# Part I: Gaussian Processes for Regression and Classification

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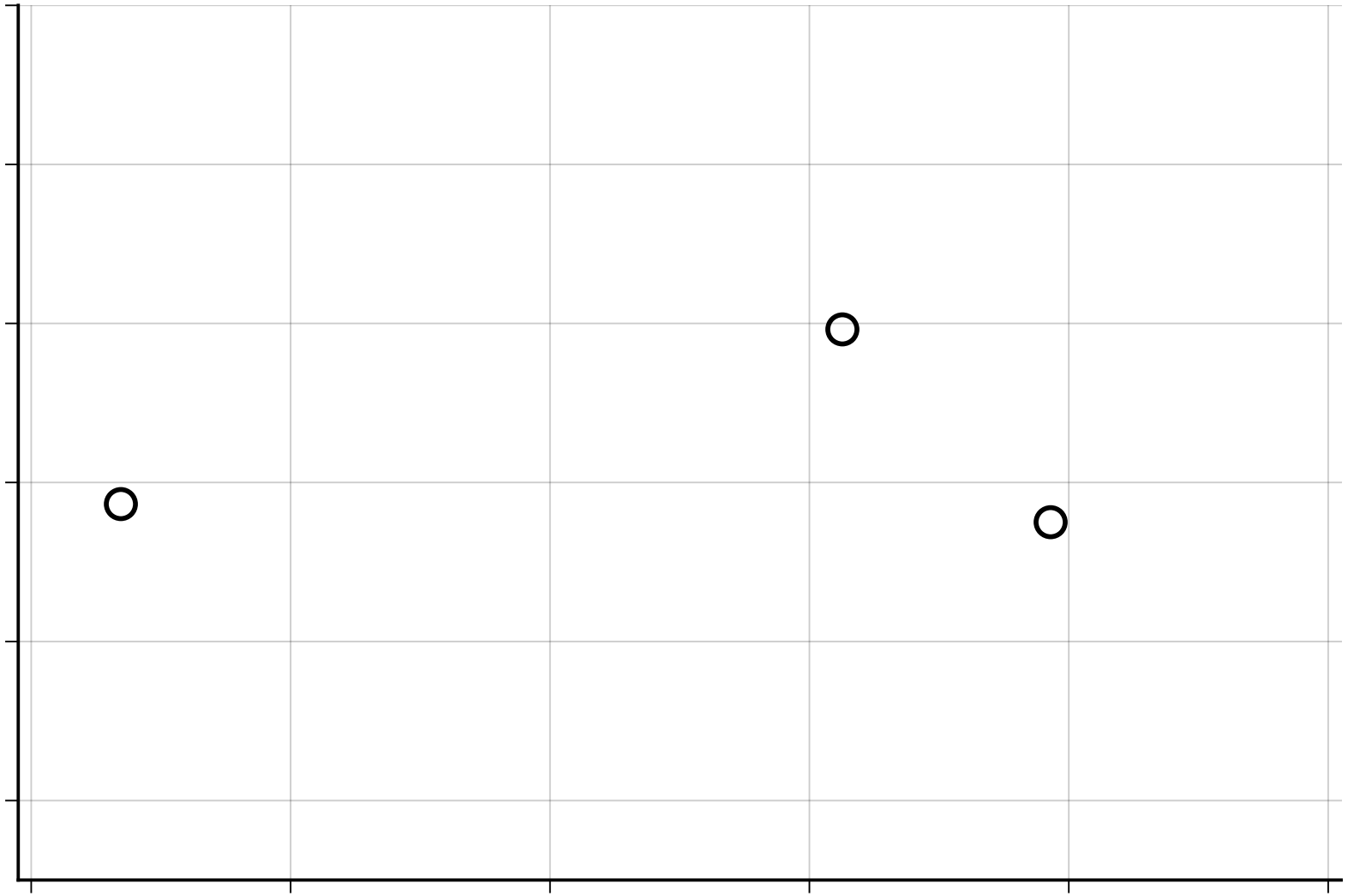
# Motivation: Regression Problems



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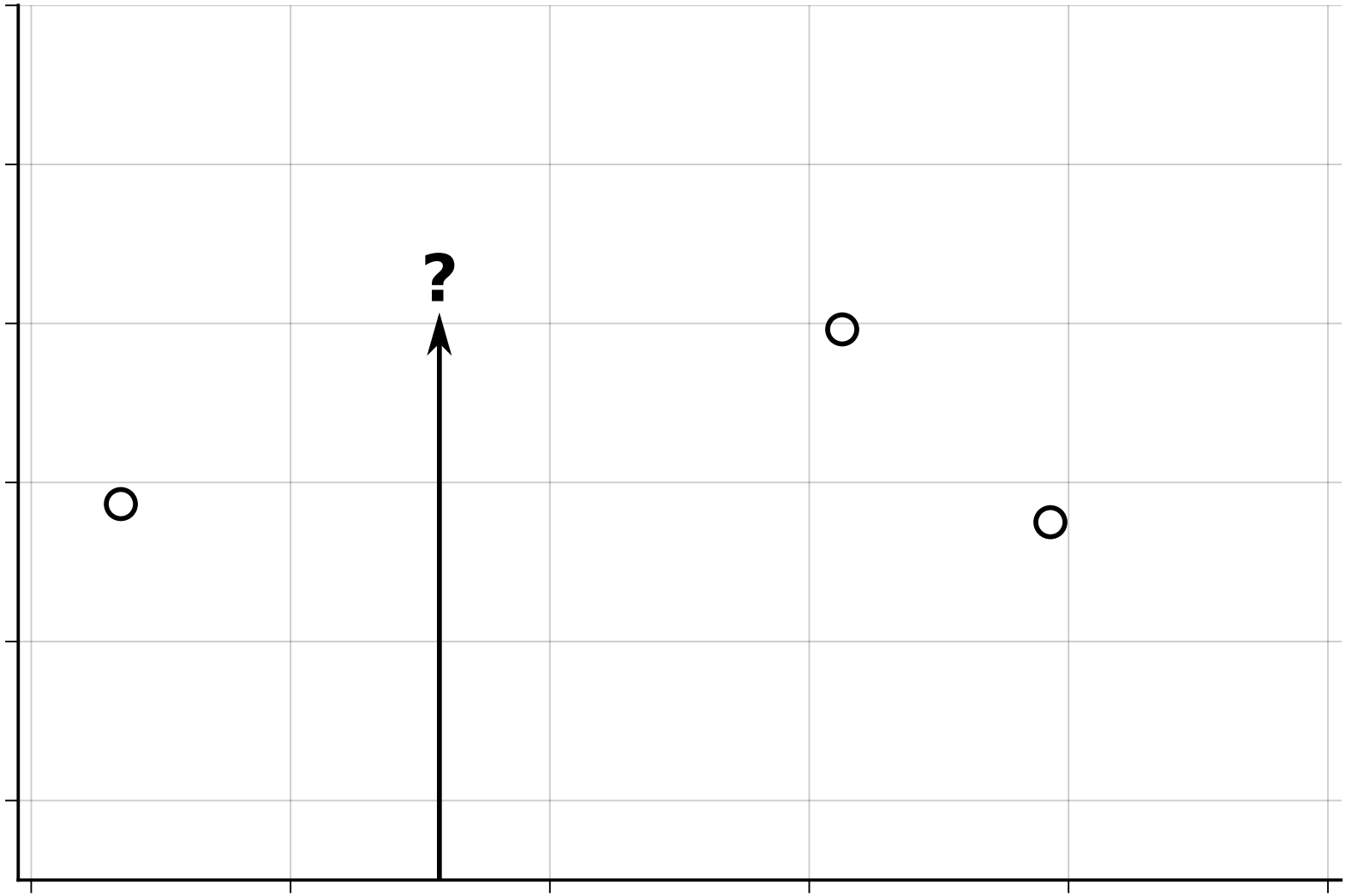

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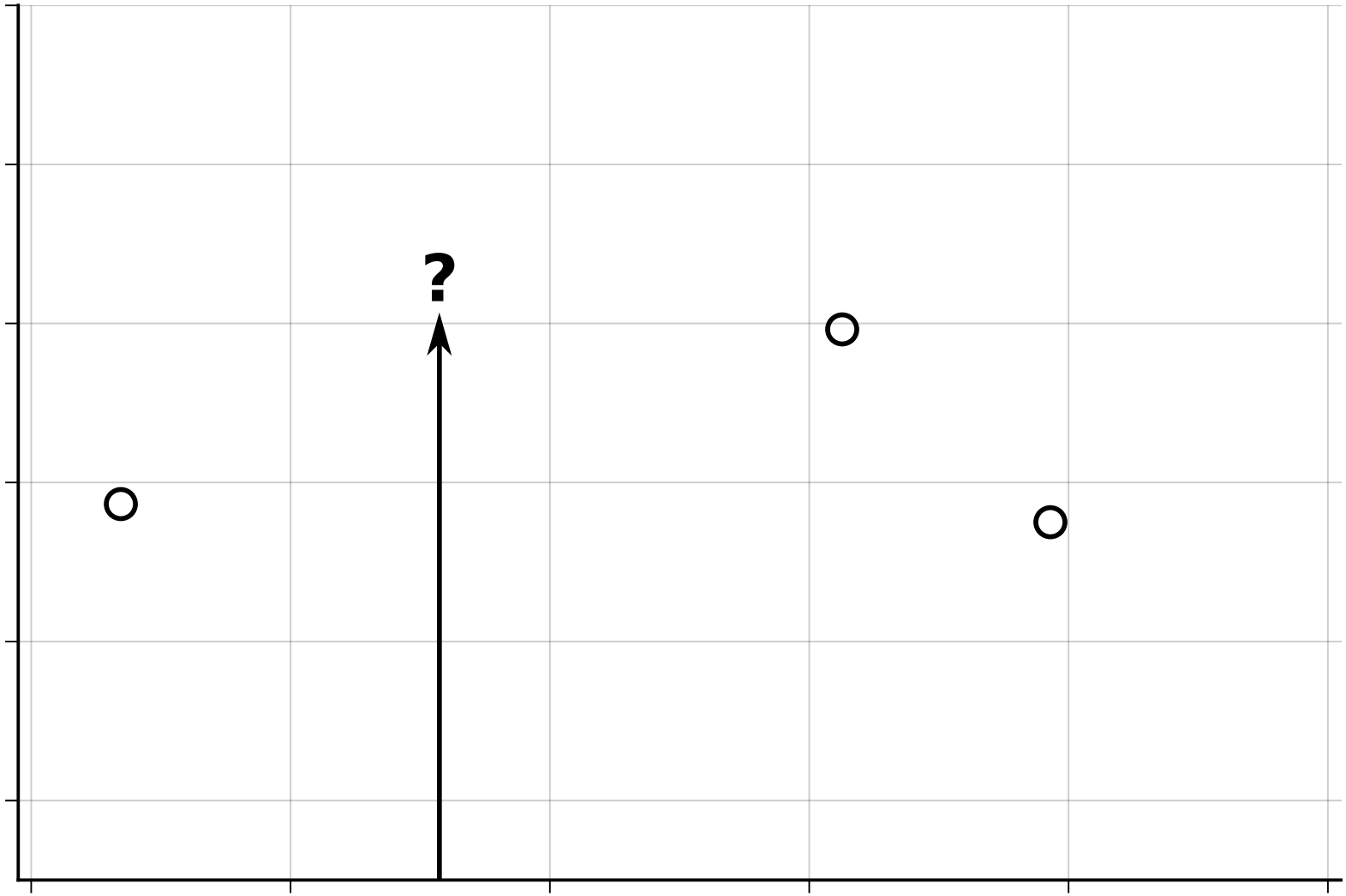


**We have to specify a model that may depend on parameters w.**

# 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 **y** under the model.

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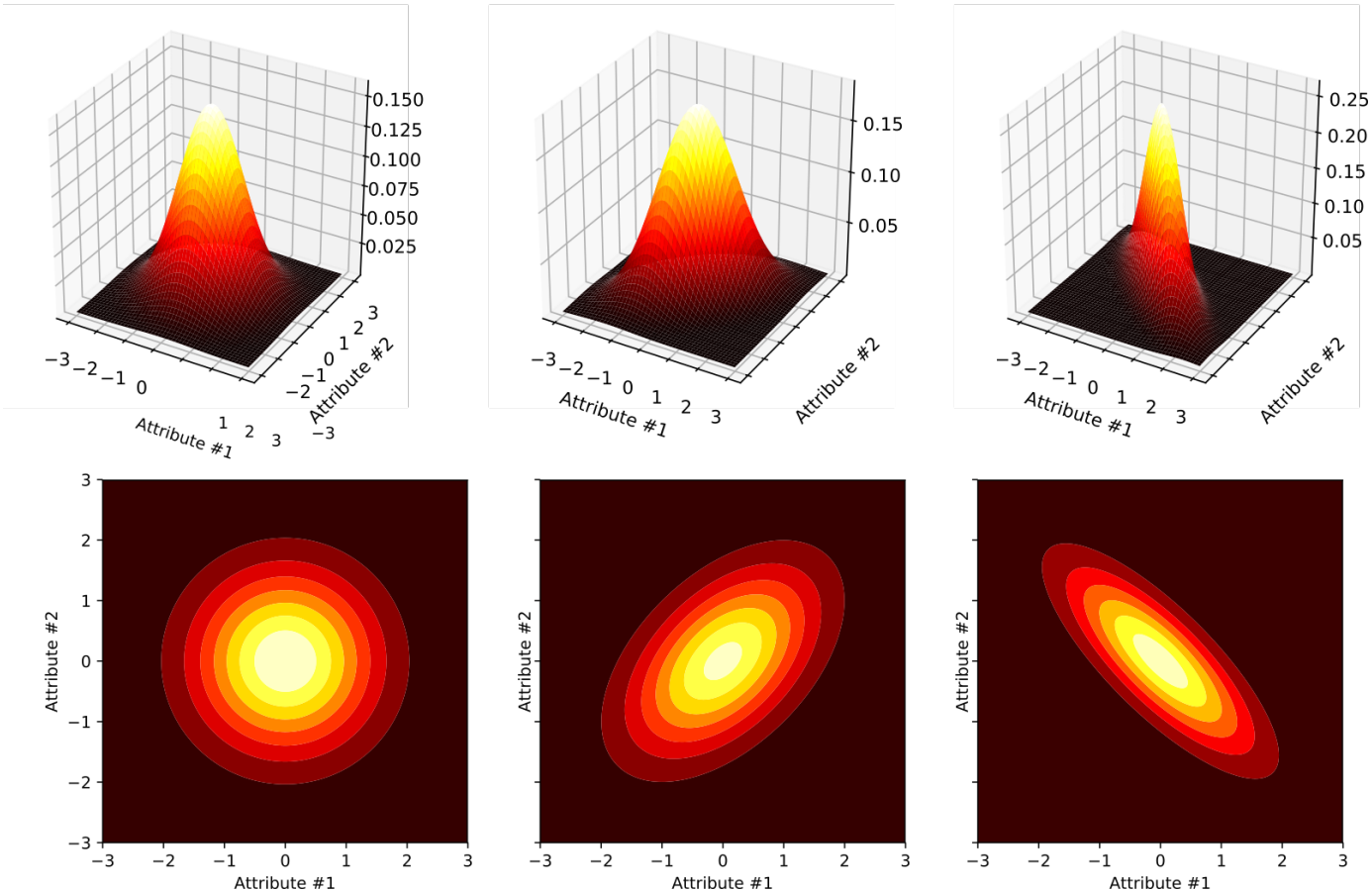
Prior: We consider an **isometric Gaussian prior** $\mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{I})$.

# Multivariate Gaussian Distribution

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

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



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(Bishop, 2006)

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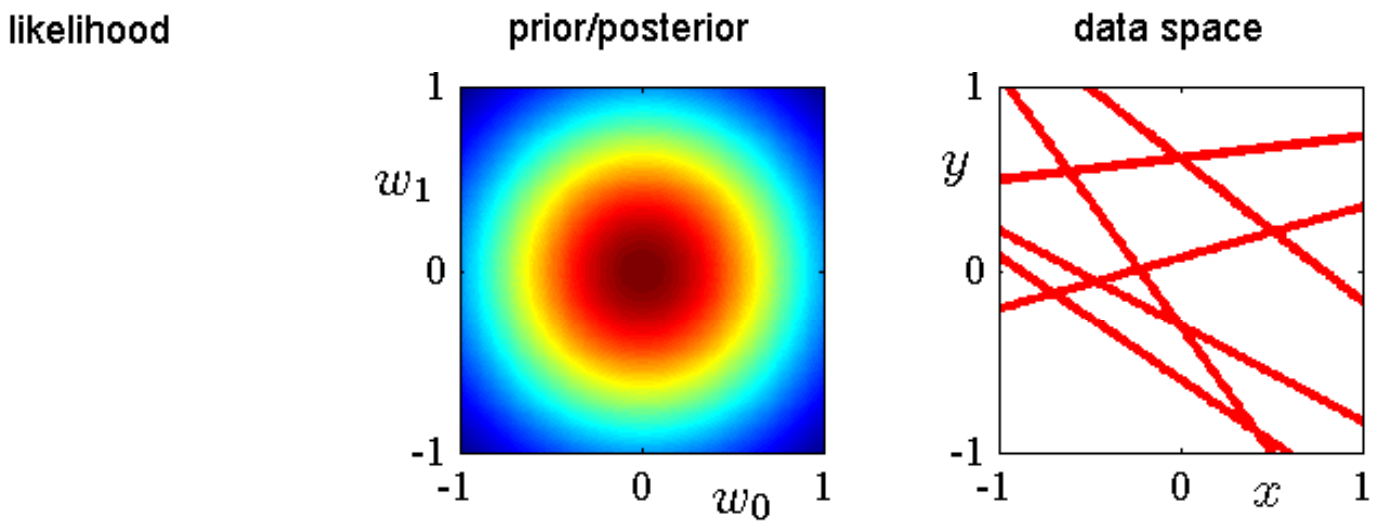


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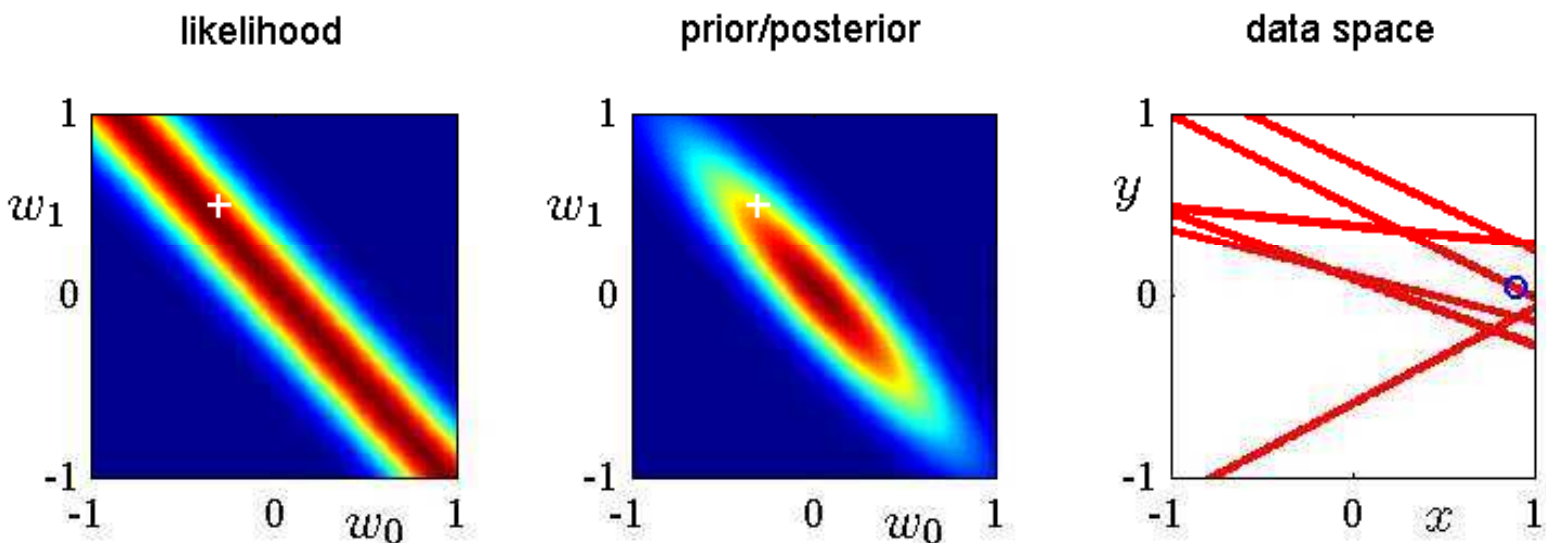


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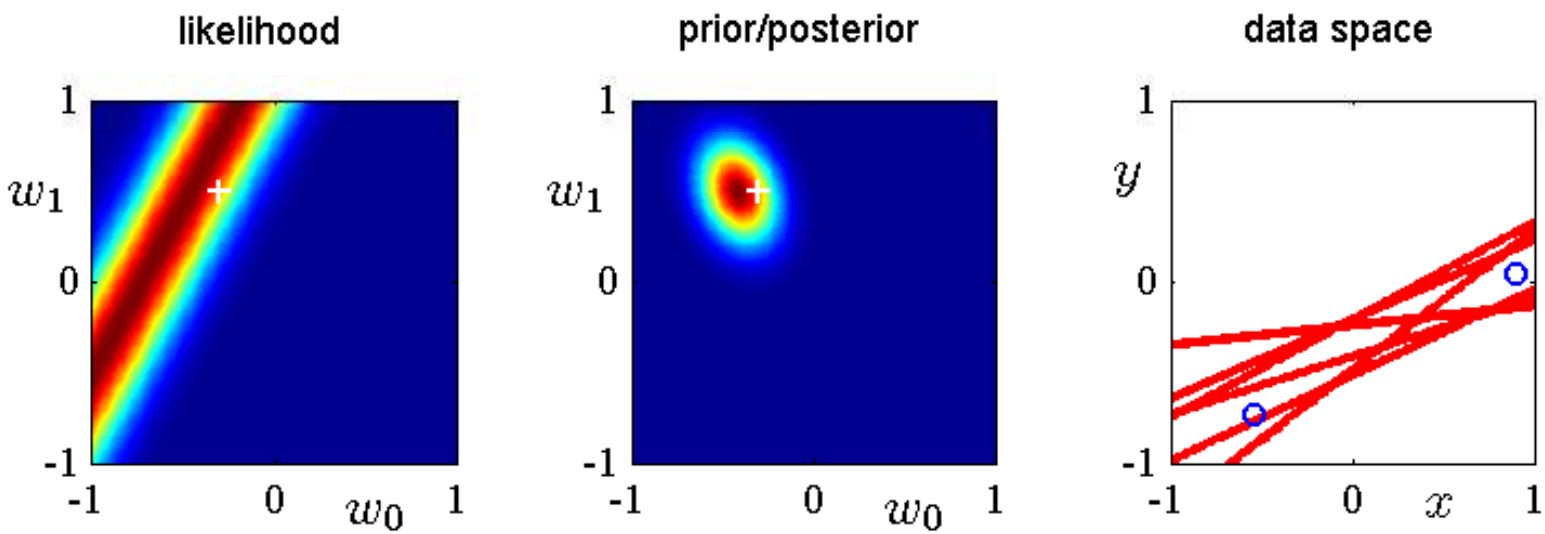


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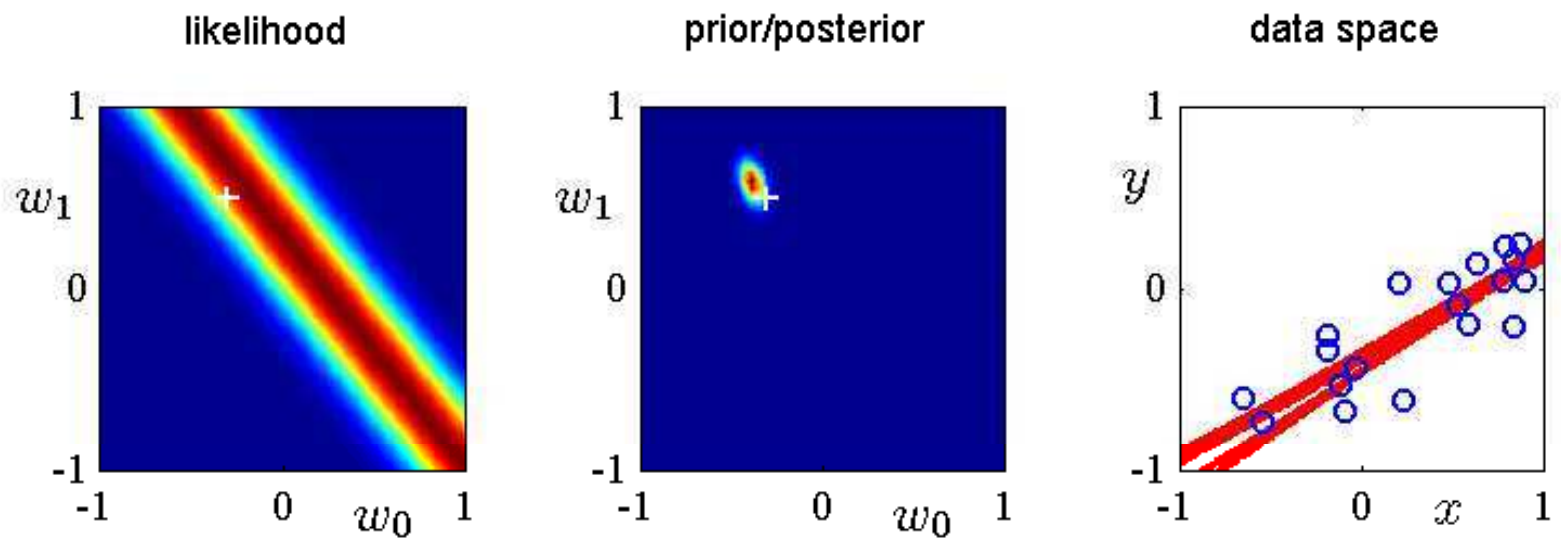


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The predictive distribution is obtained by marginalizing $\mathbf{w}$:

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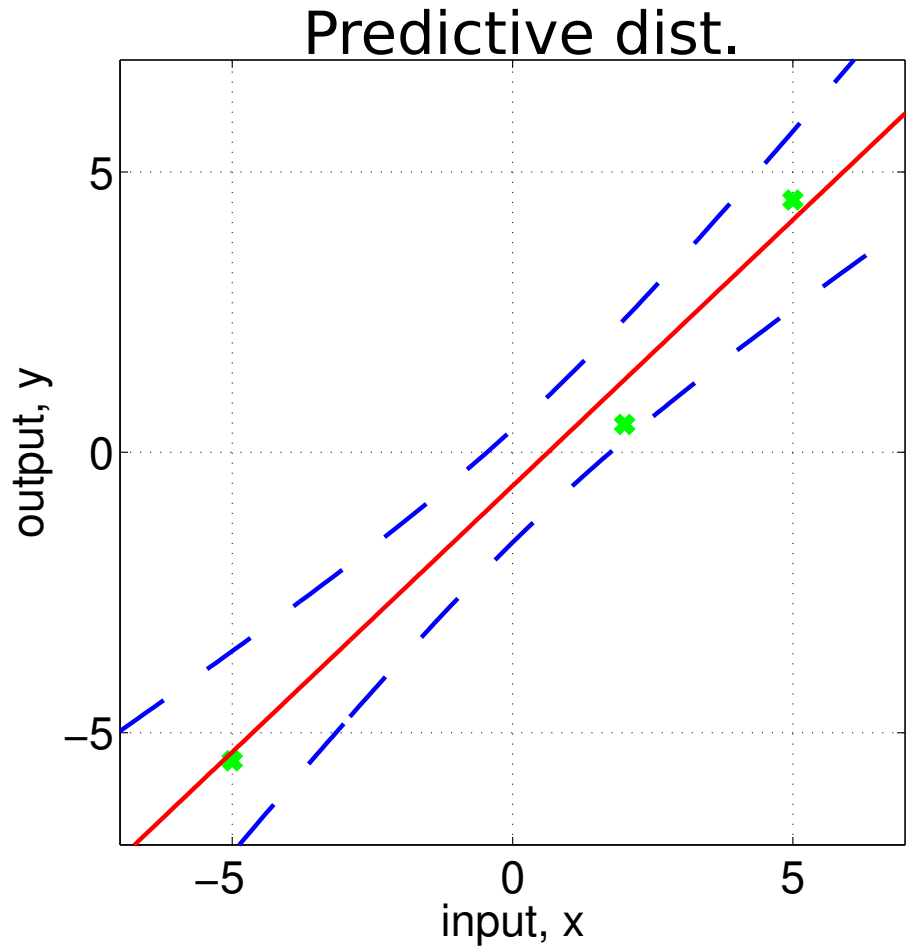


(Rasmussen & Williams, 2006)

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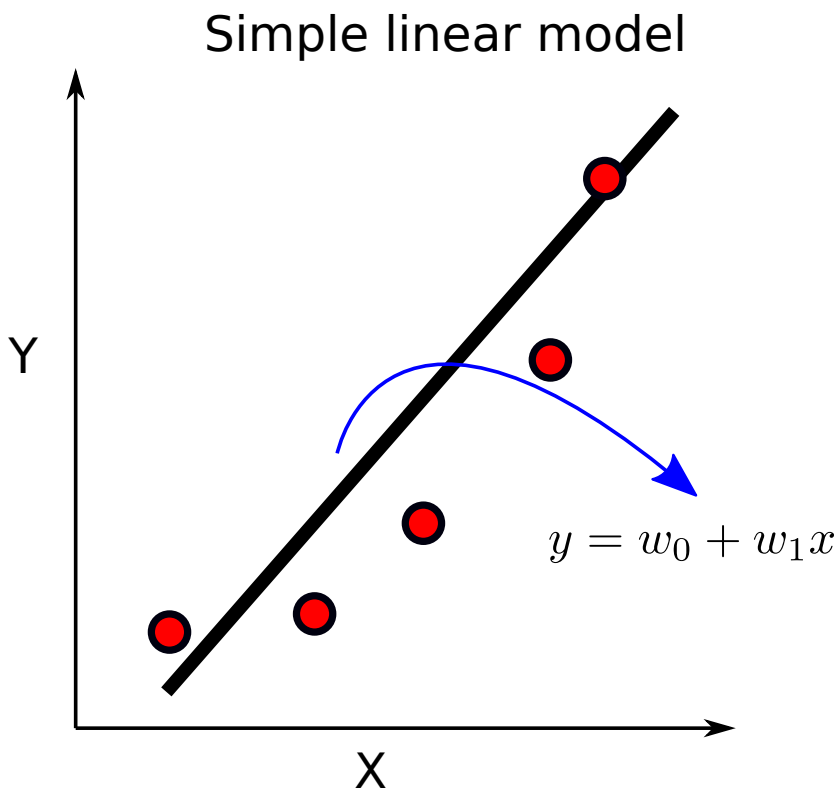


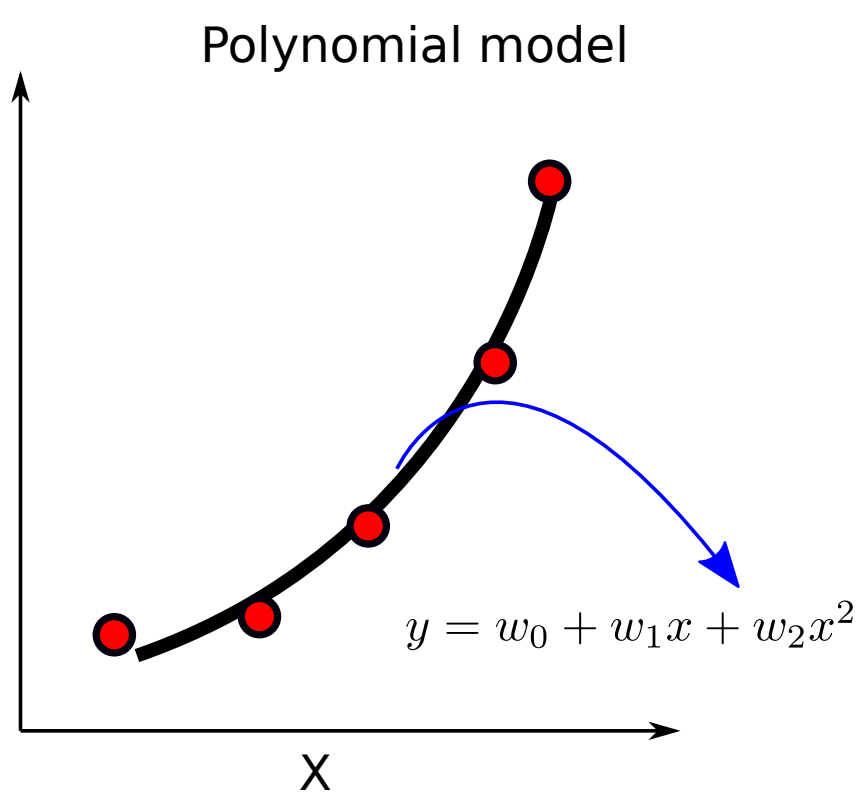

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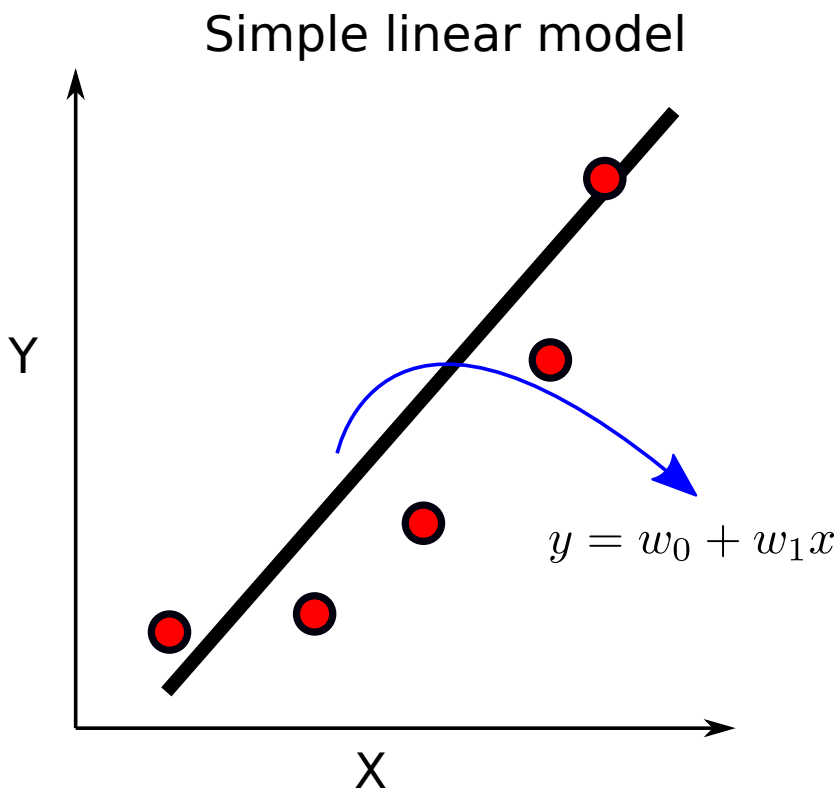


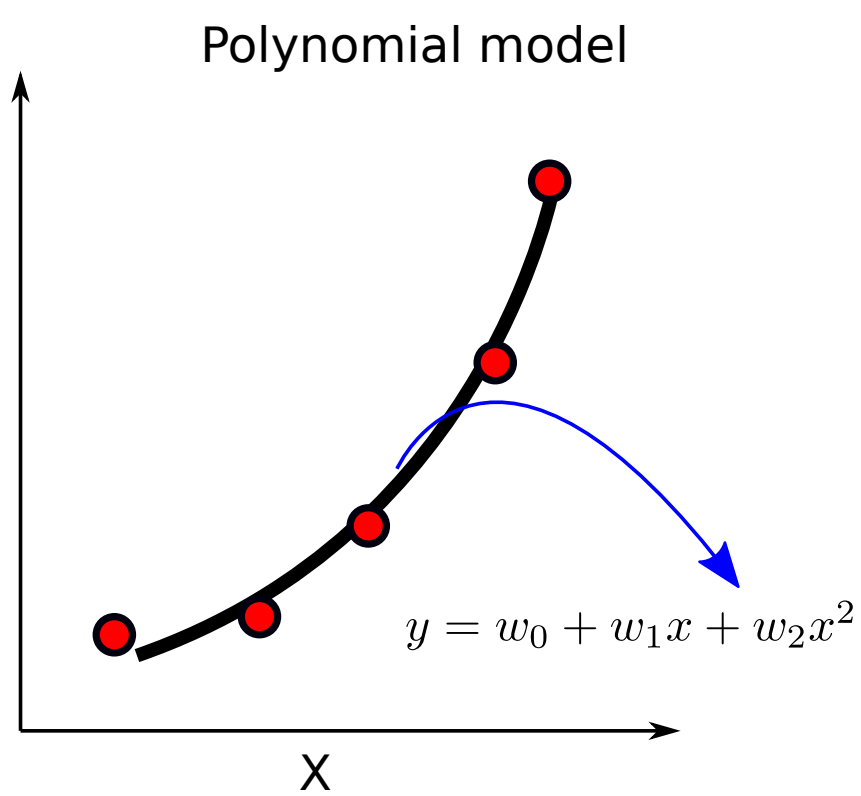


**Any other non-linear feature expansion is possible!**

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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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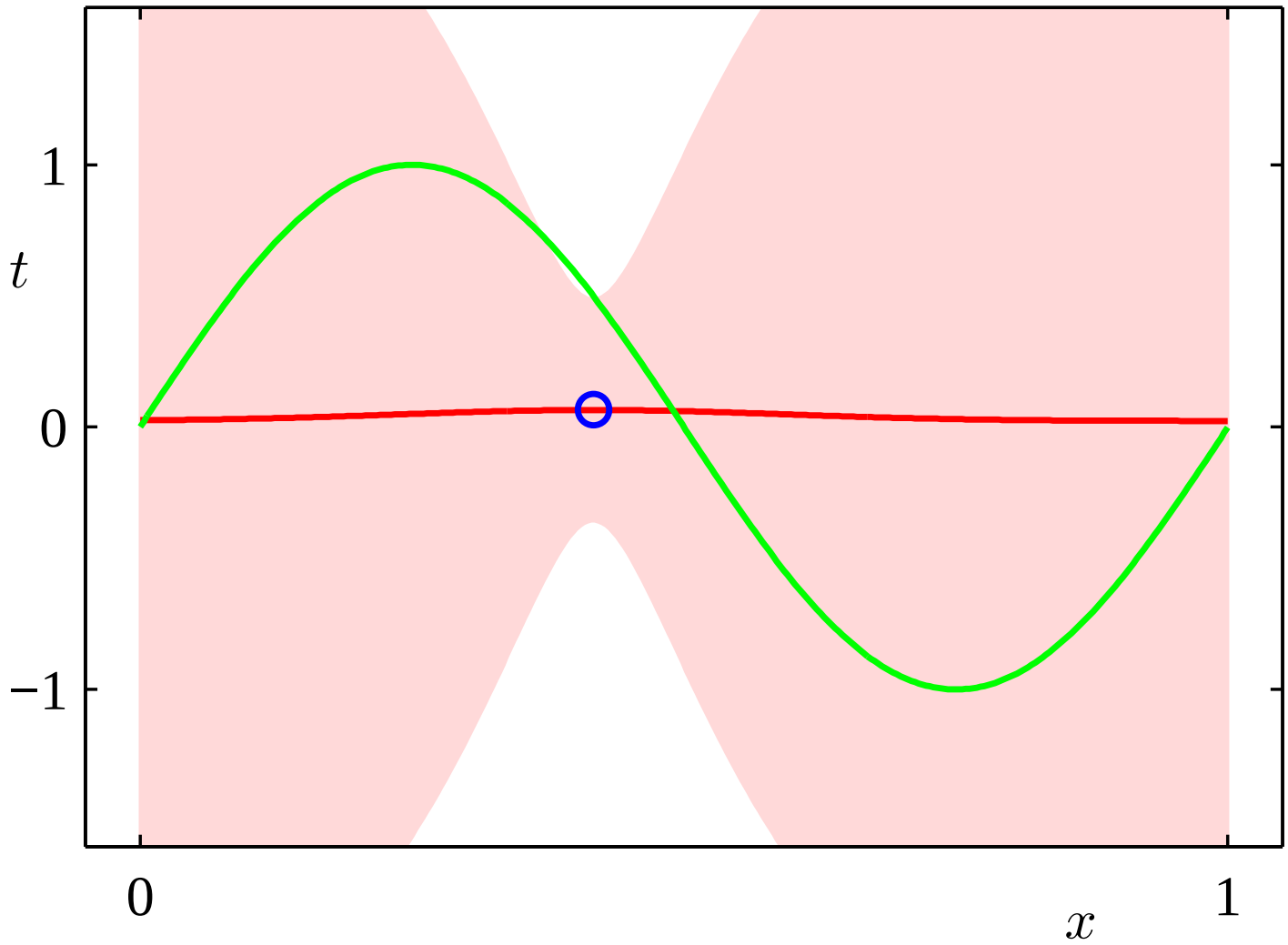


