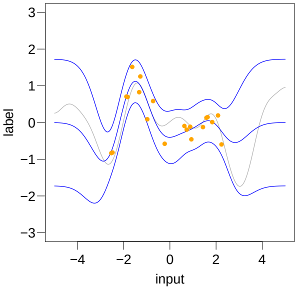
GP prior

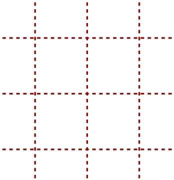


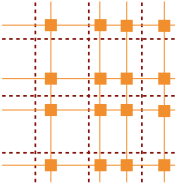
GP regression example

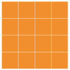


Inference result



$K_\infty =$ 

$K_\infty =$ 

$K_{\mathbf{y}} =$  $+$ 

The Squared Exponential (SE) Covariance Function

$$\kappa(\mathbf{x}, \mathbf{x}'; \boldsymbol{\theta}) = \sigma_s^2 \exp\left(-\frac{1}{2}(\mathbf{x} - \mathbf{x}')^T \mathbf{C}(\mathbf{x} - \mathbf{x}')\right)$$

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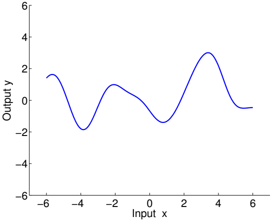

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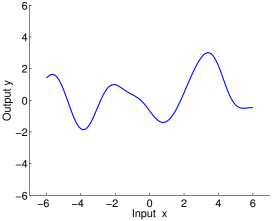

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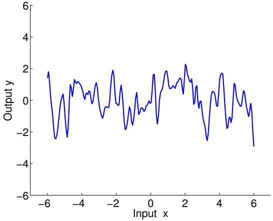

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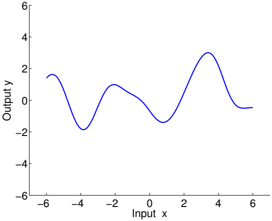

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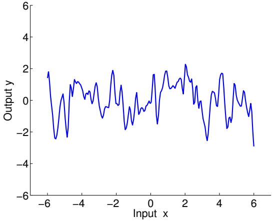

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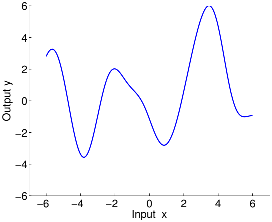

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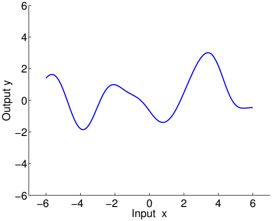

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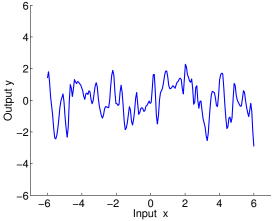

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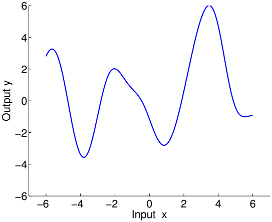

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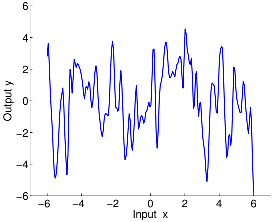

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Standard GP Regression Model: Predictions (1)

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Standard GP Regression Model: Predictions (1)

Data : $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^{N}$, $\mathbf{x} \in \mathbb{R}^D$, $y \in \mathbb{R}$

Input : $(\mathbf{X})_{D \times N}$, Targets: $(\mathbf{y})_{N \times 1}$

Goal : Make predictions $f_* = f(\mathbf{x}_*)$ at $\mathbf{x}_*$

$$
\begin{array}{llcll}
\text{Prior} & f(\mathbf{x}) & \sim & \mathcal{GP}(\mathbf{0}, \kappa(\mathbf{x}, \mathbf{x}')) & \\
\text{Noise} & y & = & f(\mathbf{x}) + \eta & \eta \sim \mathcal{N}(0, \sigma_n^2)
\end{array}
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- This is achieved simply by conditioning: $p(f_* | \mathbf{X}, \mathbf{y}, \mathbf{x}_*)$

