Part I: Gaussian Processes for Regression and Classification

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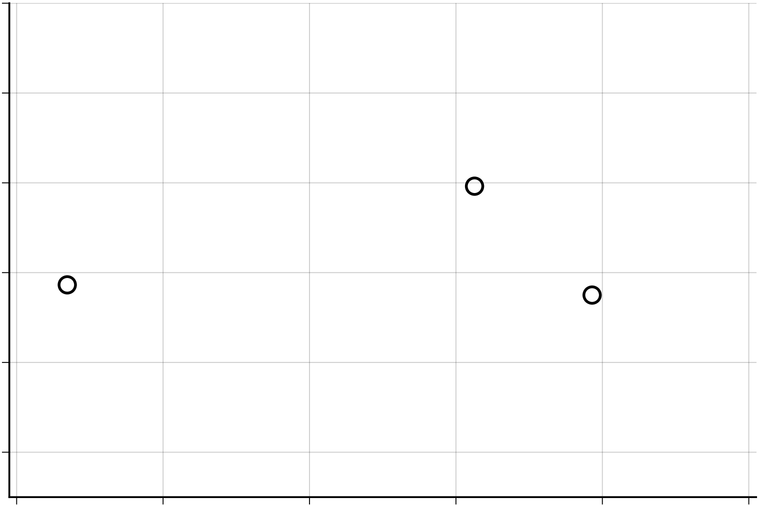
Motivation: Regression Problems



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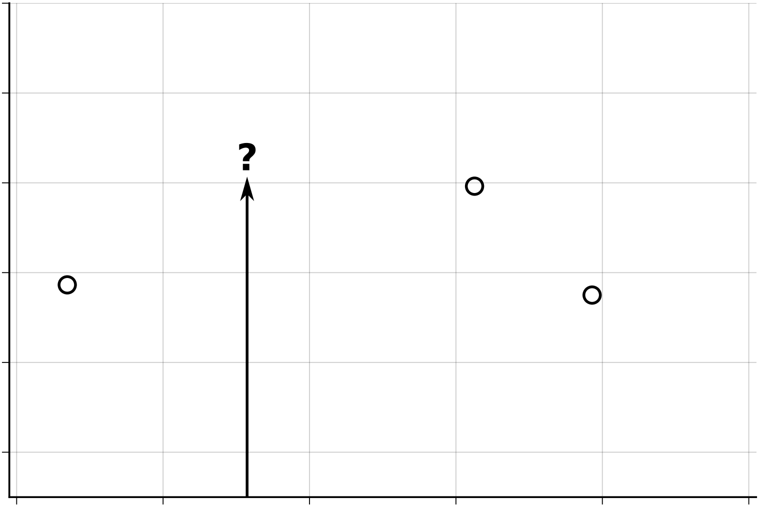

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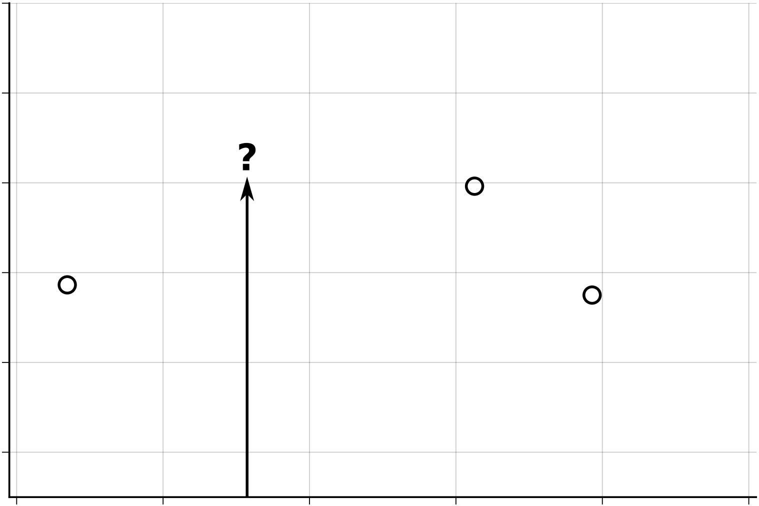

We have to specify a model that may depend on parameters w.

The Standard Linear Model

We may consider a standard linear regression model:

$$f(\mathbf{x}) = \mathbf{w}^\mathsf{T}\mathbf{x}\,, \qquad y = f(\mathbf{x}) + \epsilon\,, \qquad \epsilon \sim \mathcal{N}(0, \sigma^2)\,,$$

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We follow a Bayesian approach to machine learning:

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}\,, \qquad p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \frac{p(\mathbf{y}|\mathbf{w}, \mathbf{X})p(\mathbf{w})}{p(\mathbf{y}|\mathbf{X})}\,.$$

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Marginal Likelihood: **Probability** of observing $\mathbf{y}$ under the model.

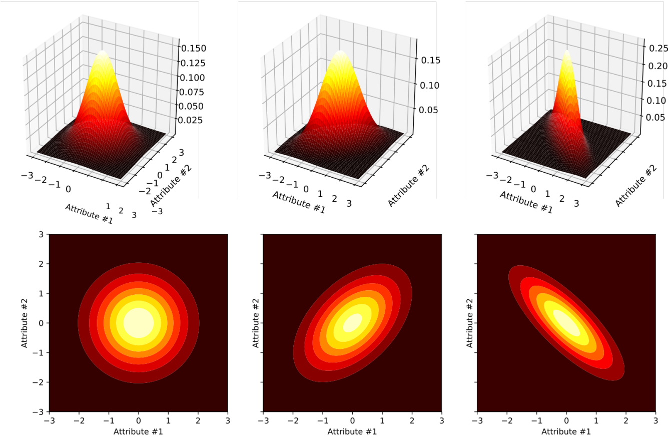
The Standard Linear Model

Prior: We consider an **isometric Gaussian prior** $\mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{I})$.

Multivariate Gaussian Distribution

$$p(\mathbf{w}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{N}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left\{-0.5 \cdot (\mathbf{w} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{w} - \boldsymbol{\mu})\right\}$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 1 & -0.8 \\ -0.8 & 1 \end{bmatrix}$$



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(Bishop, 2006)

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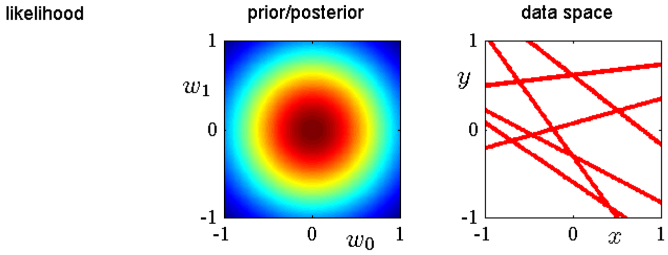

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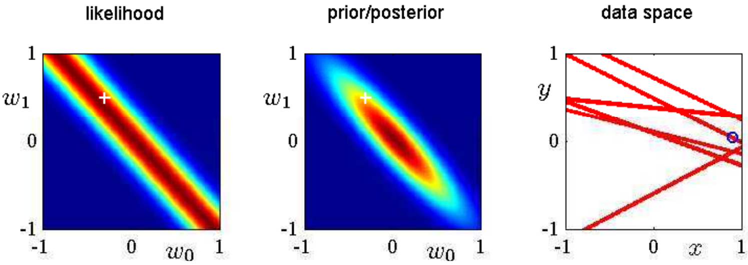

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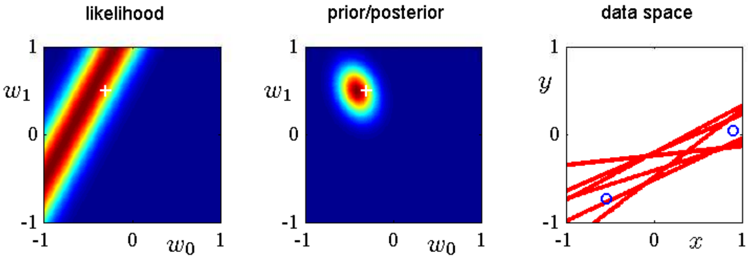

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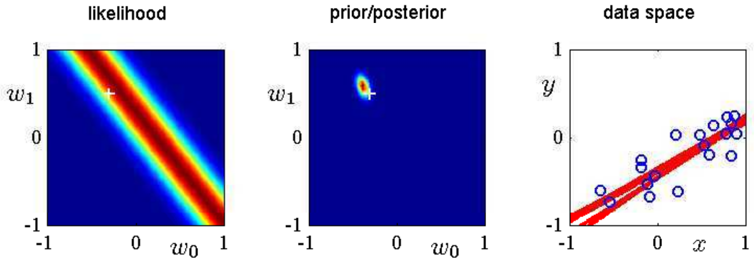

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The predictive distribution is obtained by marginalizing $\mathbf{w}$:

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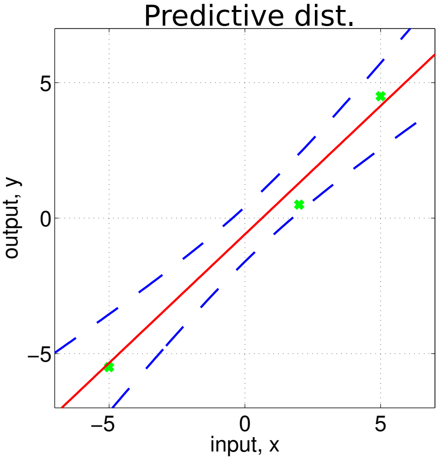

(Rasmussen & Williams, 2006)

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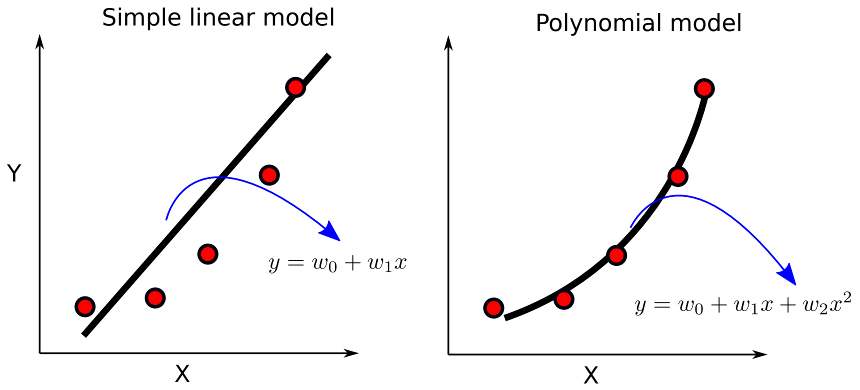

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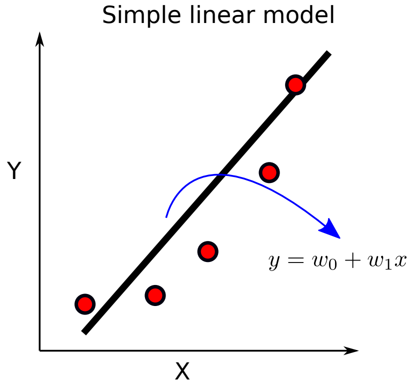

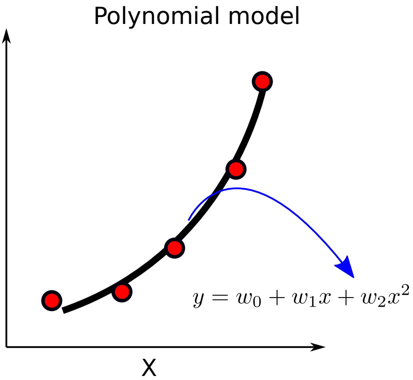

Any other non-linear feature expansion is possible!

Non-Linear Regression

Consider working with $\phi(\mathbf{x})$ instead of $\mathbf{x}$. The model is:

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All computations are tractable and result in Gaussian distributions!

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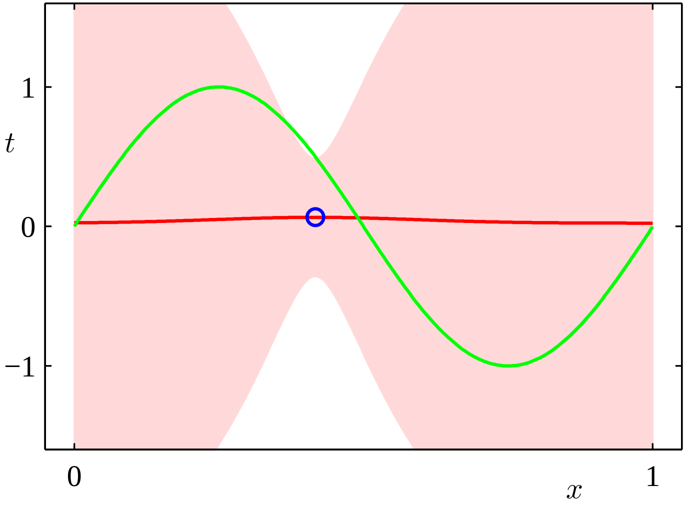

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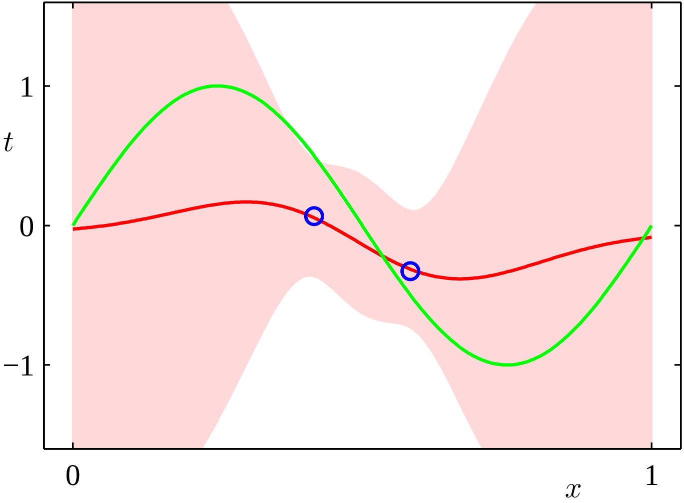

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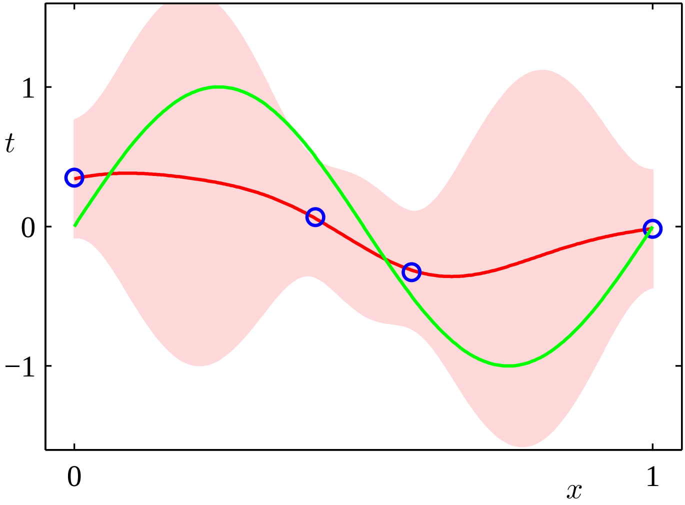

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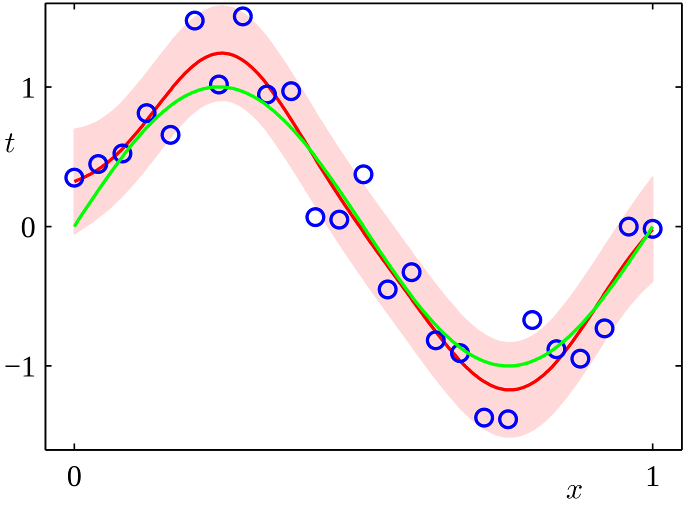

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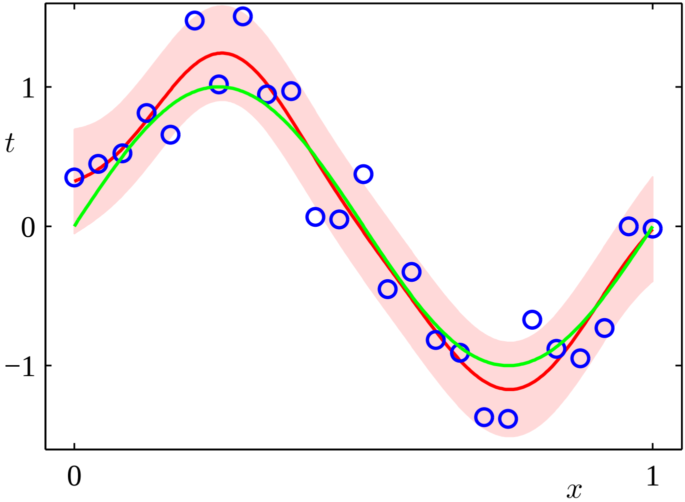

The predictive distribution tells us what our model does not know!