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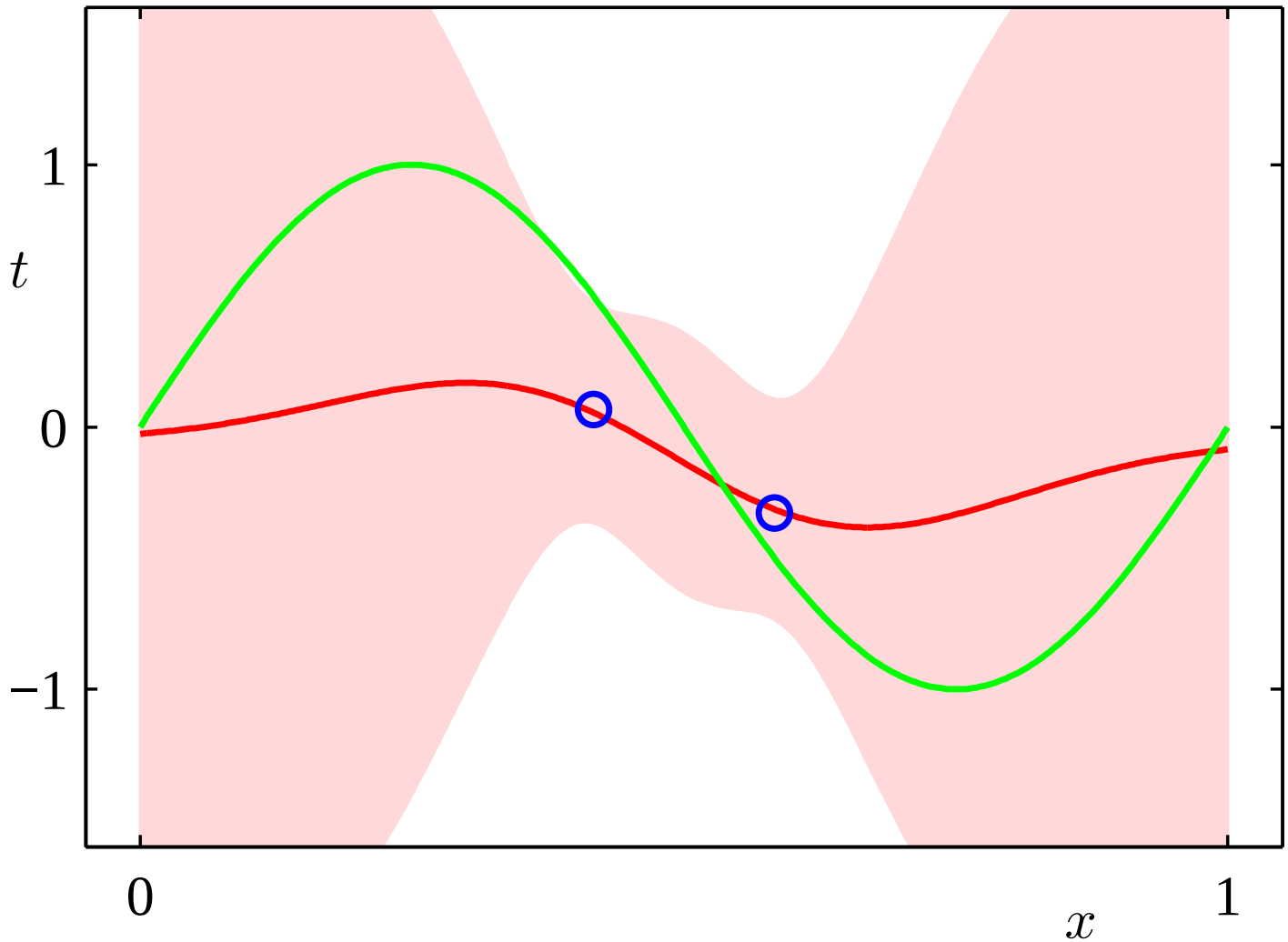


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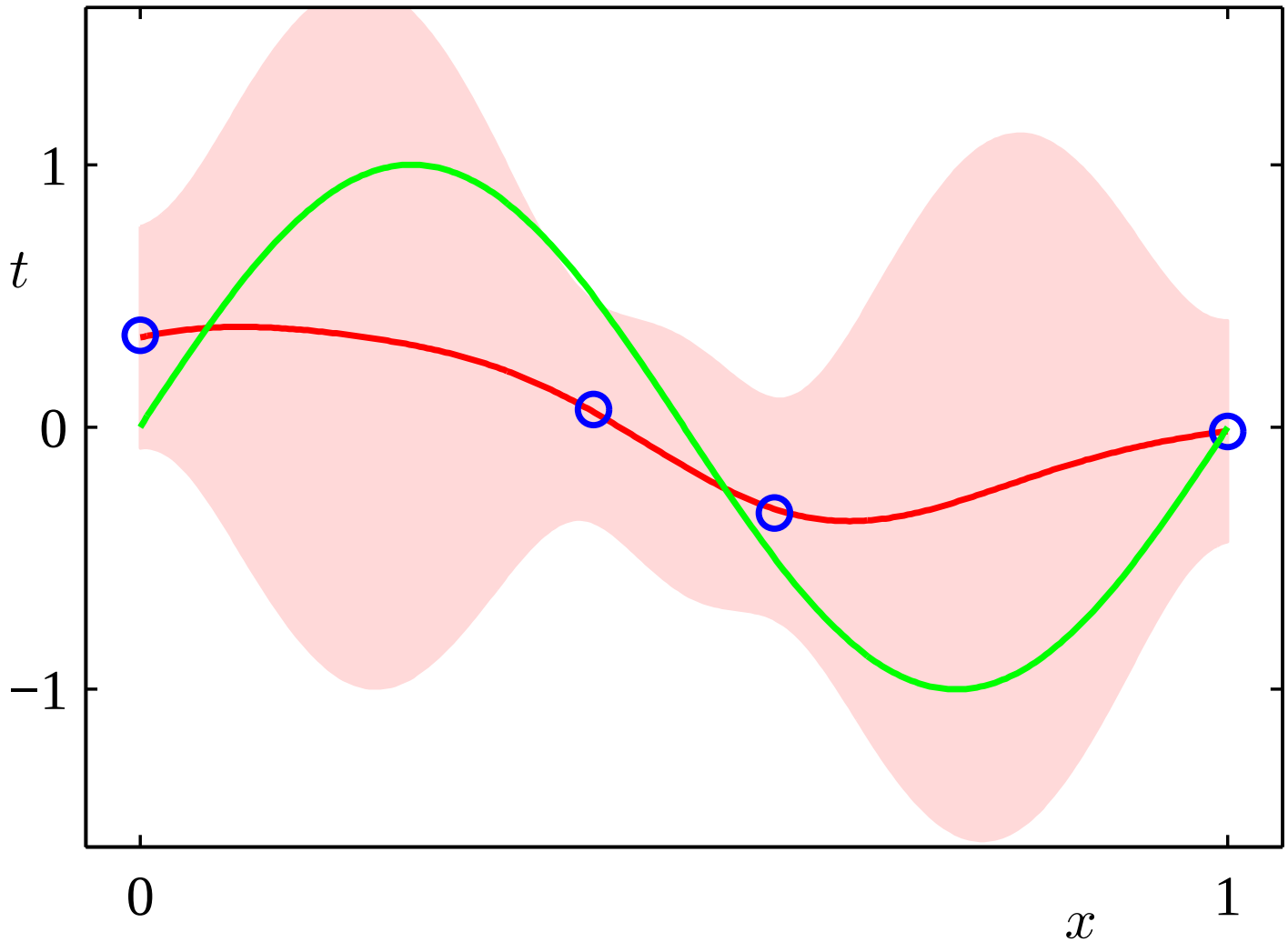


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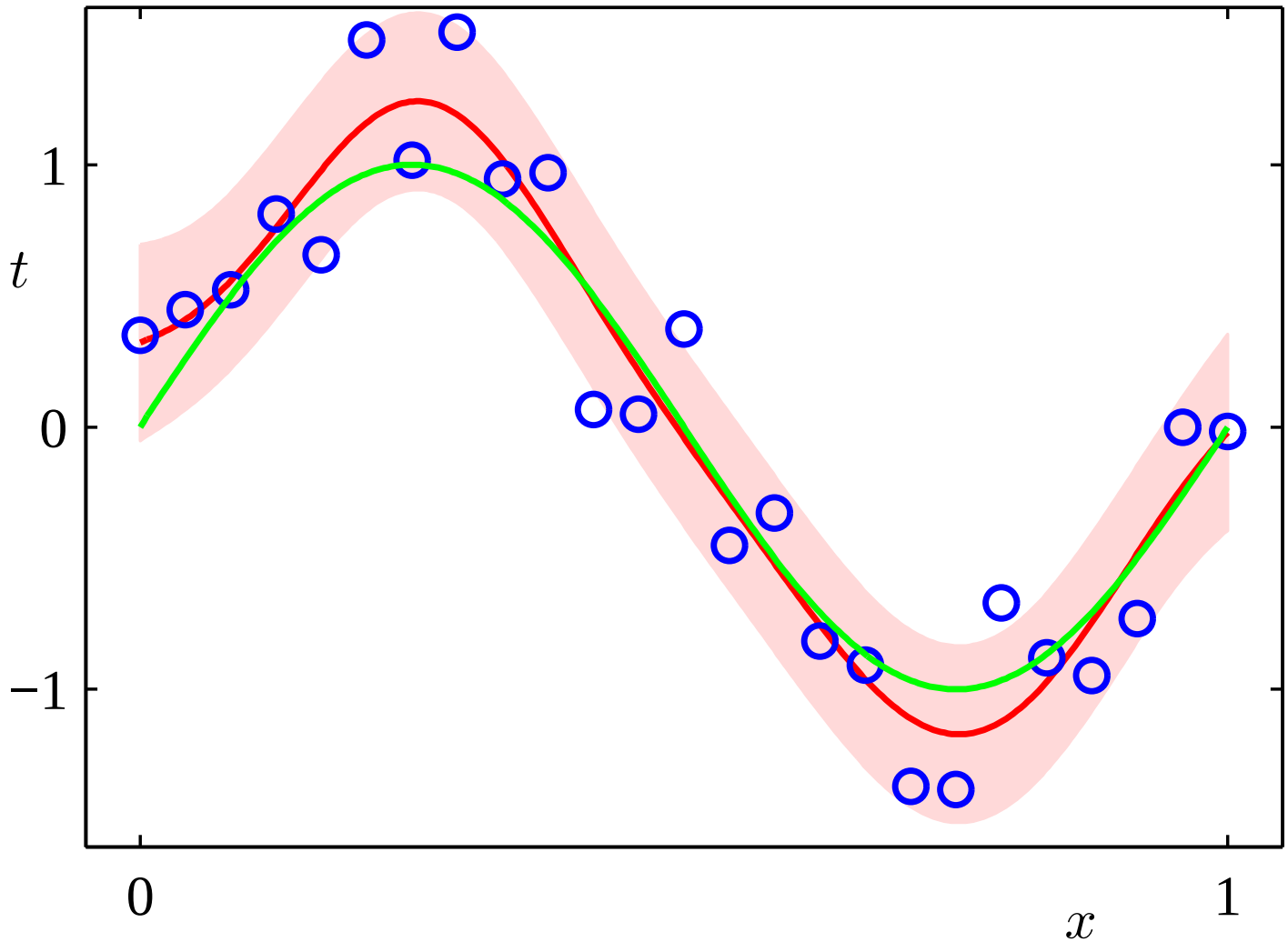


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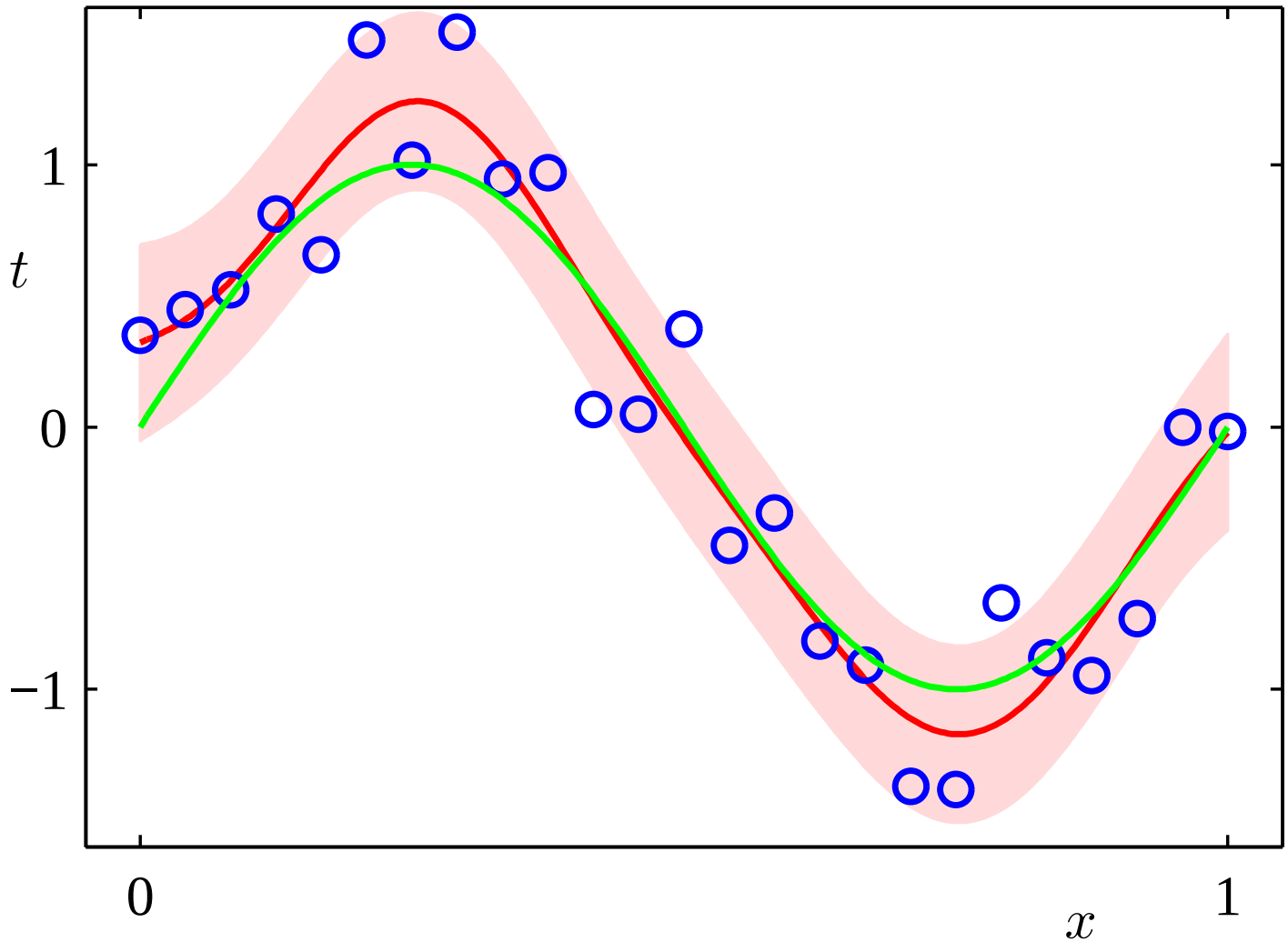


**The predictive distribution tells us what our model does not know!**

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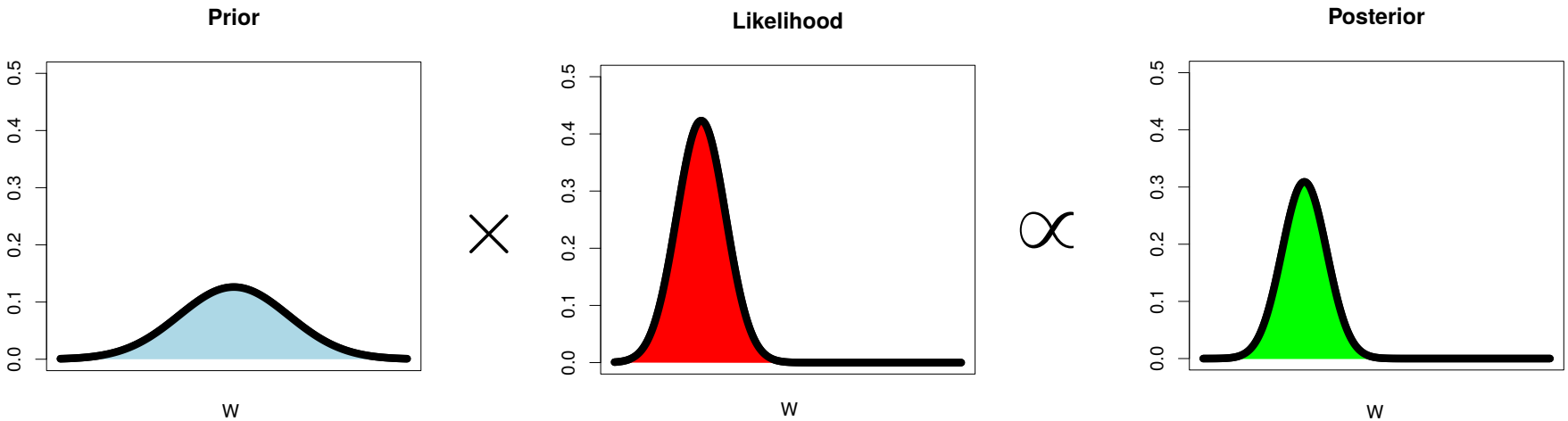

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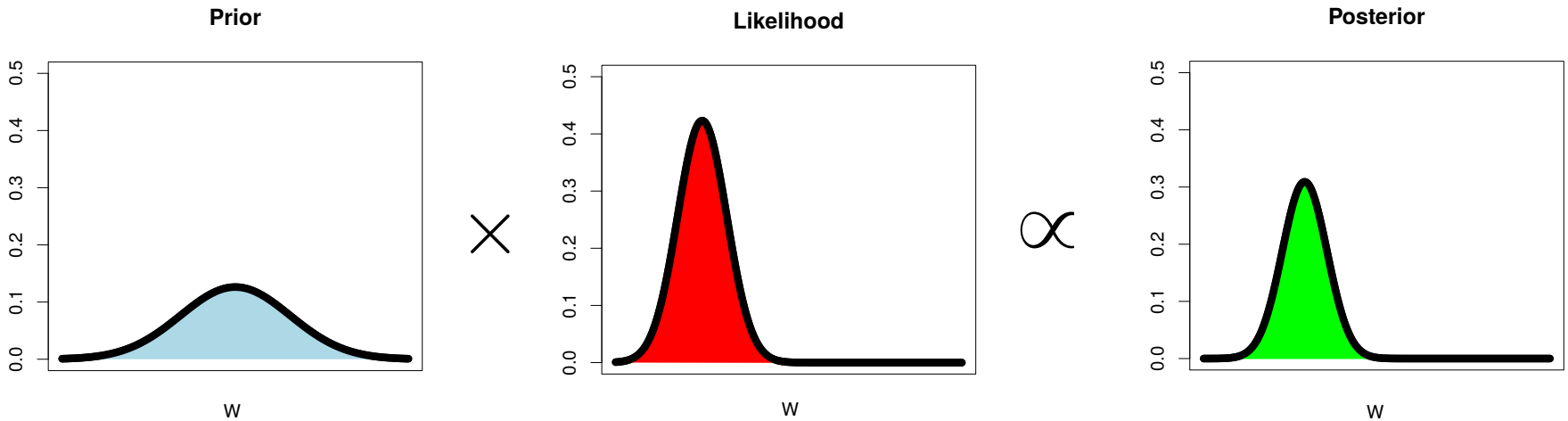


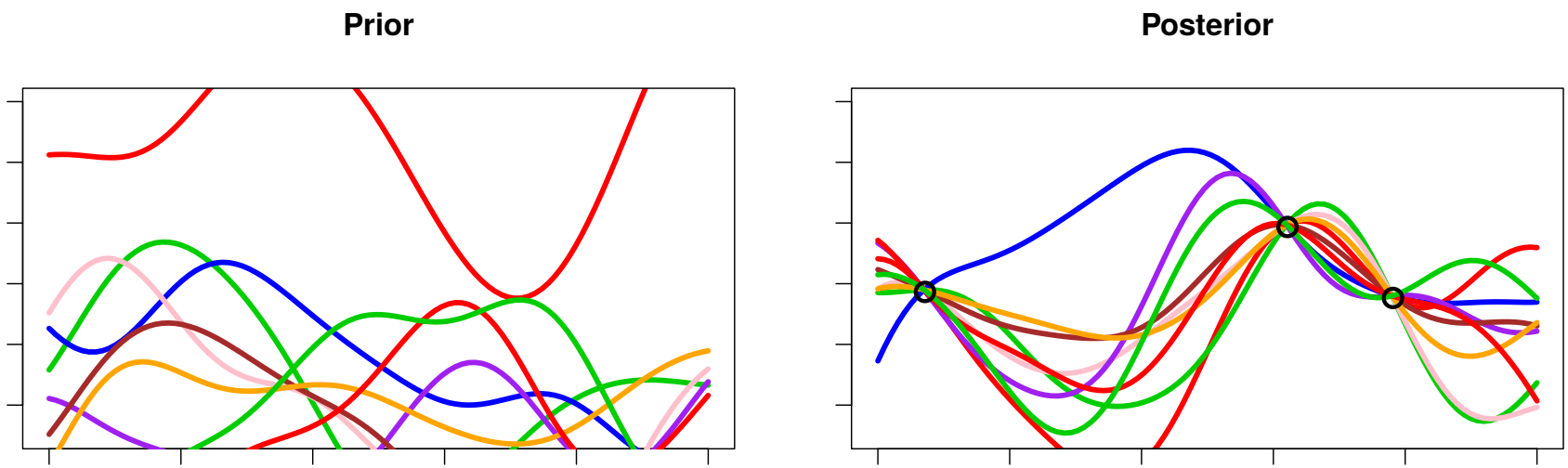

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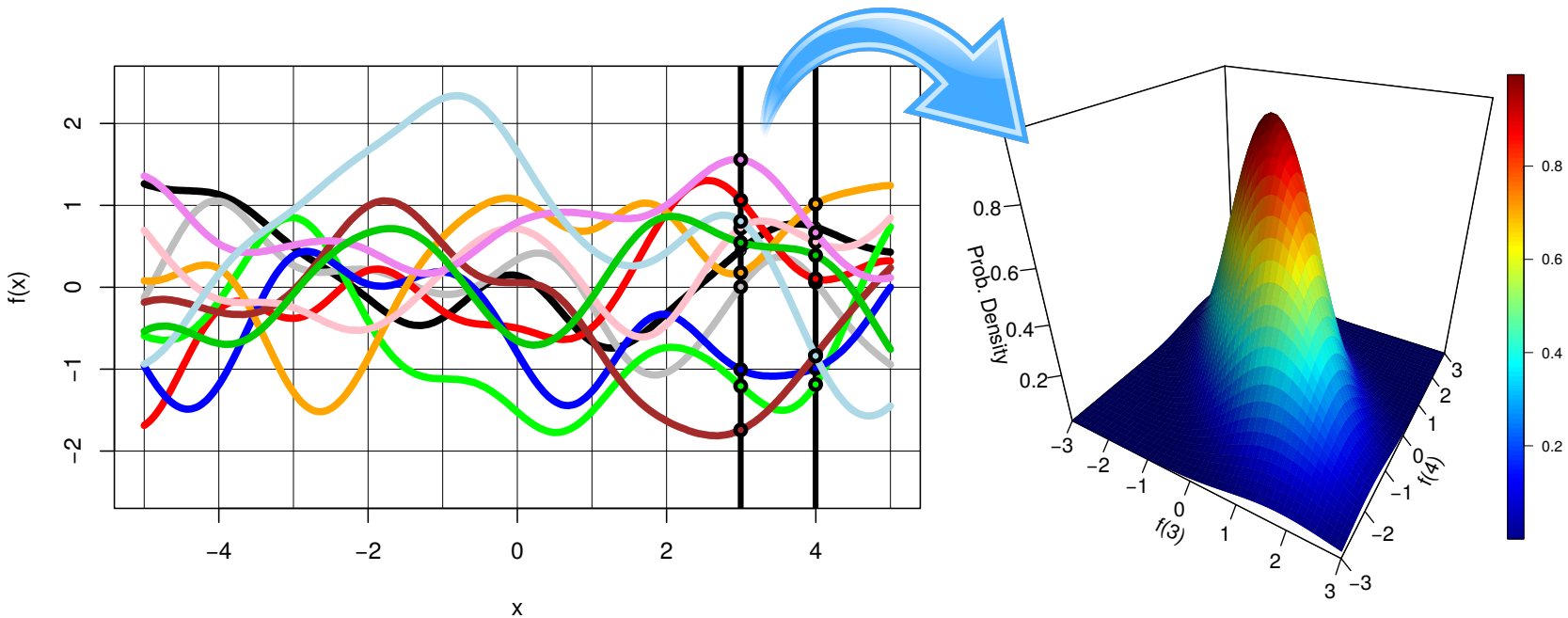

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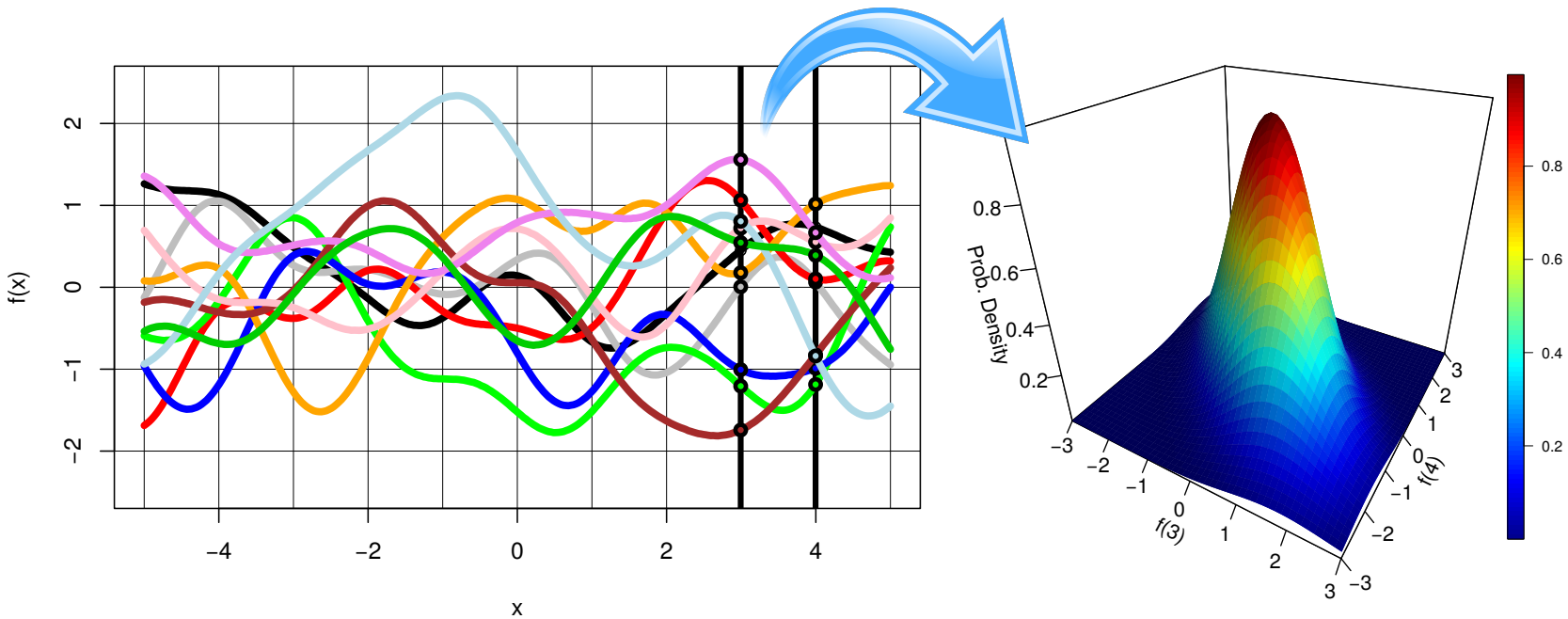


Straight-forward for the prior and posterior. Since the they are Gaussian for $\mathbf{w}$, $f$ is the sum of Gaussian random variables and is also Gaussian!

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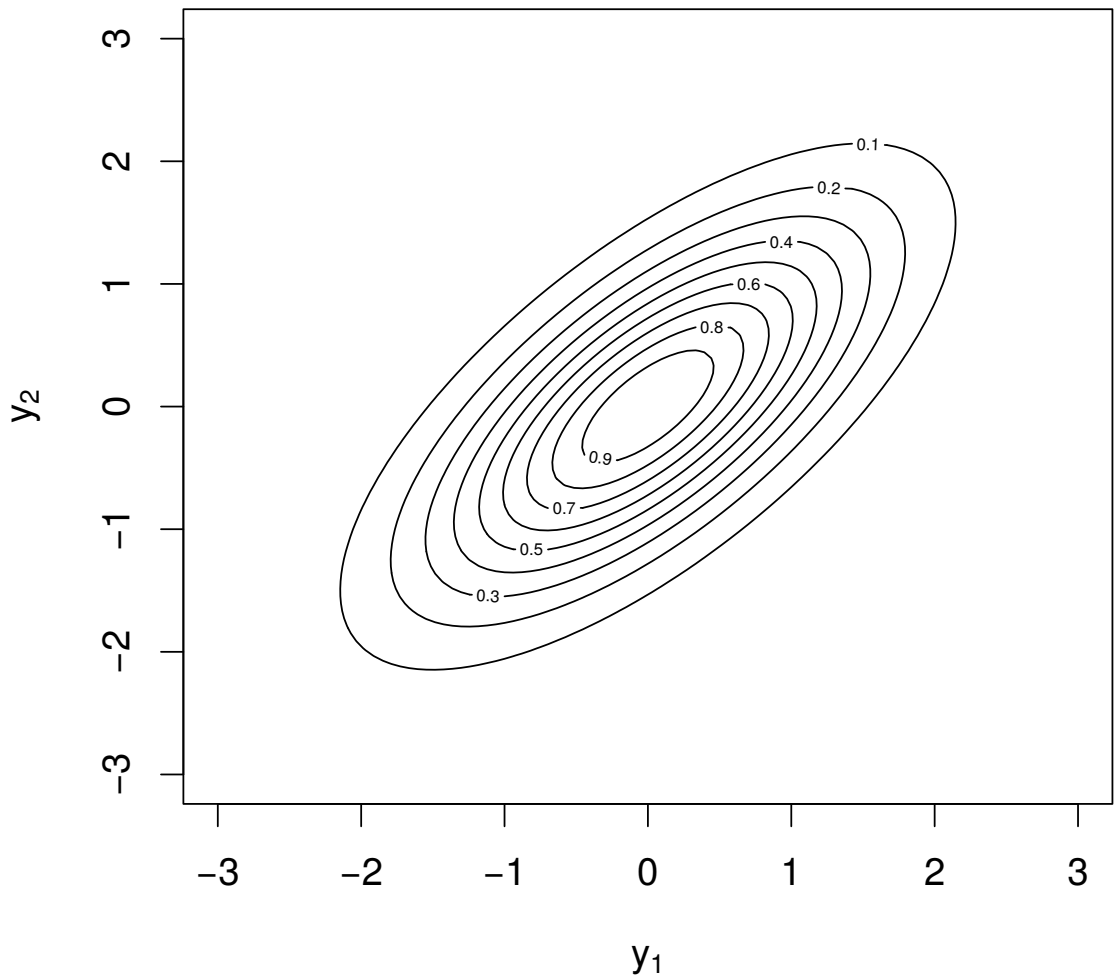
4. This results in a non-parametric model that becomes more flexible as more data is observed!