Standard GP Regression Model: Predictions (2)

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The Graphical Model for GPs

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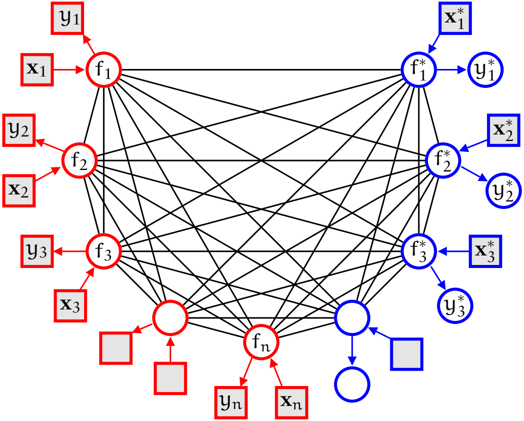

Figure from Carl Rasmussen's slides

The Graphical Model for GPs

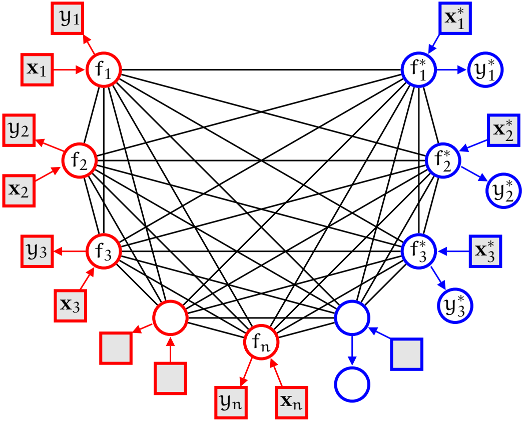

Figure from Carl Rasmussen's slides

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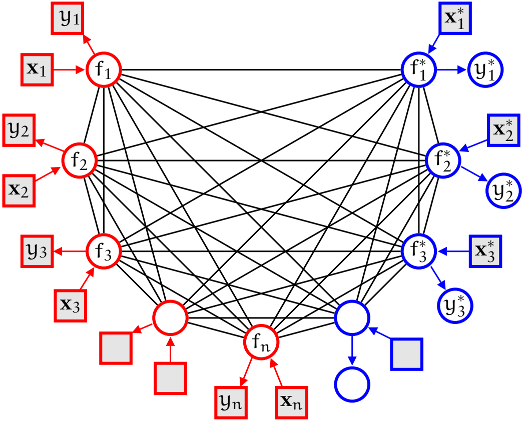

Figure from Carl Rasmussen's slides

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- The marginalization property implies that adding a new $\mathbf{x}_i^*$, f_i^*, y_i^* does not affect the distribution

1. The Gaussian Distribution Revisited
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4. Gaussian Processes for Regression
   - Function-space View
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   - **Model Selection**
   - Other Covariance Functions

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$$
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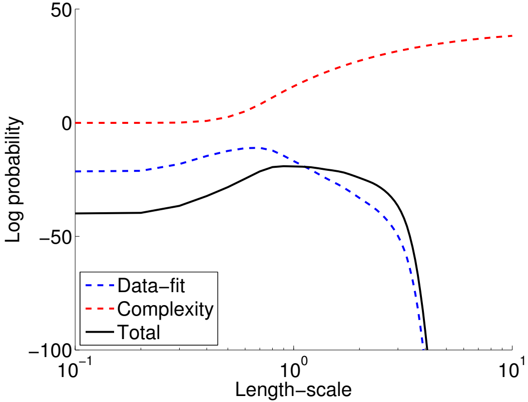

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Let $\widetilde{\mathbf{K}} = \mathbf{K} + \sigma_n^2 \mathbf{I}$:

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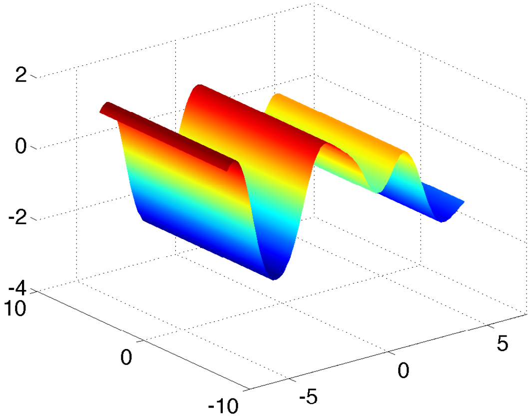

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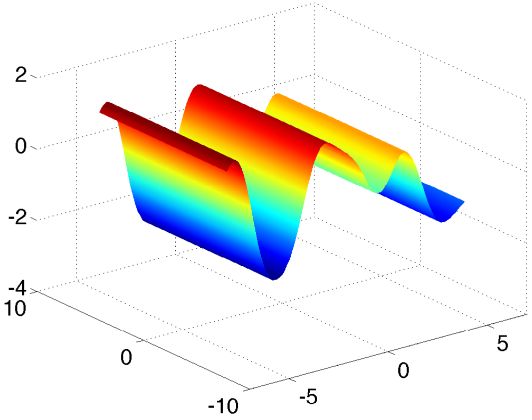

Learned lengh-scale for irrelevant dimension: 1.0557×10^5

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Other Covariance Functions: Matérn Covariance

$$\kappa(\mathbf{x}, \mathbf{x}') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}\|\mathbf{x} - \mathbf{x}'\|}{\ell} \right)^{\nu} \mathcal{K}_{\nu} \left(\frac{\sqrt{2\nu}\|\mathbf{x} - \mathbf{x}'\|}{\ell} \right)$$

where $\mathcal{K}_{\nu}$ is a modified Bessel function and $\nu > 0$, $\ell > 0$.

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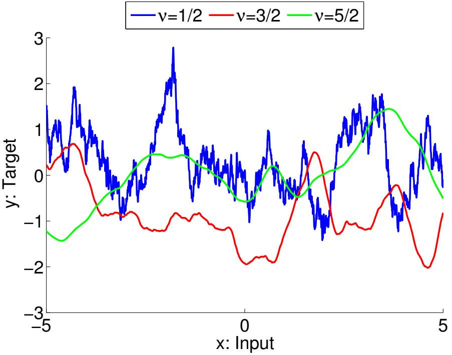

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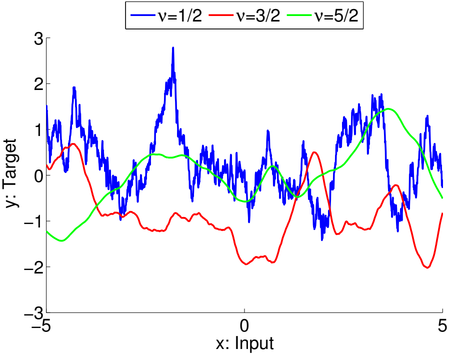

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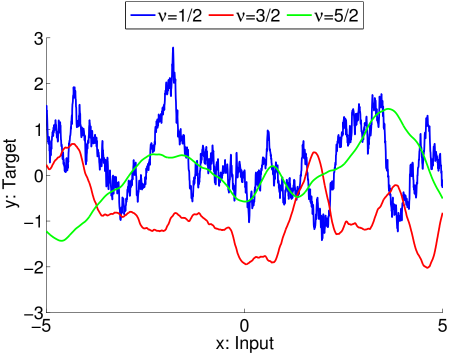

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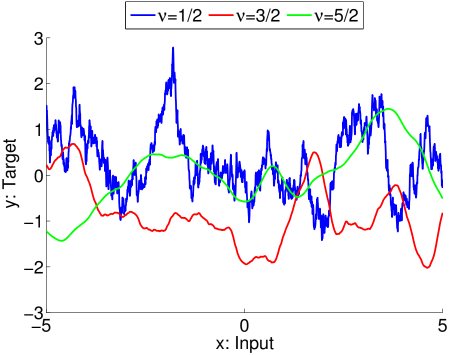