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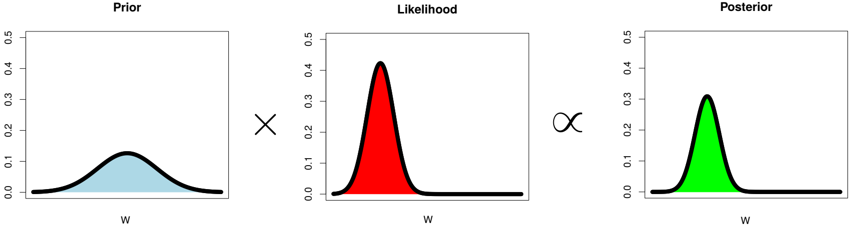

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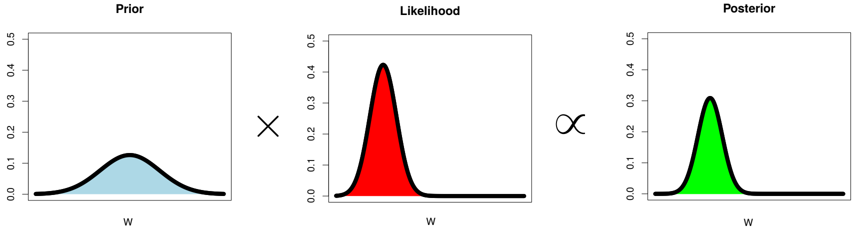

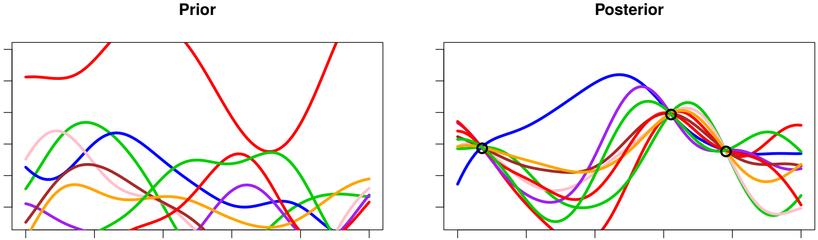

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Distribution over functions $f(\cdot)$ so that for any finite $\{\mathbf{x}_i\}_{i=1}^N$, $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N))^\mathsf{T}$ follows an N-dimensional Gaussian distribution.

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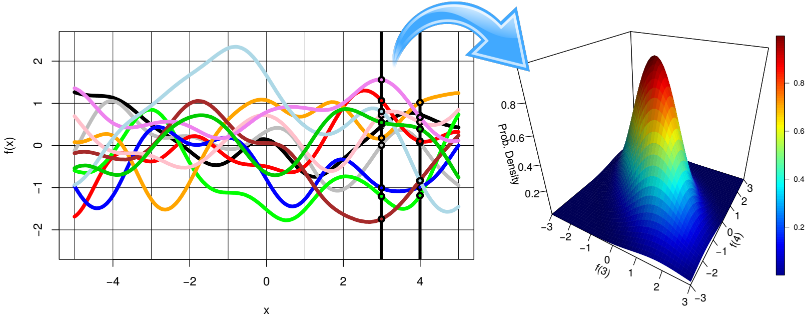

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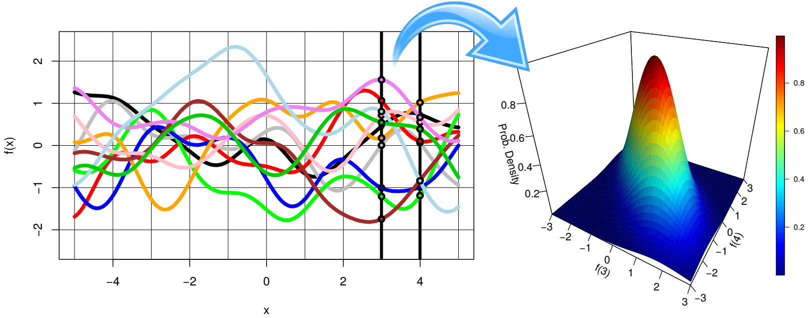

Straight-forward for the prior and posterior. Since the they are Gaussian for $\mathbf{w}$, y is the sum of Gaussian random variables and is also Gaussian!

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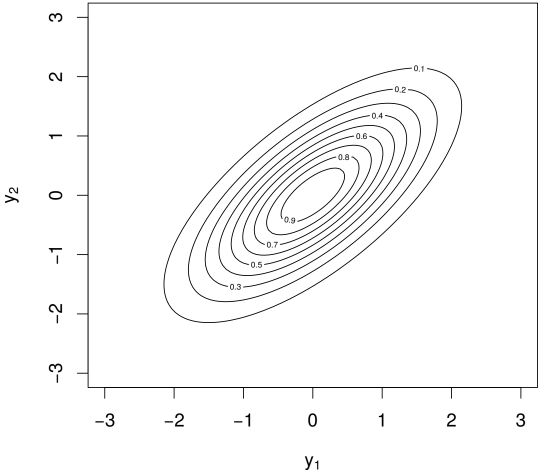
4. **This results in a non-parametric model that becomes more flexible as more data is observed!**

Gaussian Distribution

$$p(\mathbf{y}|\boldsymbol{\Sigma}) \propto \exp\left\{-0.5\mathbf{y}^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}\mathbf{y}\right\} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{bmatrix}.$$



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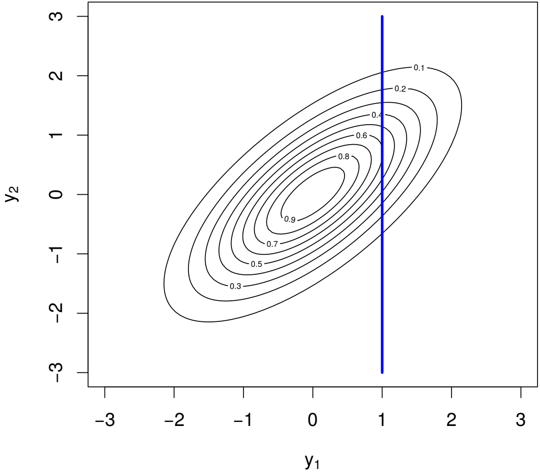

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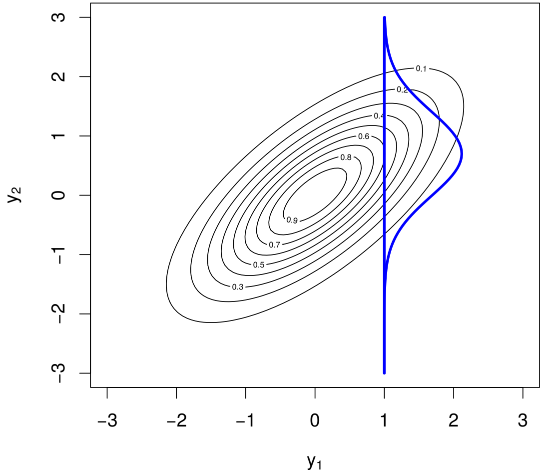

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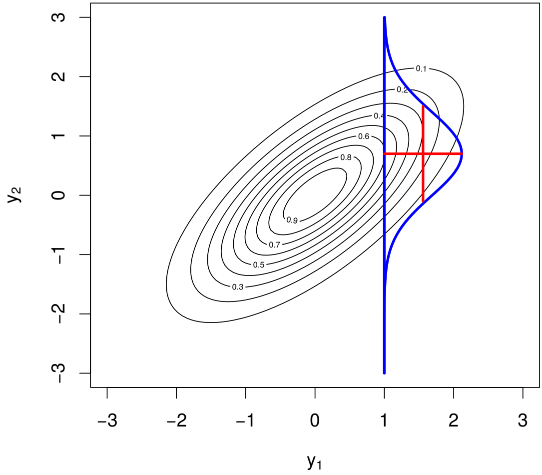

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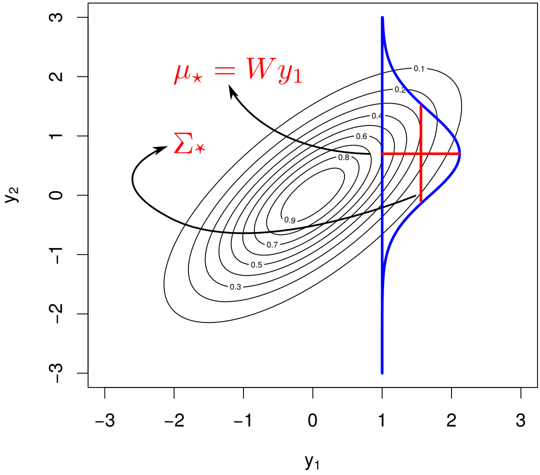
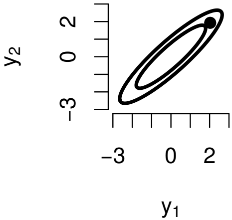


Two Dimensional Example



$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$

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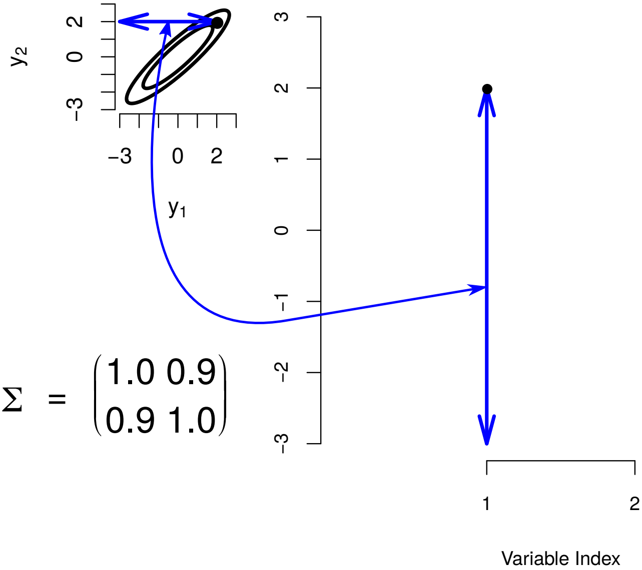

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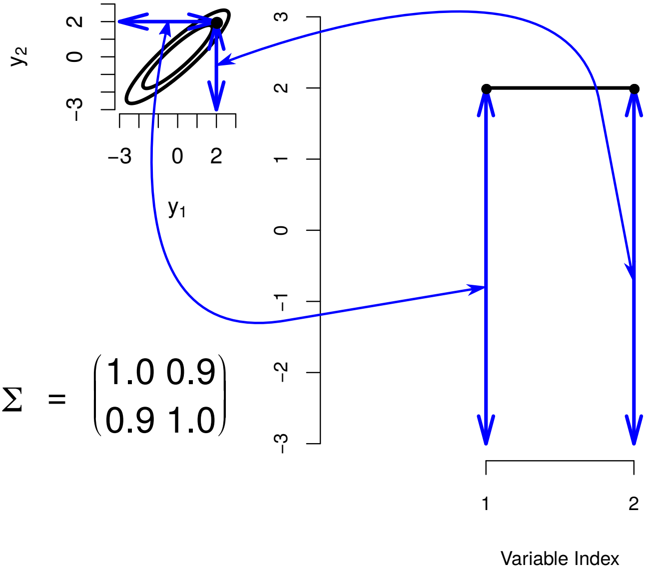

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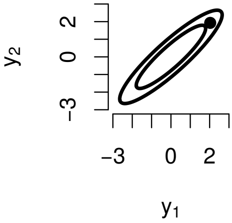

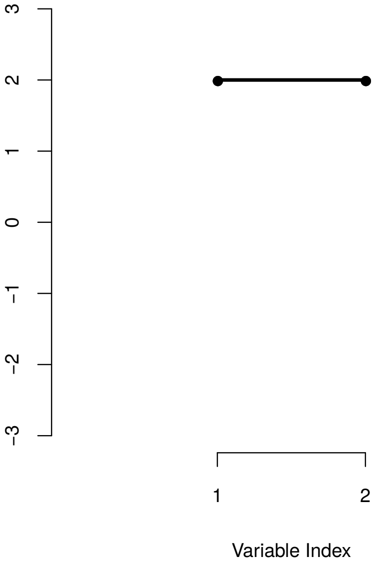

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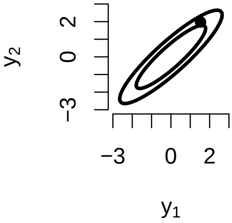

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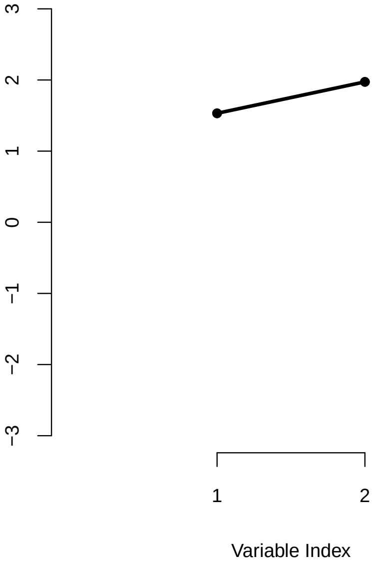

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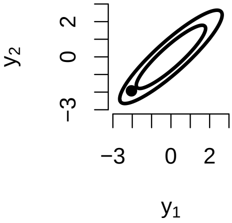

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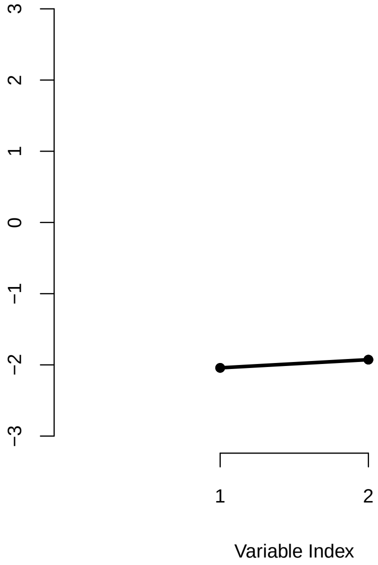

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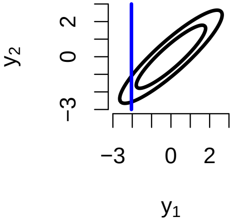

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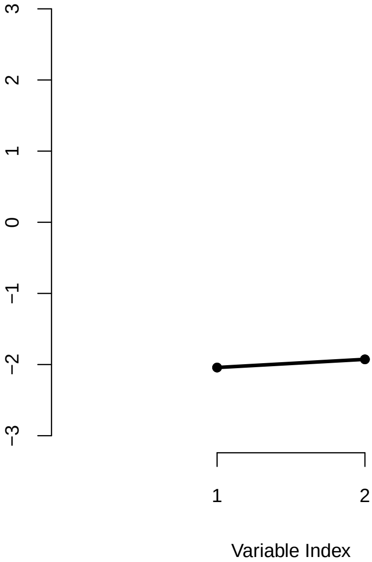

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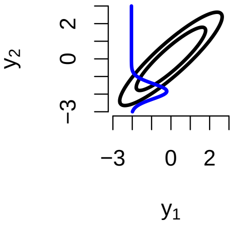

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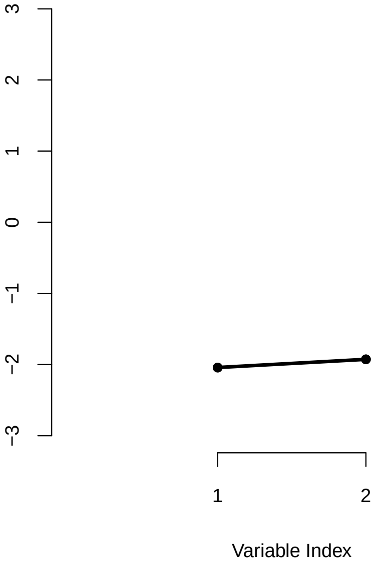

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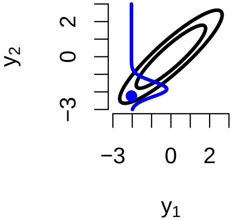

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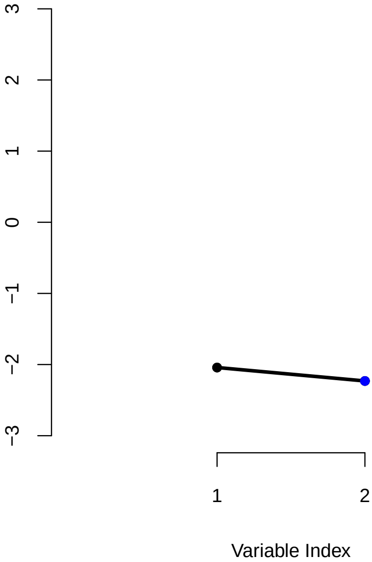
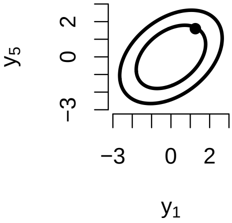
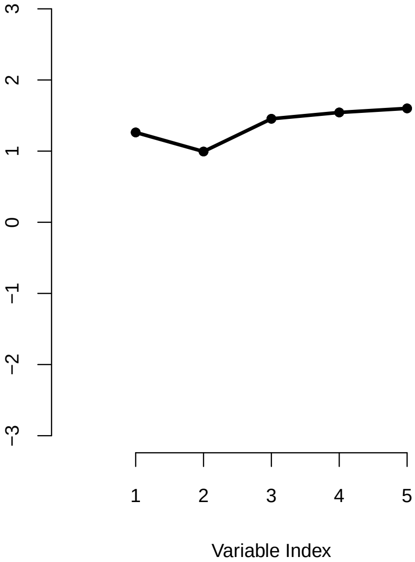