# Gaussian Distribution

$$p(\mathbf{y}|\boldsymbol{\Sigma}) \propto \exp\left\{-0.5\mathbf{y}^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}\mathbf{y}\right\}$$

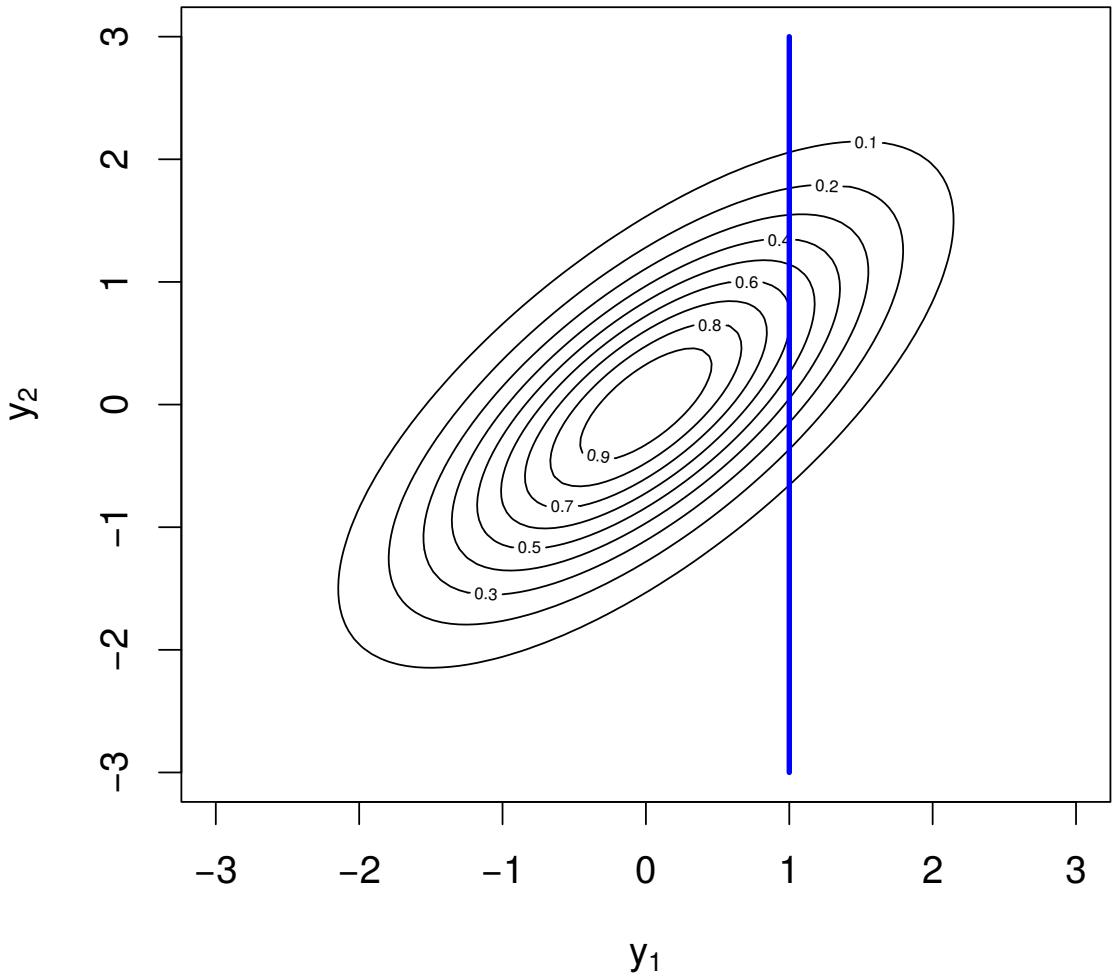
$$\boldsymbol{\Sigma} = \begin{bmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{bmatrix}.$$



# Gaussian Distribution

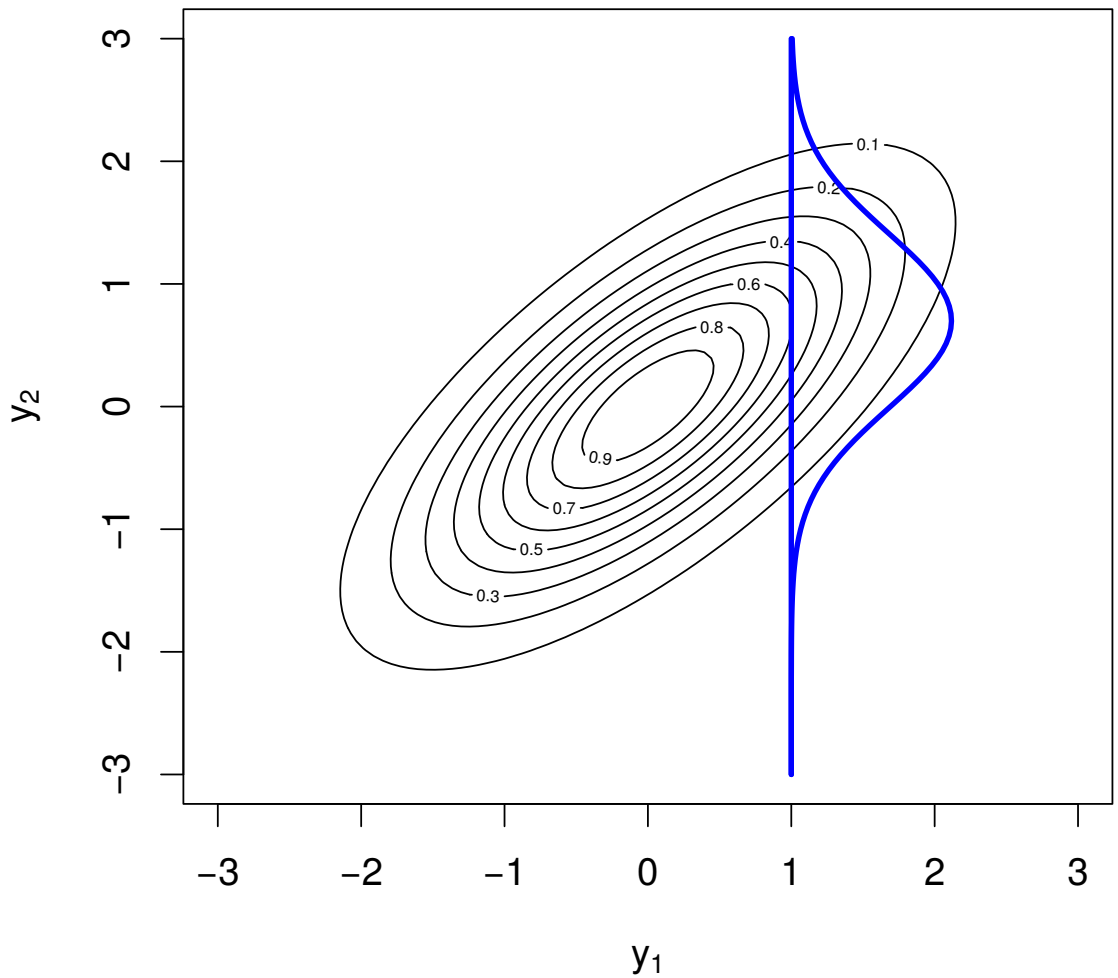
$$p(\mathbf{y}|\boldsymbol{\Sigma}) \propto \exp\left\{-0.5\mathbf{y}^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}\mathbf{y}\right\}$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{bmatrix}.$$



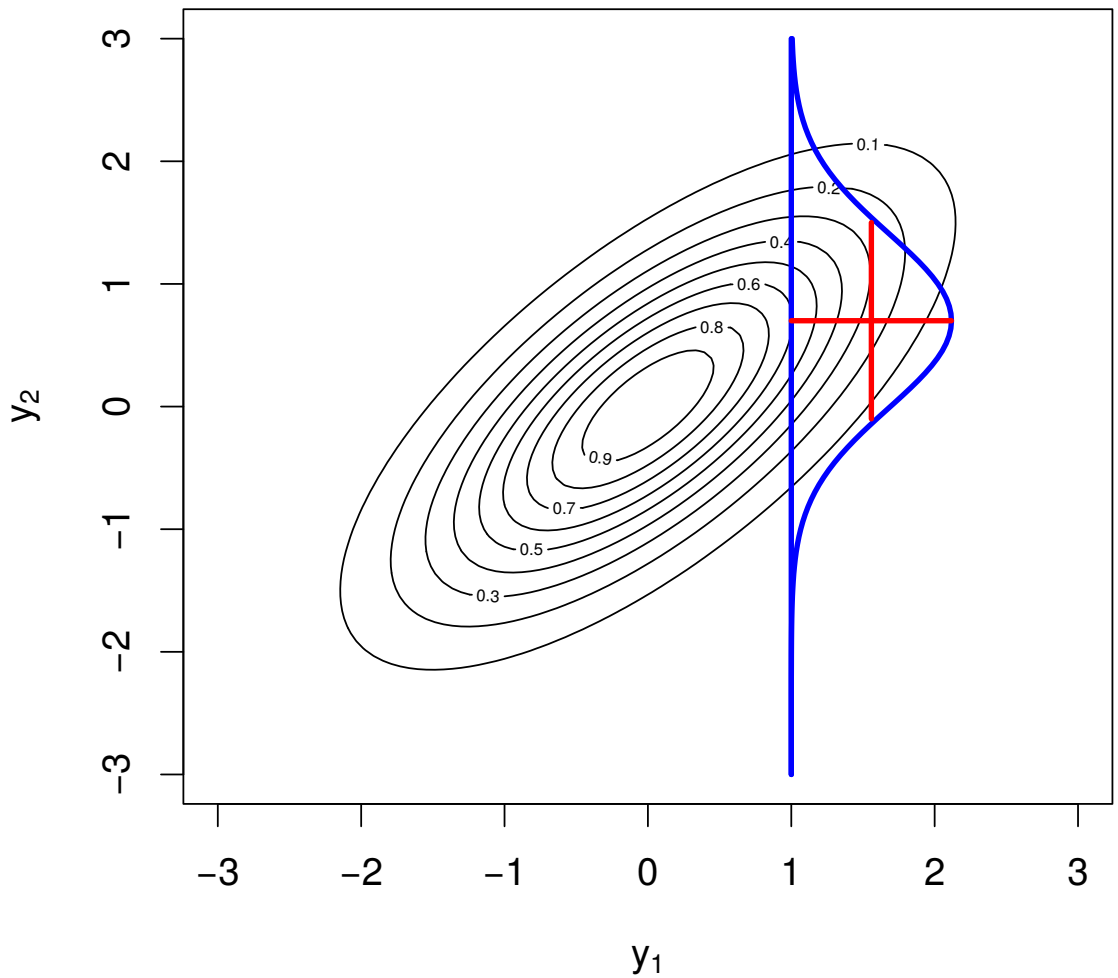
# Gaussian Distribution

$$p(y_2|y_1, \boldsymbol{\Sigma}) \propto \exp\left\{-0.5(y_2 - \mu_\star)\Sigma_\star^{-1}(y_2 - \mu_\star)\right\} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{bmatrix}.$$



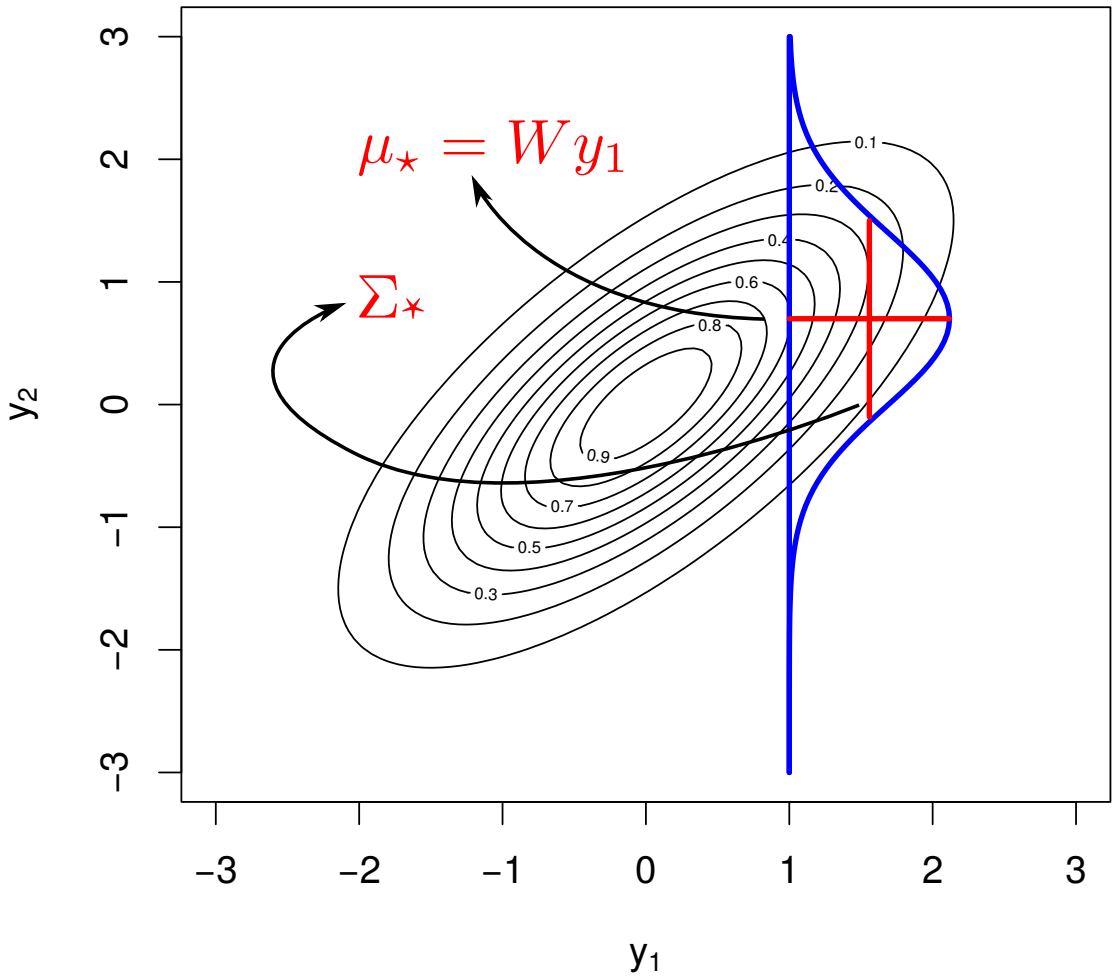
# Gaussian Distribution

$$p(y_2|y_1, \Sigma) \propto \exp\left\{-0.5(y_2 - \mu_\star)\Sigma_\star^{-1}(y_2 - \mu_\star)\right\} \qquad \Sigma = \begin{bmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{bmatrix}.$$

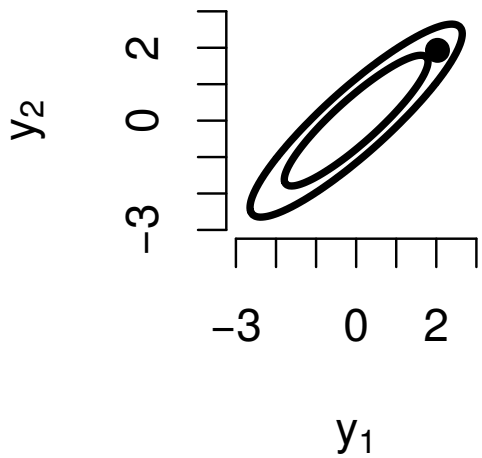


# Gaussian Distribution

$$p(y_2|y_1, \mathbf{\Sigma}) \propto \exp\left\{-0.5(y_2 - \mu_\star)\Sigma_\star^{-1}(y_2 - \mu_\star)\right\} \qquad \mathbf{\Sigma} = \begin{bmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{bmatrix}.$$

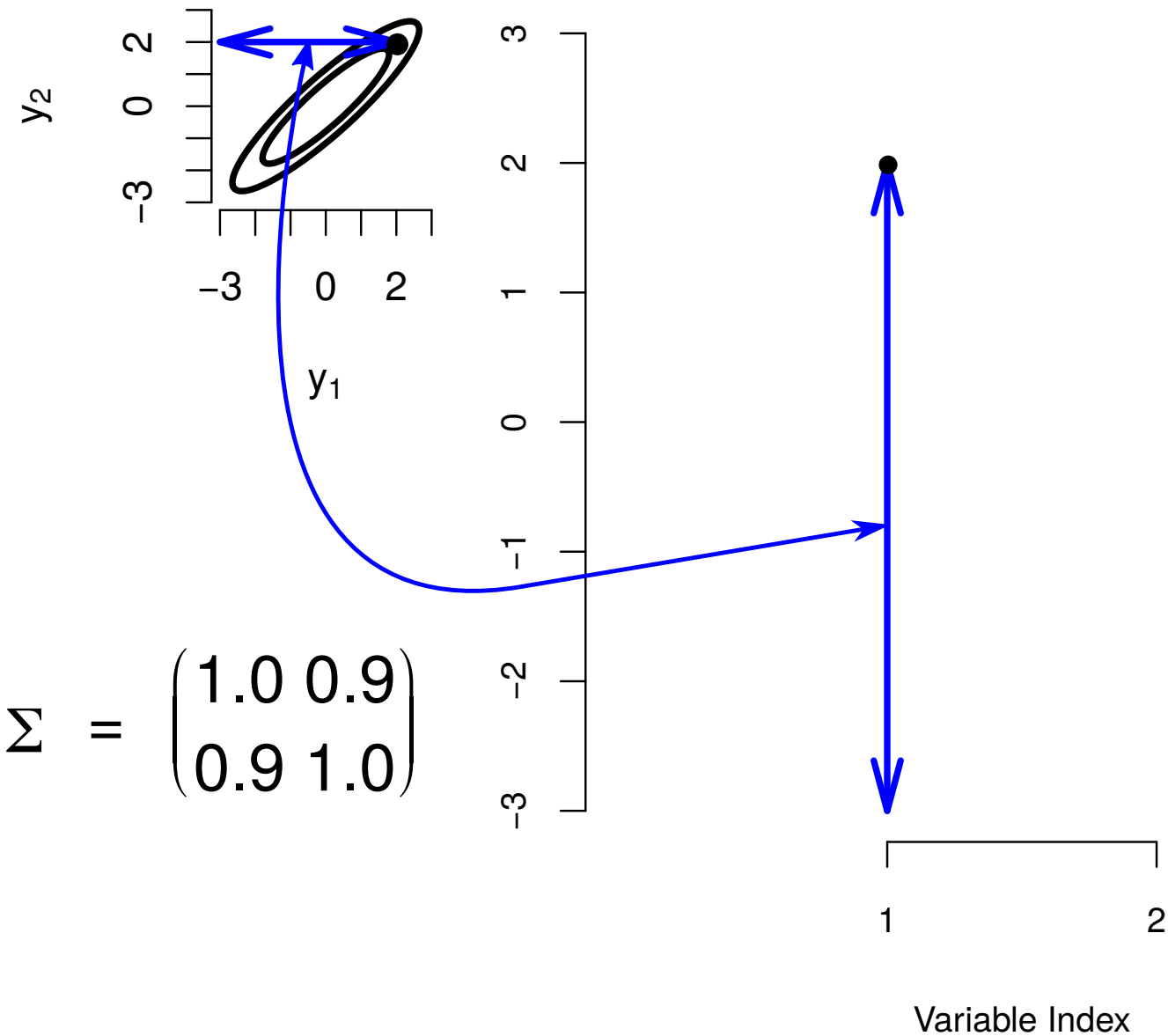


# Two Dimensional Example



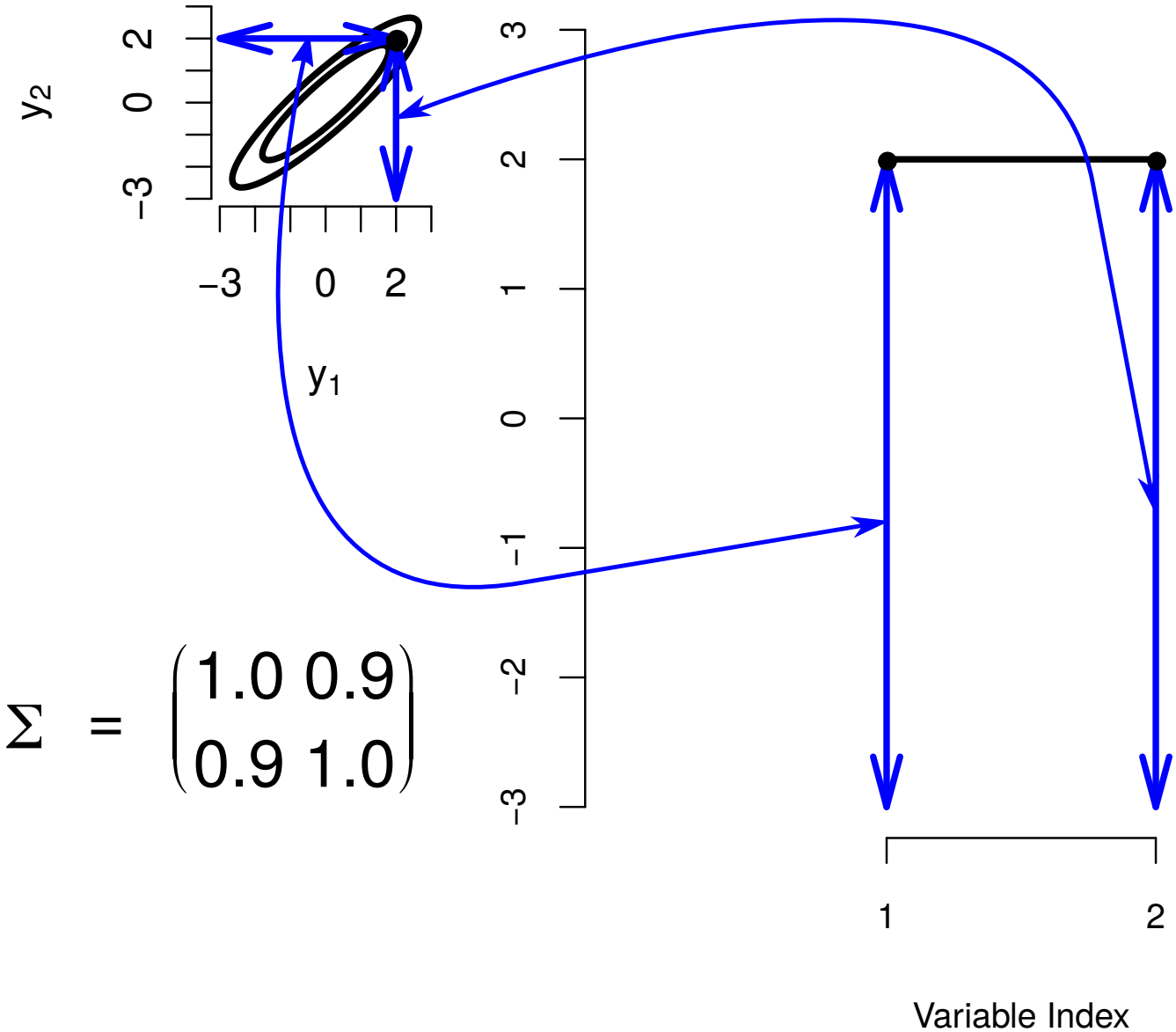

$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$

# Two Dimensional Example



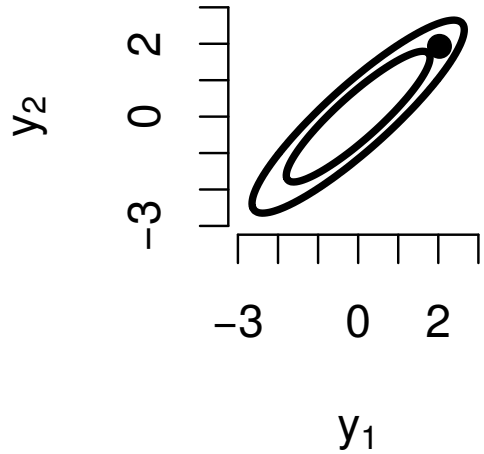

$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$

# Two Dimensional Example

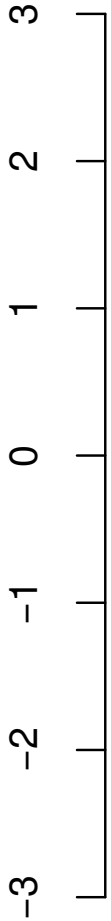



$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$

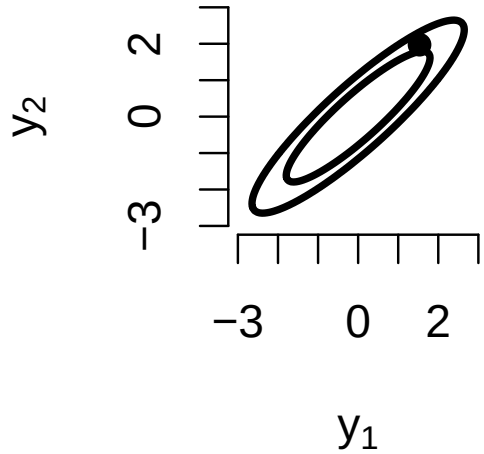
# Two Dimensional Example



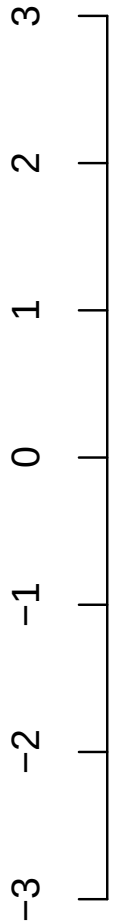

$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$



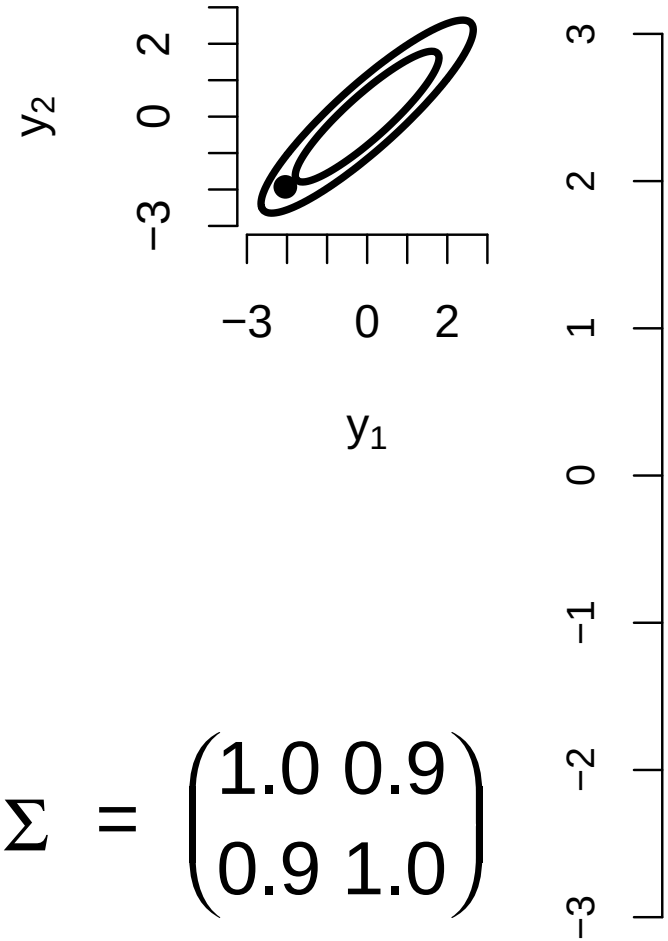

# Two Dimensional Example



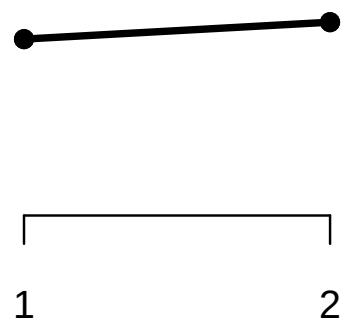

$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$



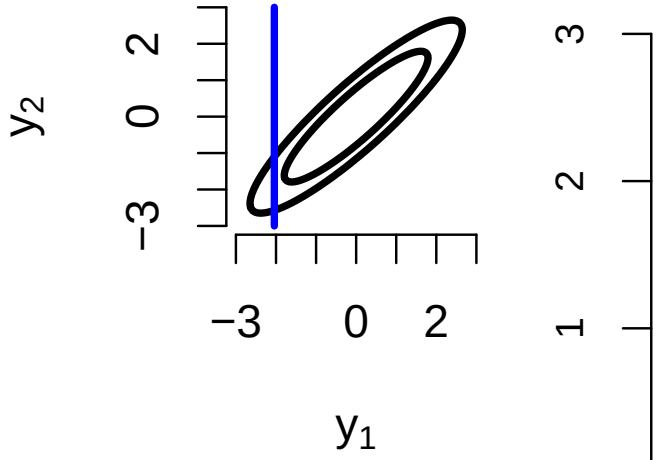

# Two Dimensional Example



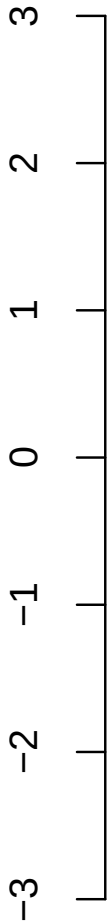

$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$

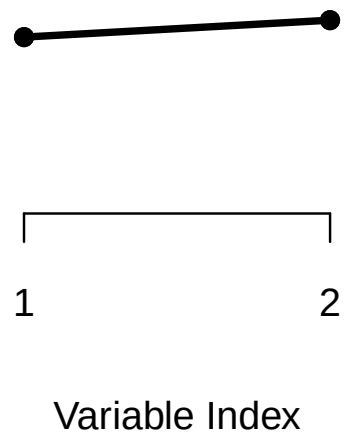


# Two Dimensional Example

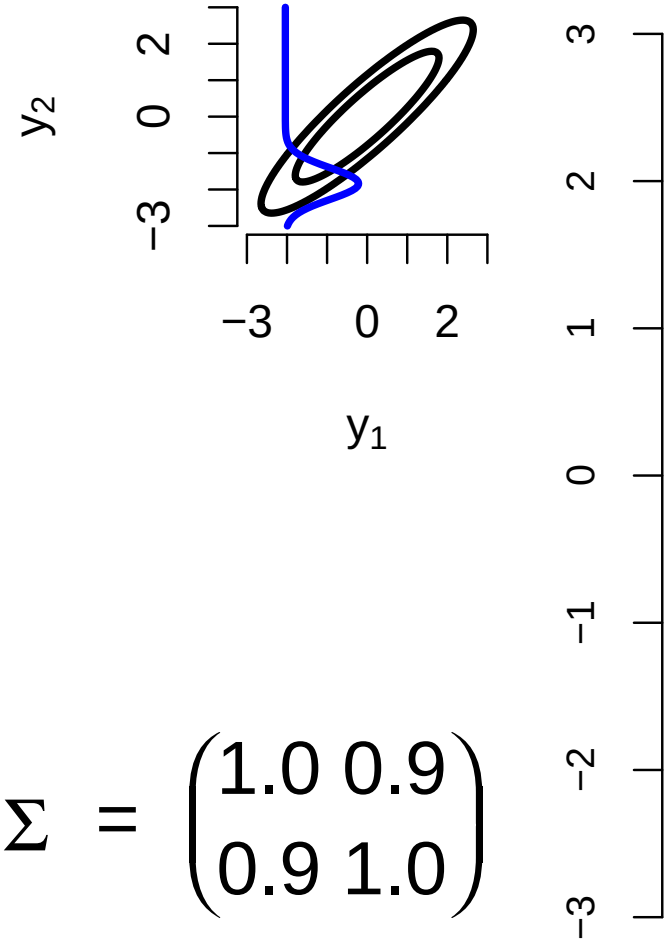



$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$

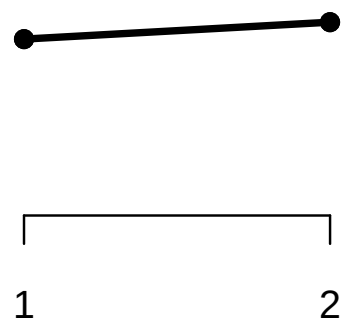


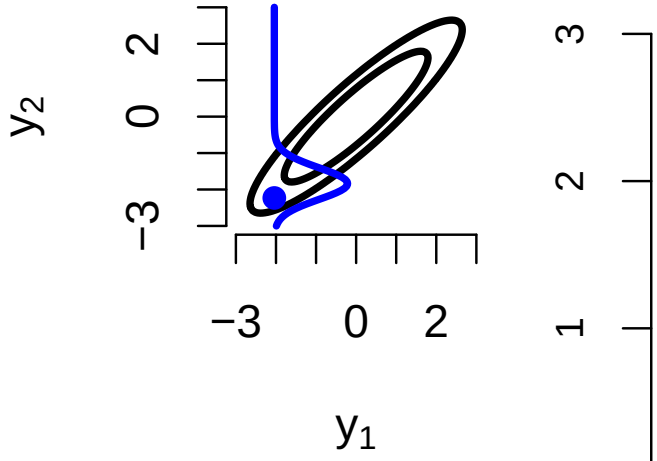
# Two Dimensional Example

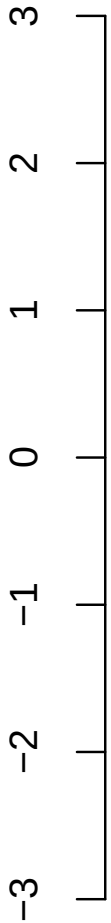



$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$

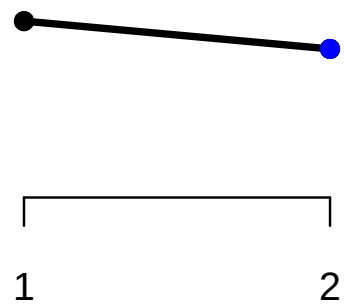


# Two Dimensional Example

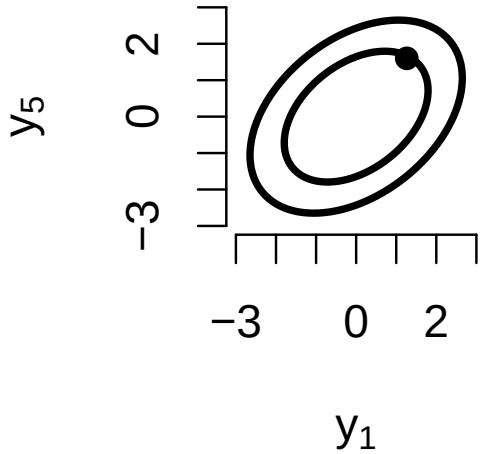


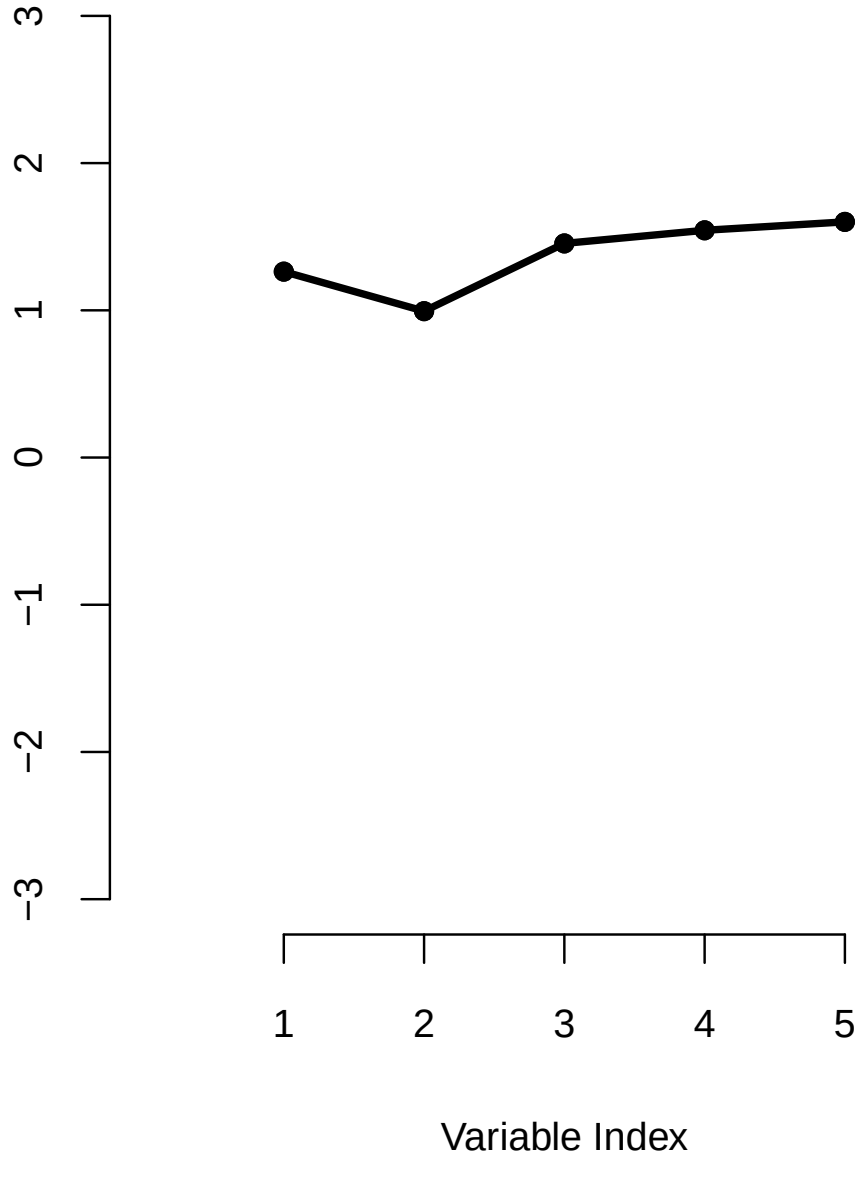

$$\Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix}$$



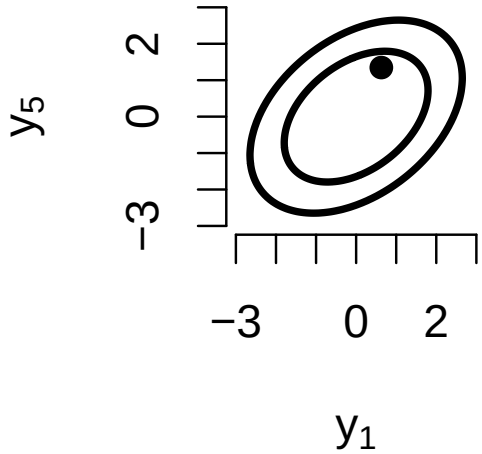
# Five Dimensional Example



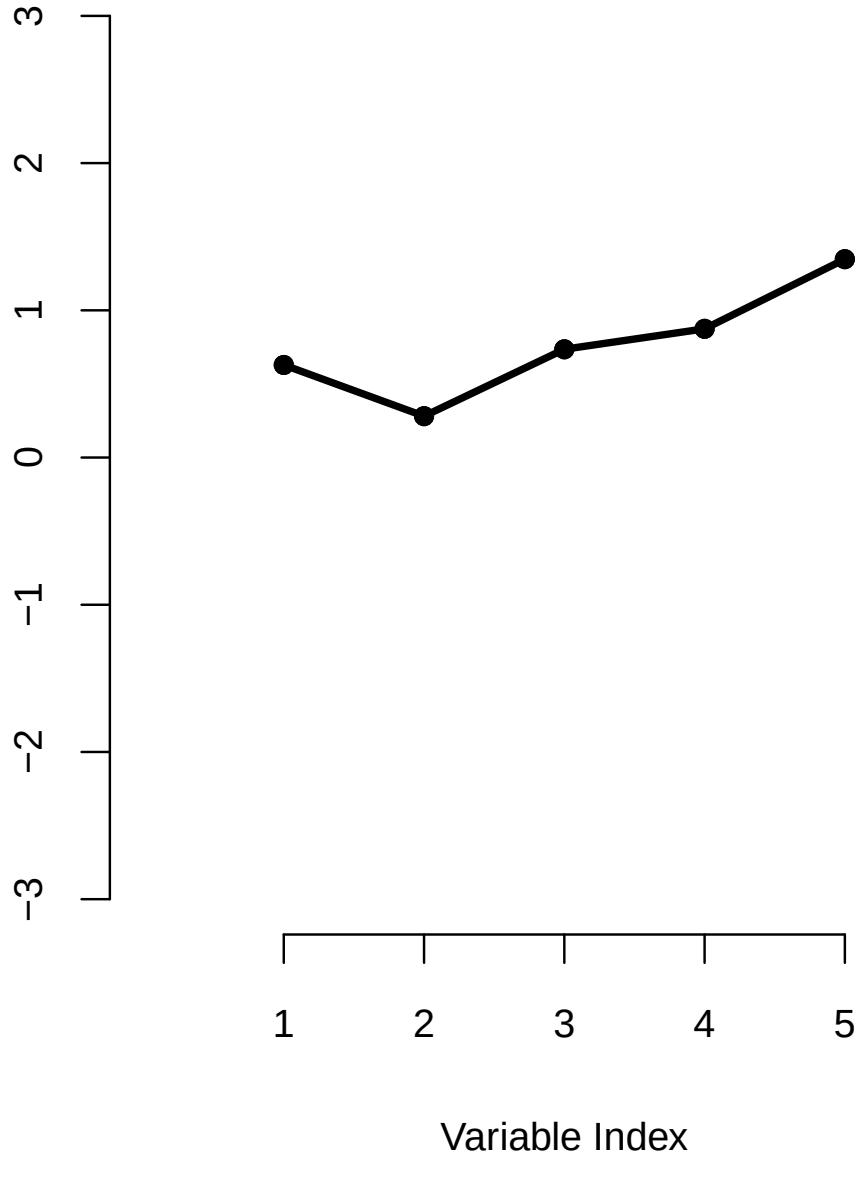

$$\Sigma = \begin{bmatrix} 1.0 & .9 & .8 & .6 & .4 \\ .9 & 1.0 & .9 & .8 & .6 \\ .8 & .9 & 1.0 & .9 & .8 \\ .6 & .8 & .9 & 1.0 & .9 \\ .4 & .6 & .8 & .9 & 1.0 \end{bmatrix}$$