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- $\nu \to \infty$: SE covariance

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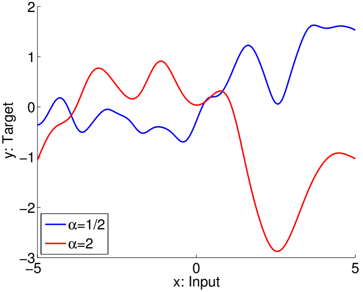

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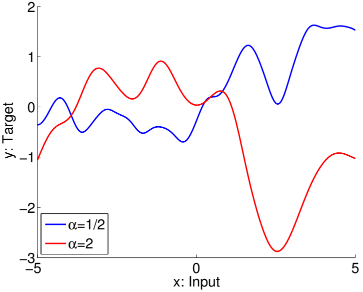

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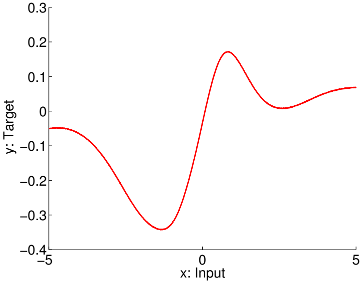
with $\alpha \to \infty$ is the SE covariance with length-scale ℓ.

Other Covariance Functions: Neural Network Covariance

- Consider a neural network with one hidden layer and N_H hidden units.
- Under certain assumptions the corresponding stochastic process will converge to a Gaussian Process as $N_H \to \infty$.
- For a specific settings of the transfer function of the neural net:

$$\kappa(\mathbf{x}, \mathbf{x}') = \frac{2}{\pi} \sin^{-1} \left(\frac{2\tilde{\mathbf{x}}^T \boldsymbol{\Sigma} \tilde{\mathbf{x}}'}{\sqrt{(1 + 2\tilde{\mathbf{x}}^T \boldsymbol{\Sigma} \tilde{\mathbf{x}})(1 + 2\tilde{\mathbf{x}}'^T \boldsymbol{\Sigma} \tilde{\mathbf{x}}')}} \right)$$



Other Covariance Functions: Periodic, Smooth Functions

We can create a distribution over periodic functions of x by using the mapping $\mathbf{u}(x) = (cos(x), sin(x))$ and then use the SE covariance on $\mathbf{u}$ space. This gives rise to:

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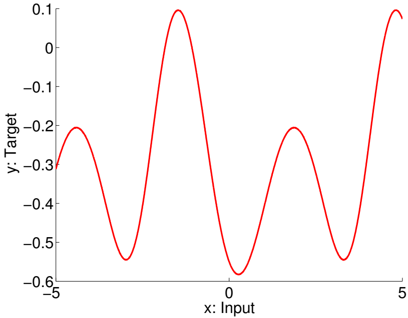

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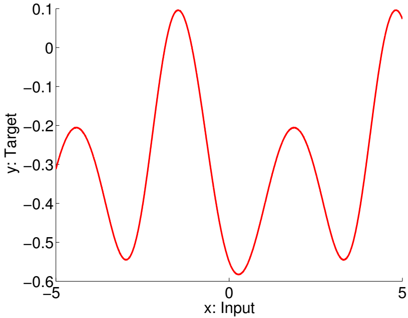

This is called warping and can also be used to introduce non-stationarity.

Conclusions

- Models based on Gaussian process (GP) priors are flexible non-parametric Bayesian approaches to non-linear regression.
- GP regression can be seen as a generalisation of Bayesian regression with non-linear feature spaces and infinite-dimensional feature maps.
- Inference in GP regression models is analytically tractable and is computable thanks to the marginalisation property underlying GPs.
- Hyper-parameter learning carried out via non-covex optimisation of the marginal likelihood.
- High computational cost in time and memory, $\mathcal{O}(N^3)$ and $\mathcal{O}(N^2)$
- Reading: Rasmussen & Williams (GPML, 2006): Ch. 1, 2, 4 (except Sec. 4.3, 4.4), Sec. 5.1, 5.2, 5.4.