Five Dimensional Example



$$\Sigma = \begin{bmatrix} 1.0 & .9 & .8 & .6 & .4 \\ .9 & 1.0 & .9 & .8 & .6 \\ .8 & .9 & 1.0 & .9 & .8 \\ .6 & .8 & .9 & 1.0 & .9 \\ .4 & .6 & .8 & .9 & 1.0 \end{bmatrix}$$



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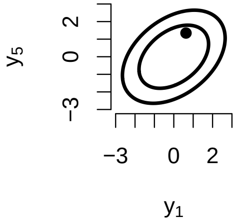
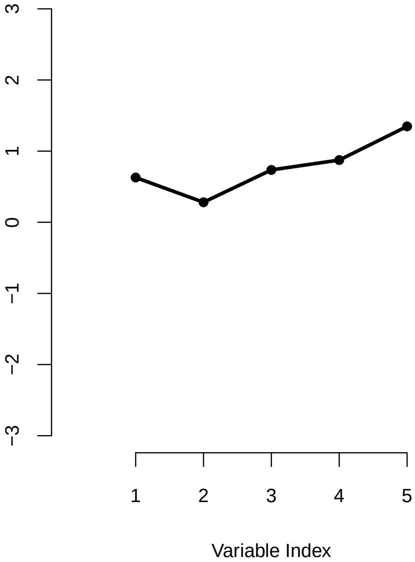


$$\Sigma = \begin{bmatrix} 1.0 & .9 & .8 & .6 & .4 \\ .9 & 1.0 & .9 & .8 & .6 \\ .8 & .9 & 1.0 & .9 & .8 \\ .6 & .8 & .9 & 1.0 & .9 \\ .4 & .6 & .8 & .9 & 1.0 \end{bmatrix}$$



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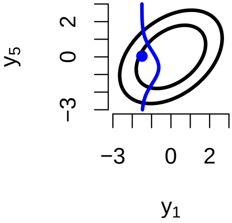

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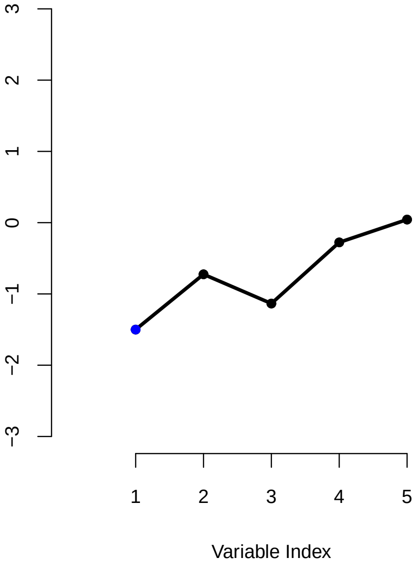
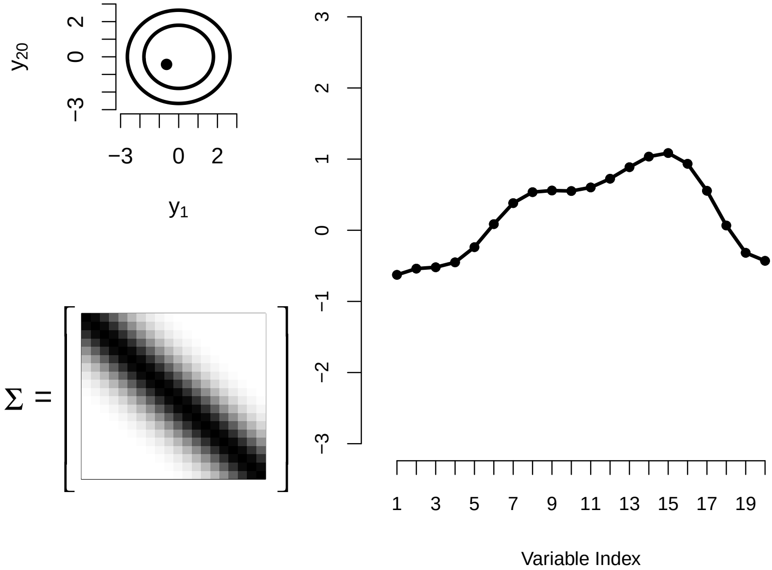


Twenty Dimensional Example



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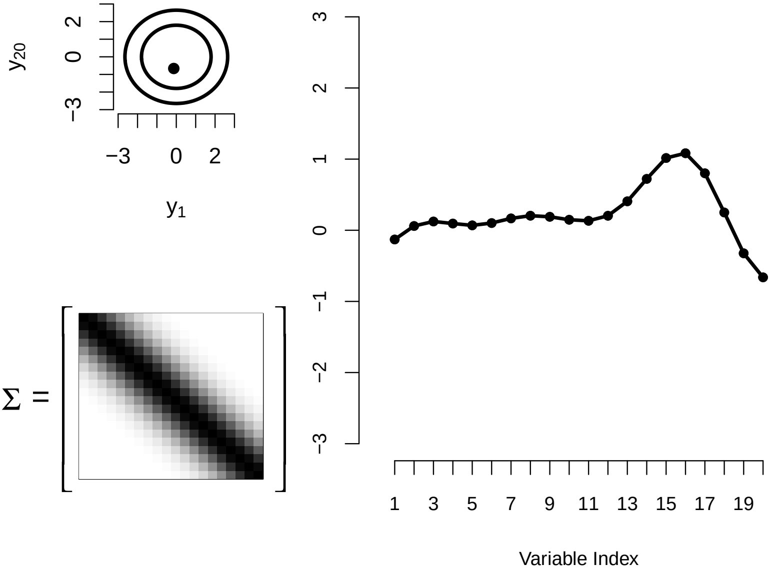

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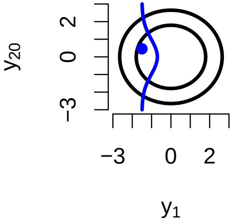

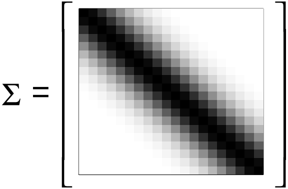

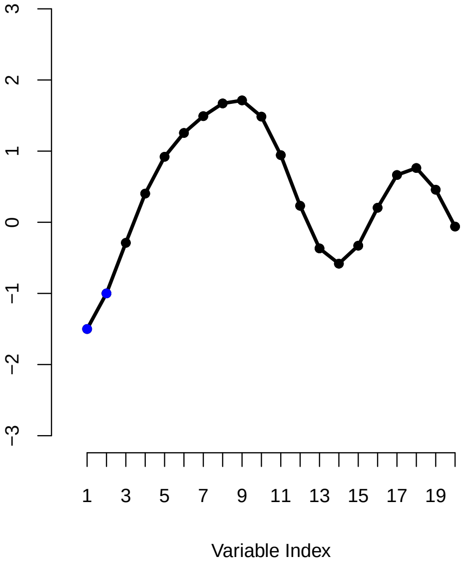

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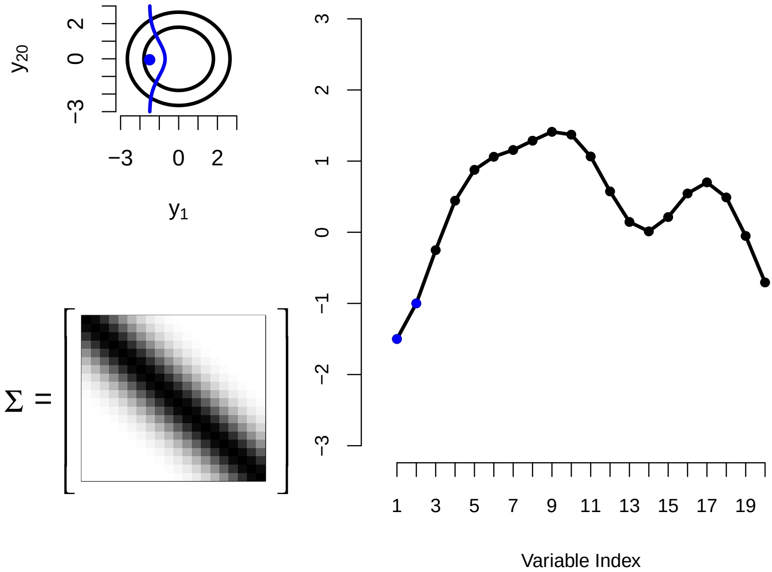
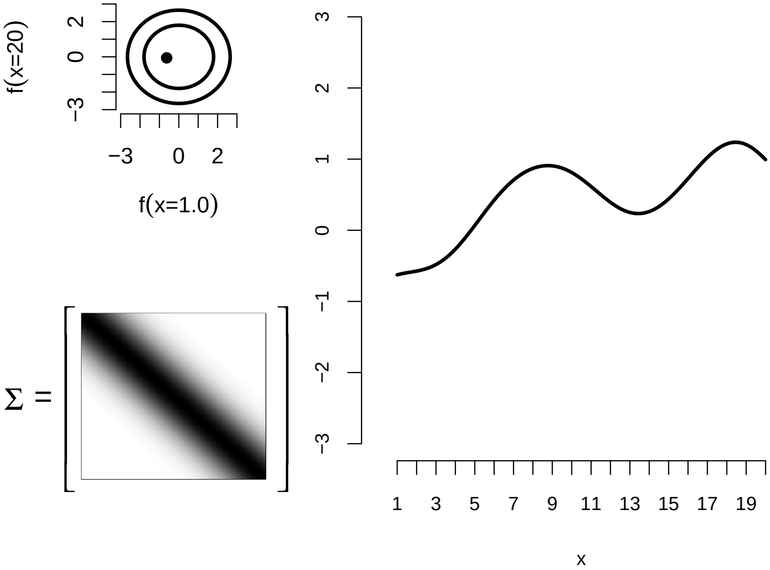


Infinite Dimensional Example



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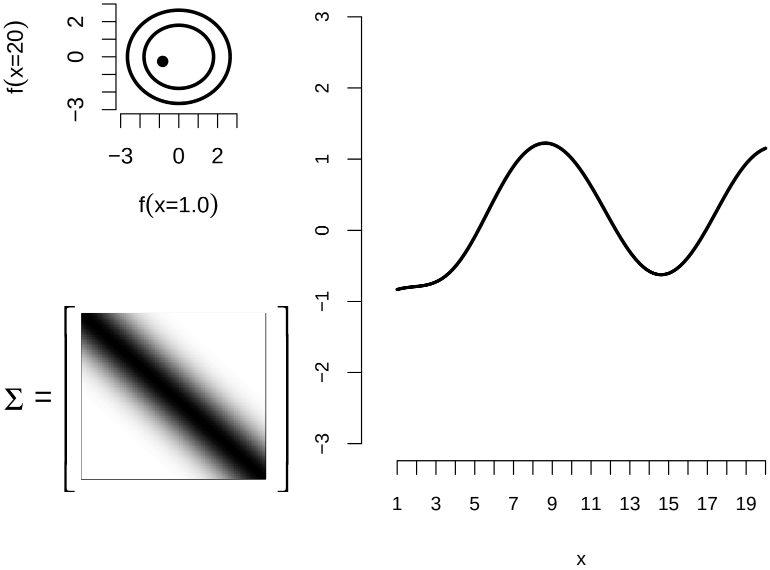

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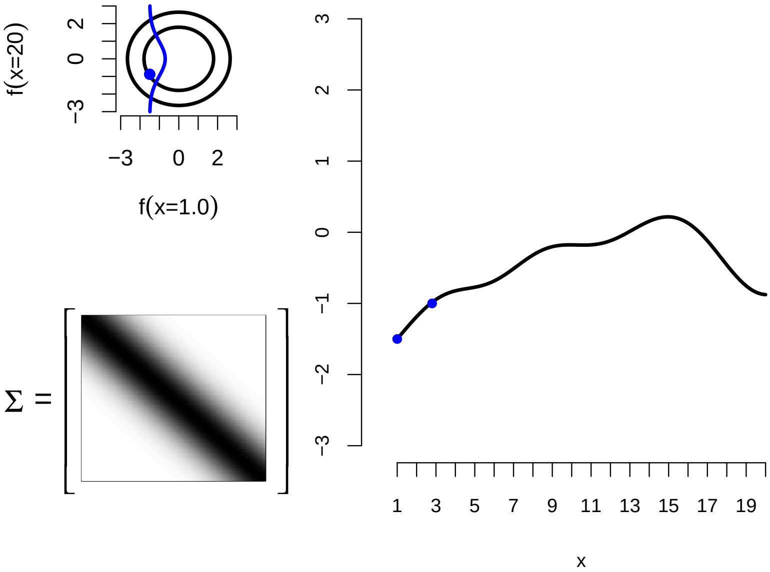

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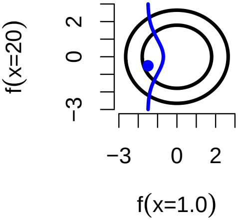
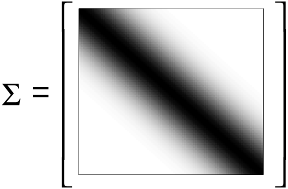
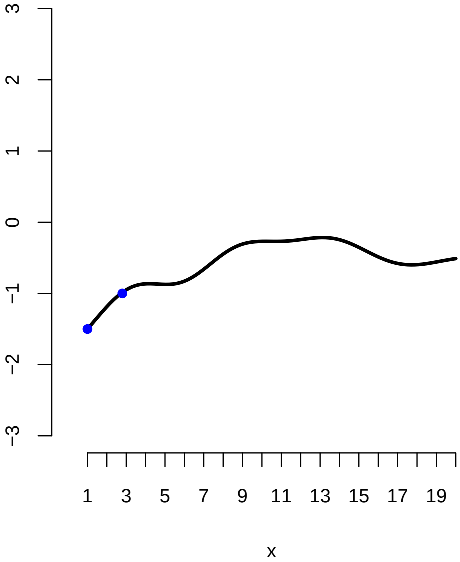
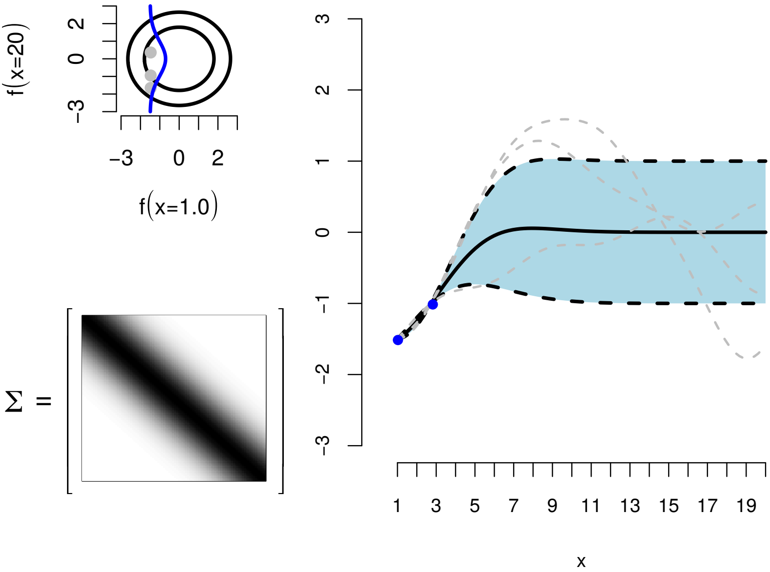






Predictive Distribution



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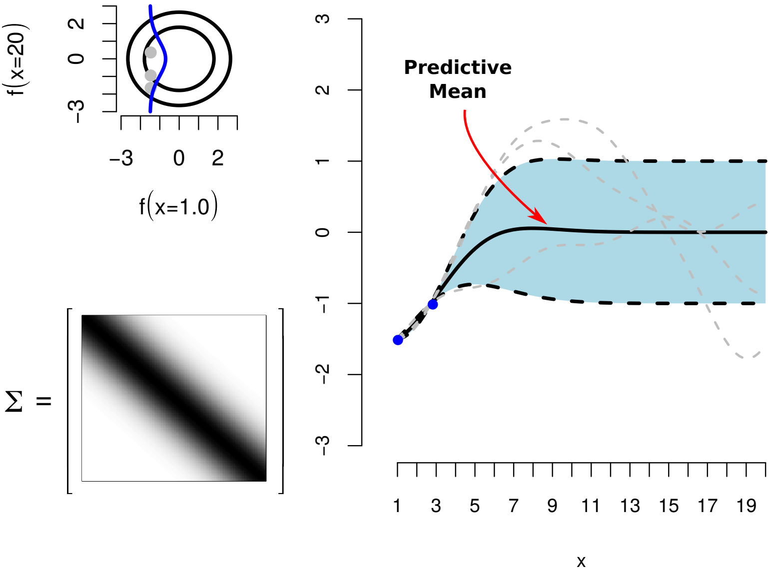

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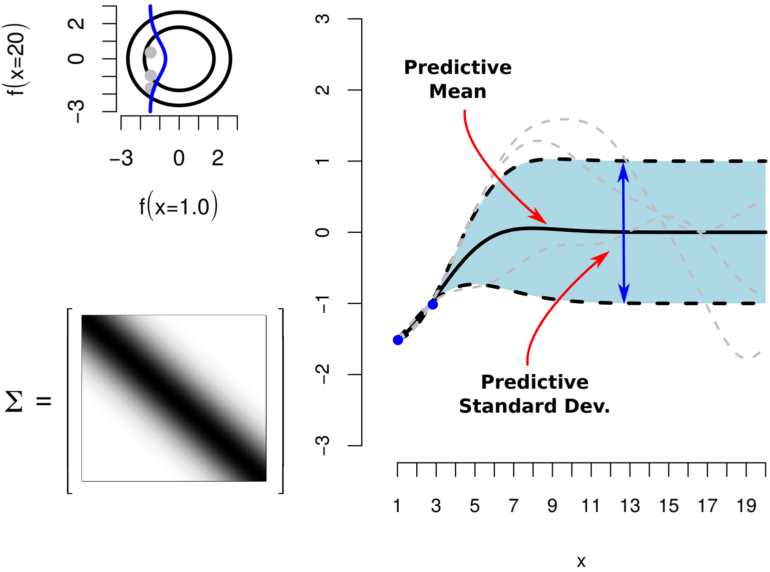