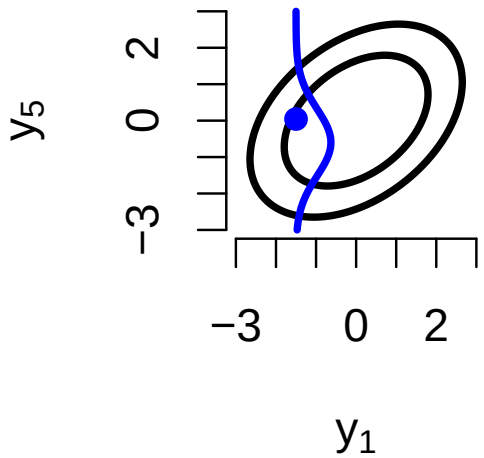
# Five Dimensional Example



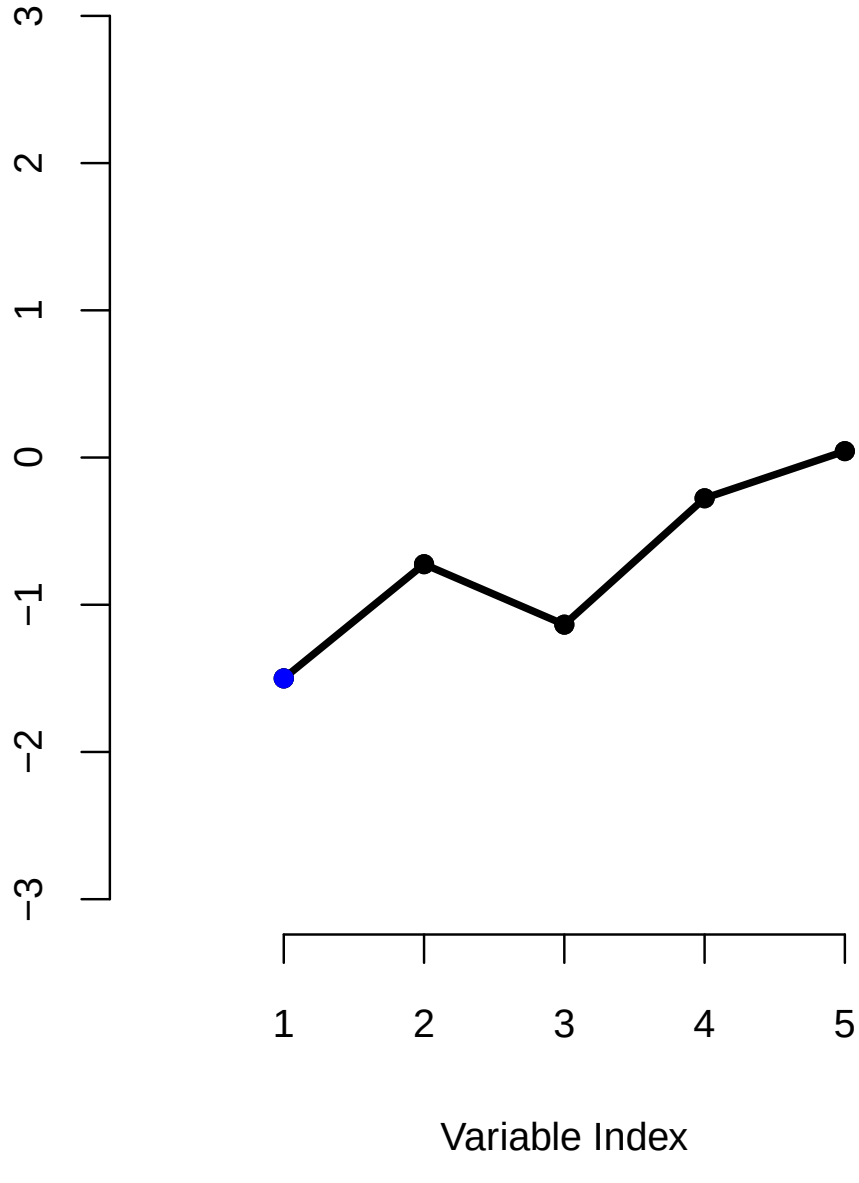

$$\Sigma = \begin{bmatrix} 1.0 & .9 & .8 & .6 & .4 \\ .9 & 1.0 & .9 & .8 & .6 \\ .8 & .9 & 1.0 & .9 & .8 \\ .6 & .8 & .9 & 1.0 & .9 \\ .4 & .6 & .8 & .9 & 1.0 \end{bmatrix}$$



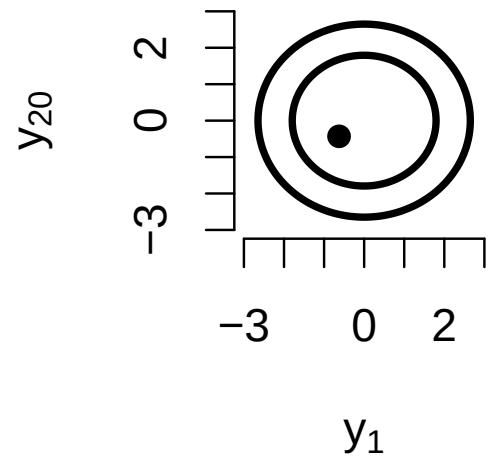
# Five Dimensional Example



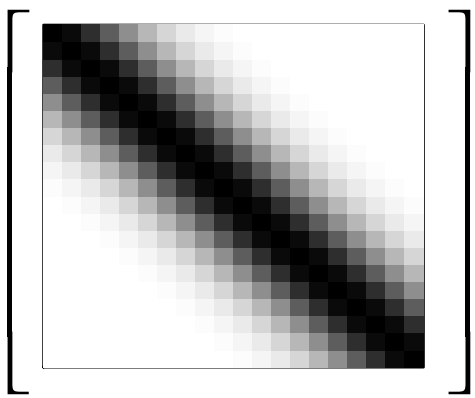

$$\Sigma = \begin{bmatrix} 1.0 & .9 & .8 & .6 & .4 \\ .9 & 1.0 & .9 & .8 & .6 \\ .8 & .9 & 1.0 & .9 & .8 \\ .6 & .8 & .9 & 1.0 & .9 \\ .4 & .6 & .8 & .9 & 1.0 \end{bmatrix}$$

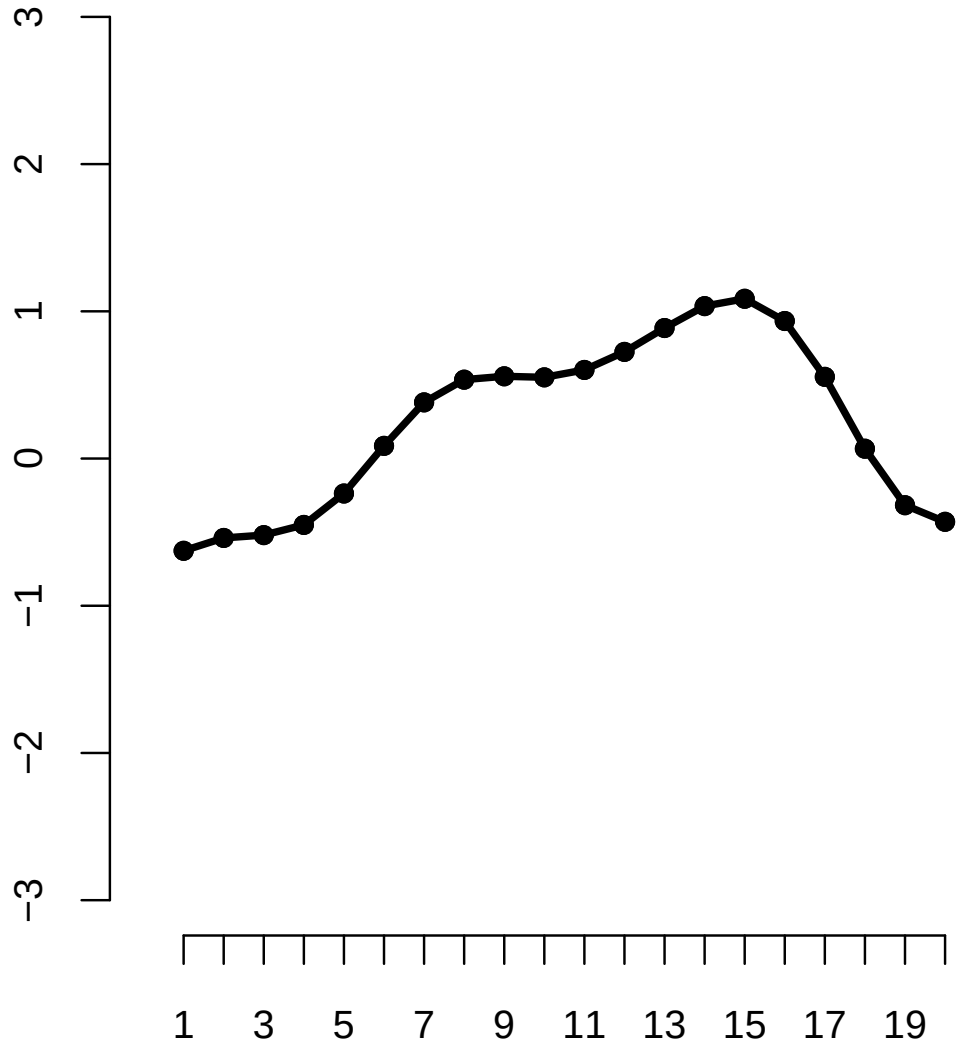


# Twenty Dimensional Example

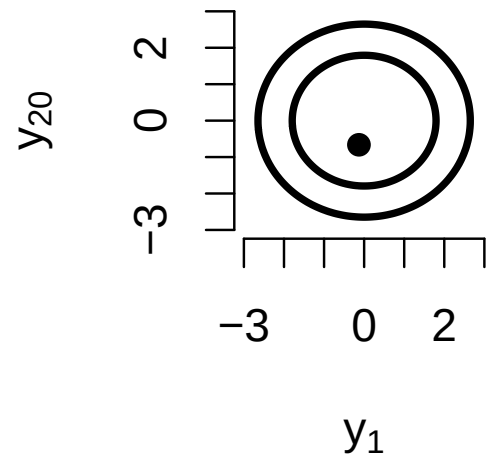



$\Sigma =$

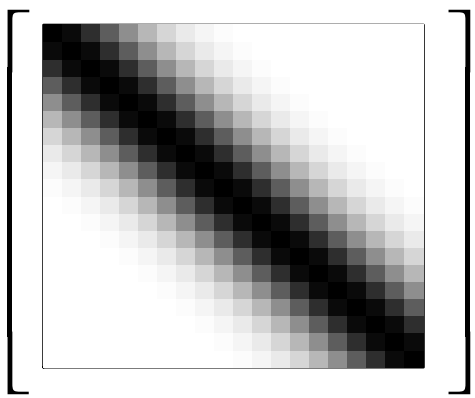


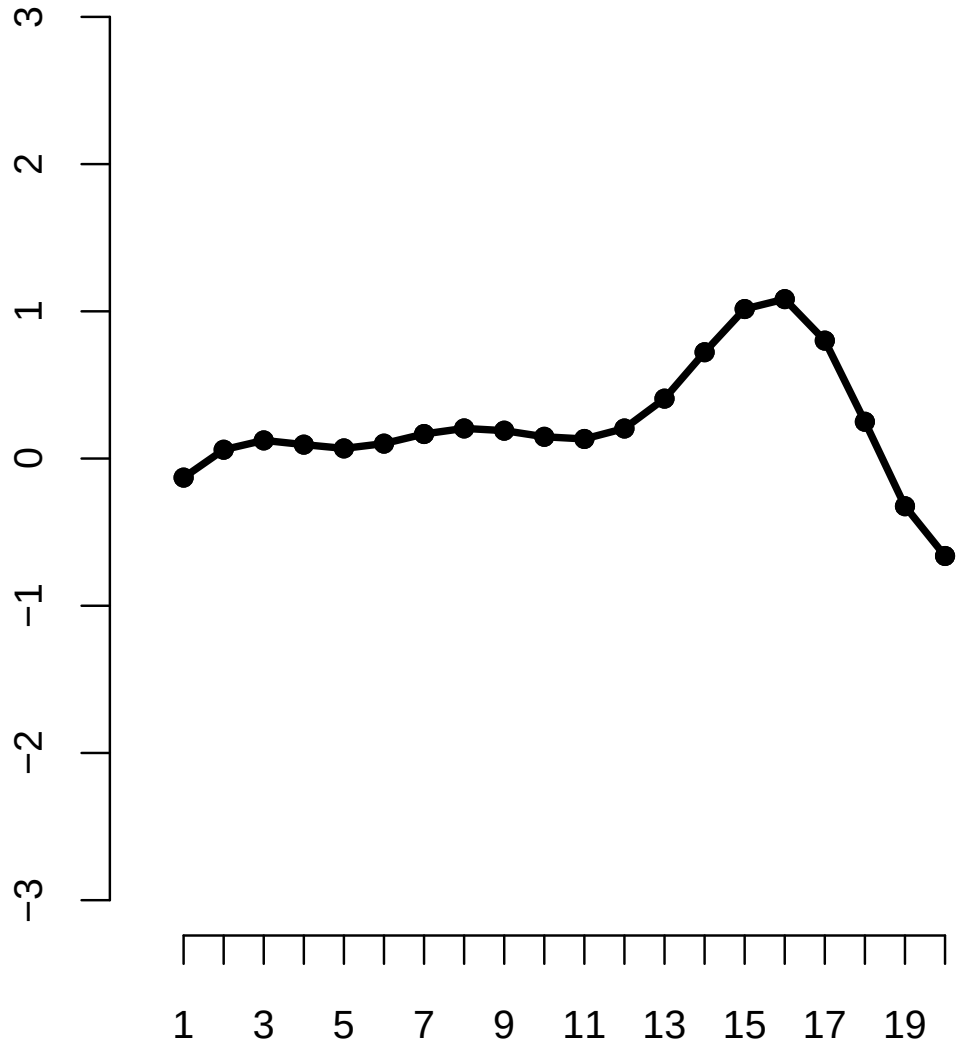


# Twenty Dimensional Example

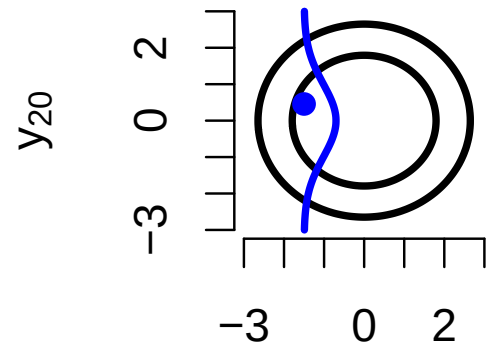


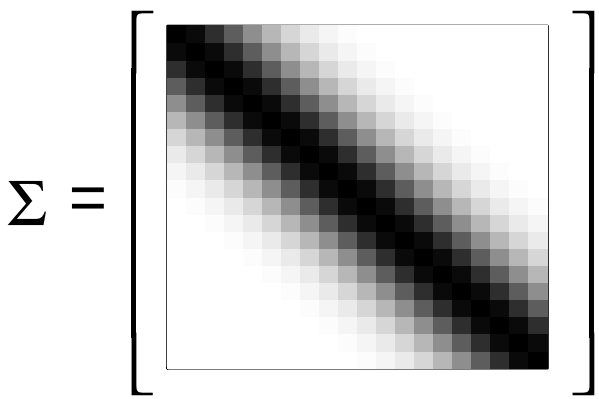

$\Sigma =$

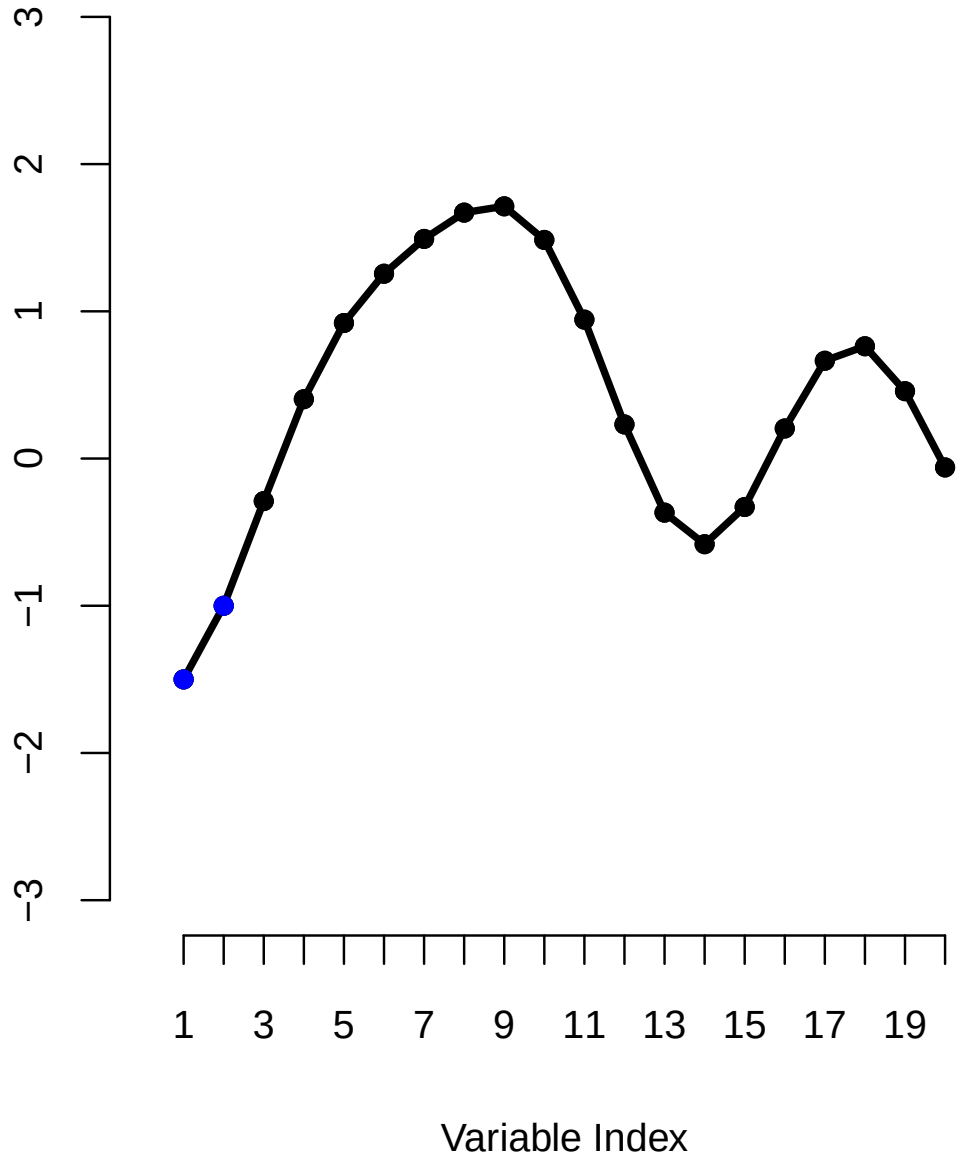




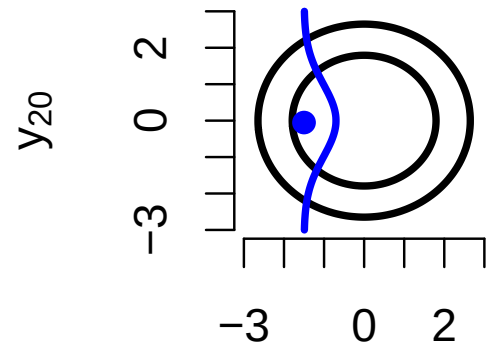
# Twenty Dimensional Example



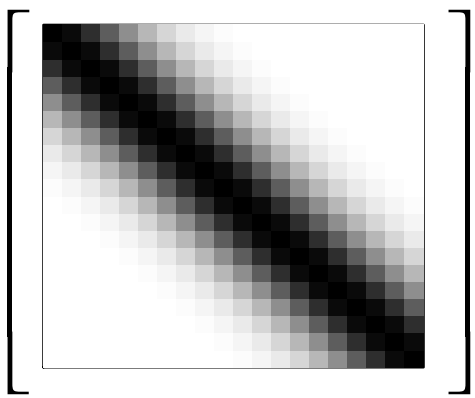



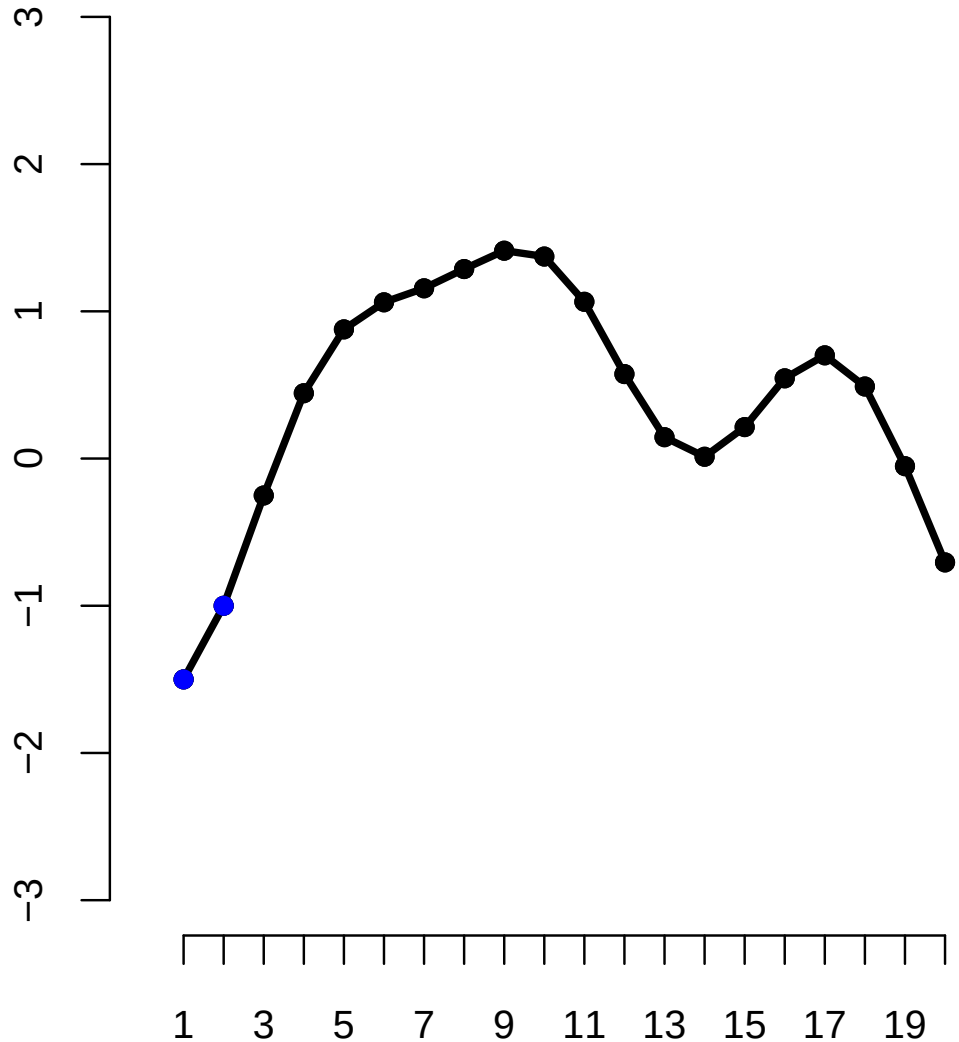



# Twenty Dimensional Example

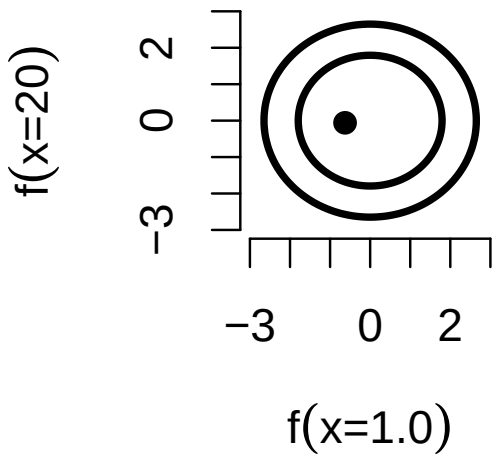


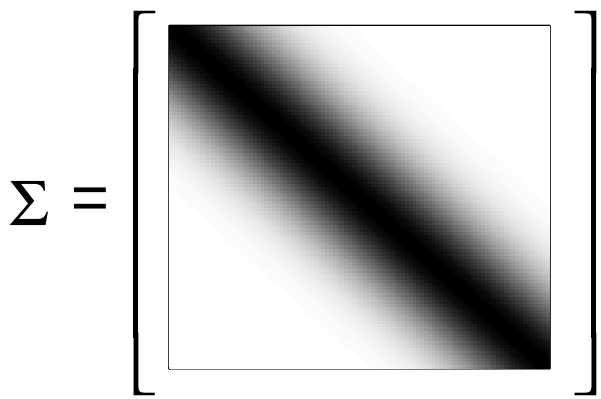

$\Sigma =$

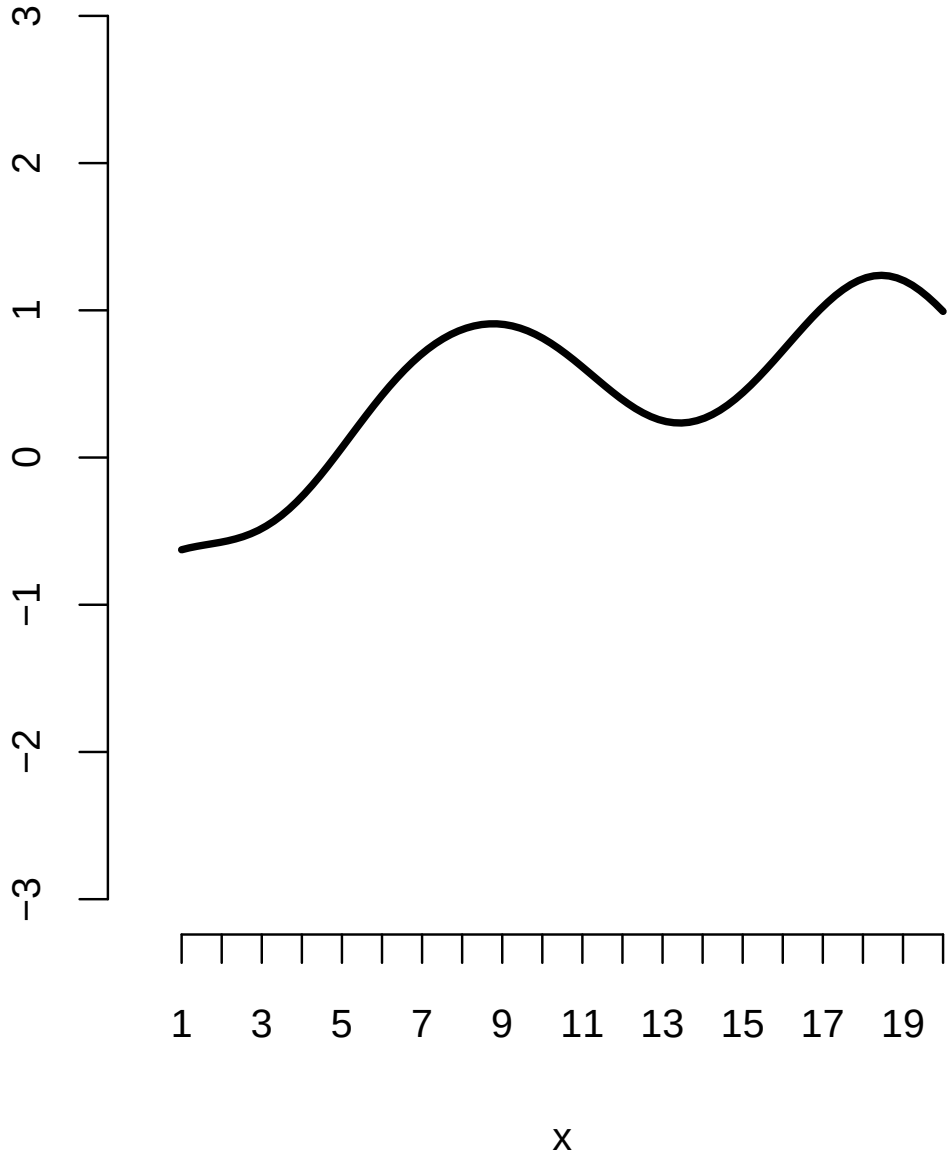




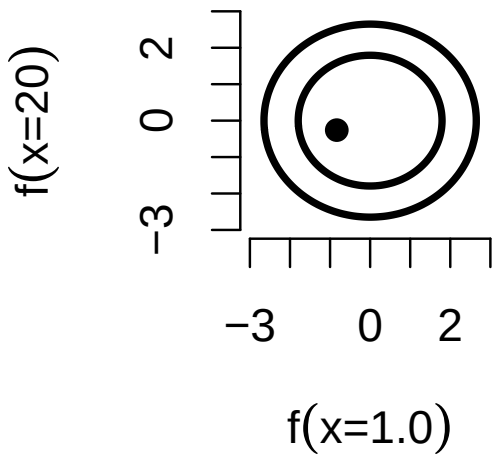
# Infinite Dimensional Example

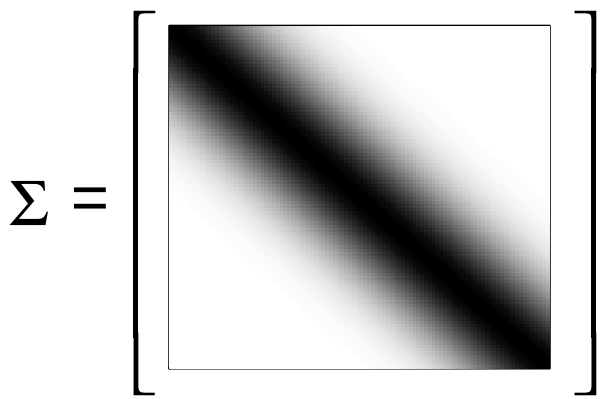


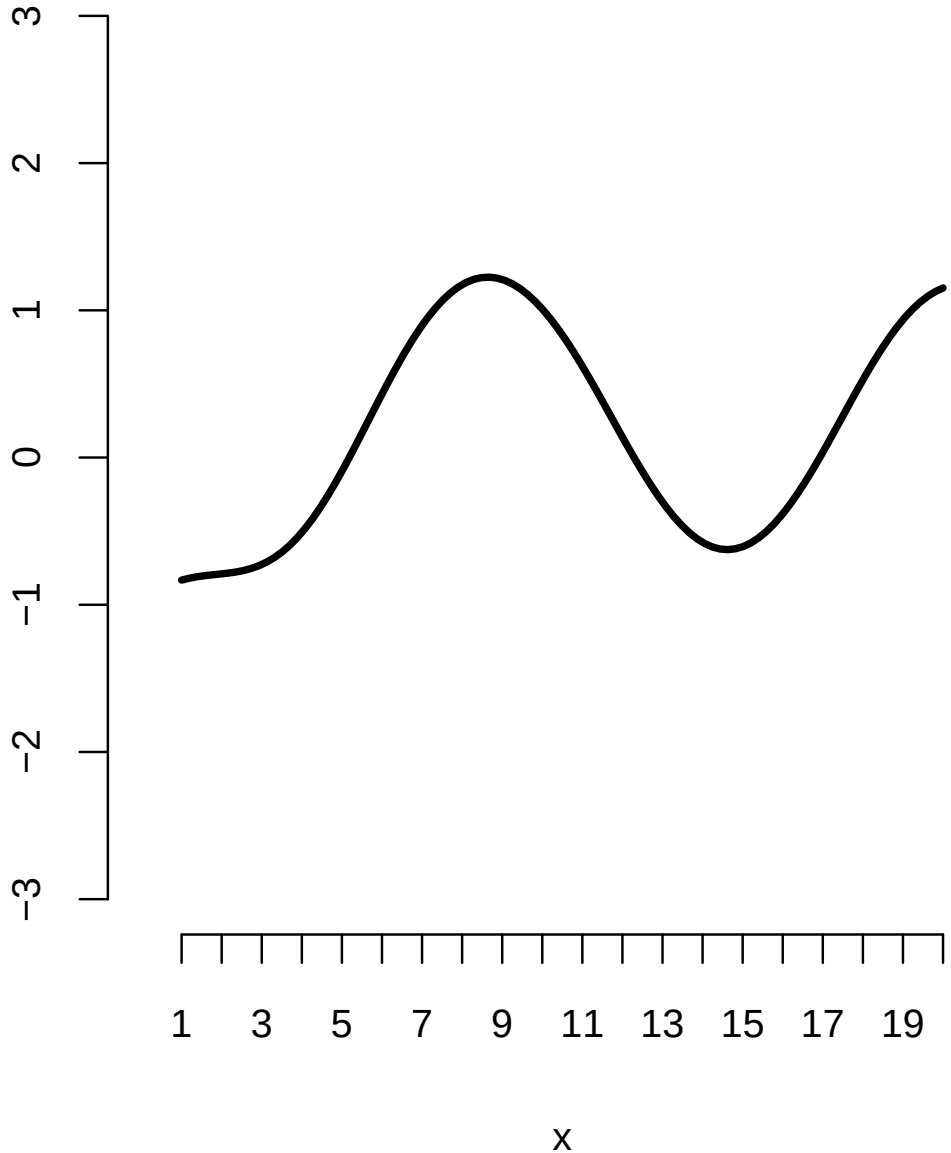



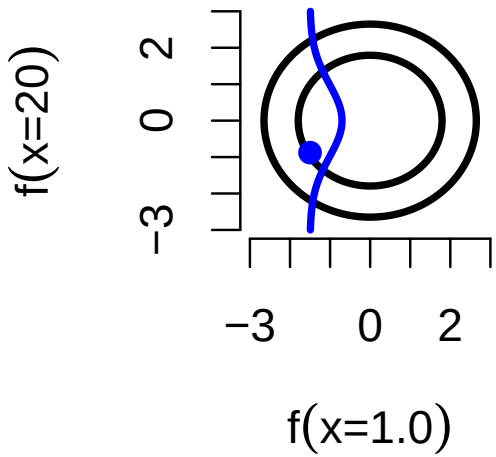
# Infinite Dimensional Example



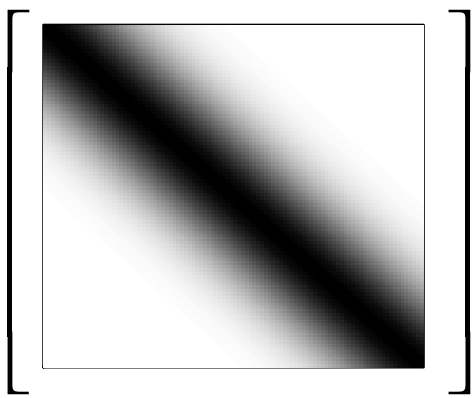



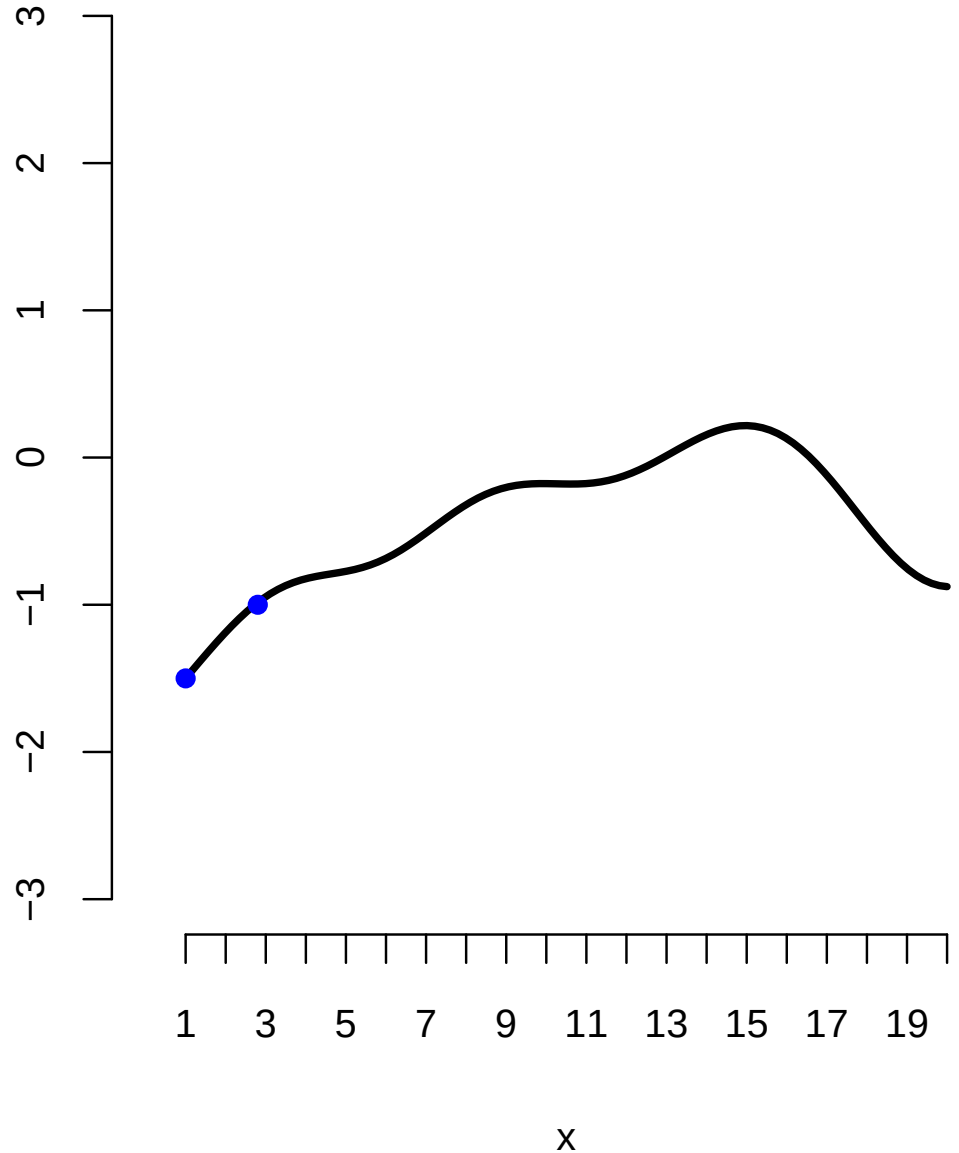



# Infinite Dimensional Example

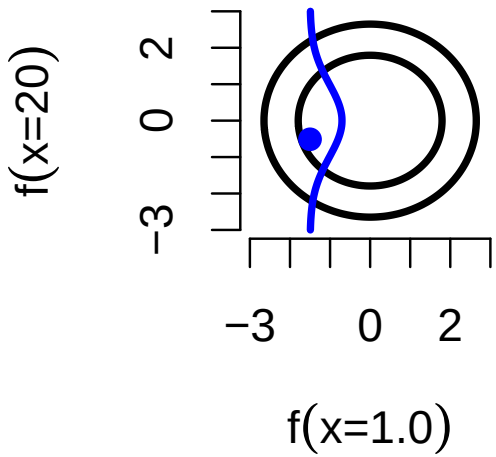



$\Sigma =$

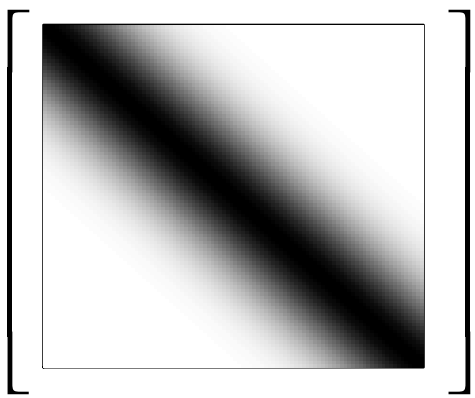


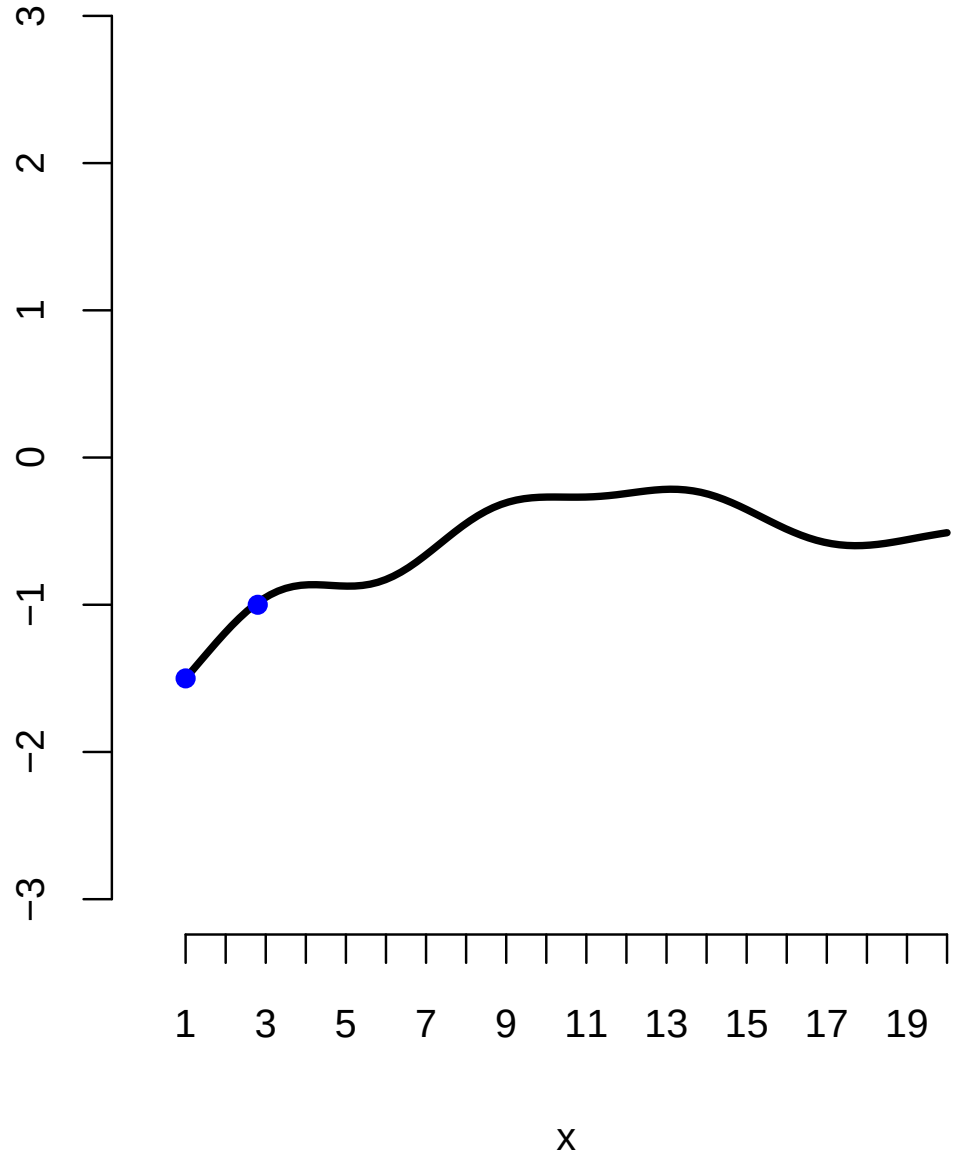


# Infinite Dimensional Example

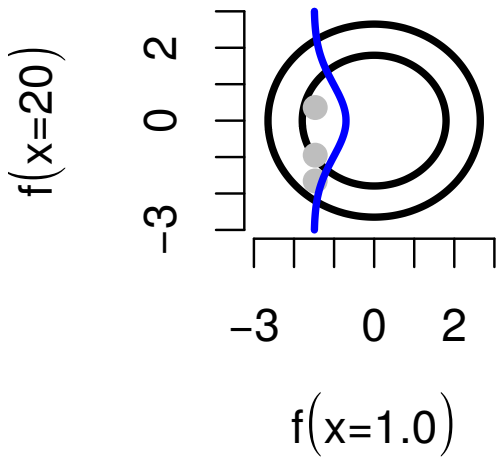


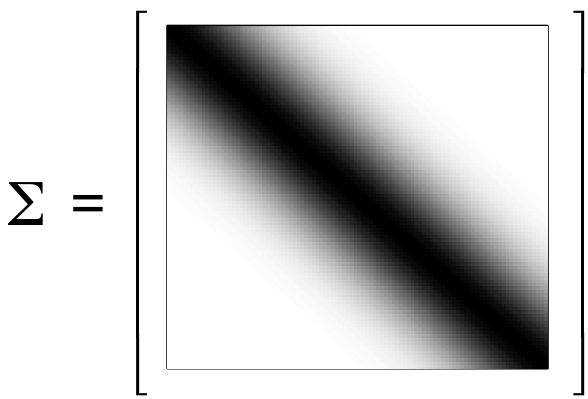

$\Sigma =$

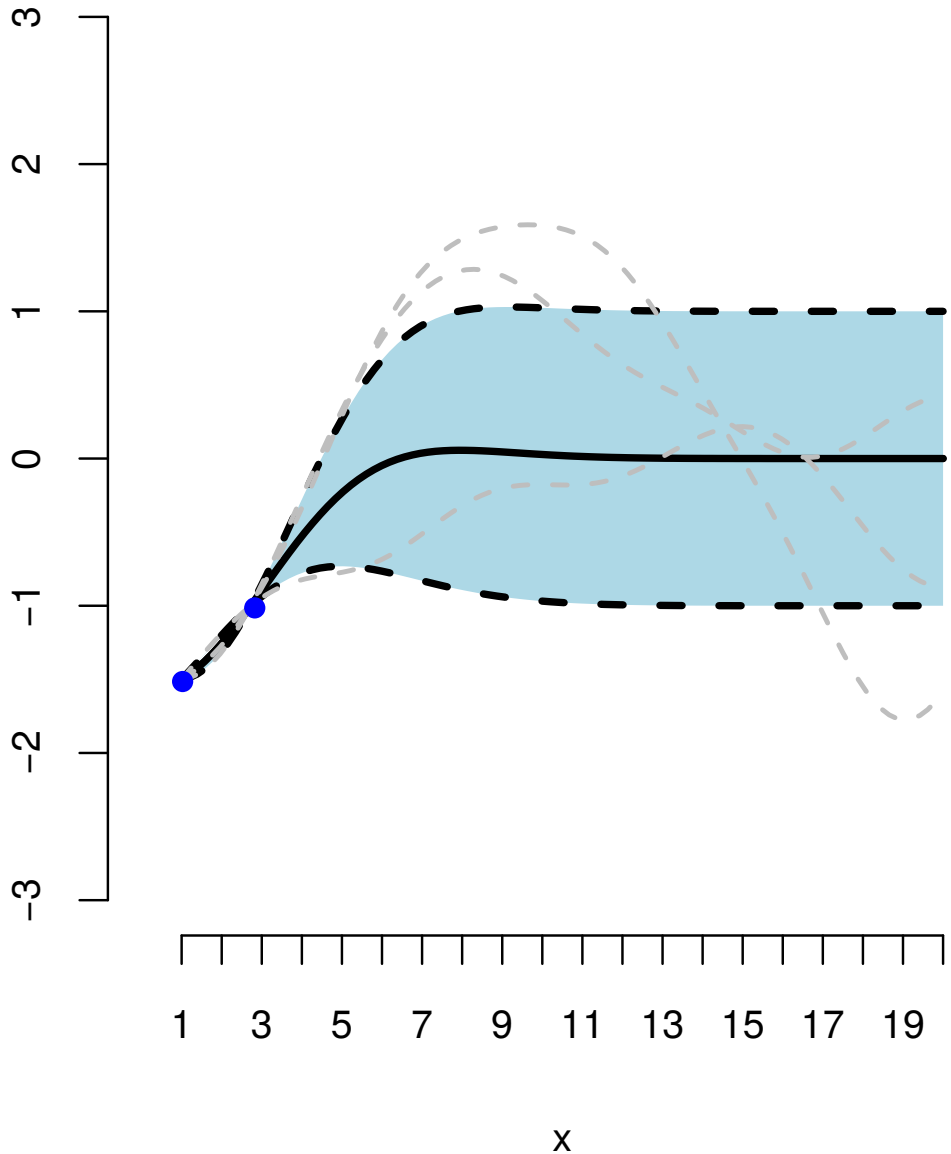




# Predictive Distribution



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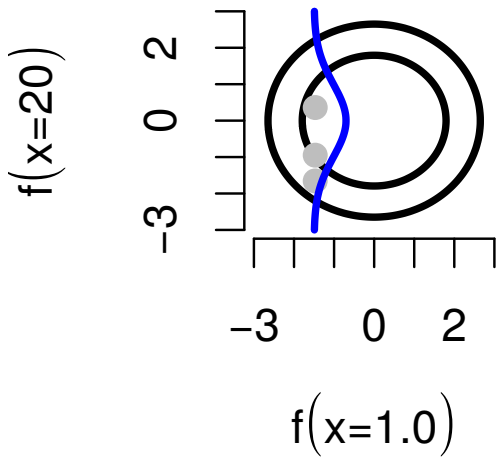


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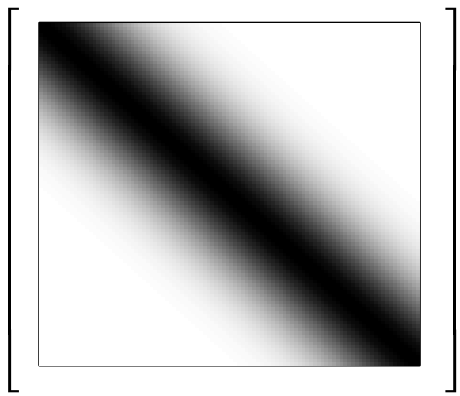

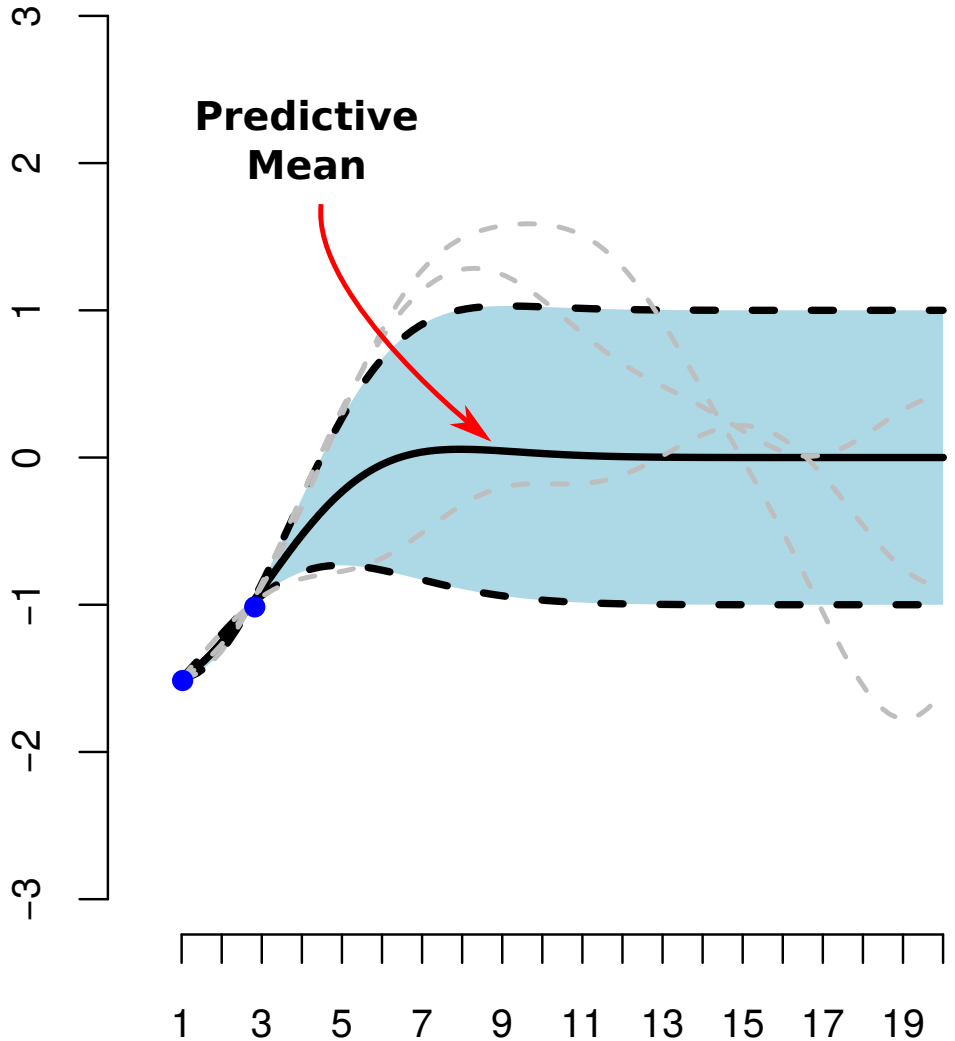

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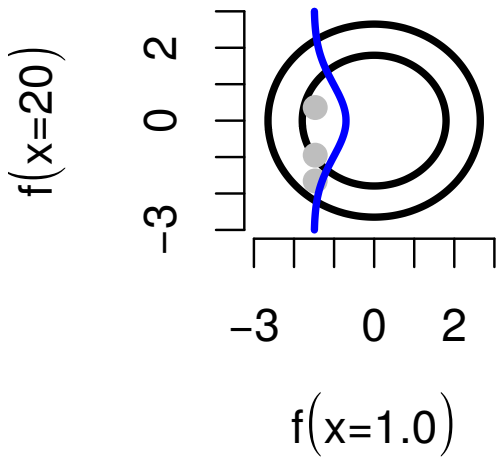


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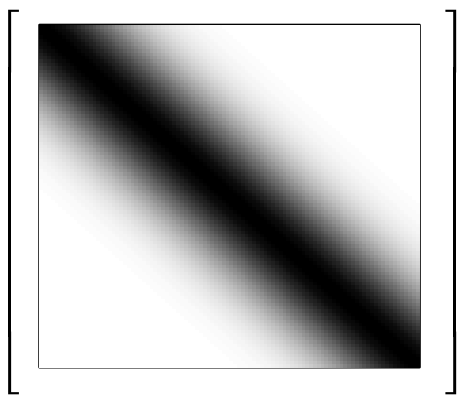

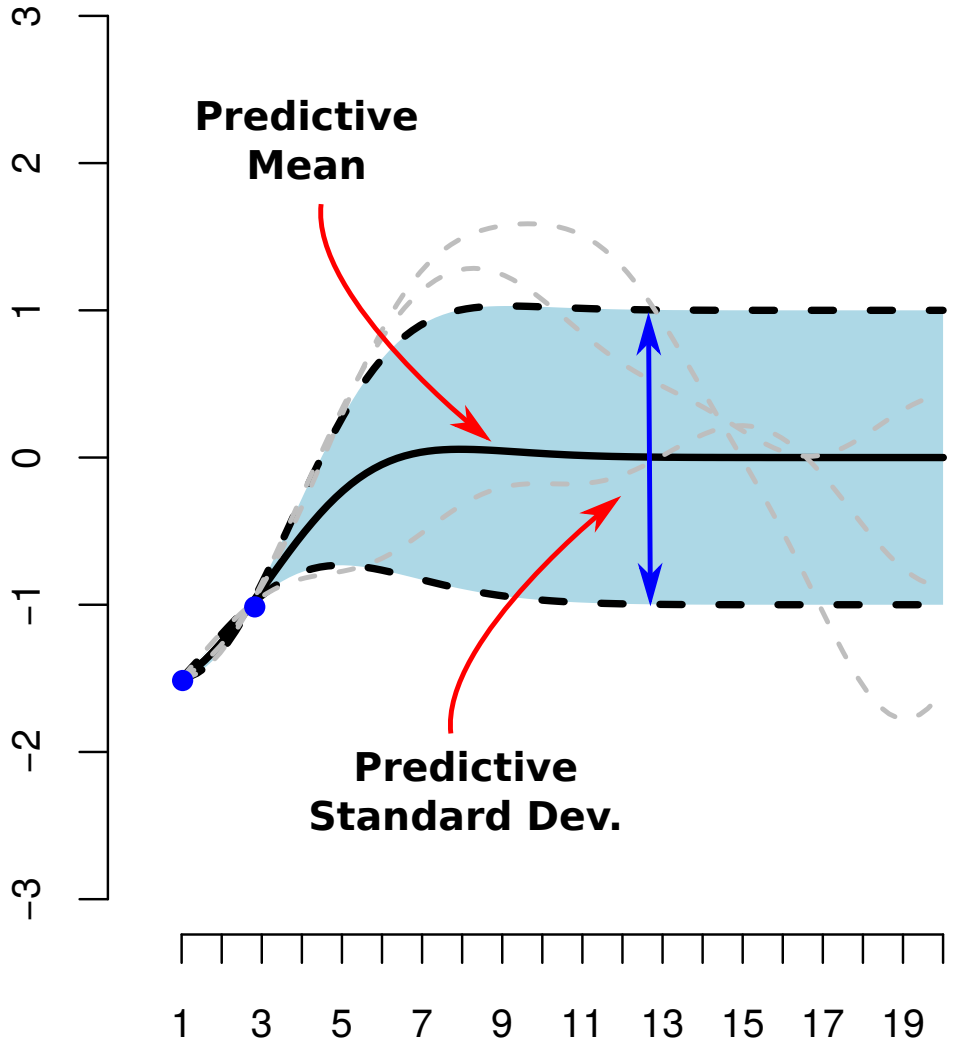

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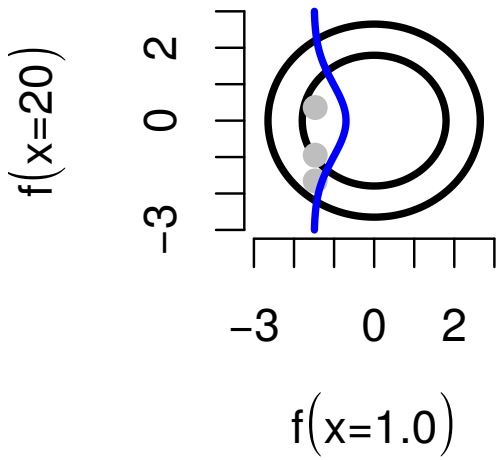


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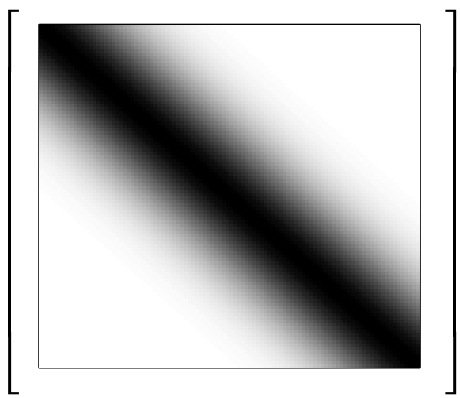

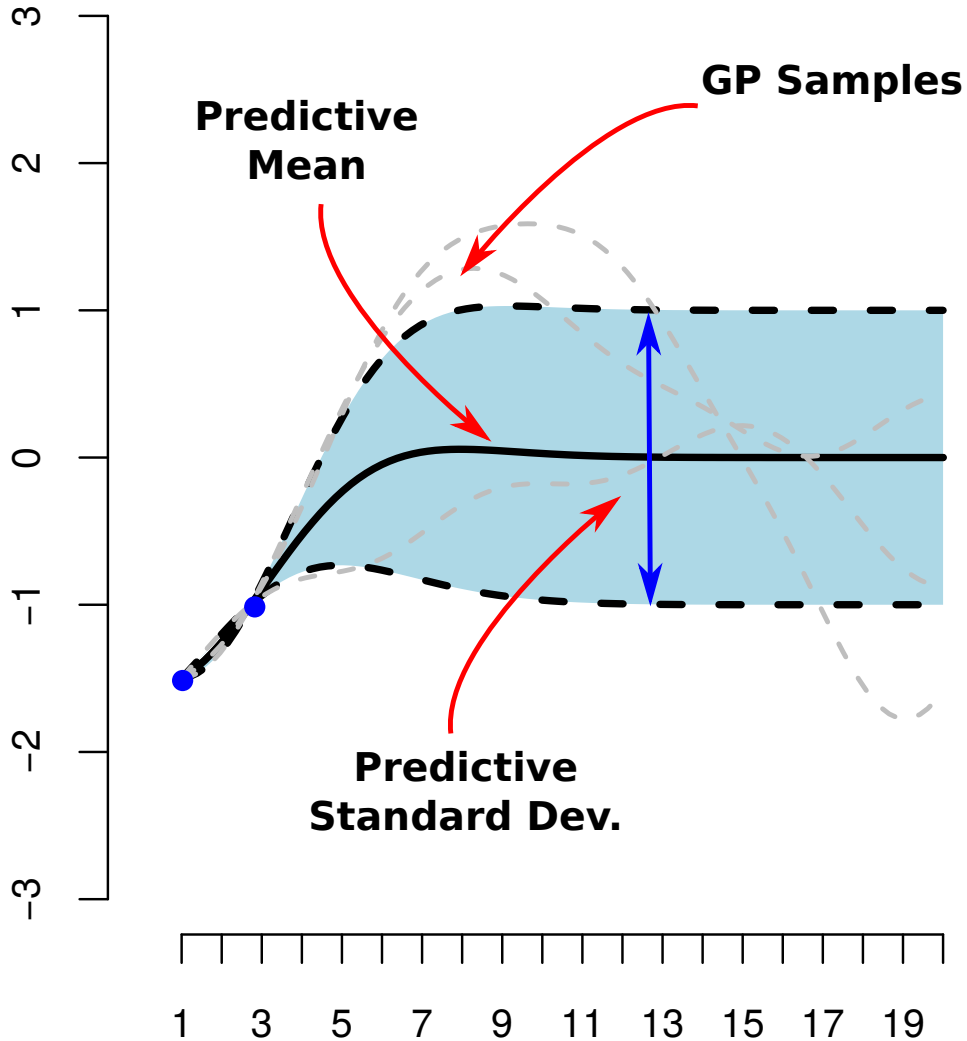

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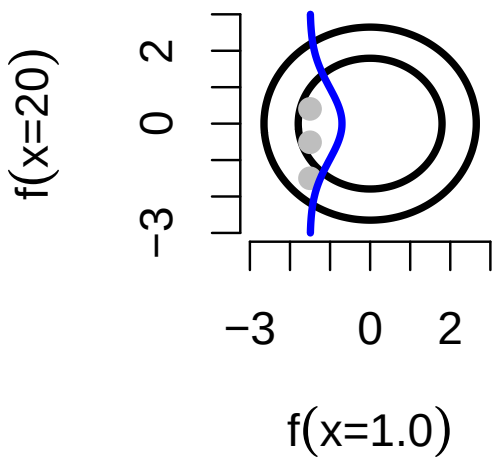


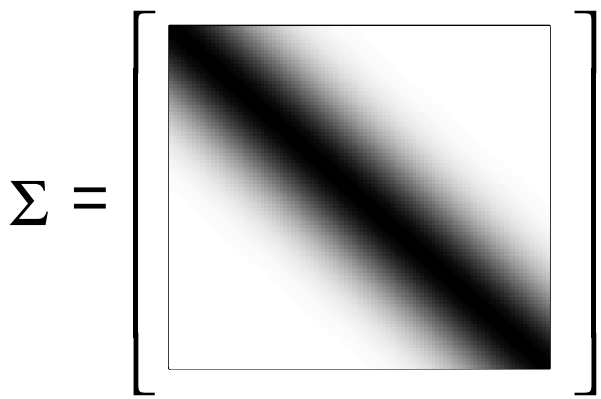


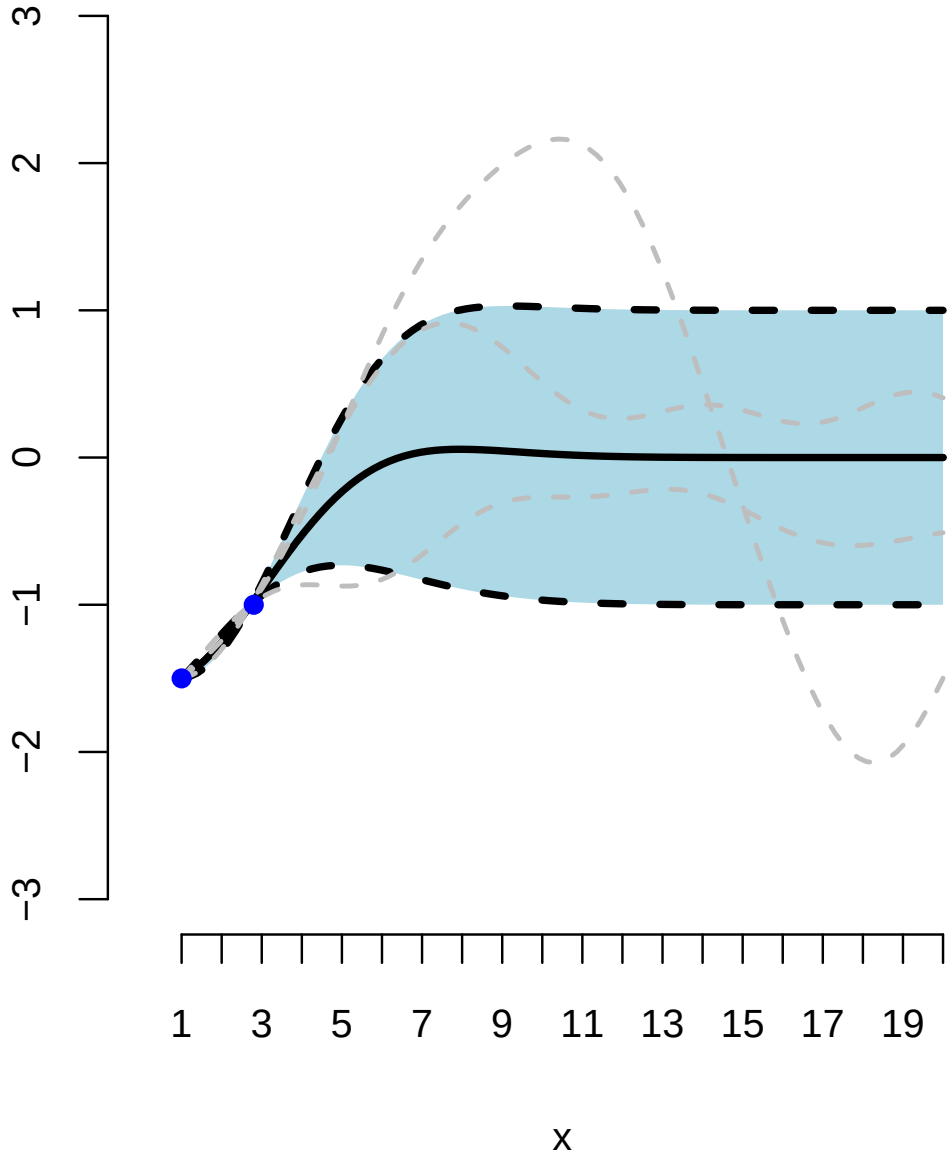

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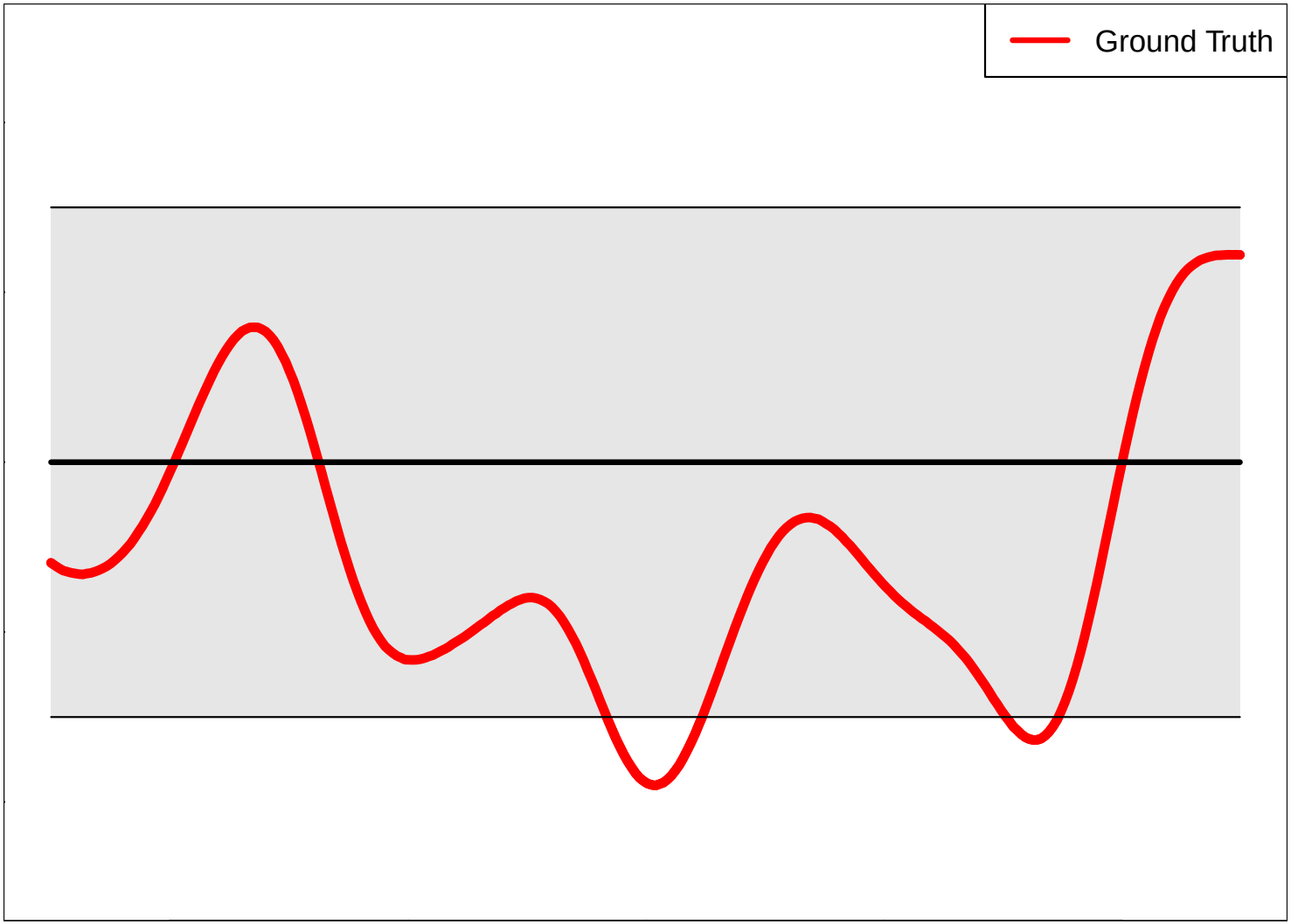

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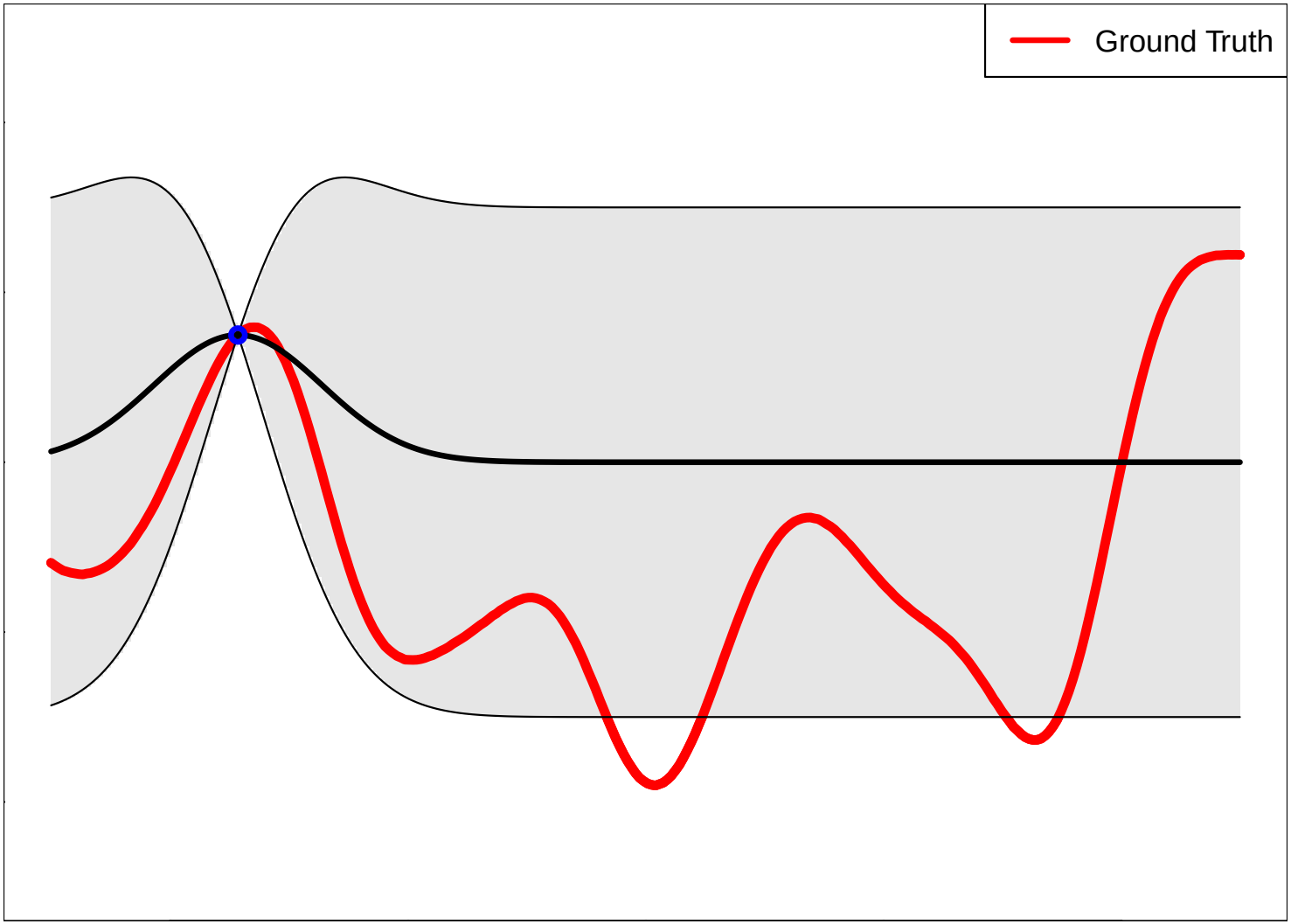

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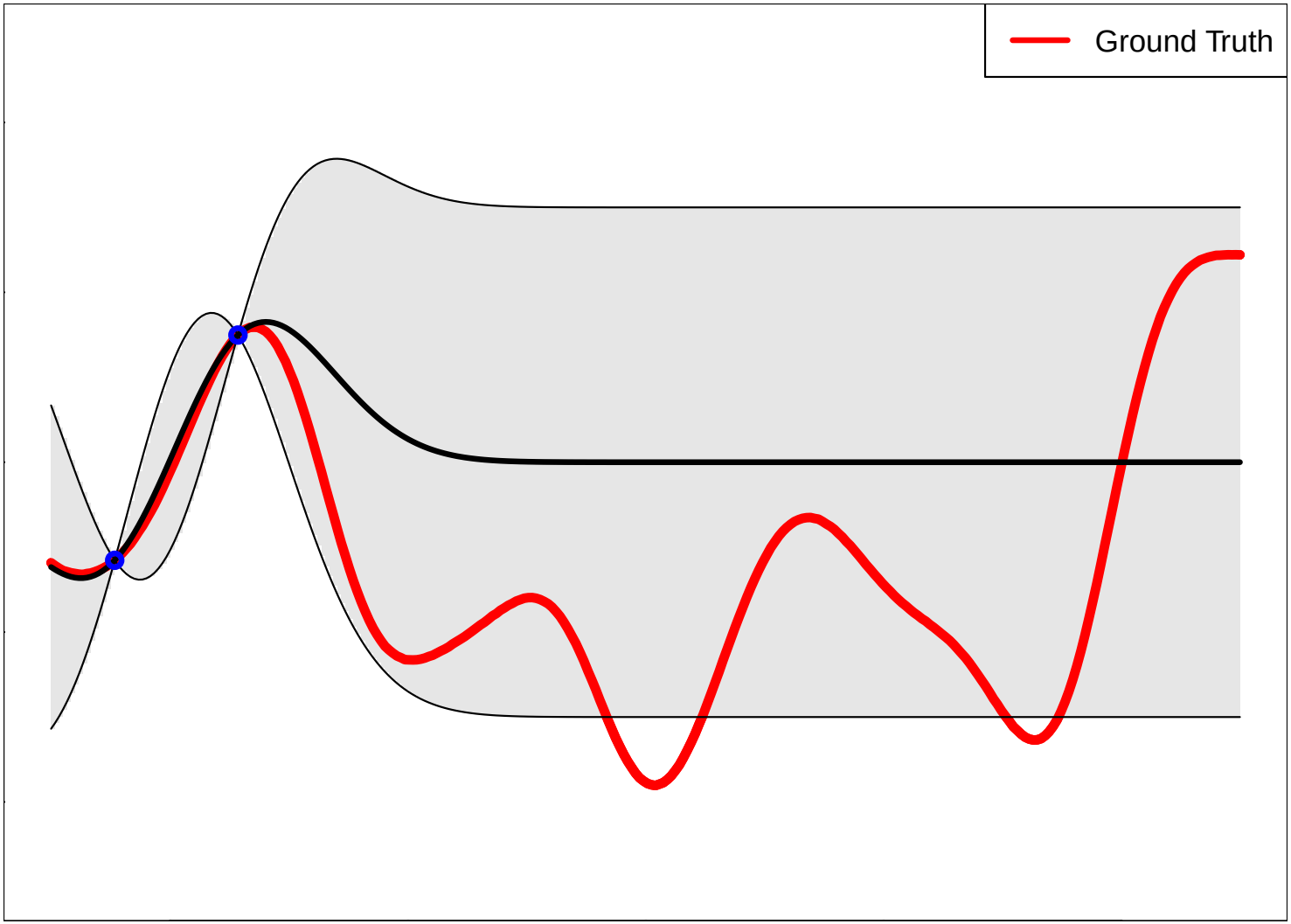