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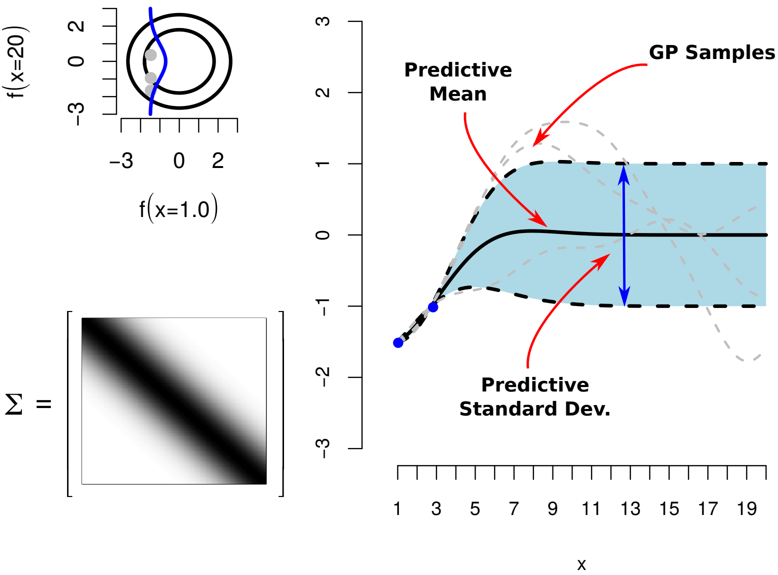

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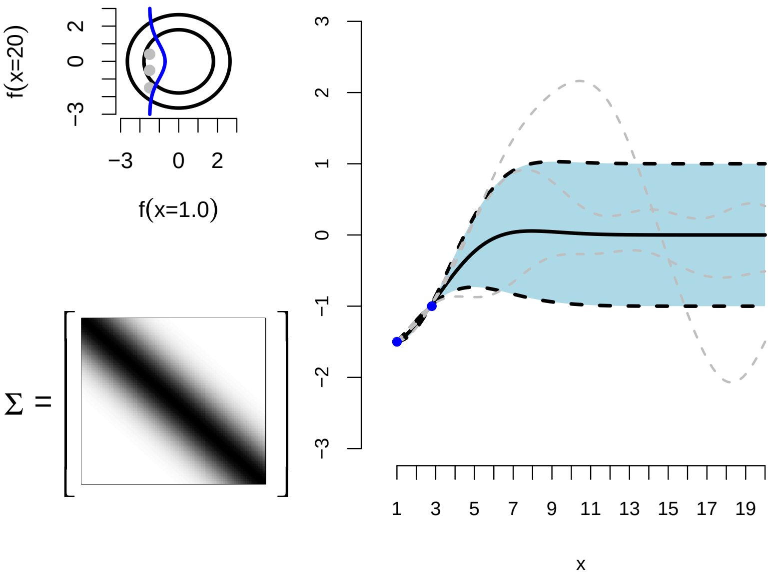

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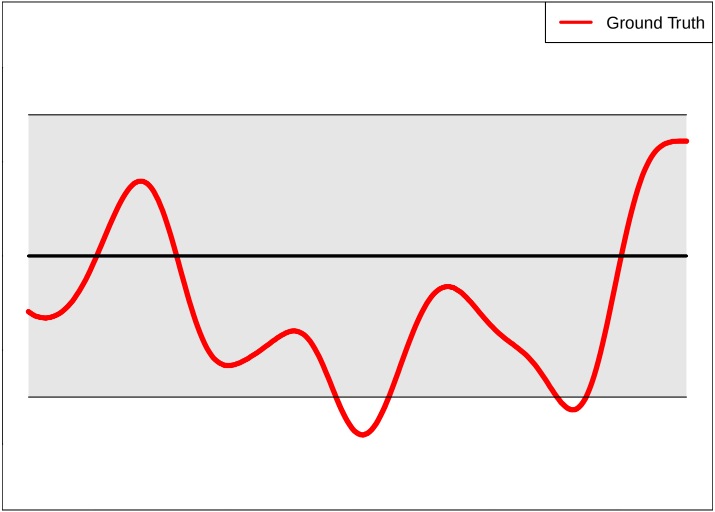

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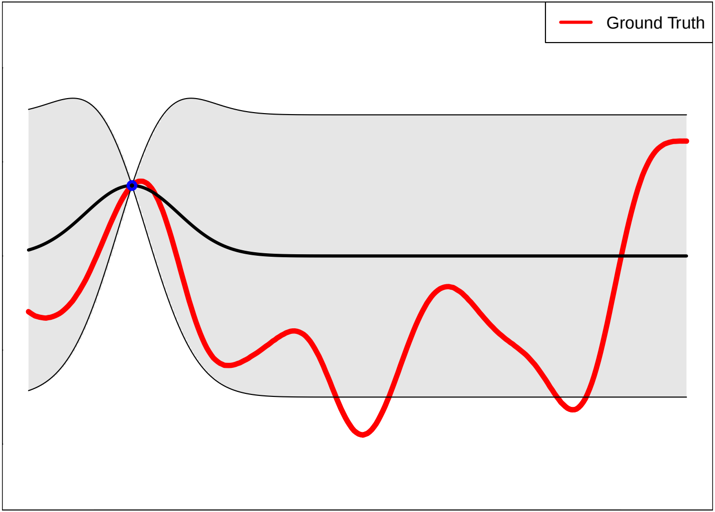

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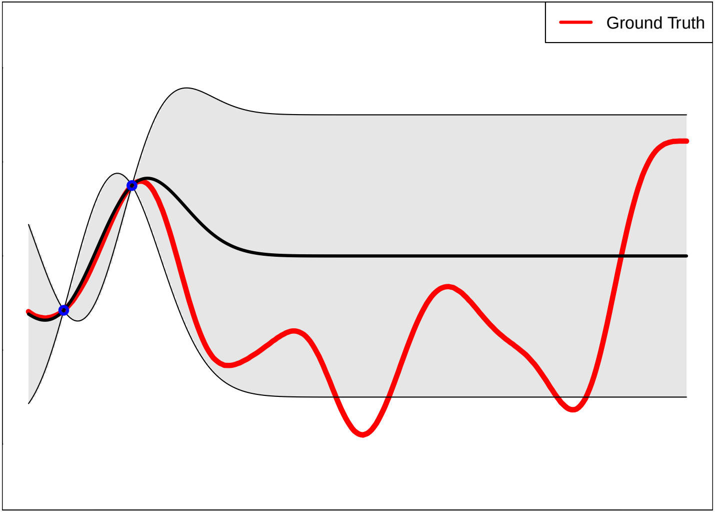

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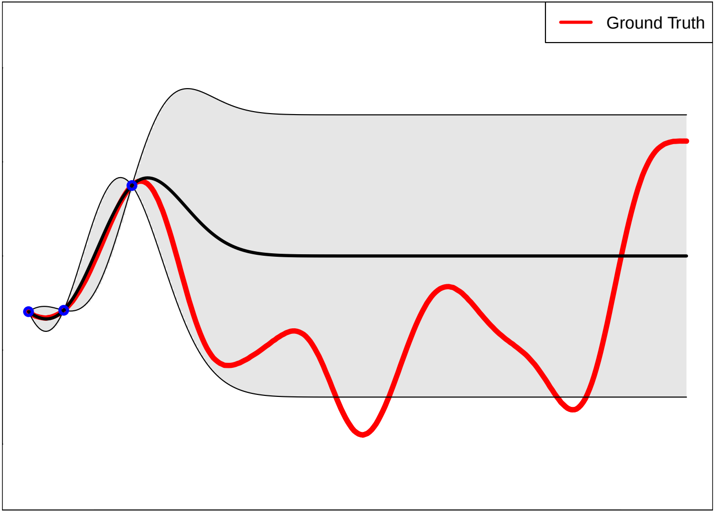

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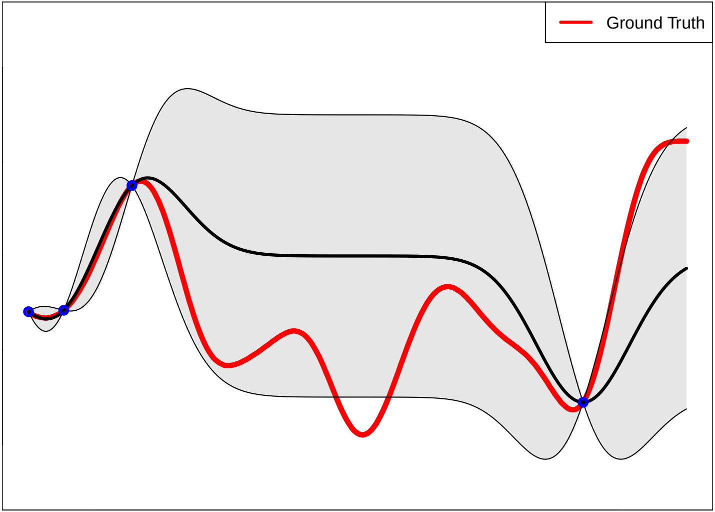

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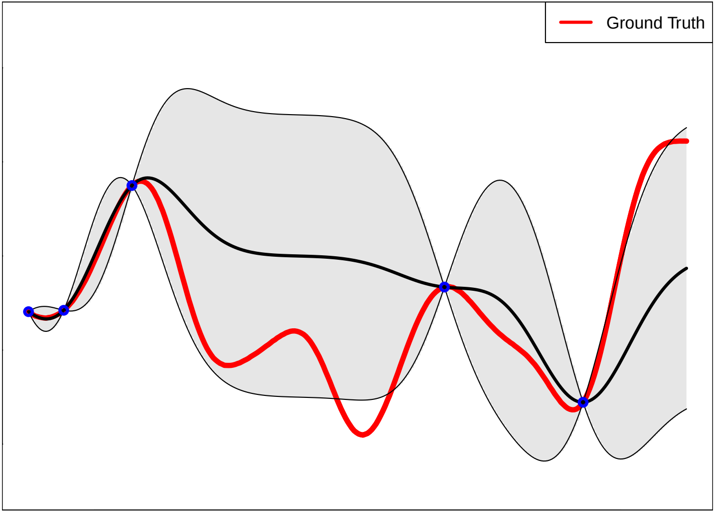

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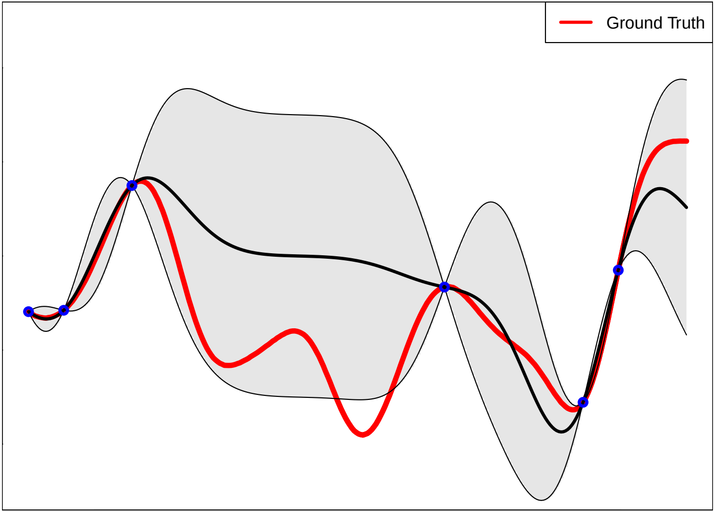

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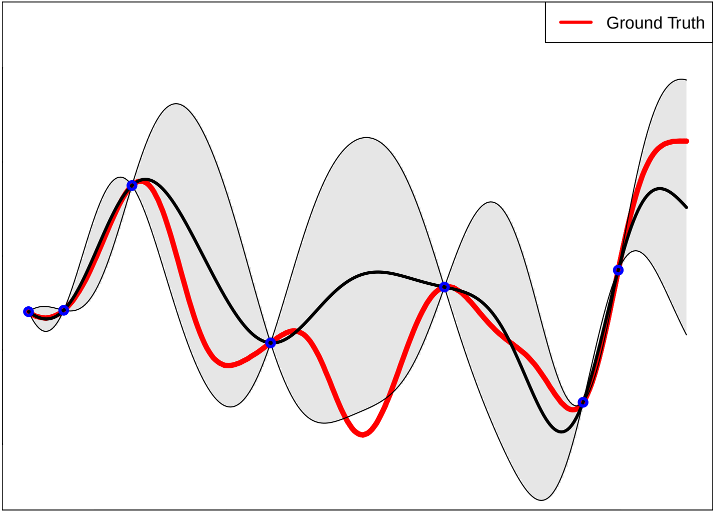

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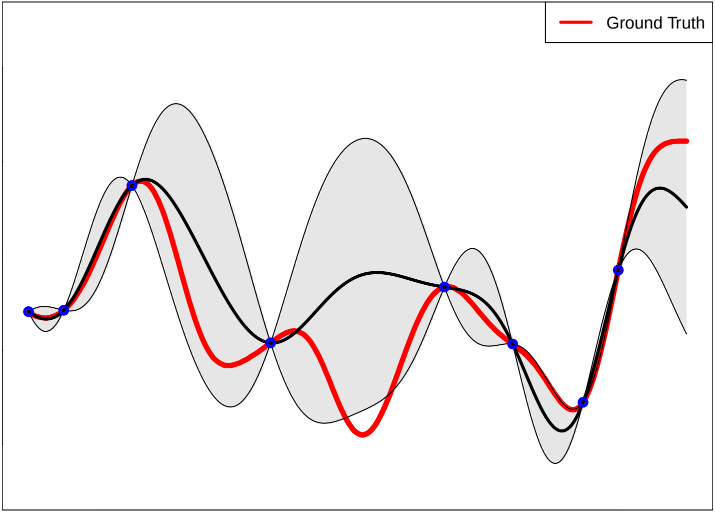

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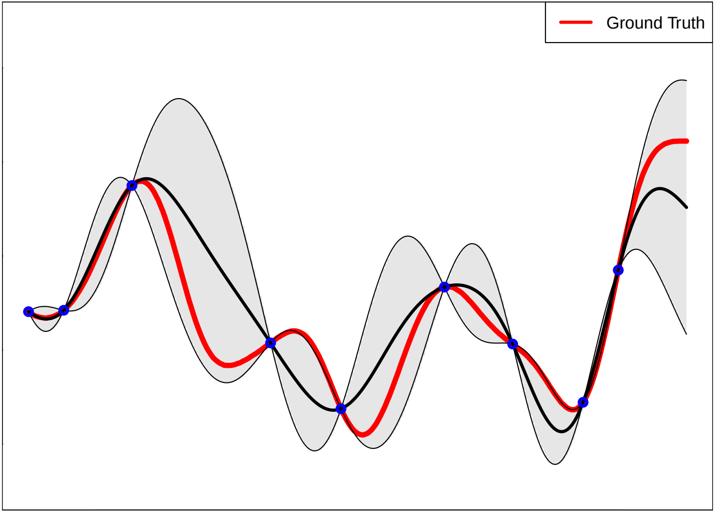

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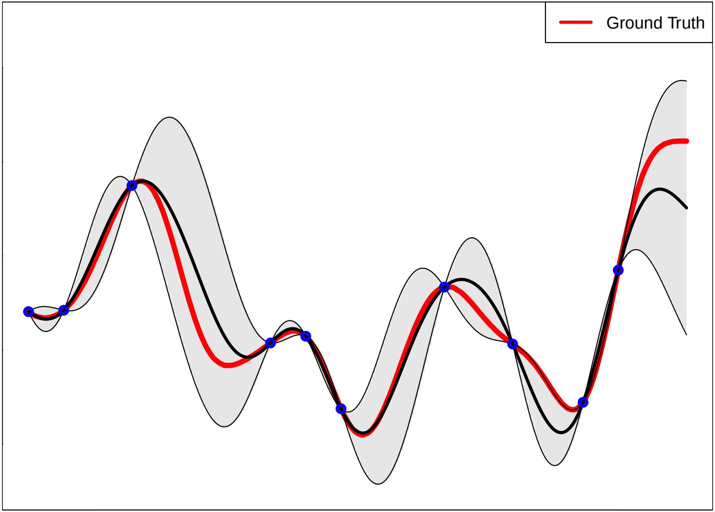

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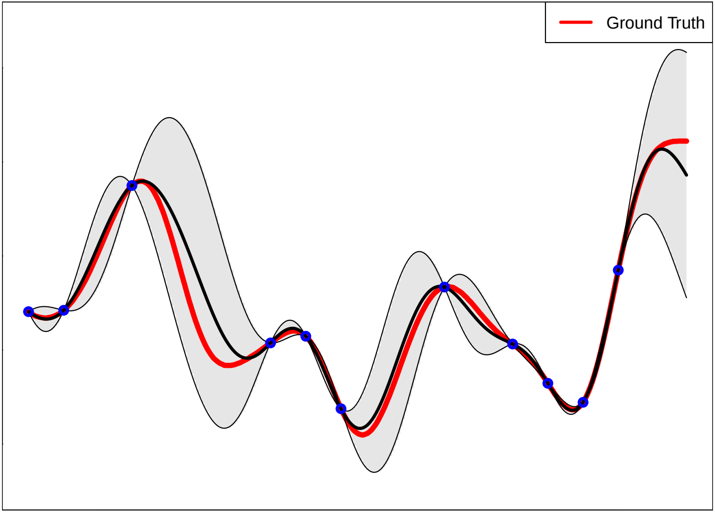