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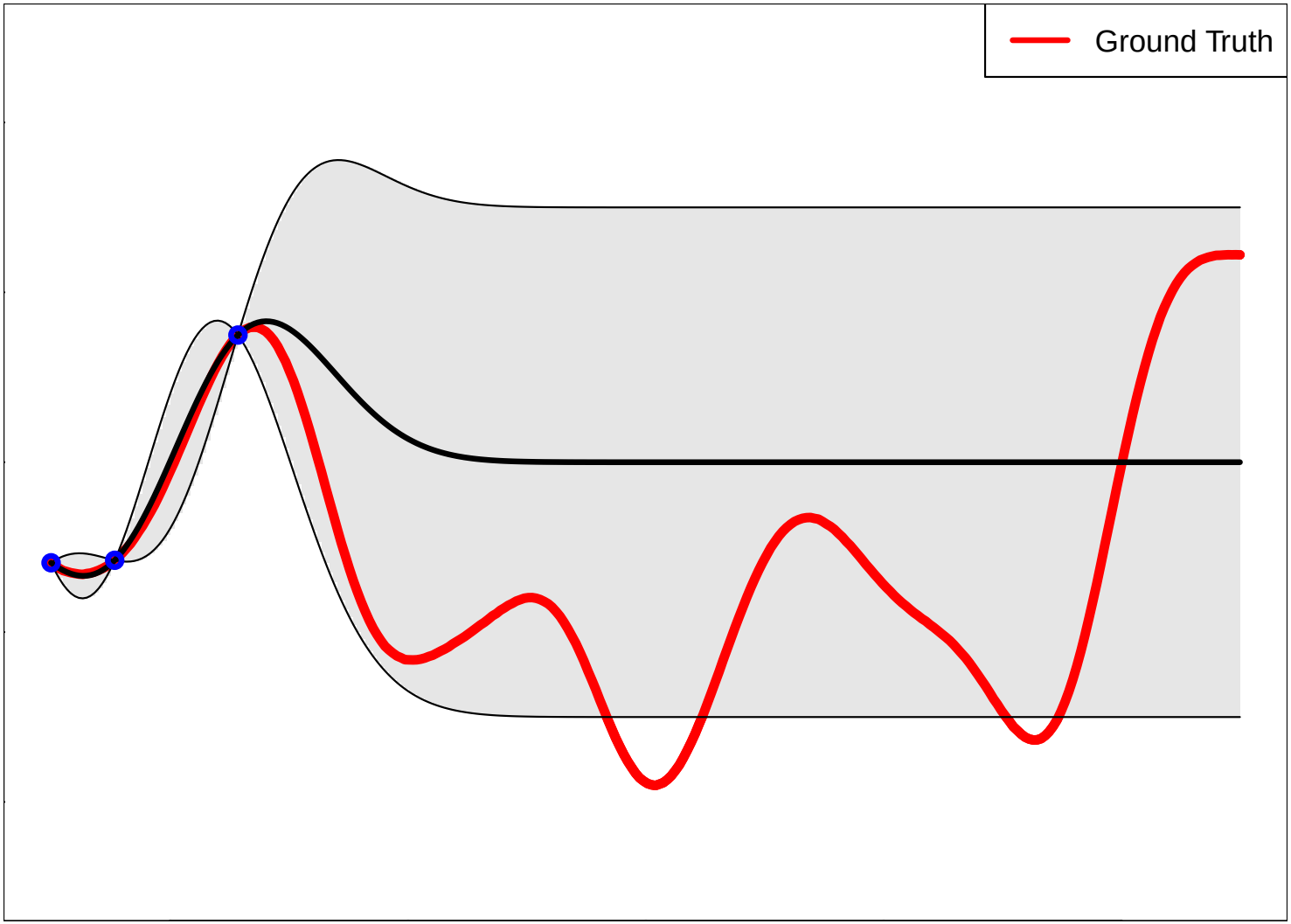

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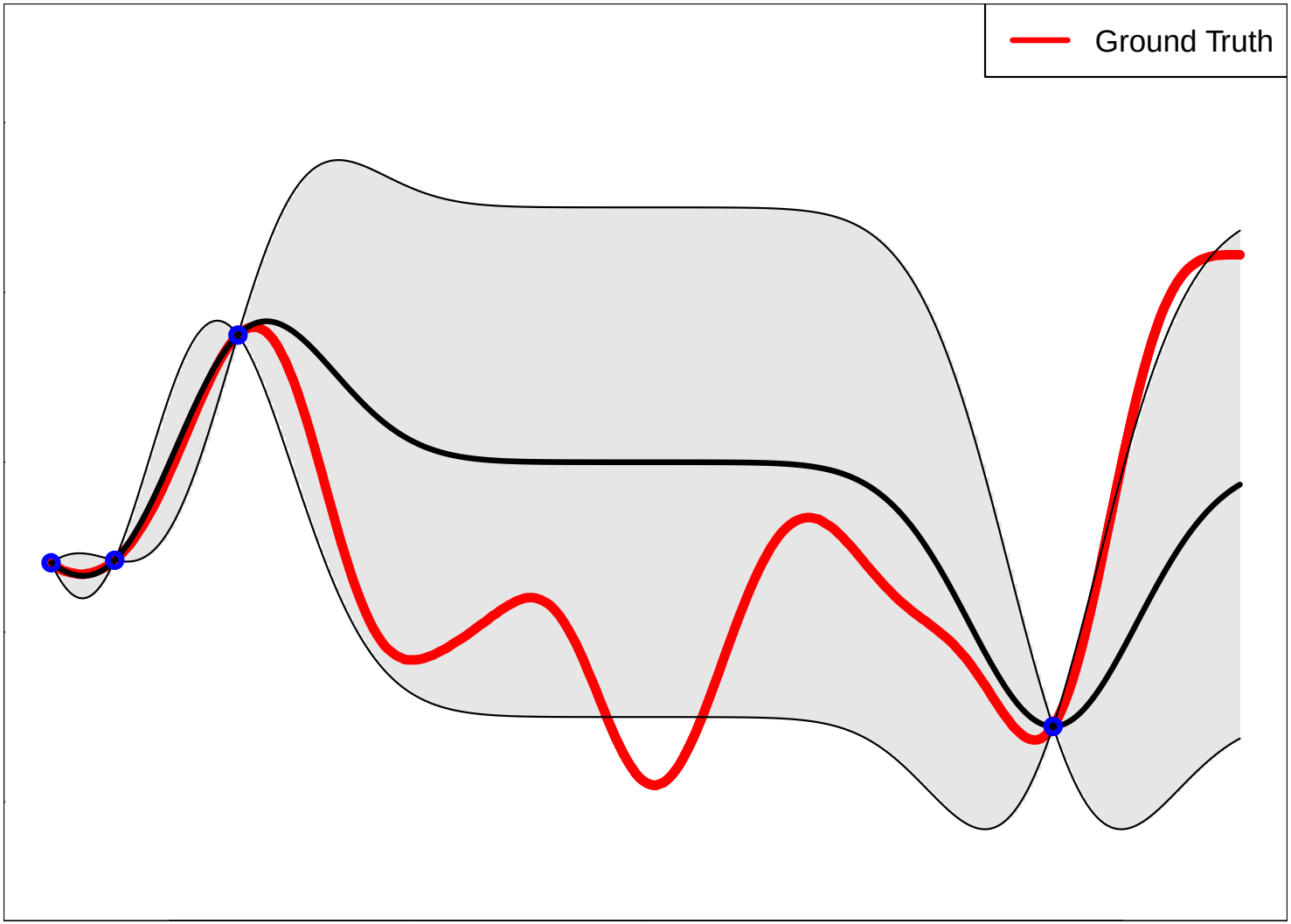

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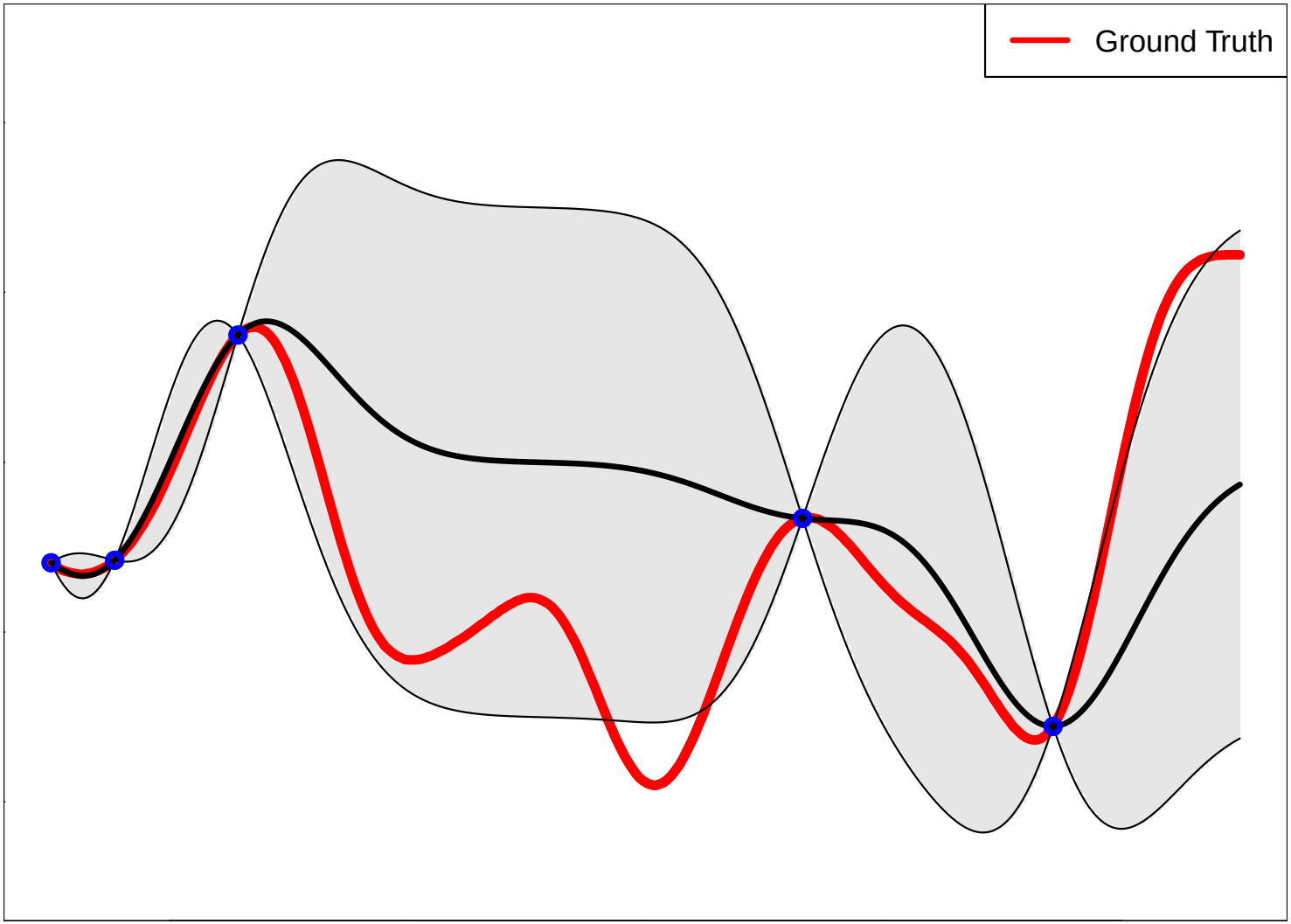

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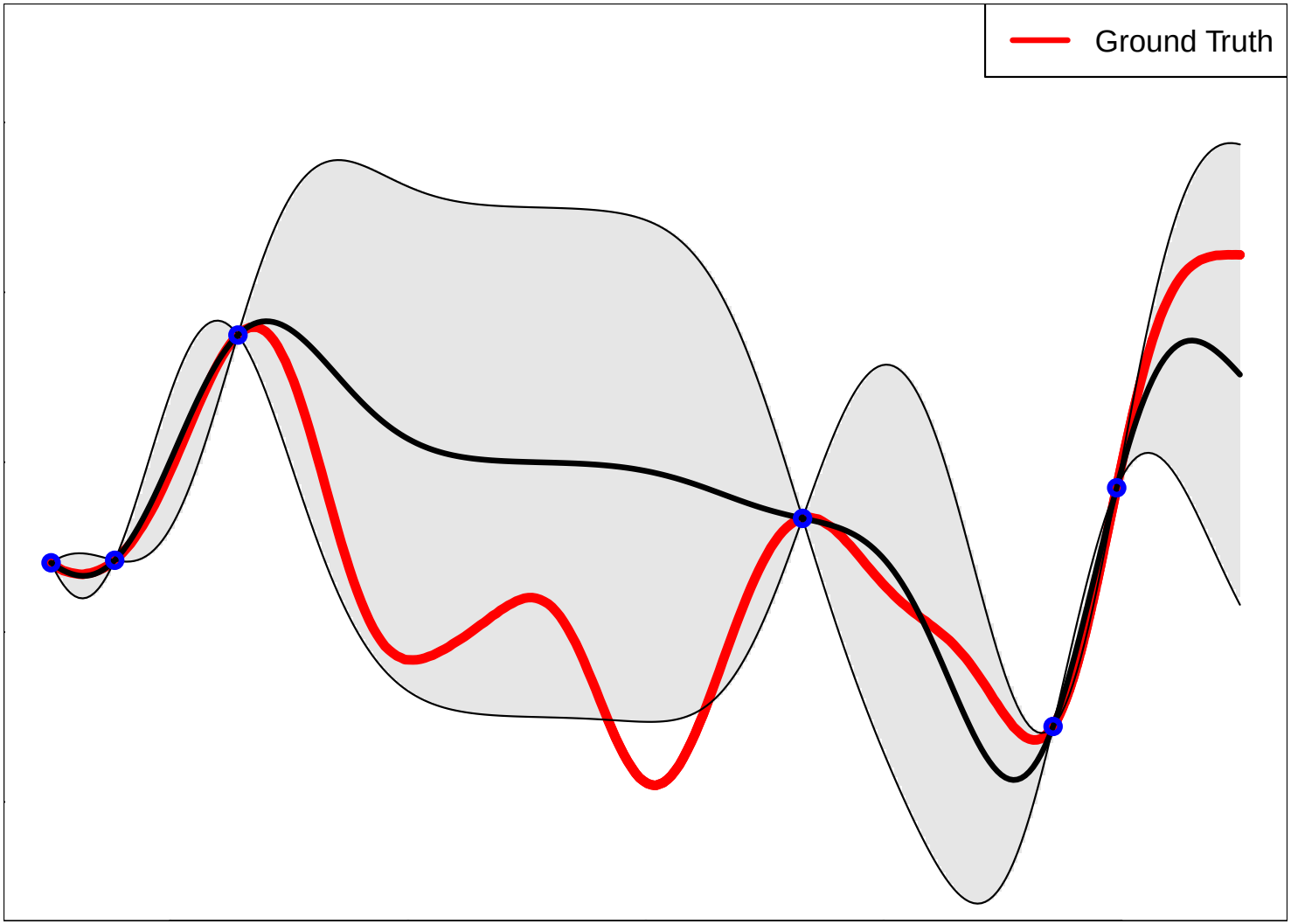

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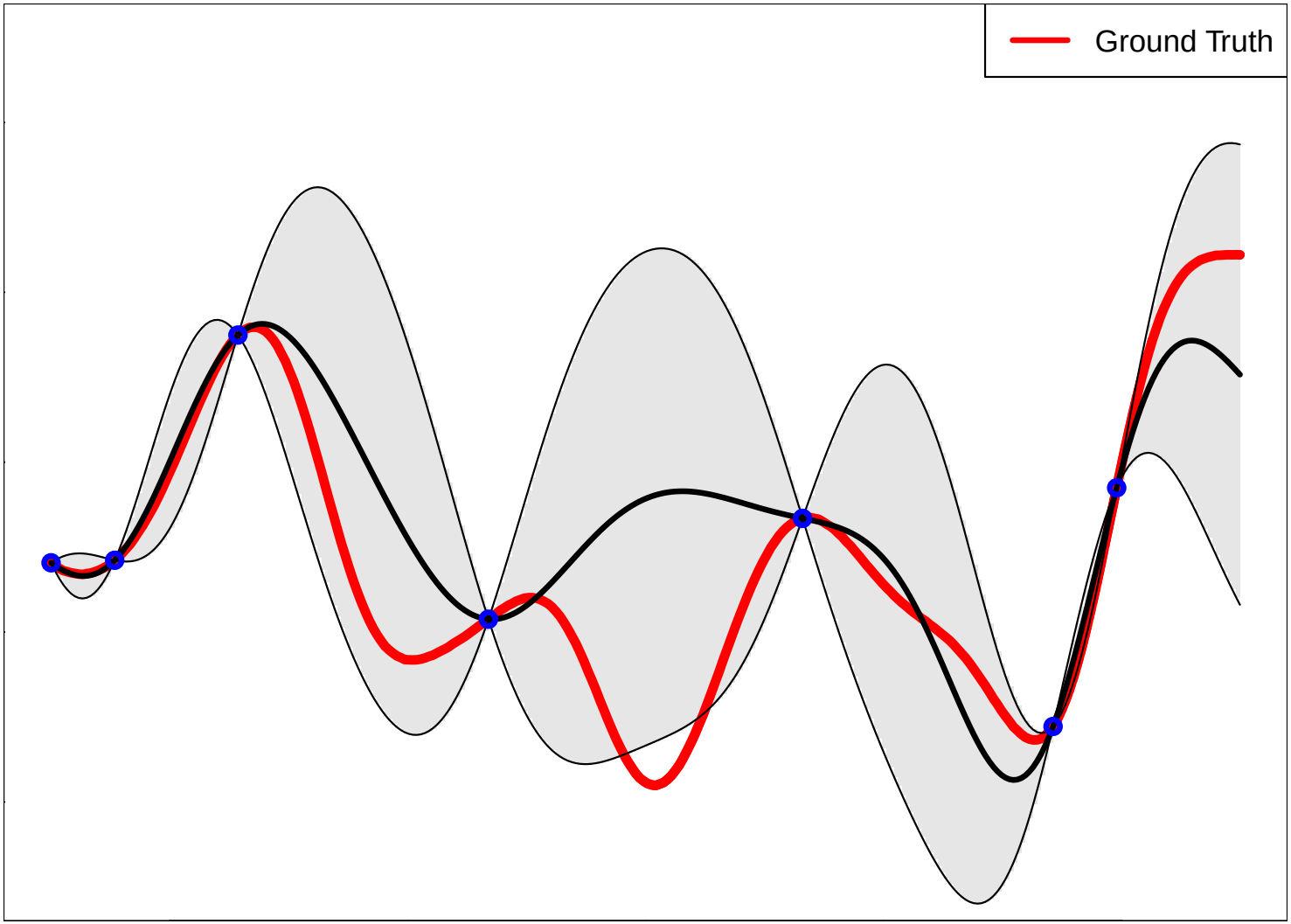

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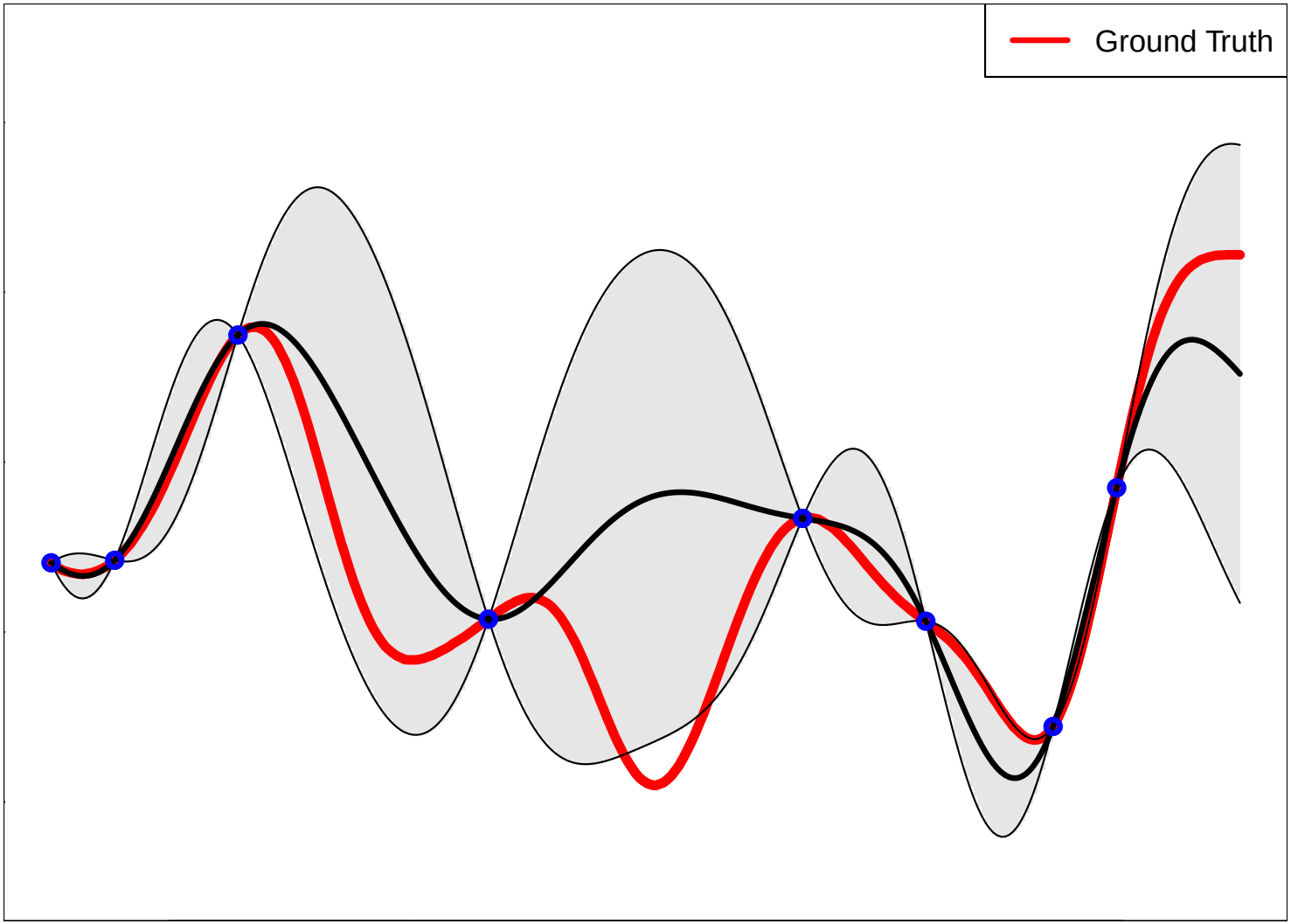

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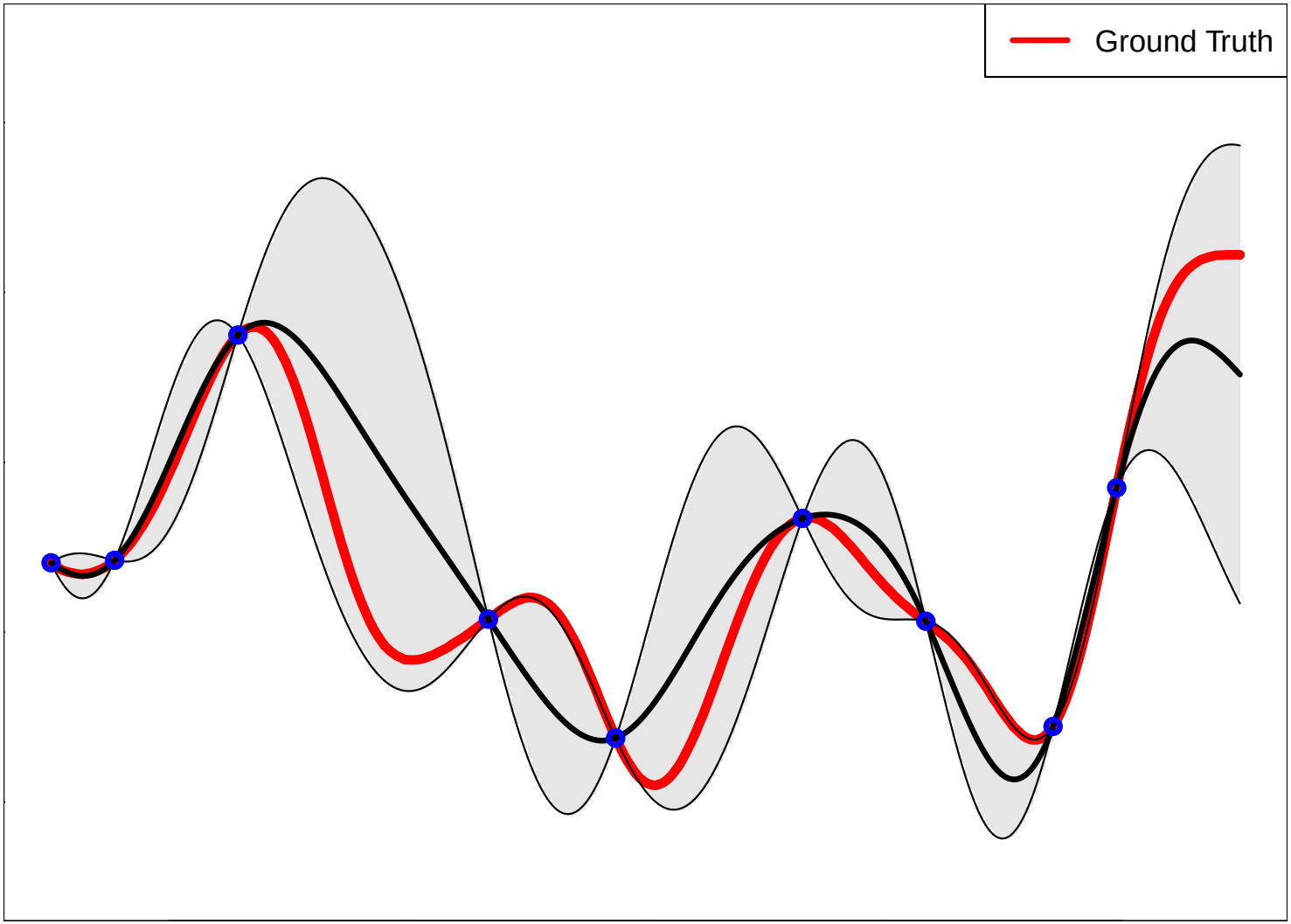

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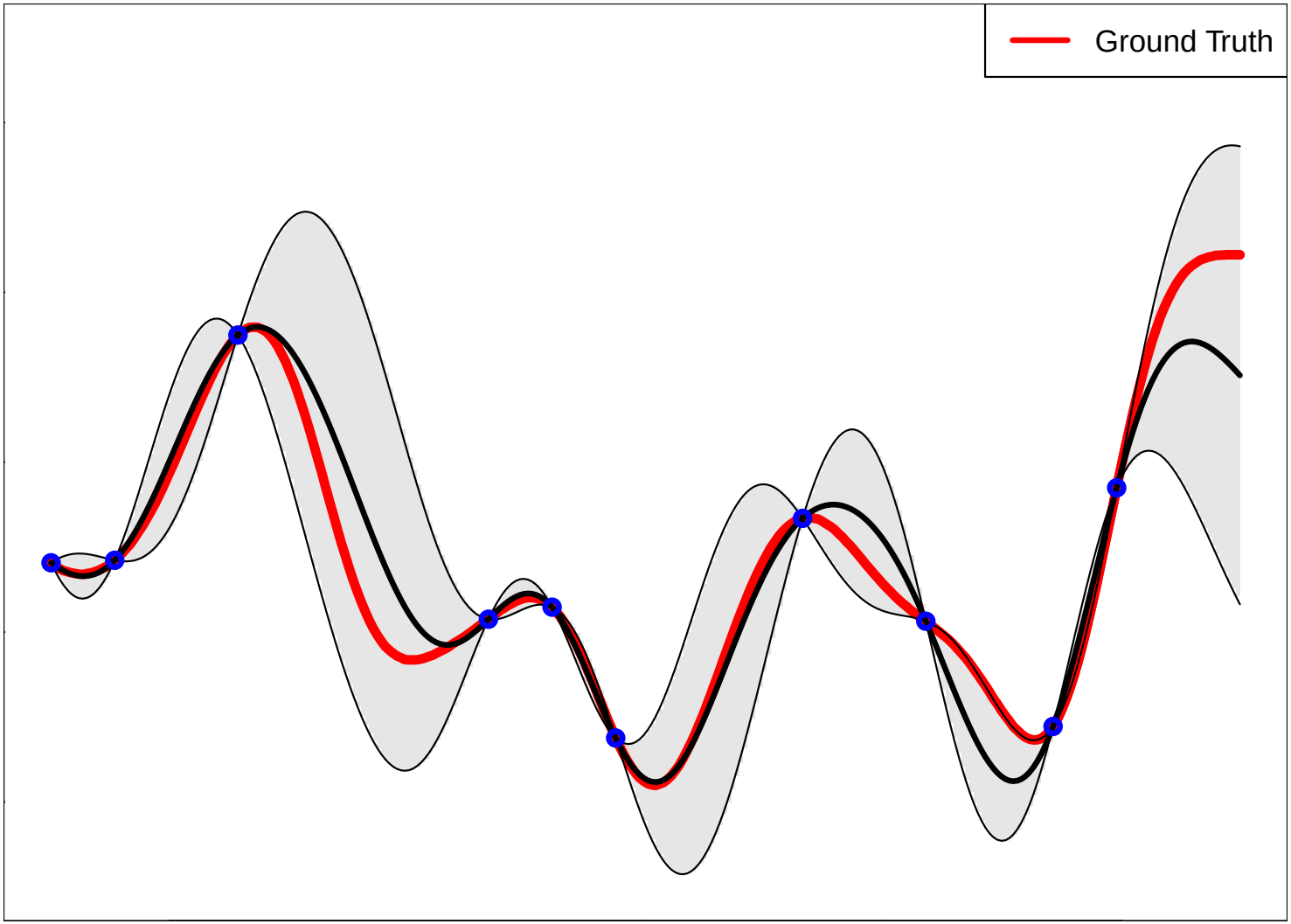

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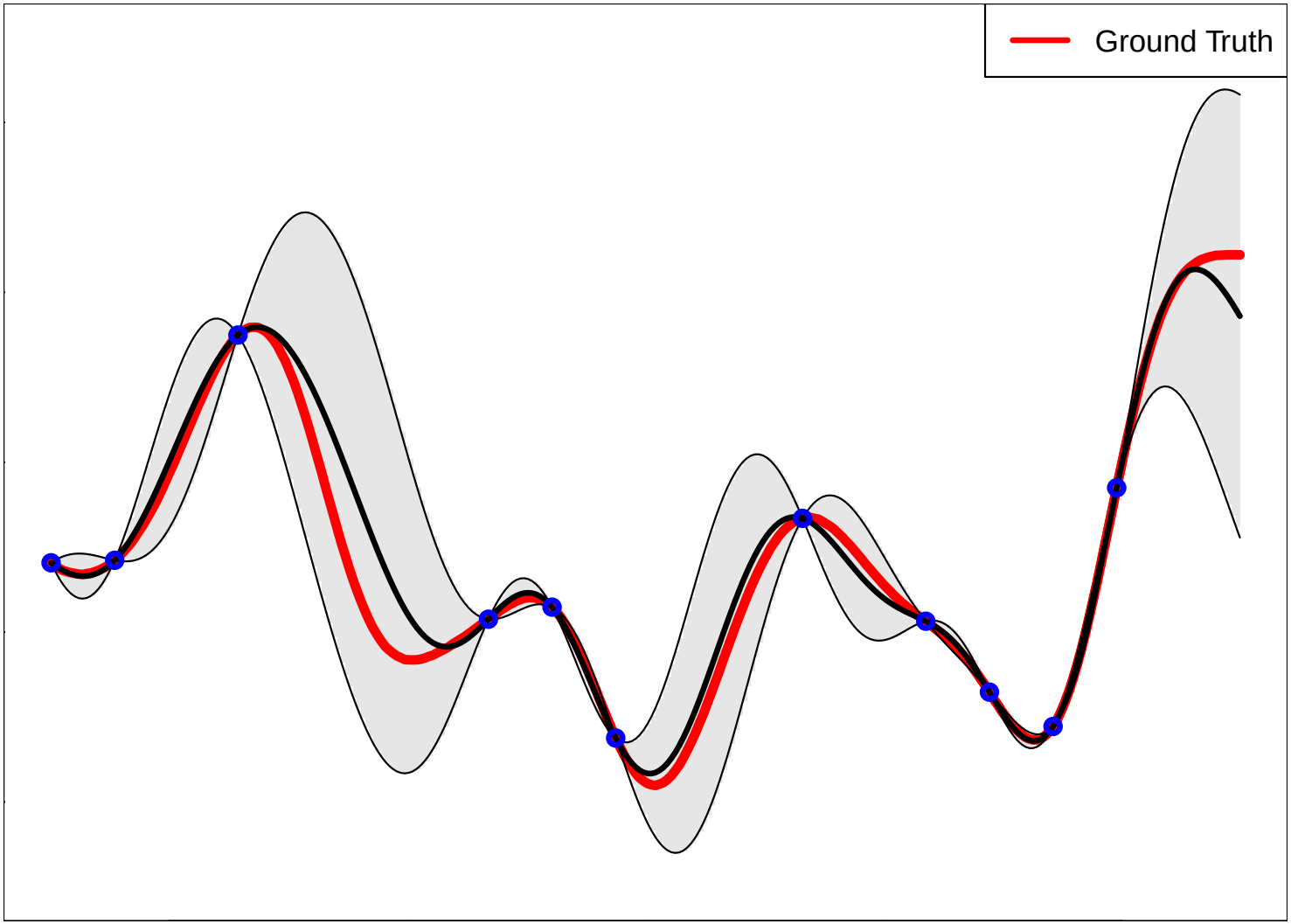

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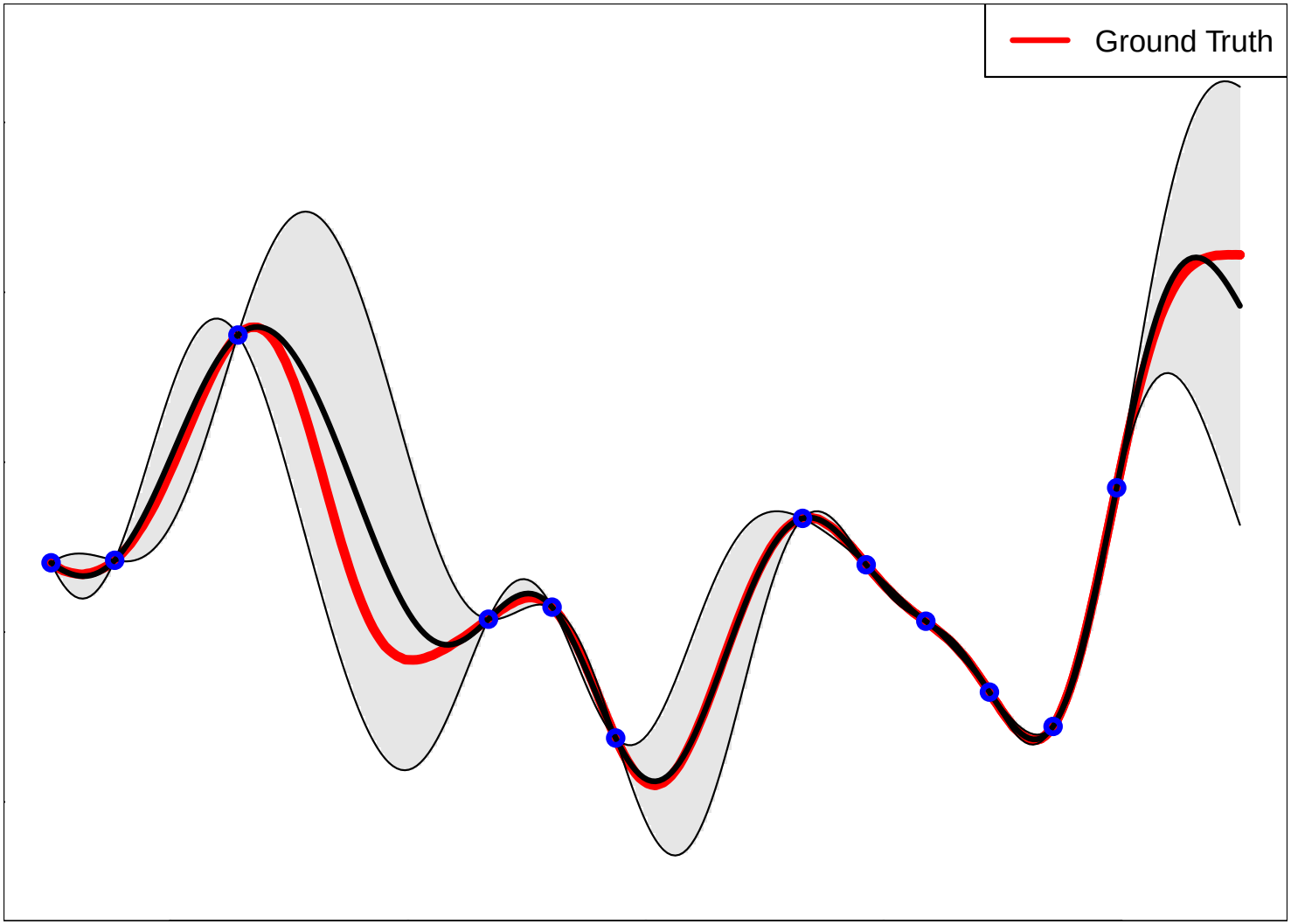

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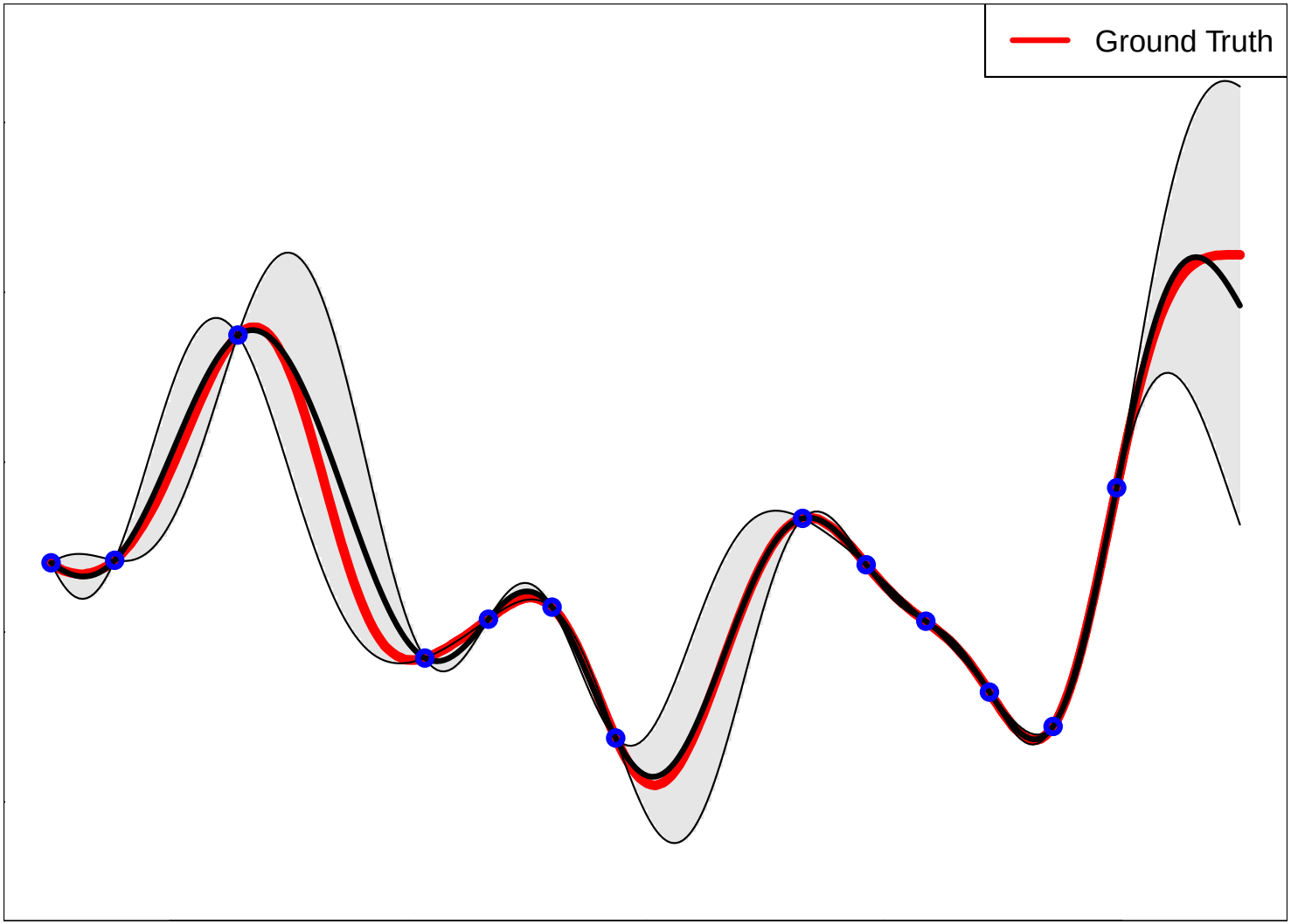

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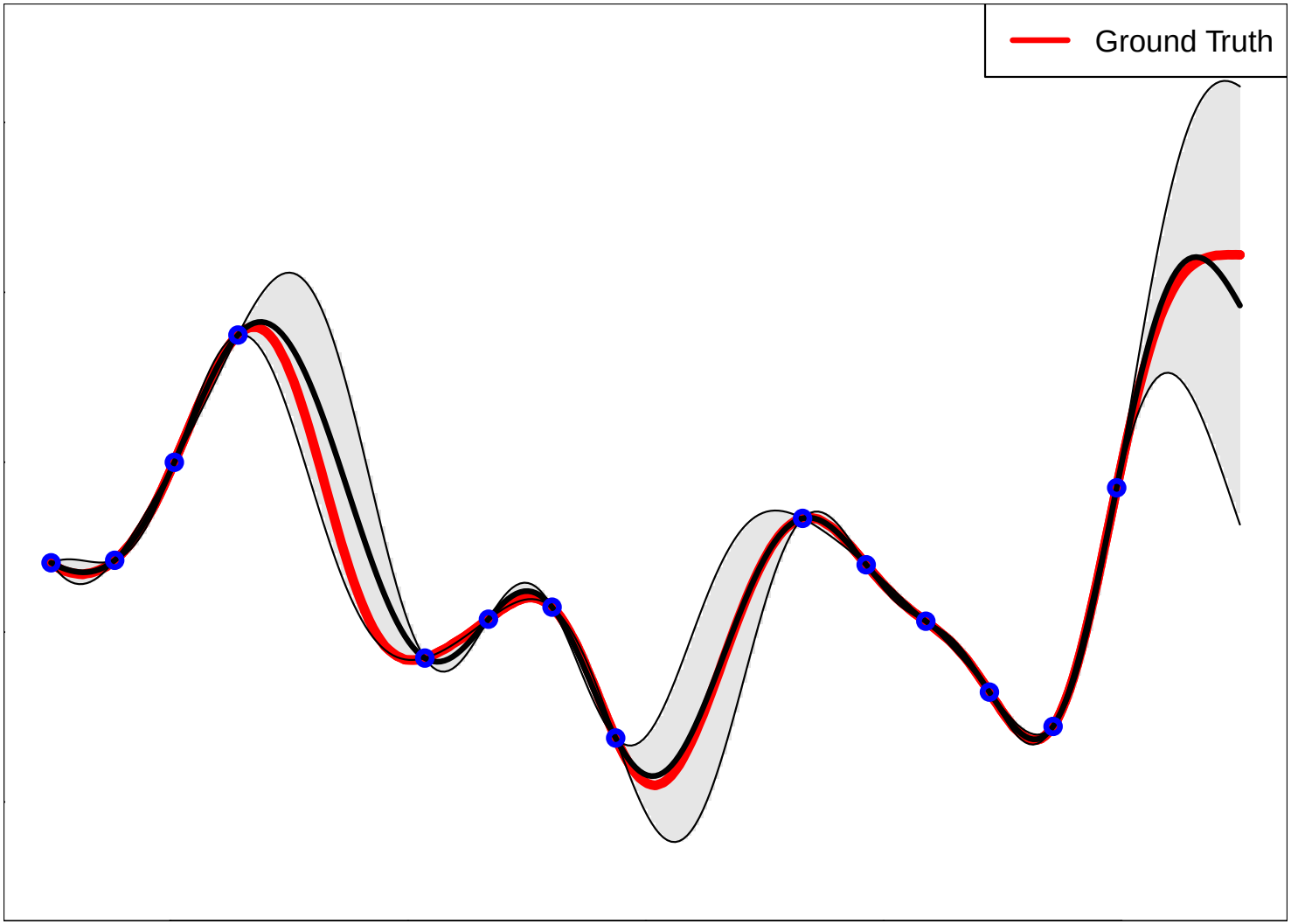

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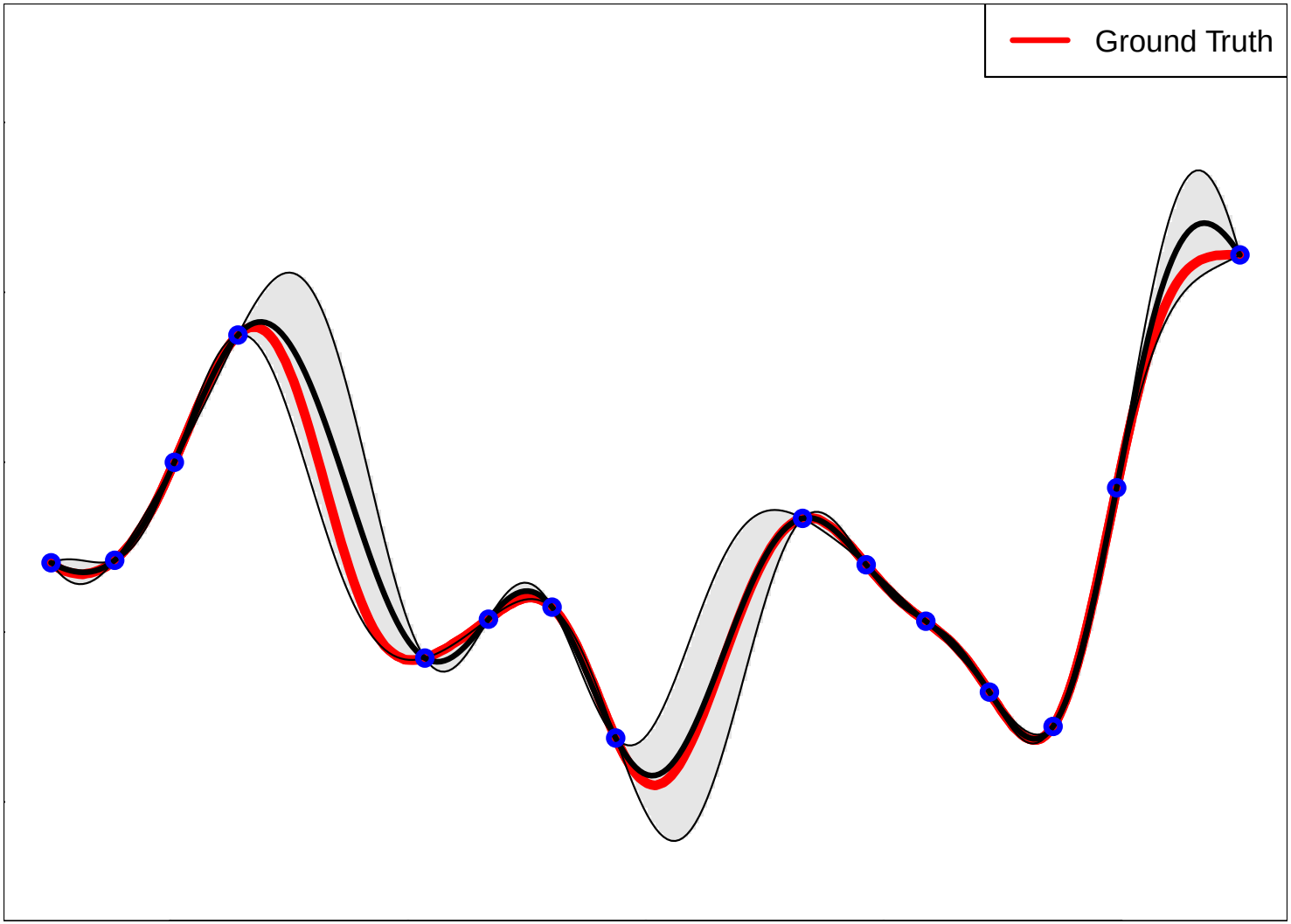

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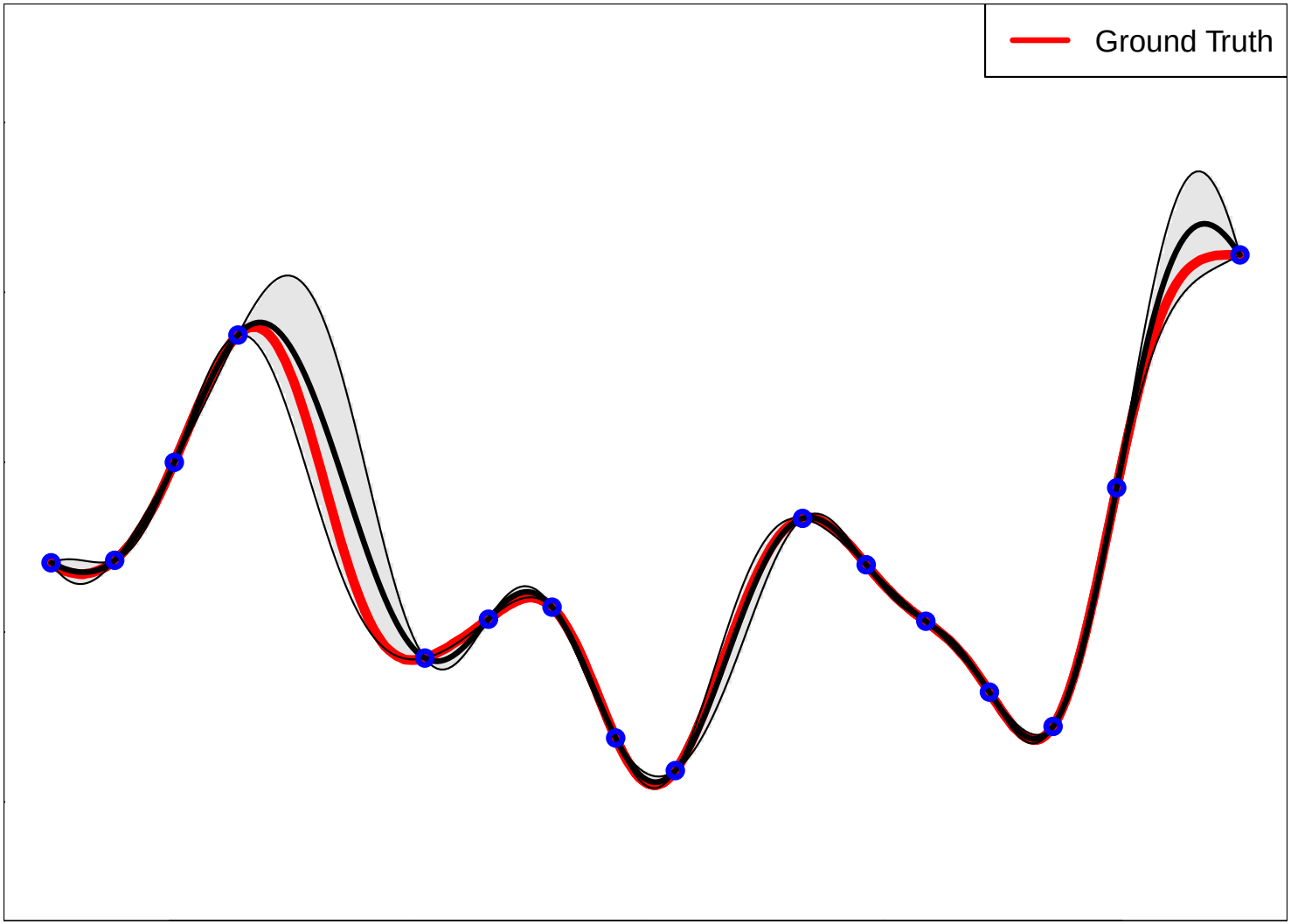

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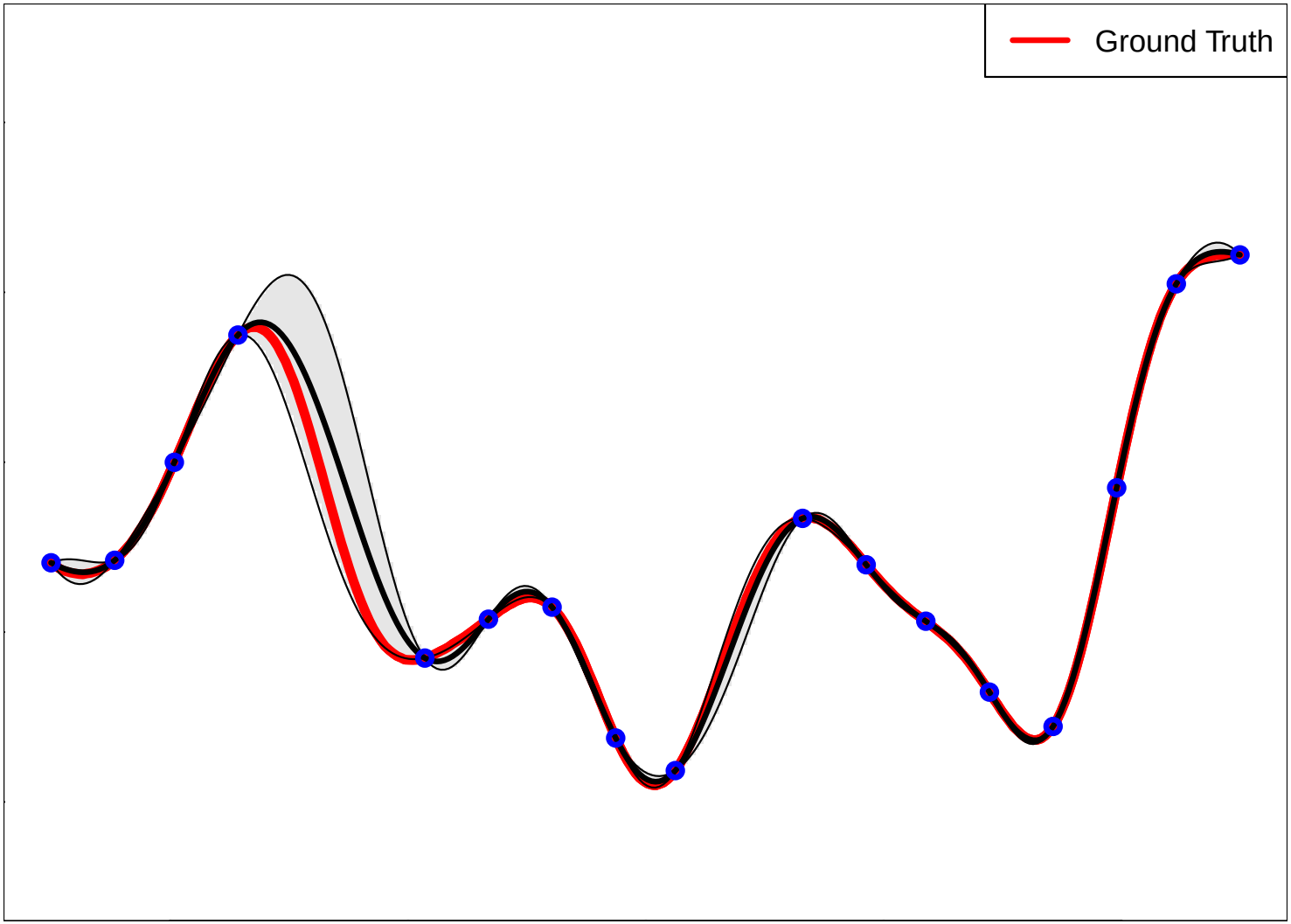

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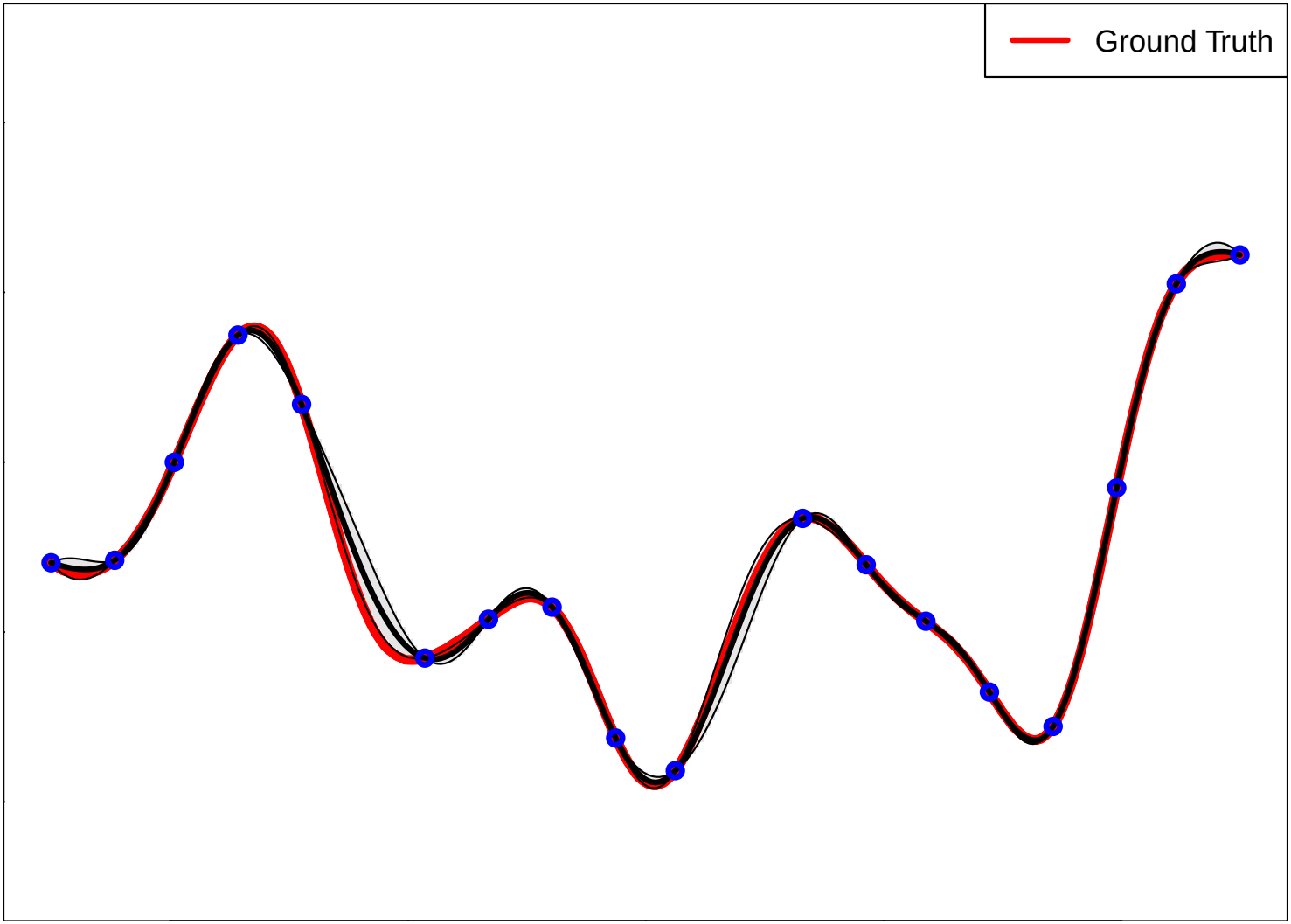

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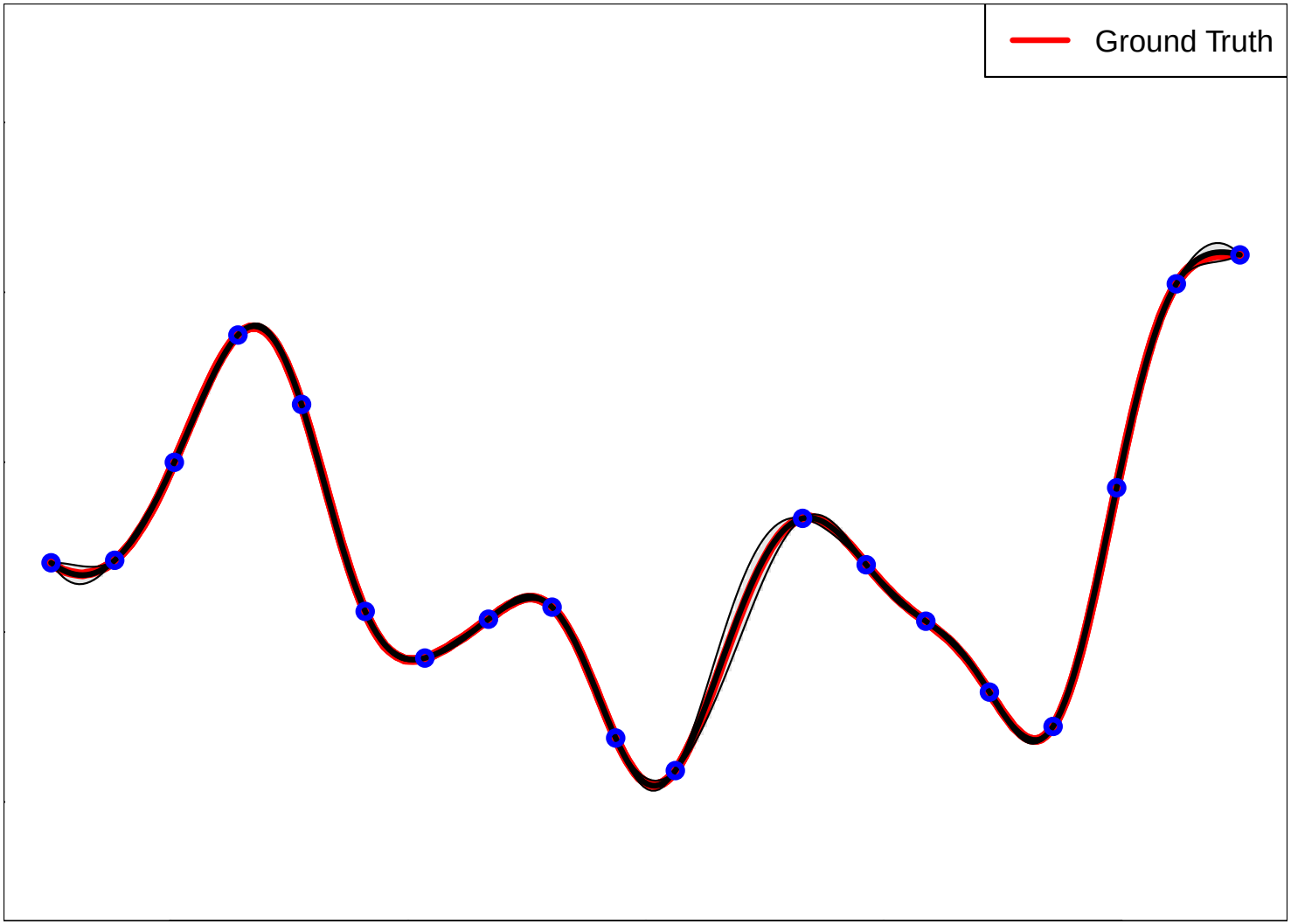

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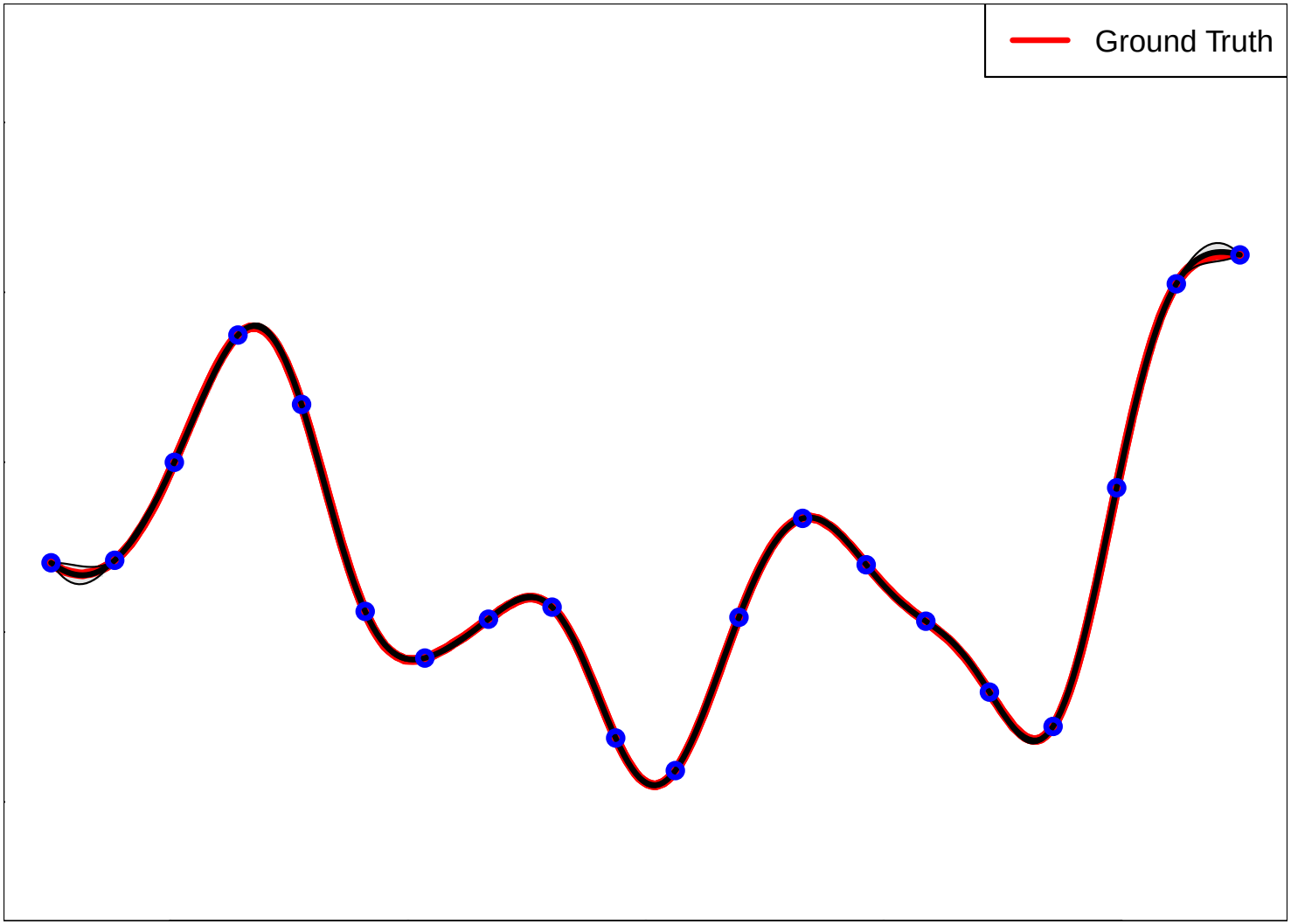

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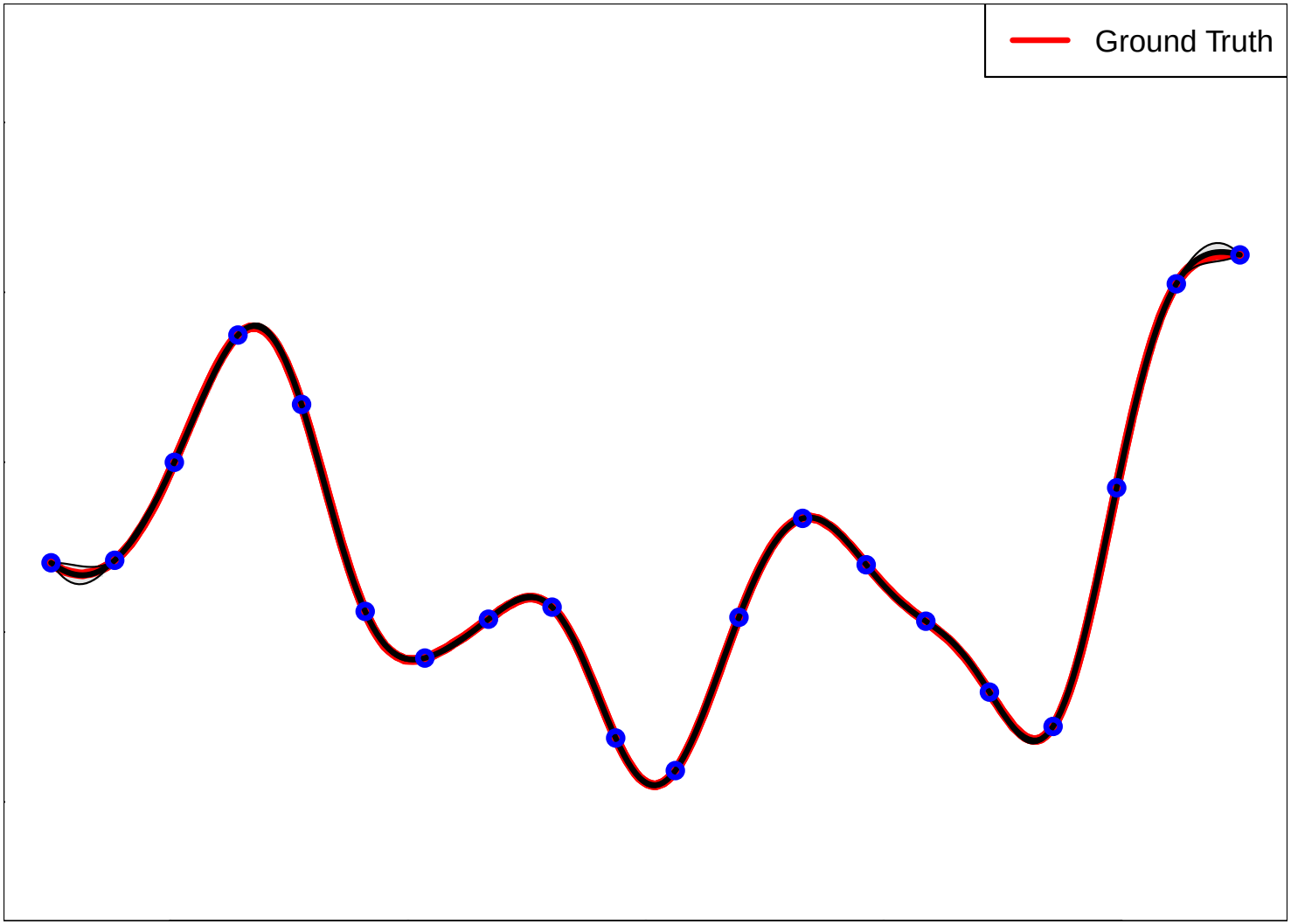


**The model becomes more flexible as we observe more data!**

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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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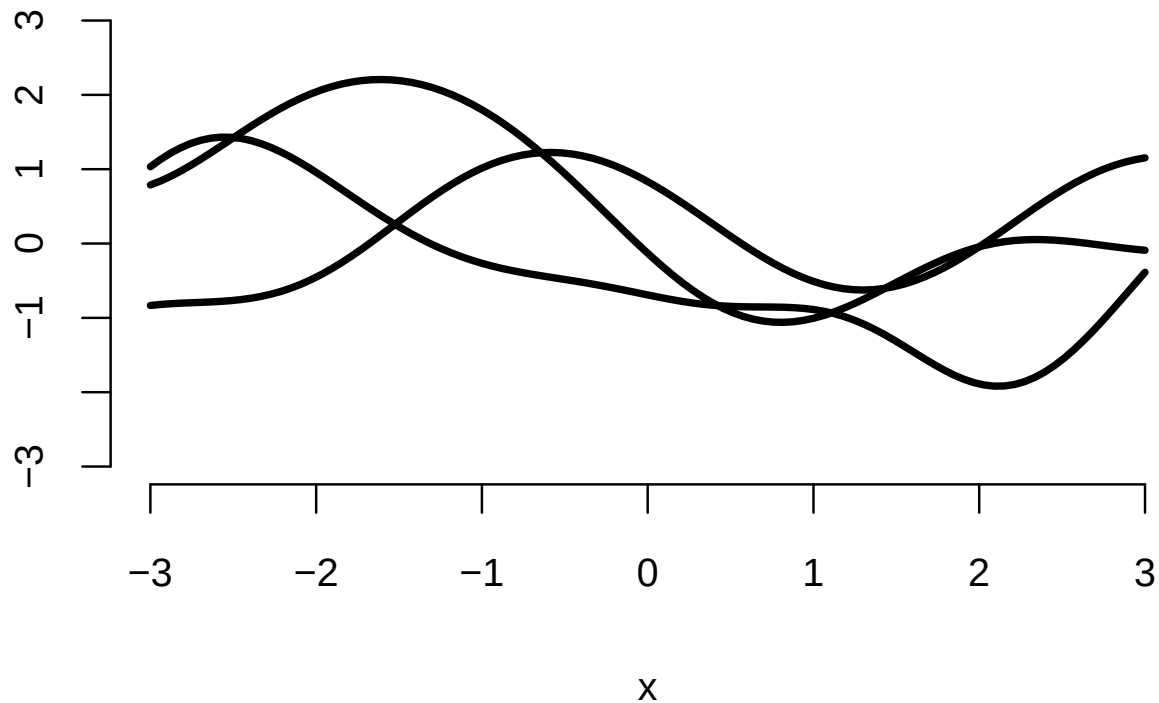

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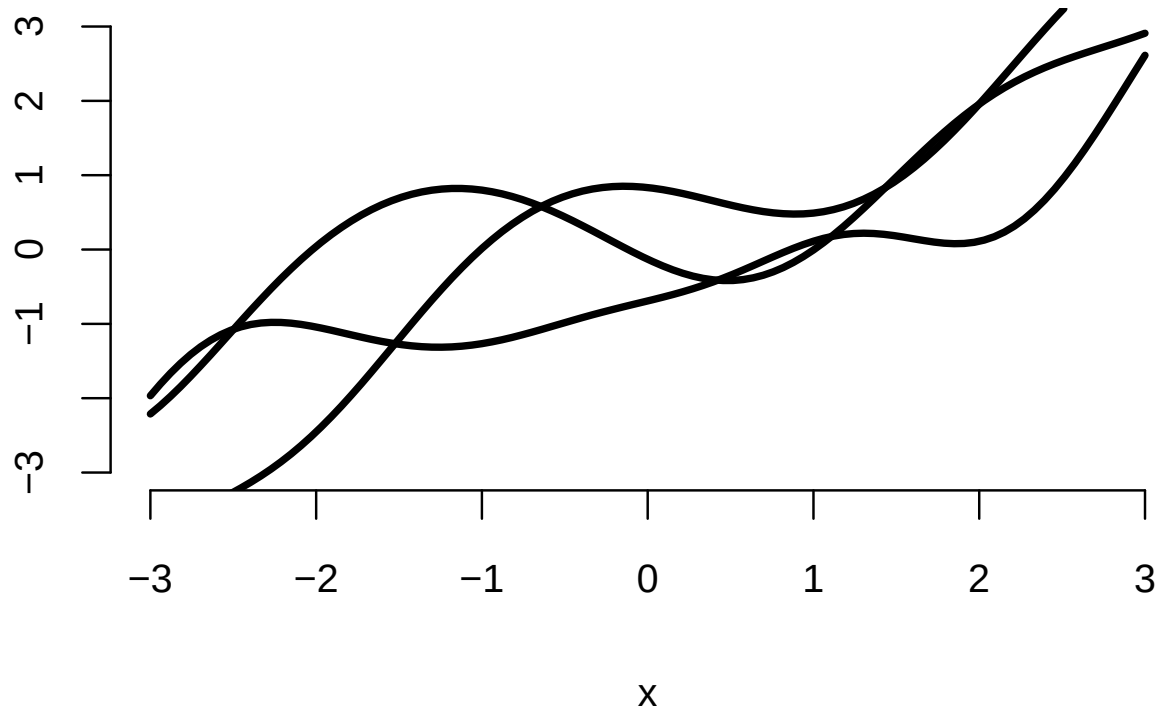

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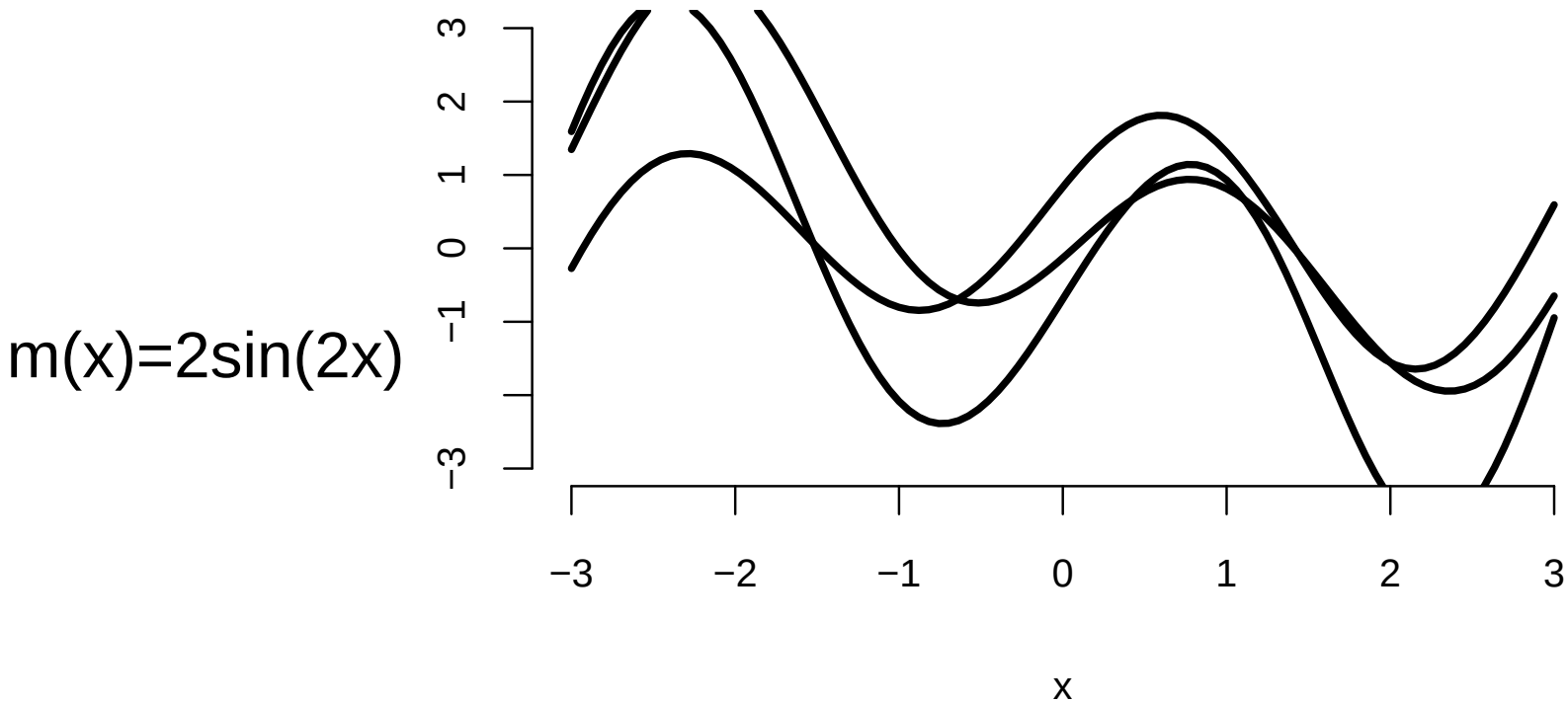