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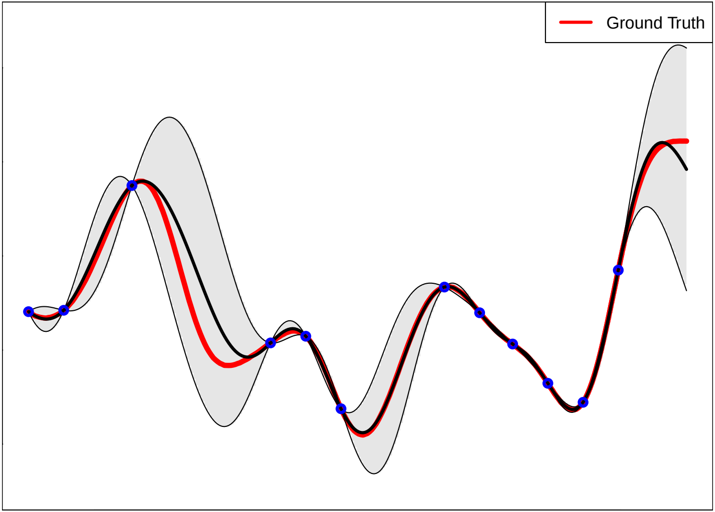

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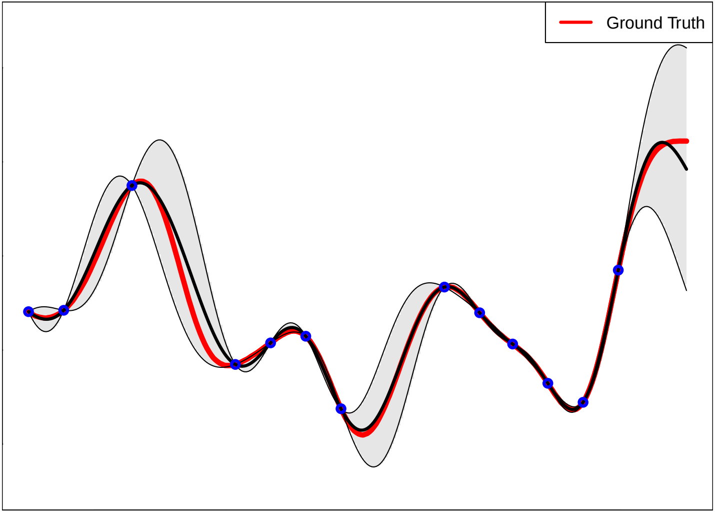

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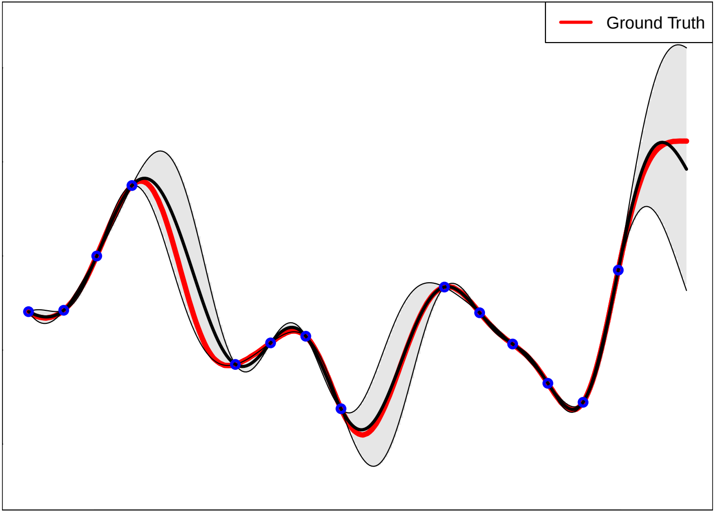

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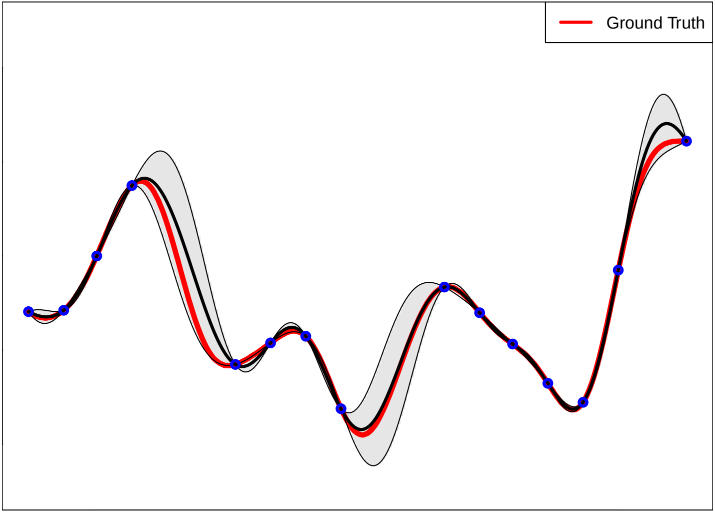

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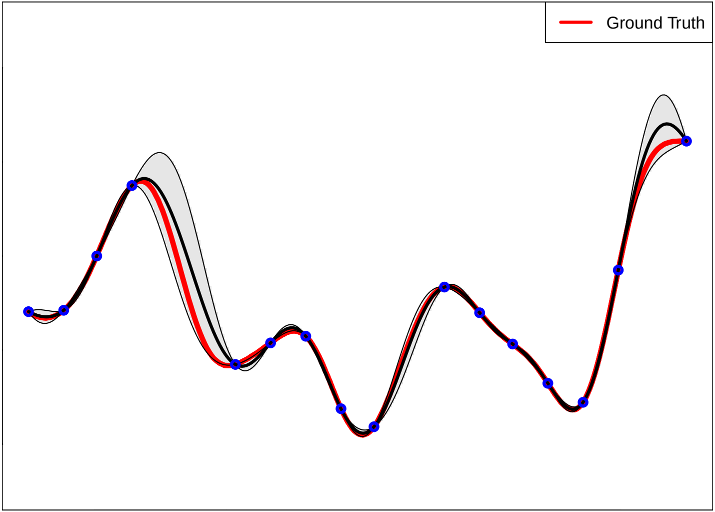

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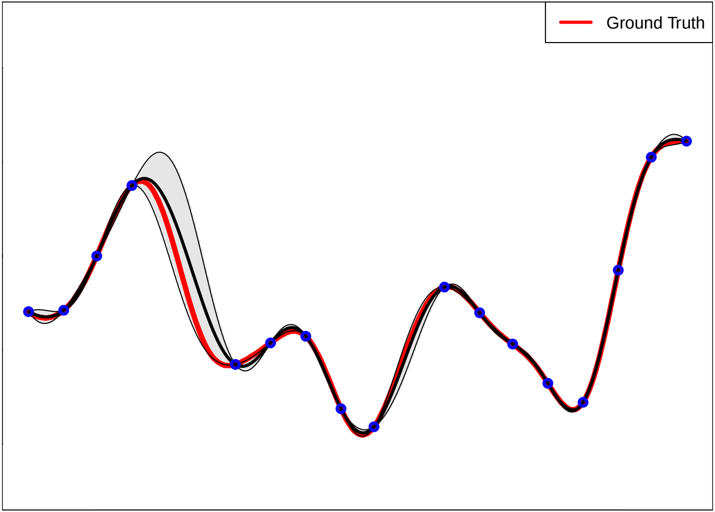

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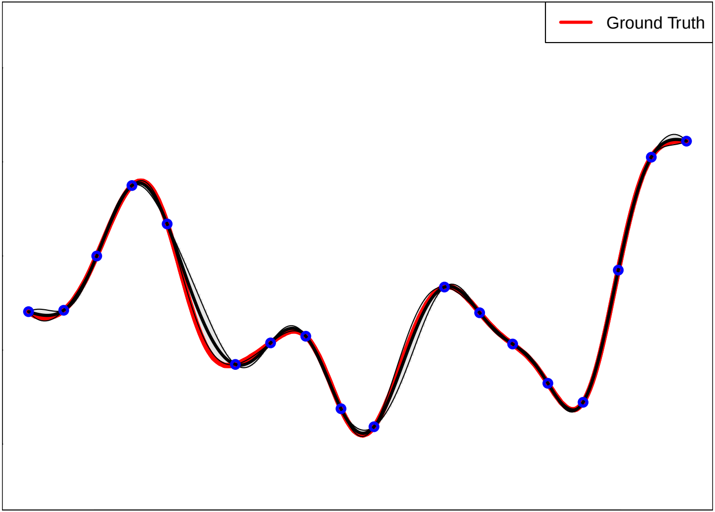

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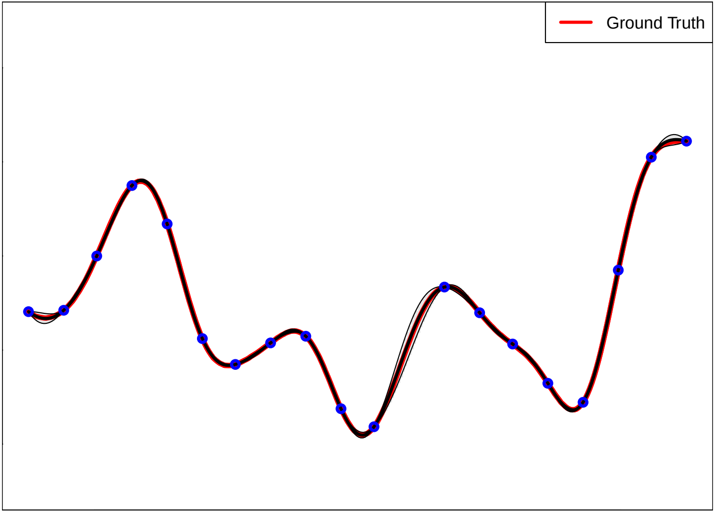

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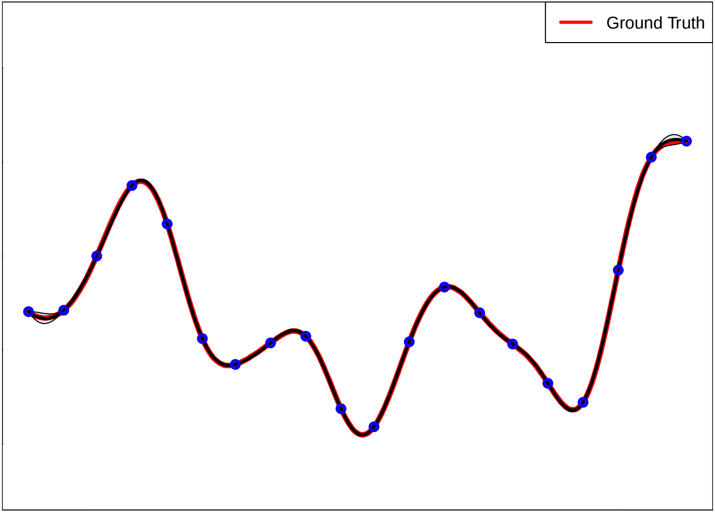

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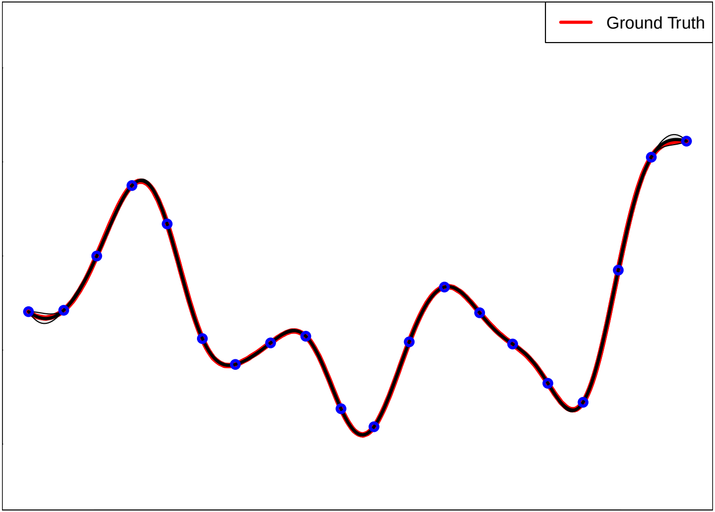

The model becomes more flexible as we observe more data!

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A Gaussian process is fully specified by a mean function $m(\mathbf{x})$ and covariance function $C(\mathbf{x}, \mathbf{x}')$:

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), C(\mathbf{x}, \mathbf{x}')), \quad \text{indices} \quad \mathbf{x}\,.$$

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It determines the global tendency of the latent function before observing the data. Often, simply set to zero.

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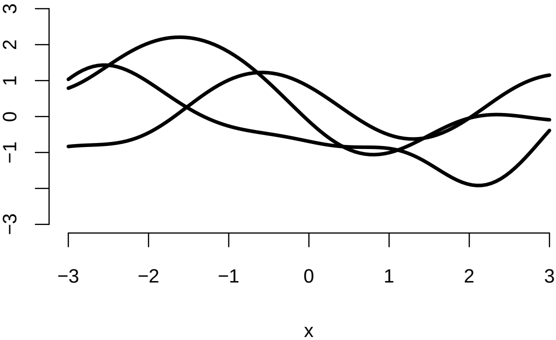

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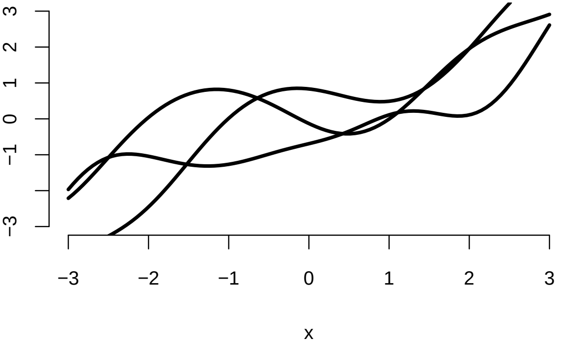

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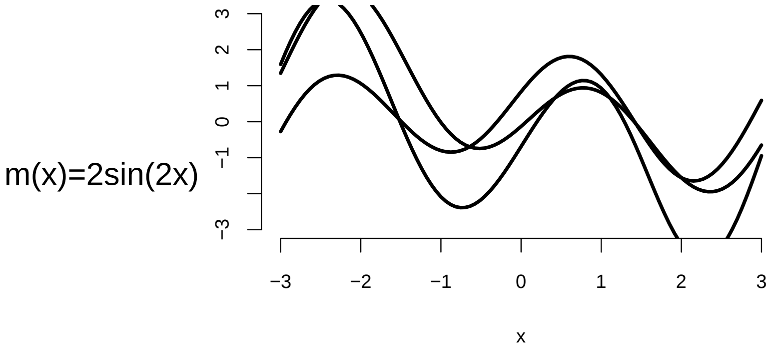

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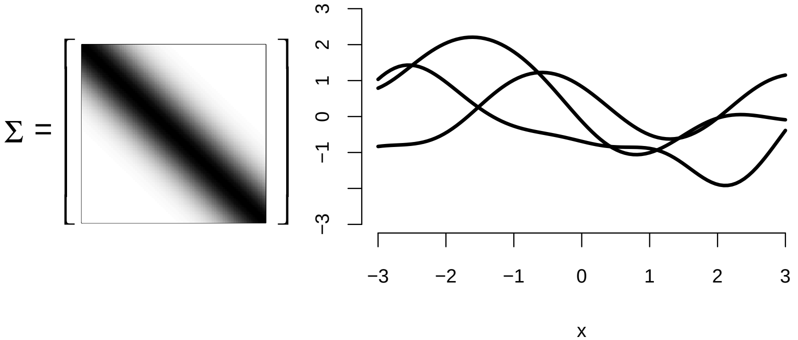

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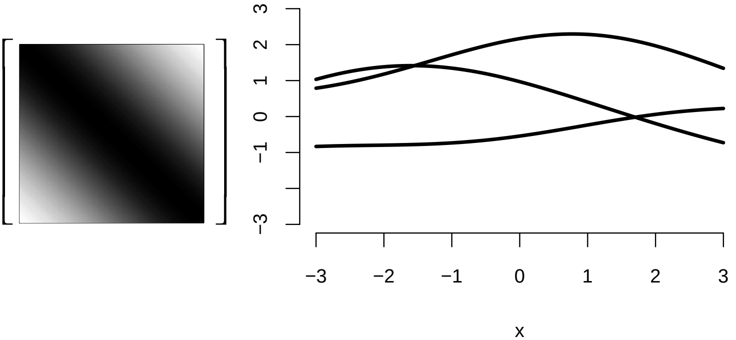

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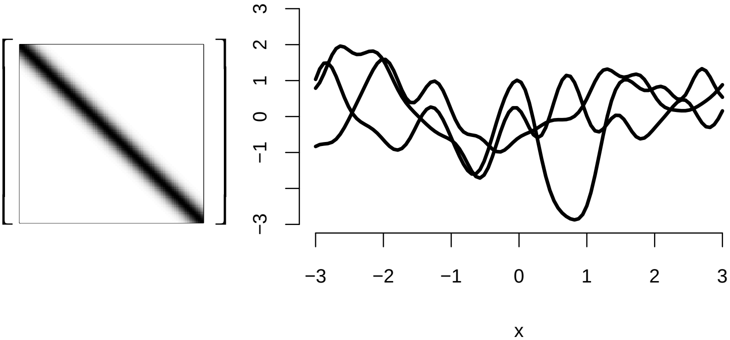

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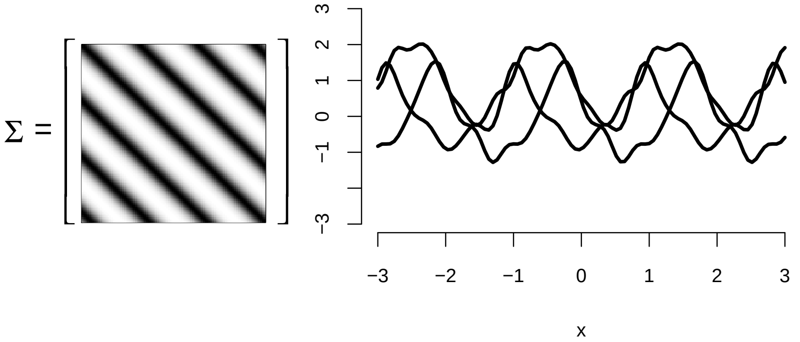

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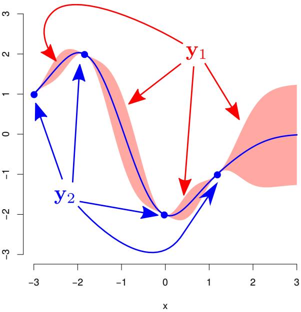
We only need to work with finite sets of random variables!

Computing the Predictive Distribution



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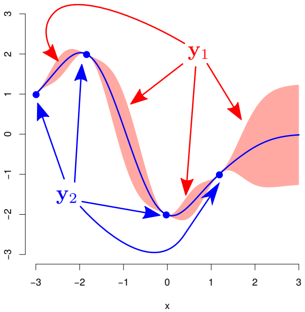

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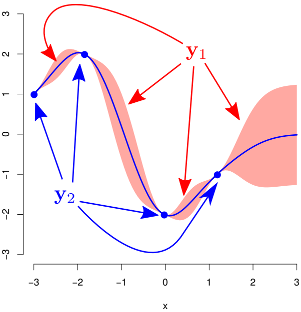

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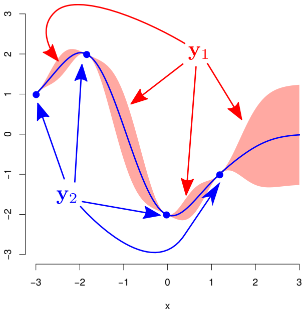

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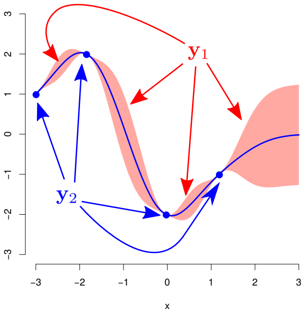

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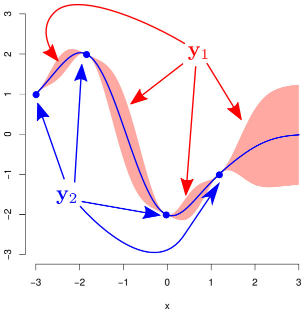

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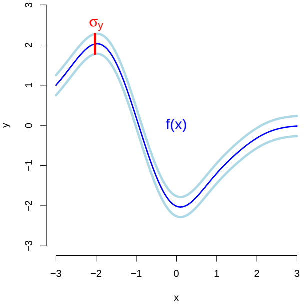
Considering Additive Noise



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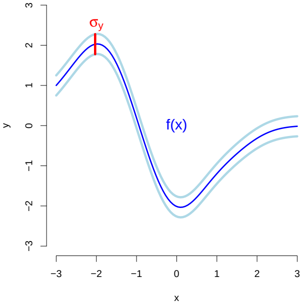

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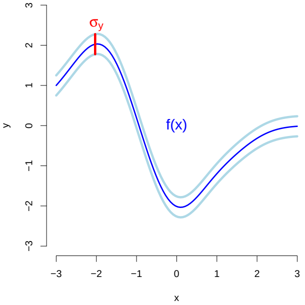

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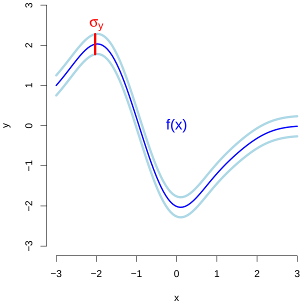

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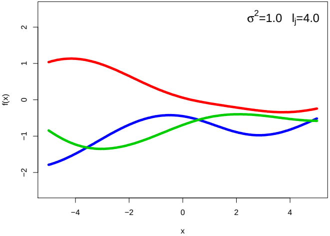

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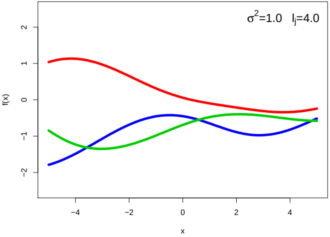

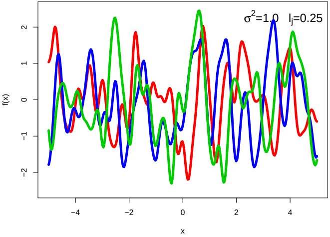

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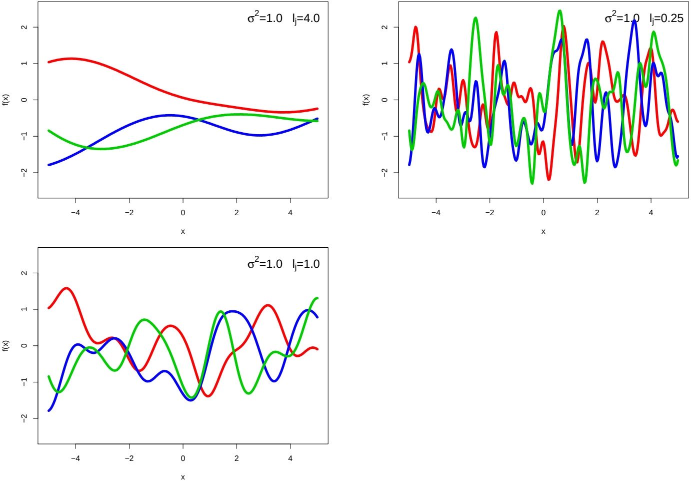

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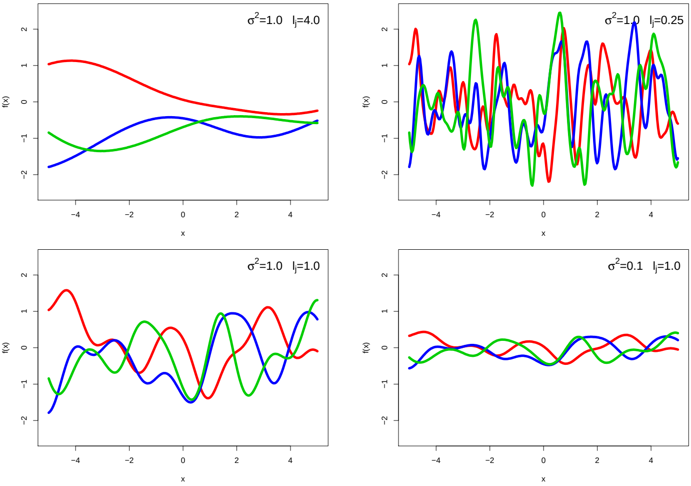

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Often, with a reasonable amount of data, maximizing $p(\mathbf{y}|\theta)$ w.r.t. θ gives good results as it favors the right model!

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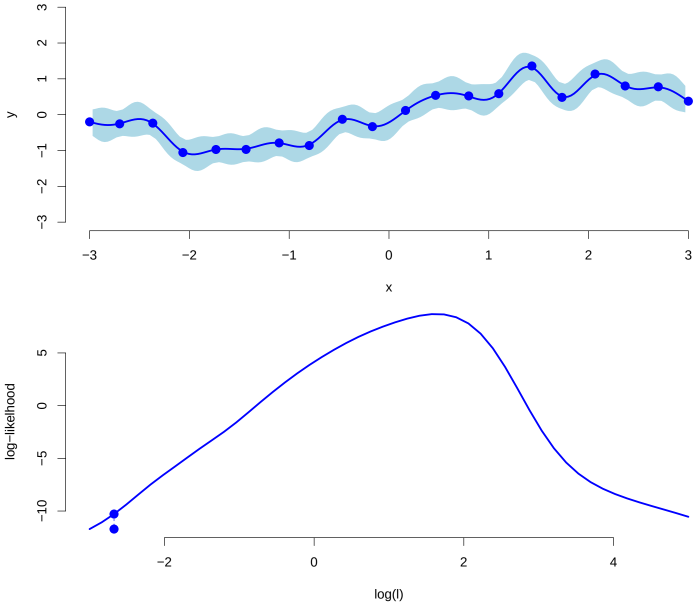

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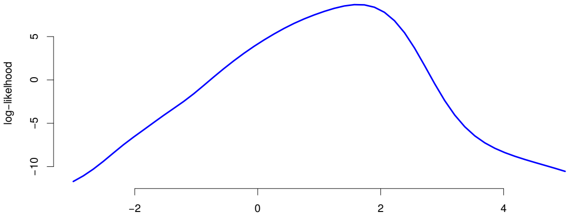

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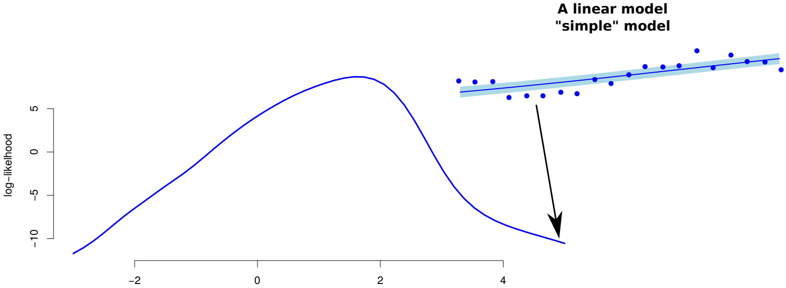

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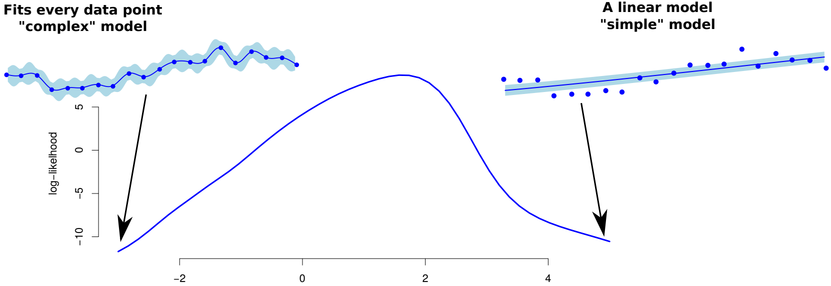

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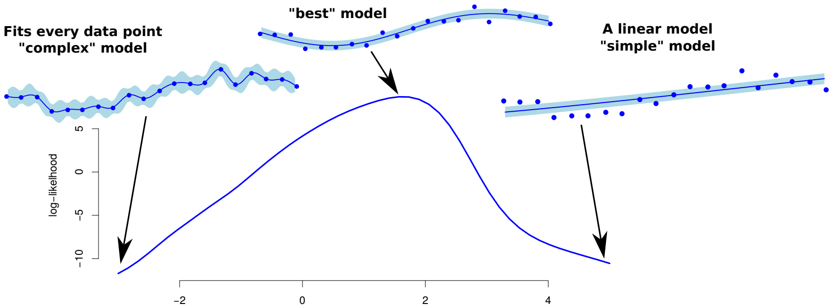

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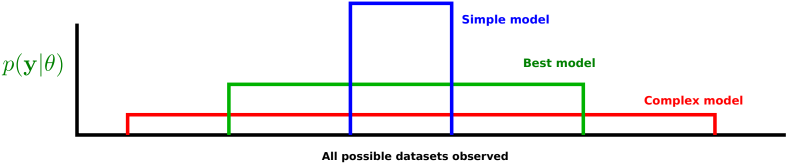

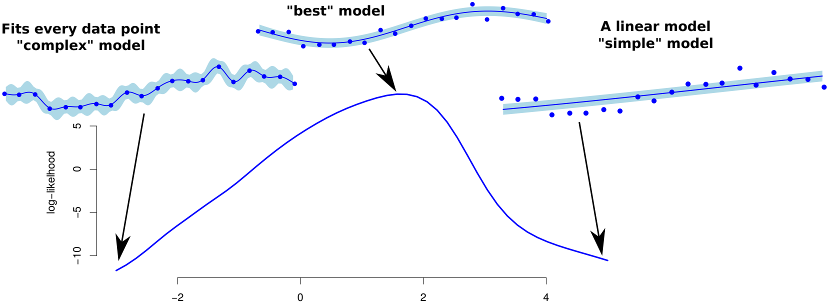

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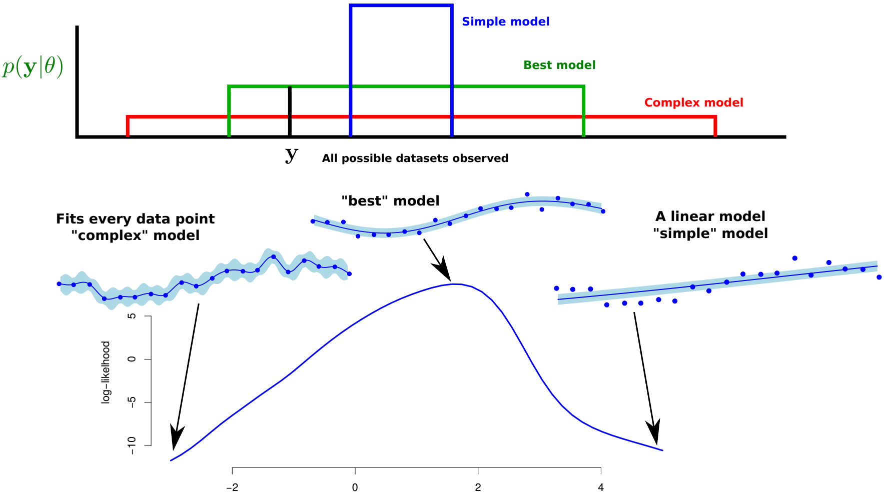

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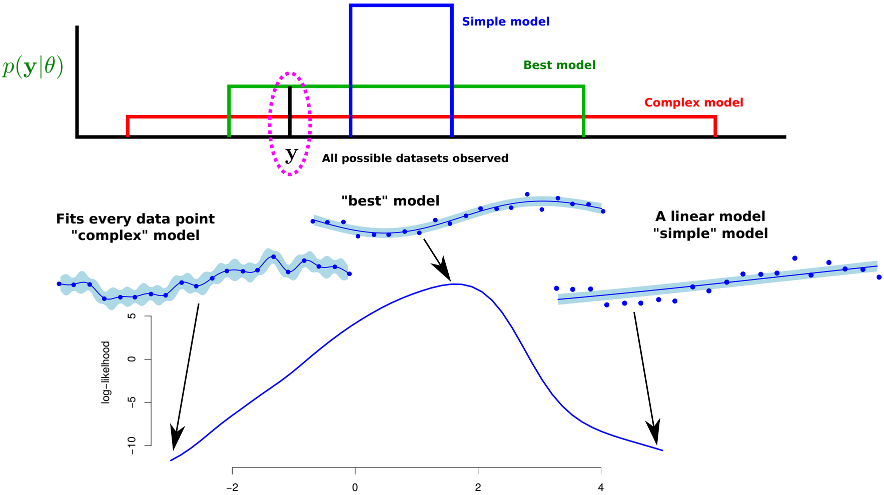

Covariance Functions: Matérn

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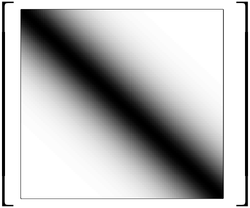
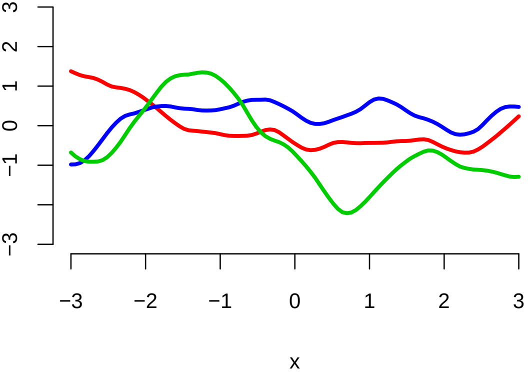
$\Sigma =$ 



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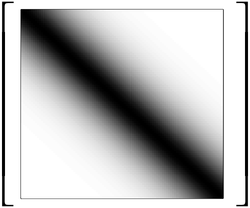
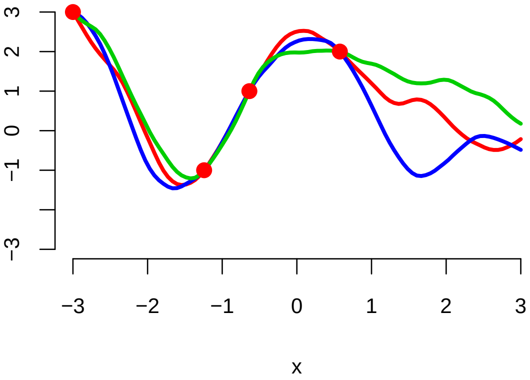
$\Sigma =$ 



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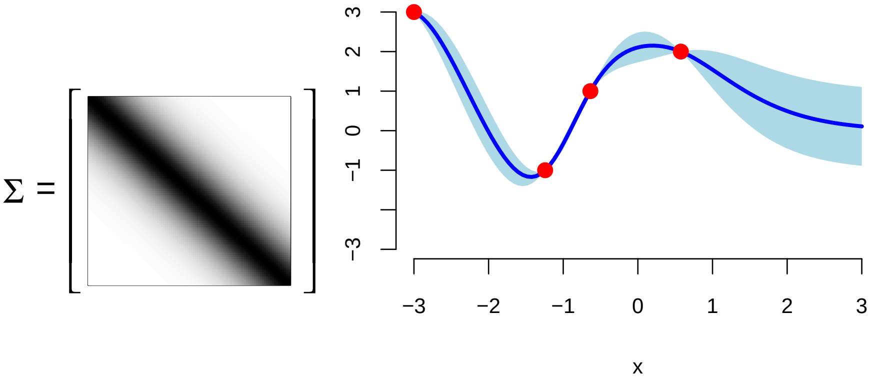
$$C(\mathbf{x}, \mathbf{x}') = \sigma^2 \frac{2^{1-\nu)}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu r}}{l} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu r}}{l} \right)$$



Covariance Functions: Neural Network

$$C(\mathbf{x}, \mathbf{x}') = \sigma^2 \frac{2}{\pi} \sin^{-1} \left(\frac{\mathbf{x}^\top \boldsymbol{\Sigma} \mathbf{x}'}{\sqrt{(1 + 2\mathbf{x}^\top \boldsymbol{\Sigma} \mathbf{x}')(1 + 2\mathbf{x}^\top \boldsymbol{\Sigma} \mathbf{x}')}} \right)$$

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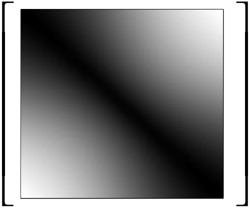
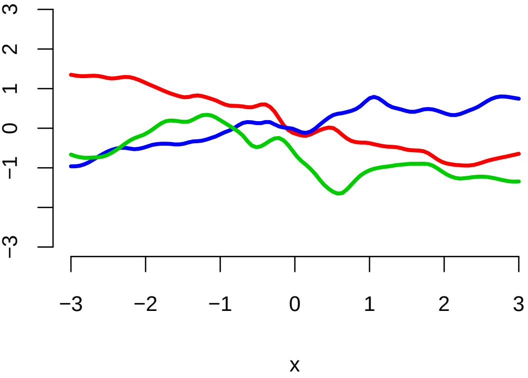
$\Sigma =$ 



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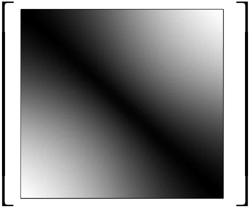

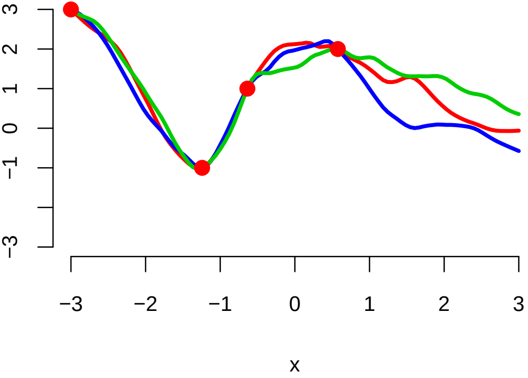

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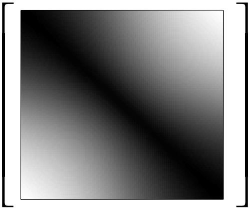
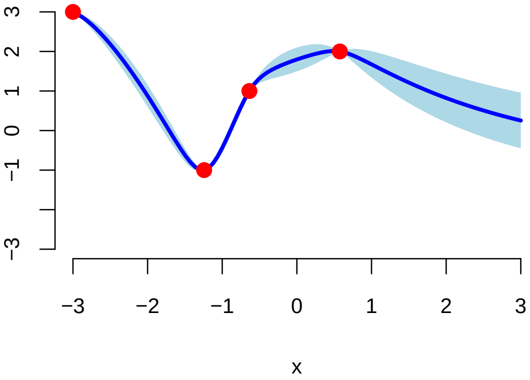
$\Sigma =$ 



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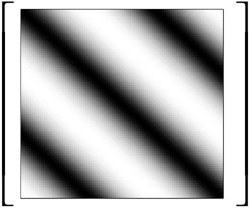
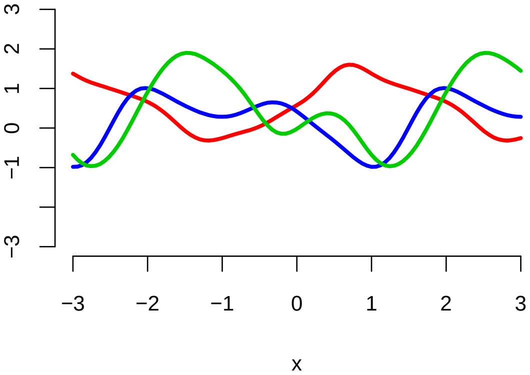
$\Sigma =$ 



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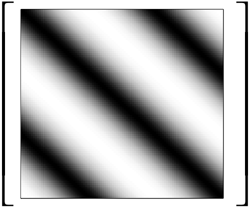
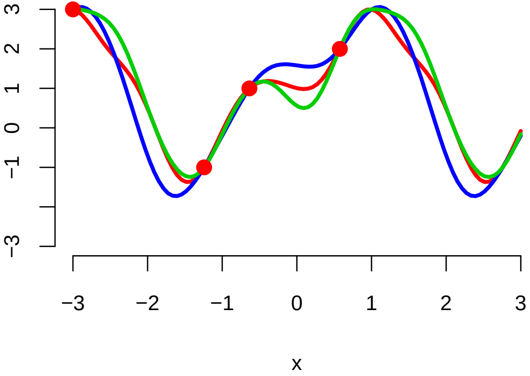
$\Sigma =$ 



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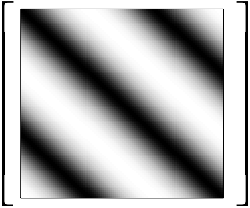
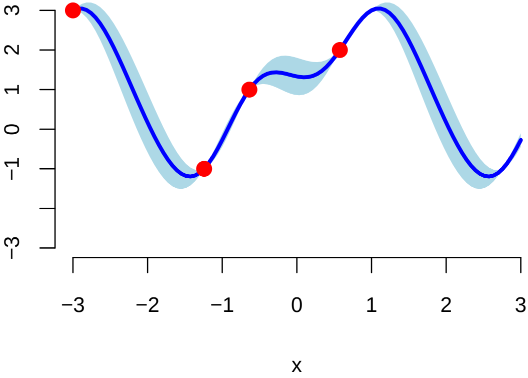
$\Sigma =$ 



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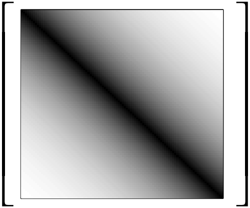
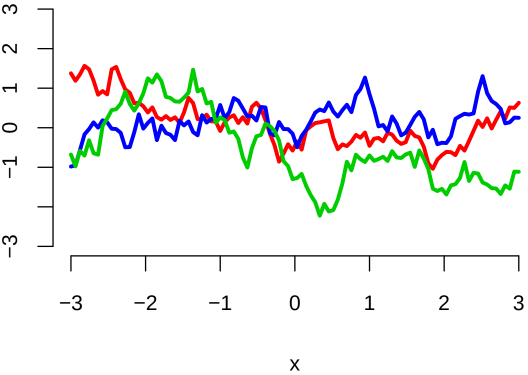
$\Sigma =$ 



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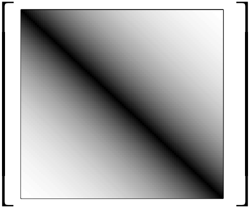
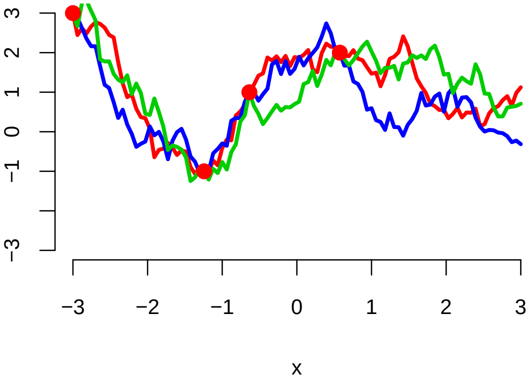
$\Sigma =$ 



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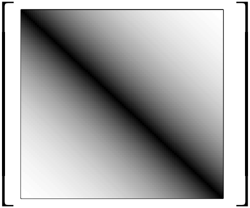
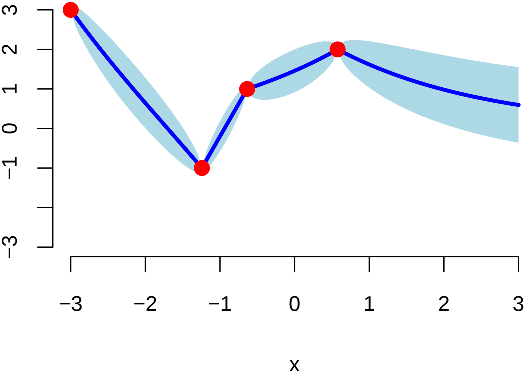
$\Sigma =$ 



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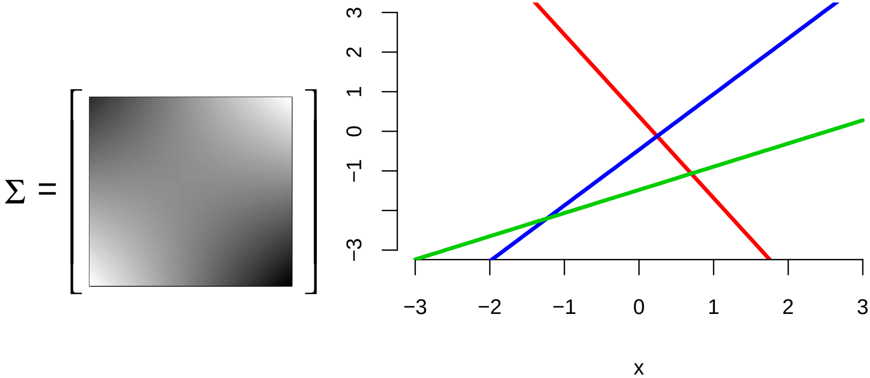

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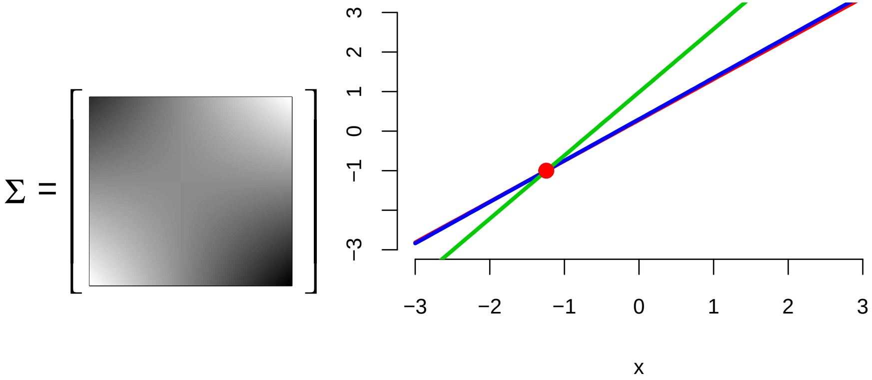

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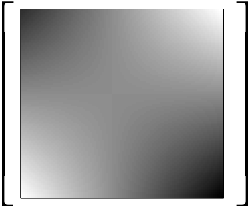
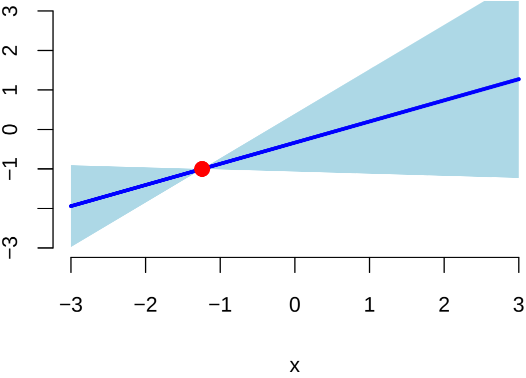
$\Sigma =$ 



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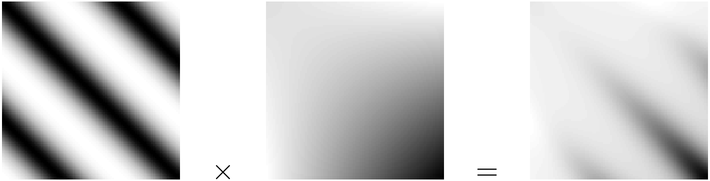

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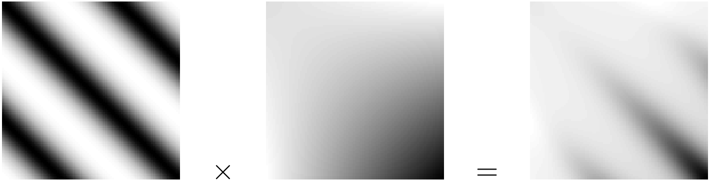

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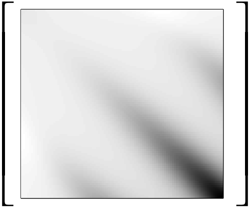
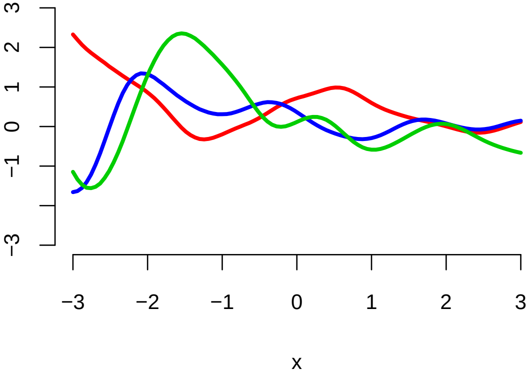
$\Sigma =$ 



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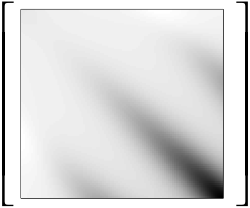
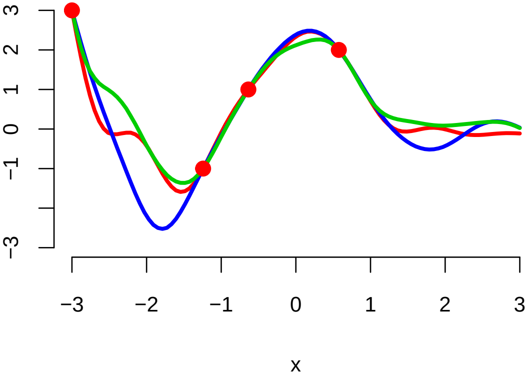
$\Sigma =$ 



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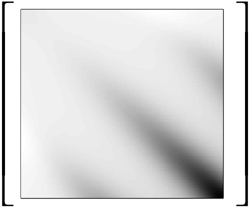
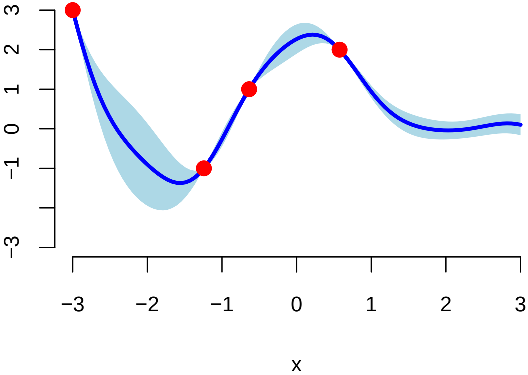
$\Sigma =$ 



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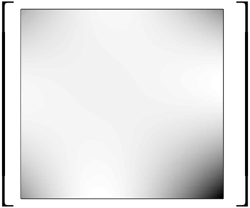
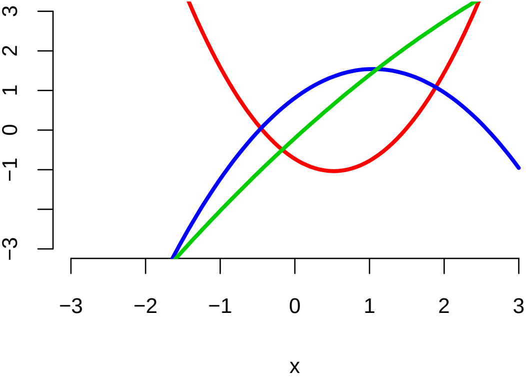
$\Sigma =$ 



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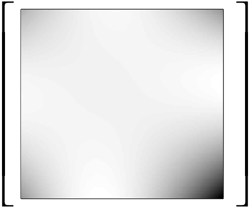
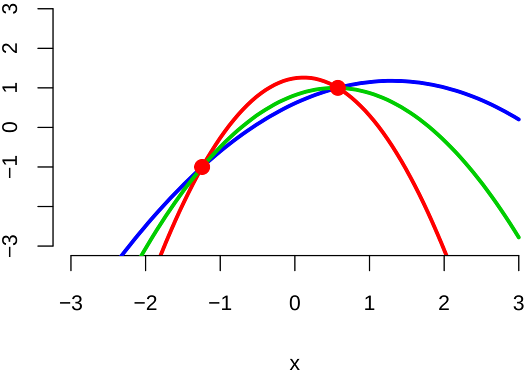
$\Sigma =$ 



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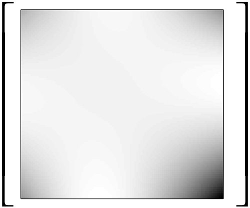
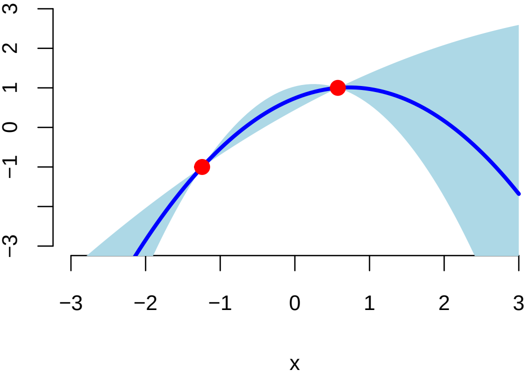
$\Sigma =$ 



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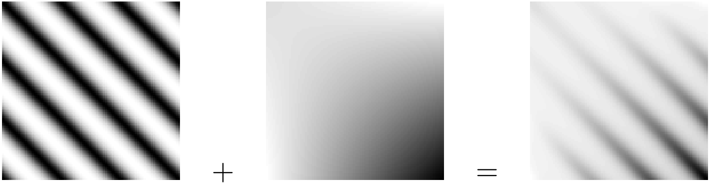

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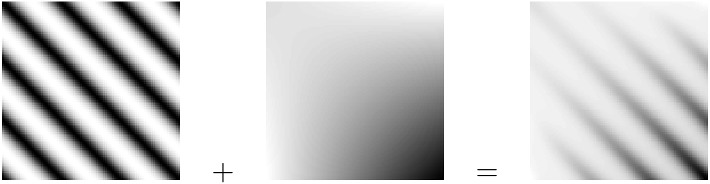

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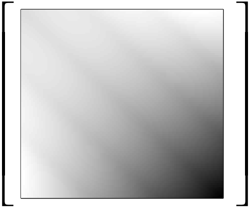
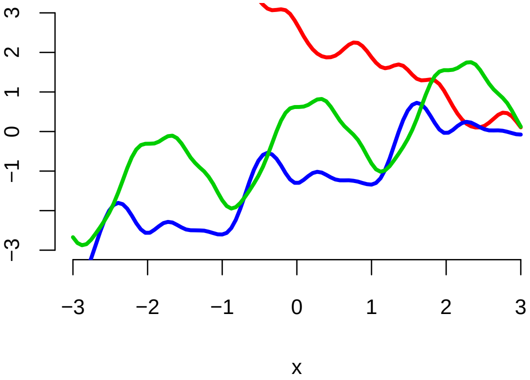
$\Sigma =$ 



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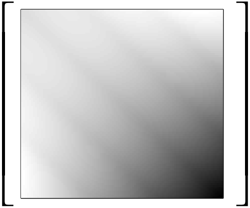
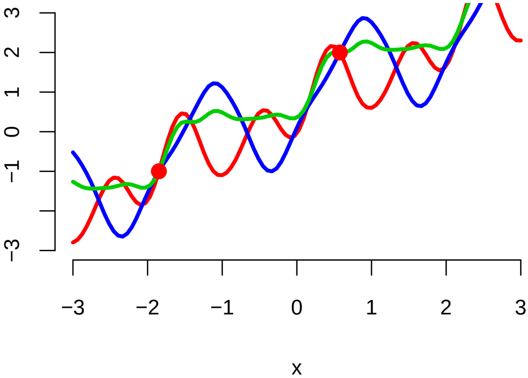
$\Sigma =$ 



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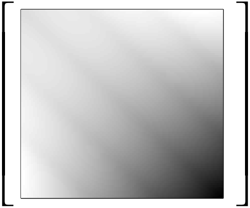

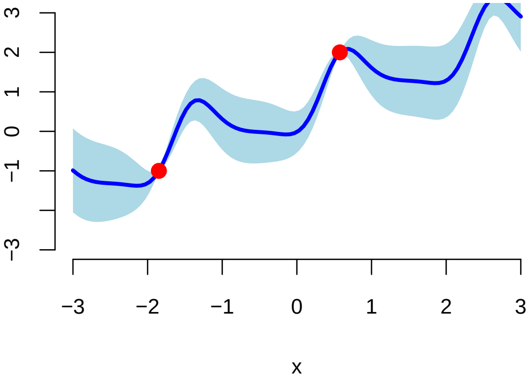

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i.e., we should assign the class for which $p(\mathcal{C}_k|\mathbf{x}) \propto p(\mathbf{x}, \mathcal{C}_1)$ is larger.

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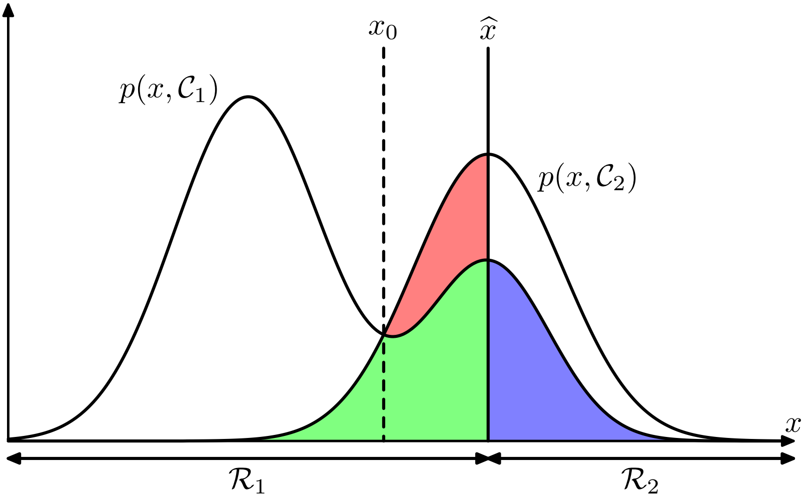

(Bishop, 2006)

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with $f(\cdot)$ a latent function modeled by a GP.

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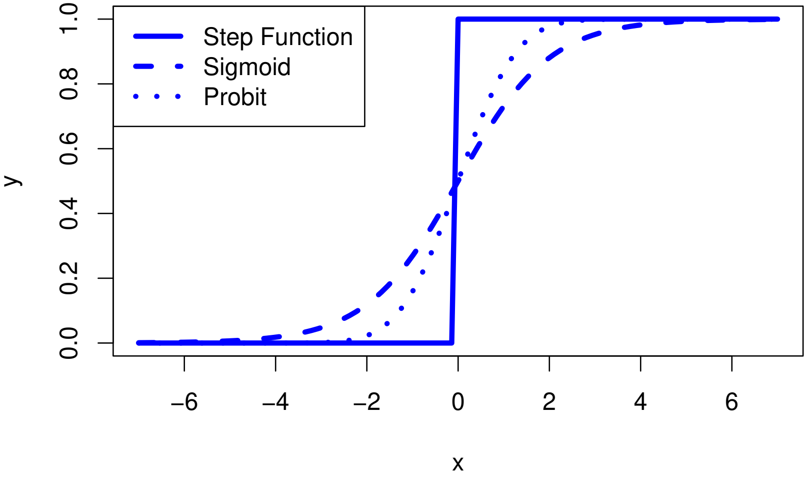

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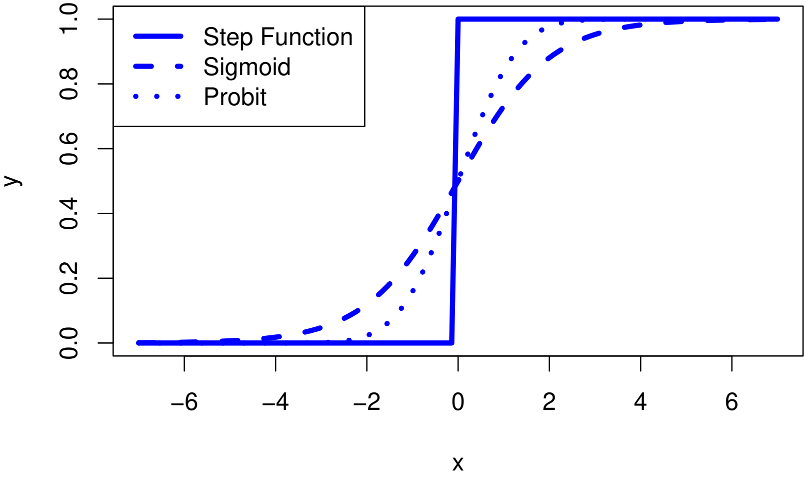
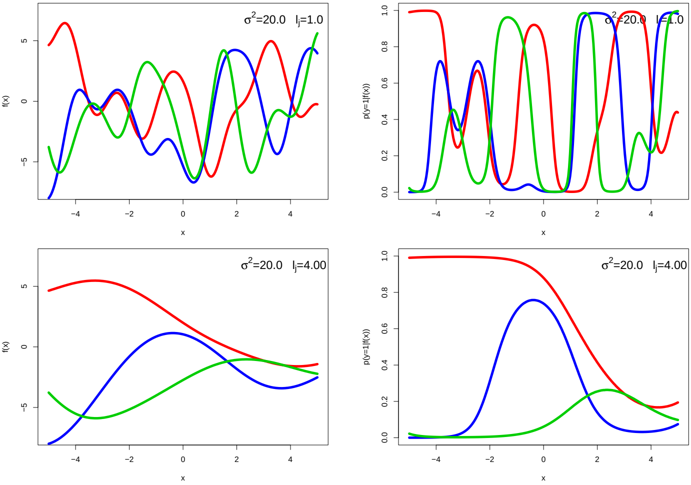


The sigmoid and probit consider logistic and standard Gaussian noise! $p(y_i = 1|\mathbf{x}_i) = I(f(\mathbf{x}_i) + \epsilon_i > 0)$

Prior Samples Squashed via the Sigmoid Function



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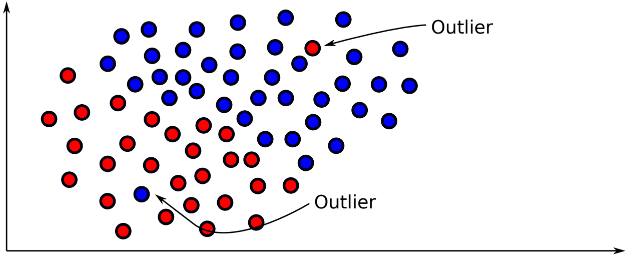

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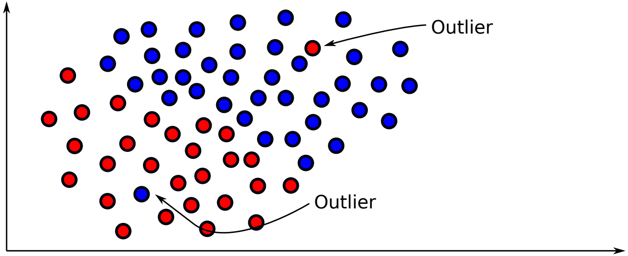

Robust likelihood with probability ϵ of label flip:

$$p(y|f(\mathbf{x}_i), \epsilon) = (1 - \epsilon) \cdot \sigma(f(\mathbf{x}_i)) + \epsilon \cdot (1 - \sigma(f(\mathbf{x}_i)))$$

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Unfortunately, the posterior is intractable since the likelihood is not Gaussian and must be approximated!

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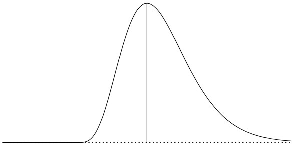

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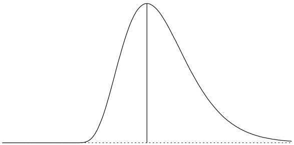

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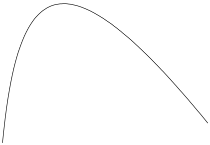

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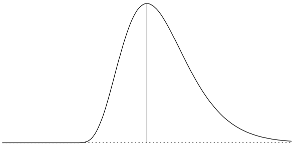

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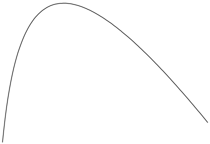

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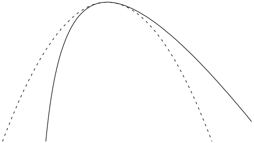

$\log f(z)$ and $\log \tilde{q}(z)$

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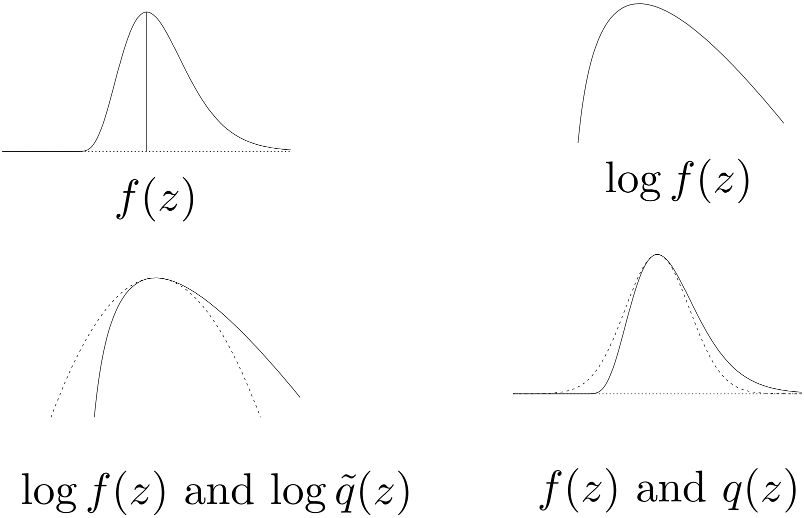

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The posterior is unimodal and hence $\mathbf{A}$ is positive semidefinite.

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with this last integral evaluated via quadrature and

$$q(f(\mathbf{x}_\star)) = \mathcal{N}(f(\mathbf{x}_\star)|\mathbf{c}_\star^\mathsf{T}\mathbf{C}^{-1}\mathbf{f}_0, C(\mathbf{x}_\star, \mathbf{x}_\star) - \mathbf{c}_\star^\mathsf{T}\mathbf{C}^{-1}\mathbf{c}_\star + \mathbf{c}_\star^\mathsf{T}\mathbf{C}^{-1}\mathbf{A}^{-1}\mathbf{C}^{-1}\mathbf{c}_\star)\,,$$

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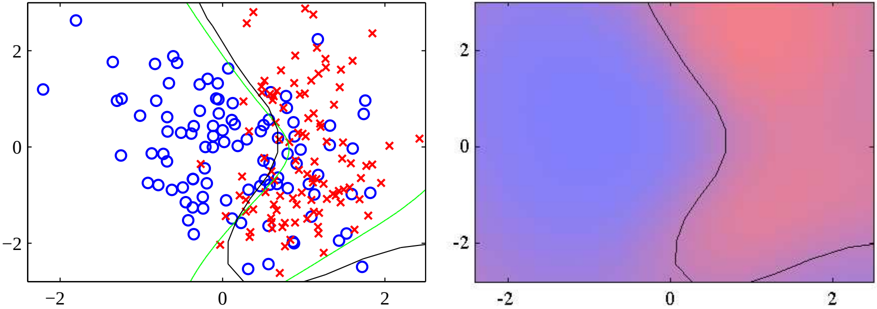
Decision boundary and prediction uncertainty:



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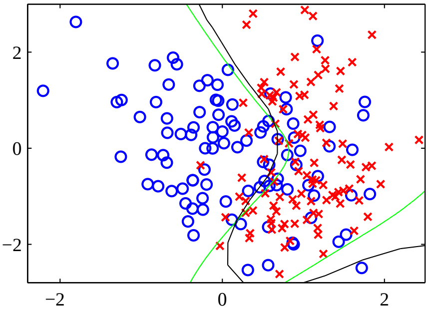

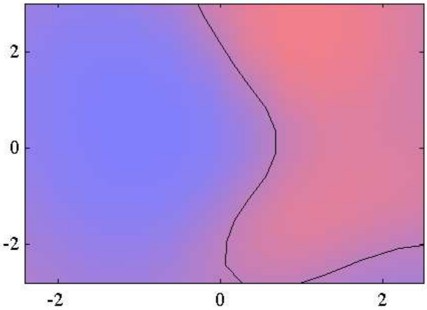

Prediction uncertainty is higher in regions with no observed data.

(Bishop, 2006)

Multi-class Classification

There are latent process values at N training points for all C classes:

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The posterior is approximated using the Laplace approximation with linear cost in C!

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Software for GPs and Deep GPs

There are several packages providing implementations of GPs:

- **GPy**: Gaussian Processes in Python. Easy-to-use and extend. Supports multi-output GPs, different noise models and different approximate inference methods.
- **GPML**: Gaussian Processes in Matlab. No longer maintained. Implements the models and methods from the book "Gaussian Process for Machine learning".
- **GPflow**: Gaussian processes in python using Tensorflow. Supports GPU acceleration. Focuses on variational inference and MCMC for approximate inference.
- **GPyTorch**: Gaussian processes in python using PyTorch. Supports GPU acceleration. Also supports deep GPs.

Deep GPs: uses doubly stochastic variational inference and GPflow.

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5. GPs can address **classification problems** too, but **approximate inference** is needed.

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