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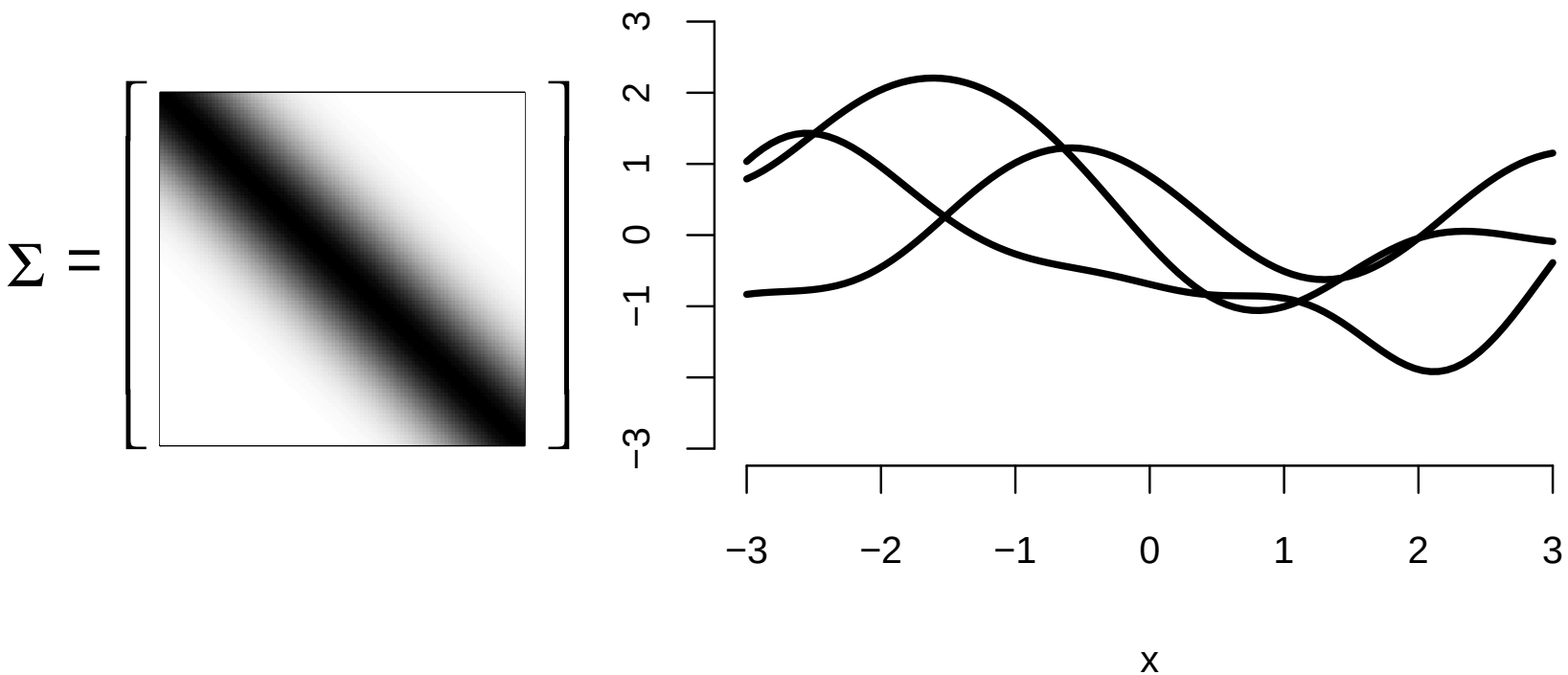

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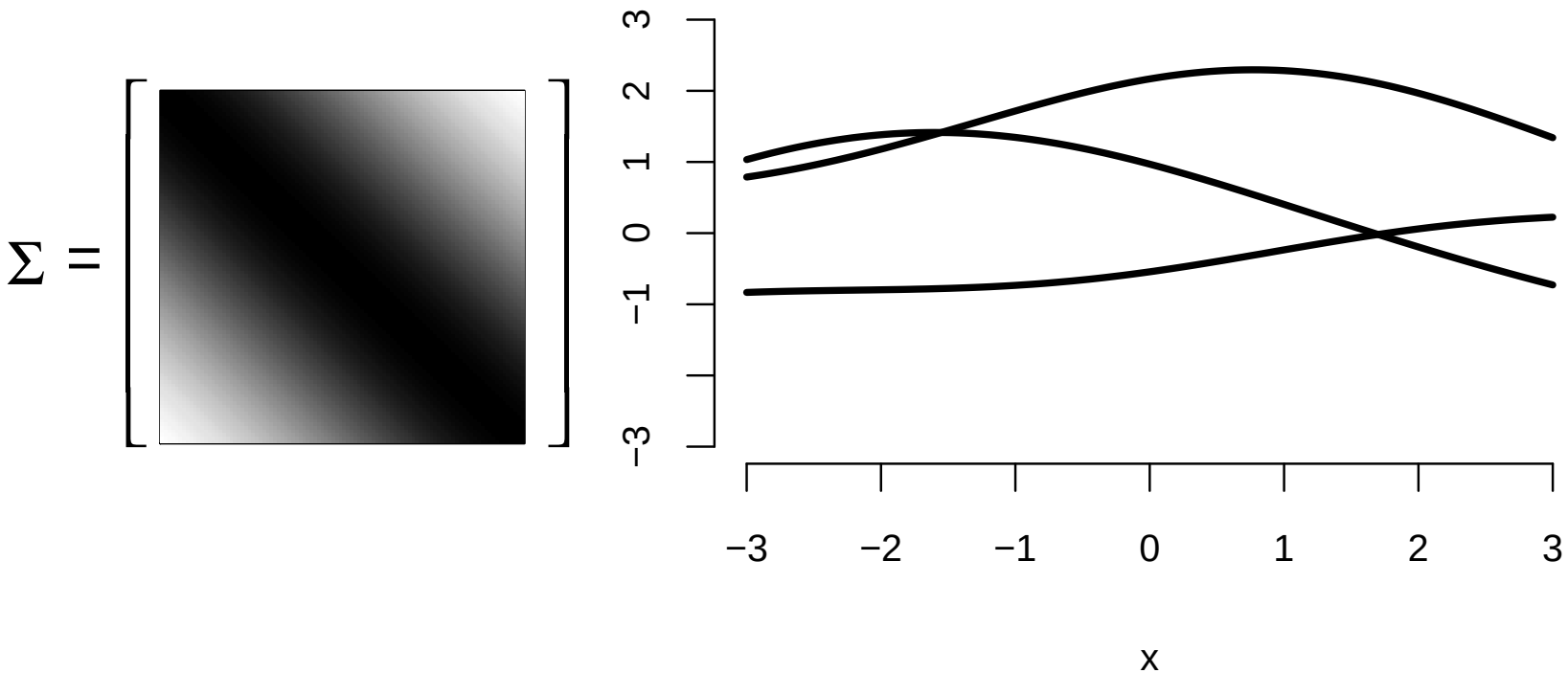

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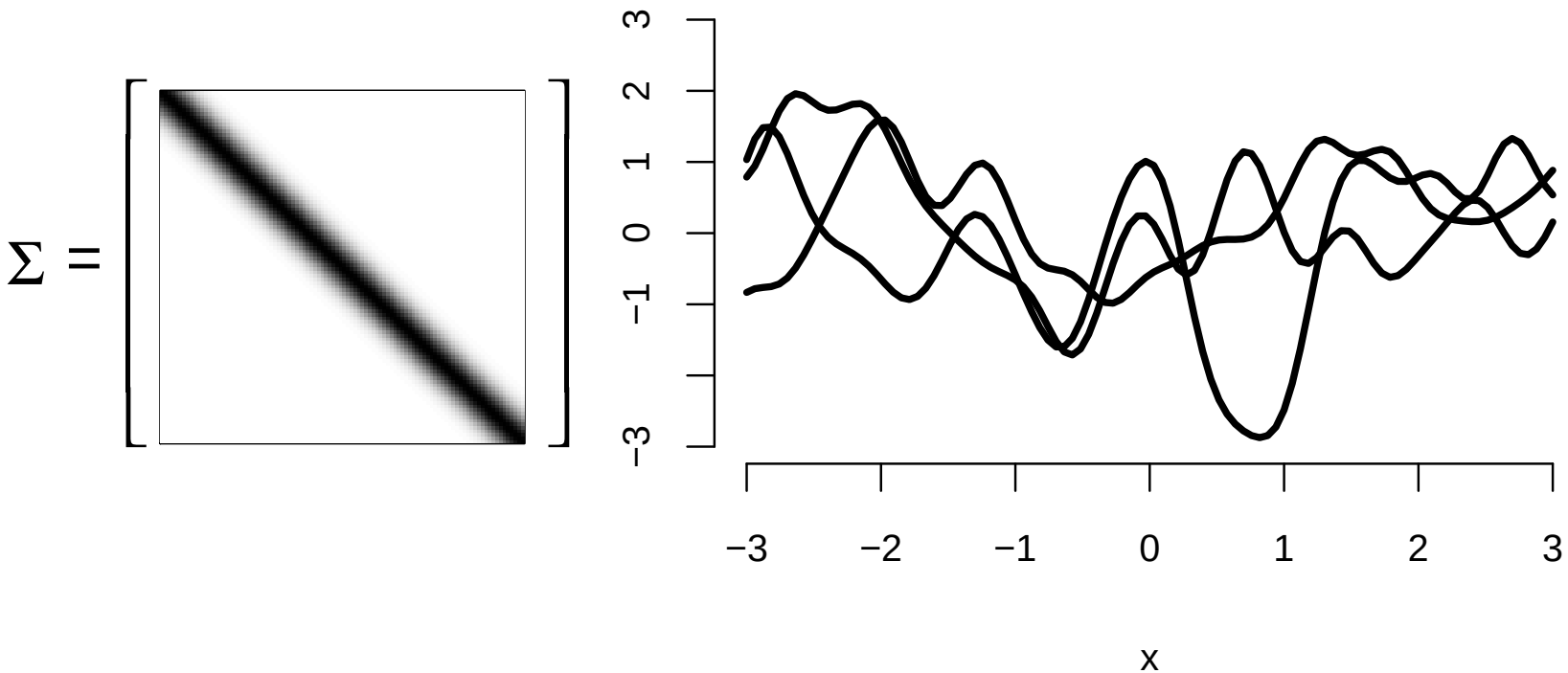

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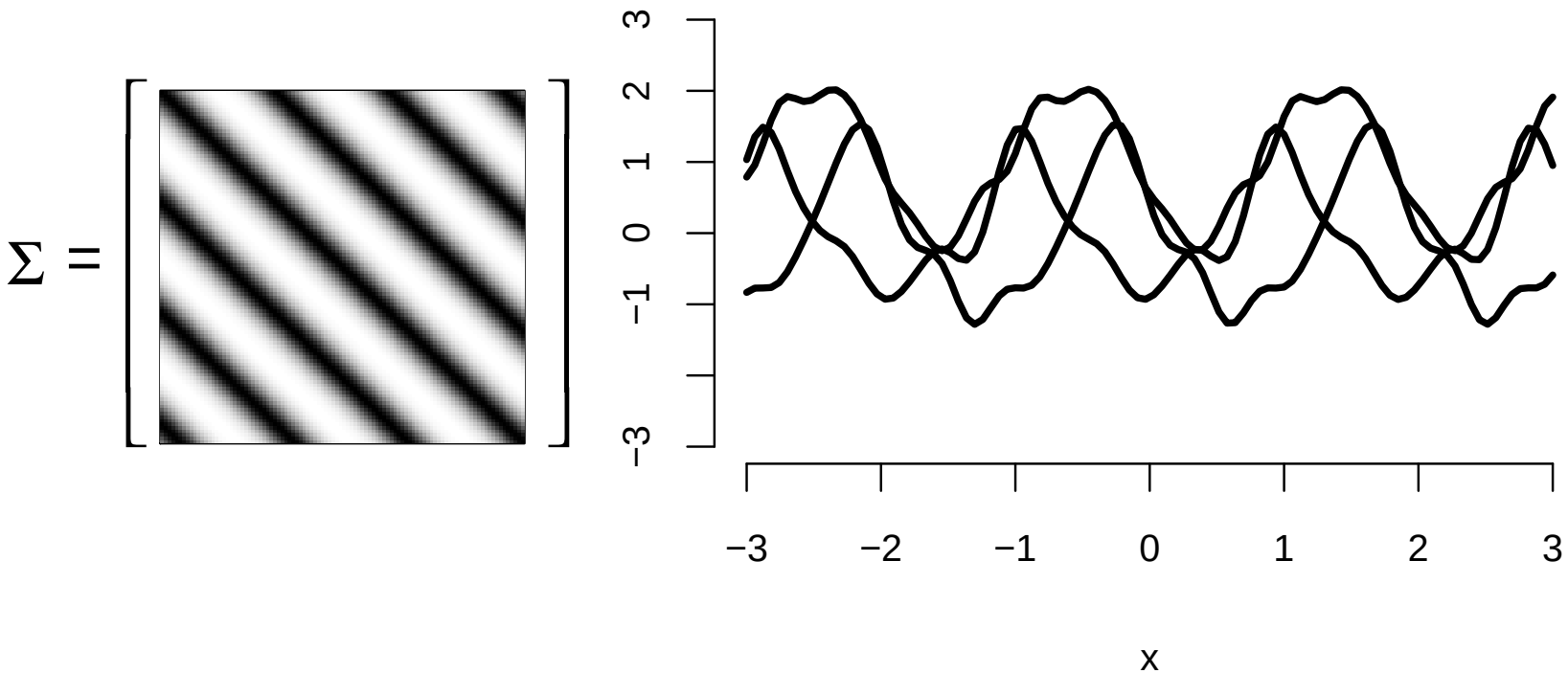

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# Marginalization

**If the GP mean has infinite length and the GP covariance matrix is $\infty \times \infty$, how do we represent a GP on a computer?**

We can use the marginalization property of distributions:

$$p(\mathbf{y}_1) = \int p(\mathbf{y}_1, \mathbf{y}_2) d\mathbf{y}_2 \,,$$

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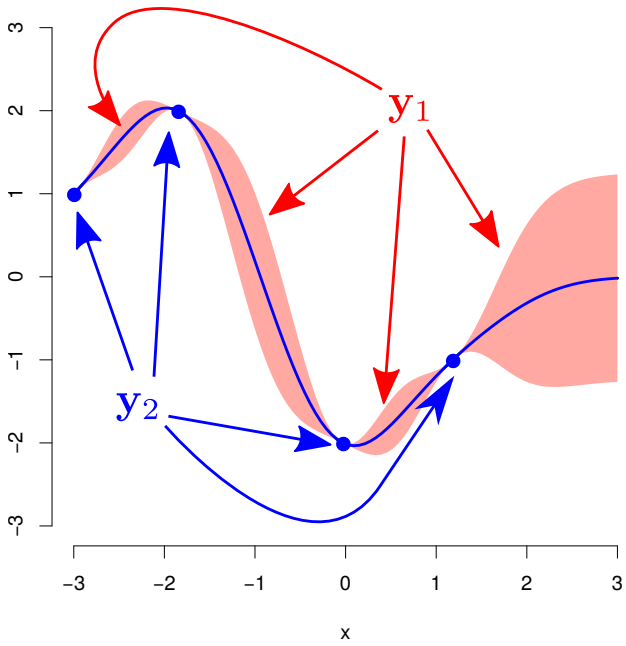
**We only need to work with finite sets of random variables!**

# Computing the Predictive Distribution



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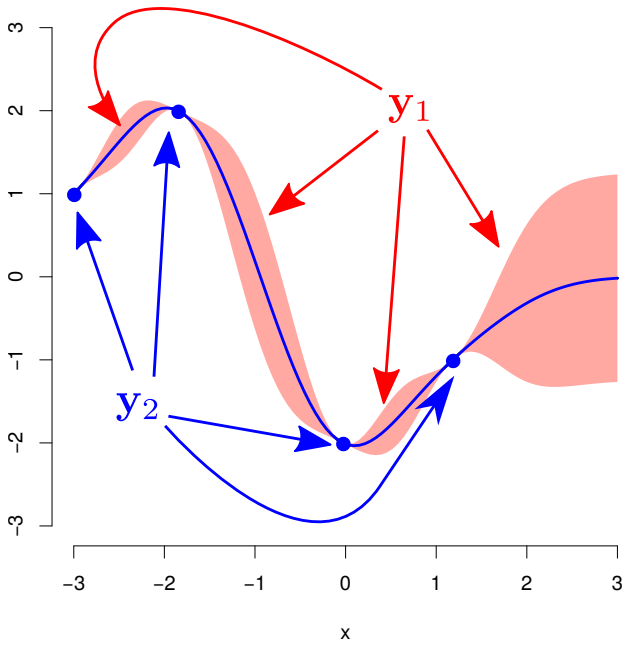


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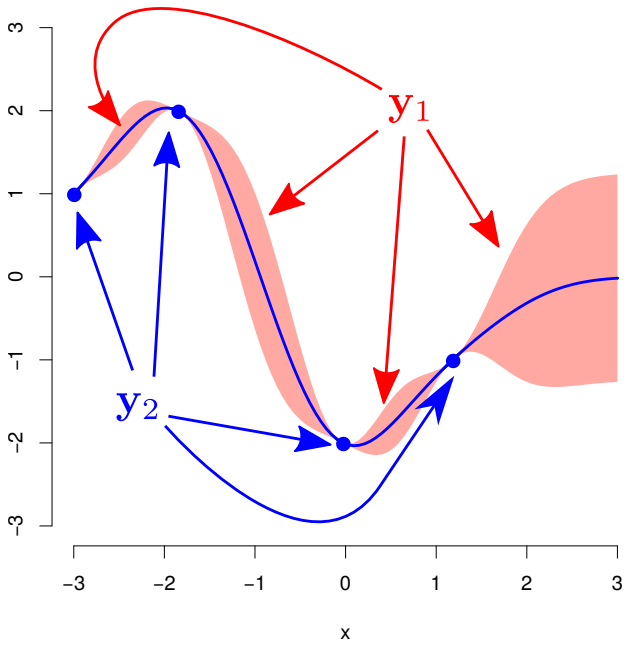


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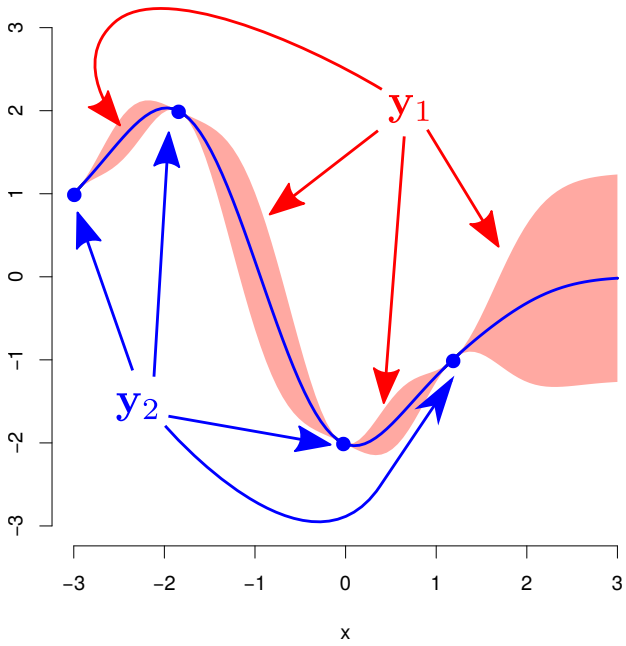


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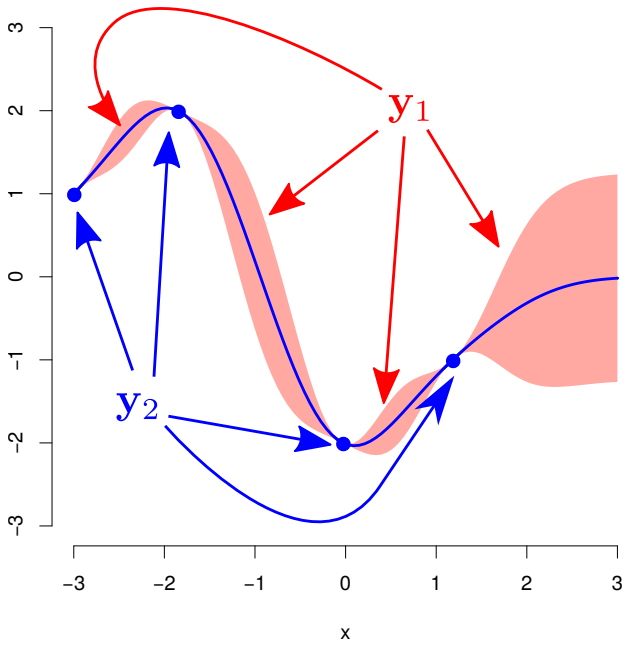


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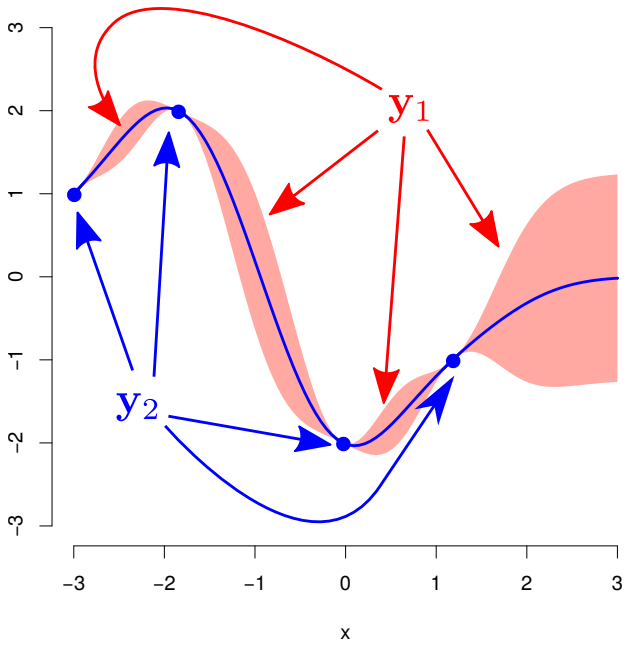


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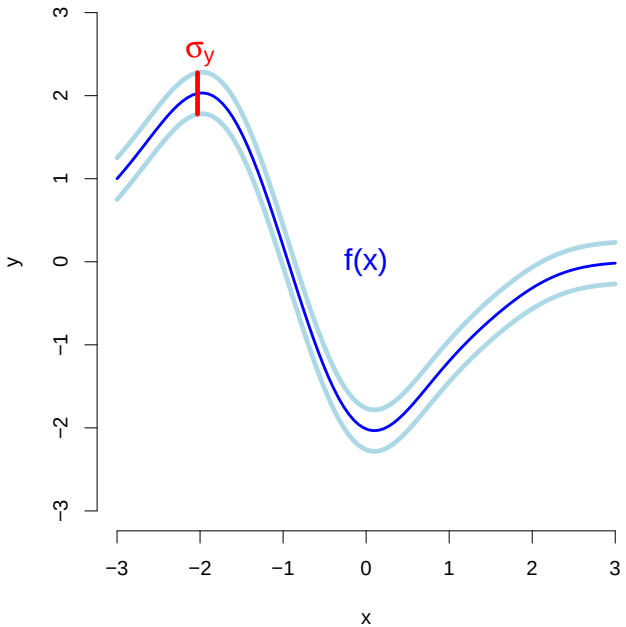
- The predictive covariance is **more confident** than the prior!.

# Considering Additive Noise

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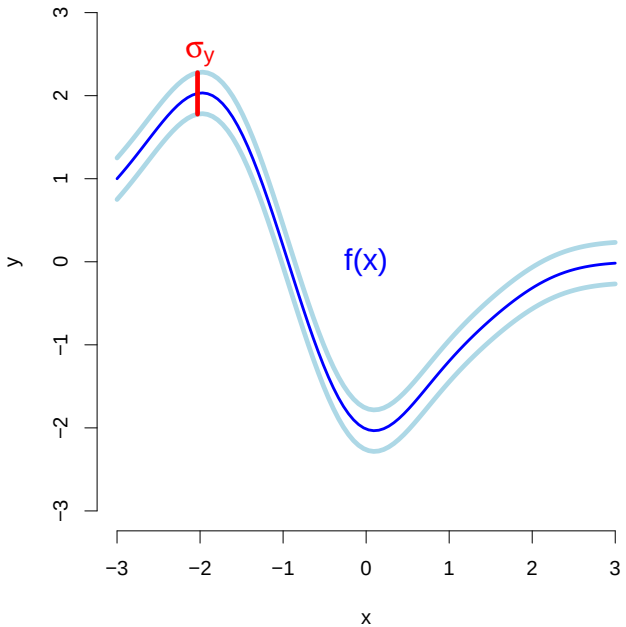


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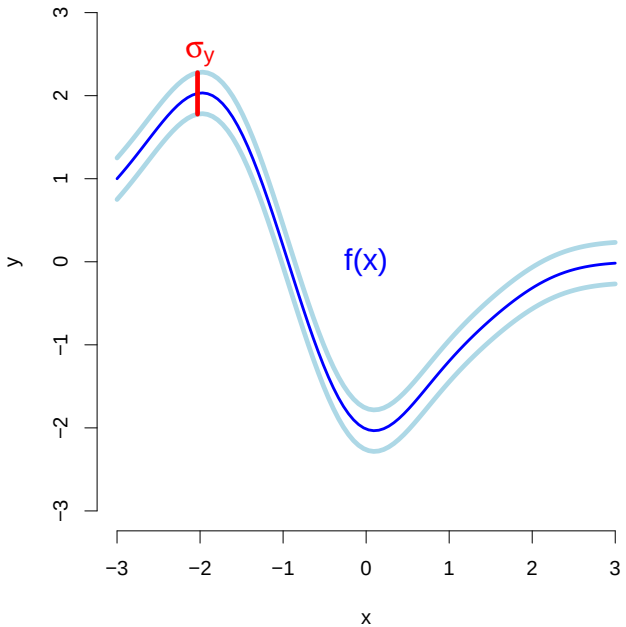


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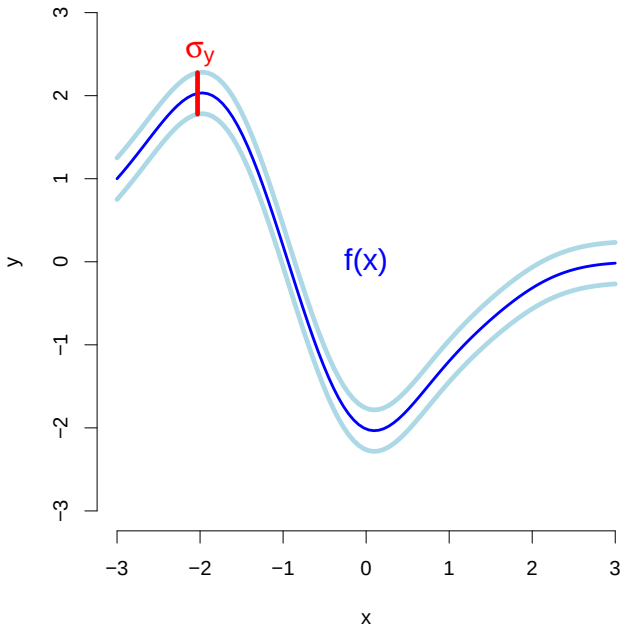


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# An Example of a Covariance Function

**Squared Exponential**: $$C(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left\{-\frac{1}{2}\sum_{j=1}^{d}\left(\frac{x_j - x_j'}{l_j}\right)^2\right\}$$

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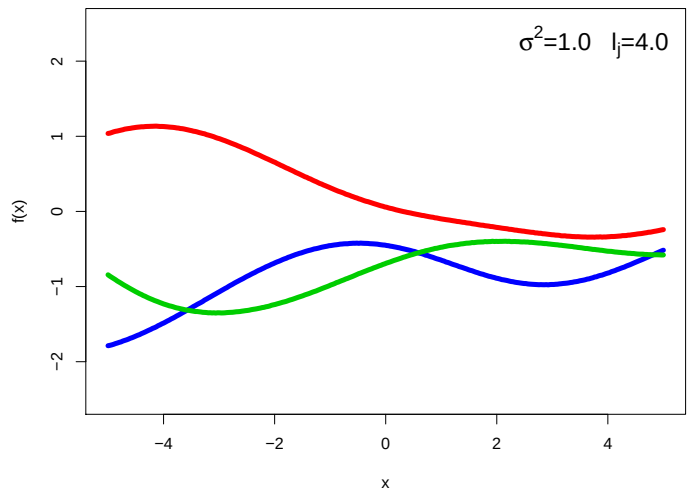

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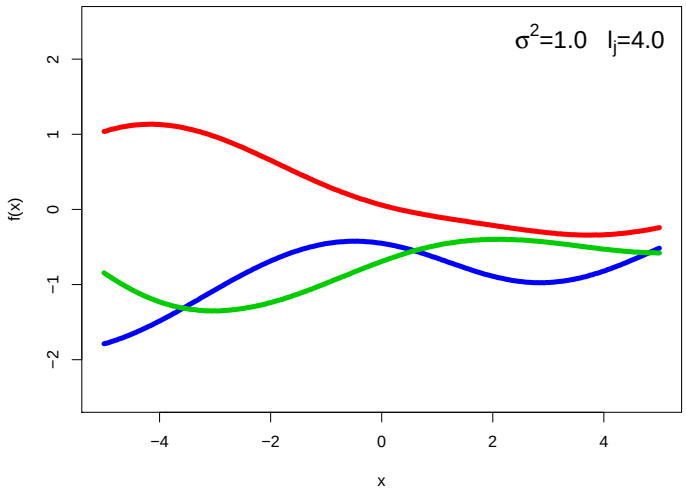


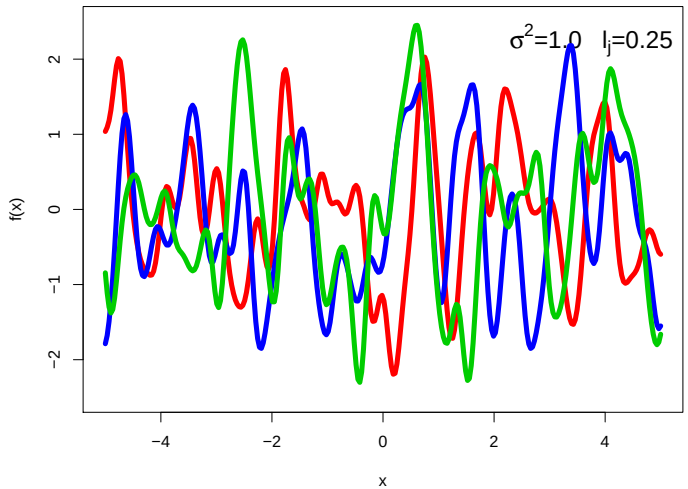

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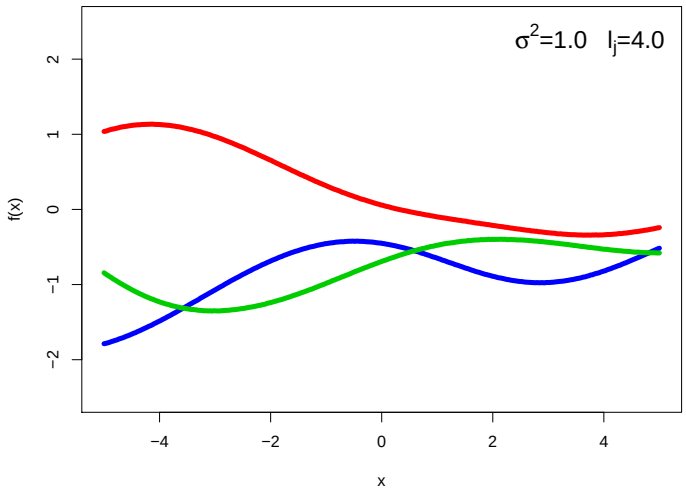


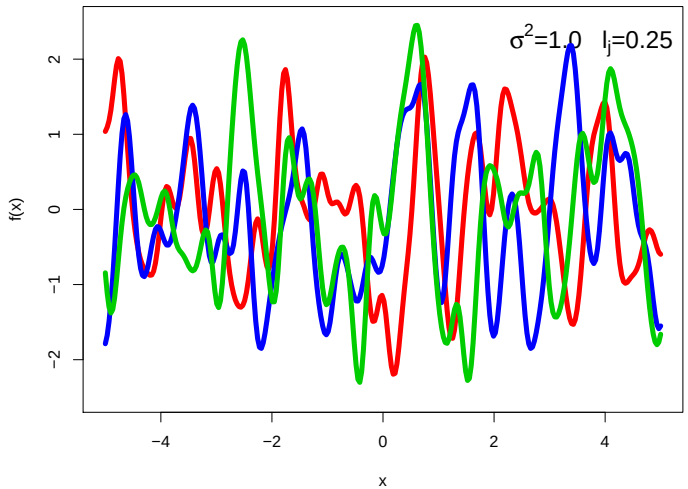


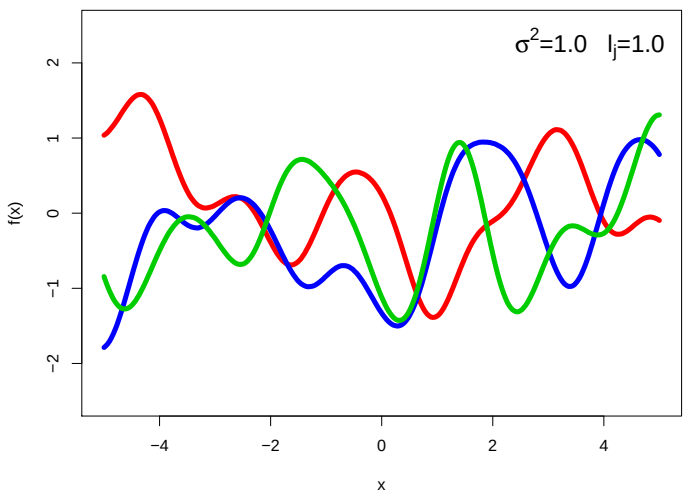

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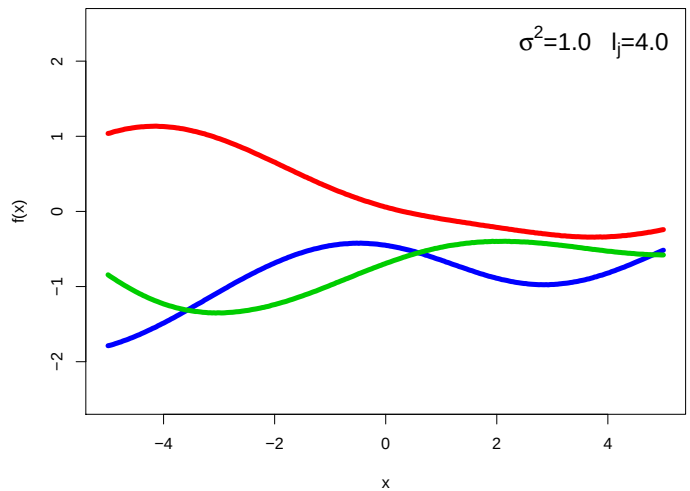


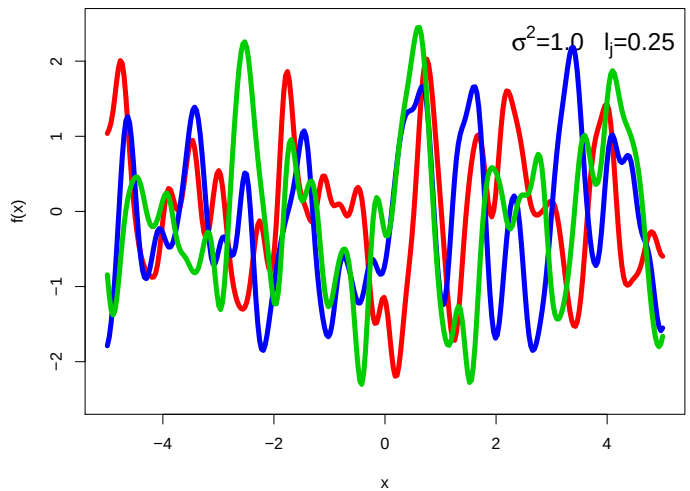


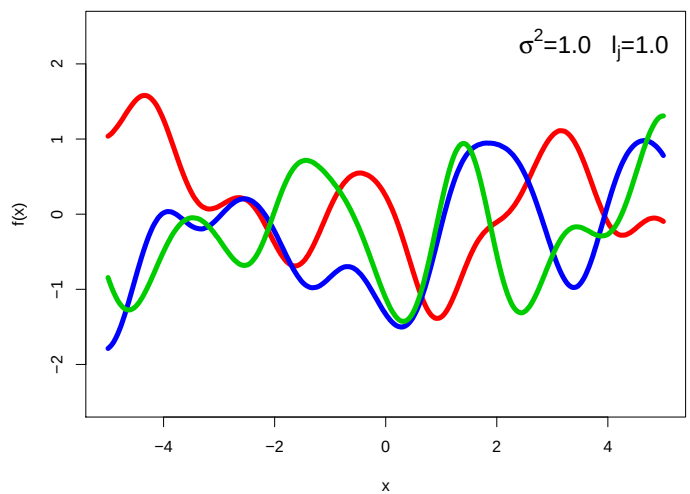


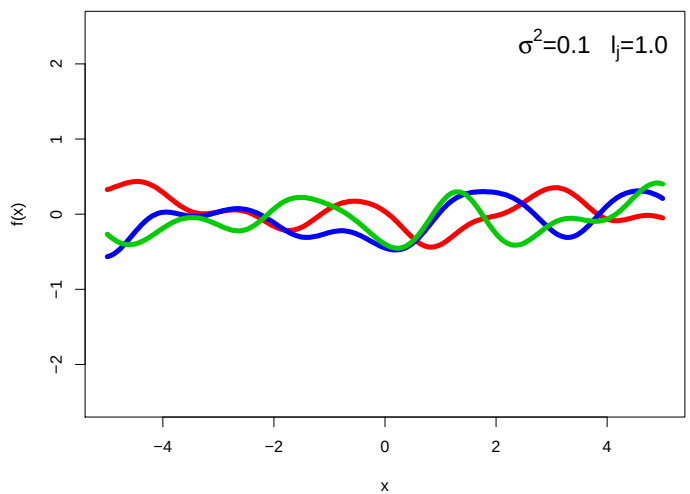

**Run the first cells of the notebook to sample functions from a GP prior and complete task 1!**

# How do we choose the hyper-parameters?

**Intuition**: find parameters $\theta$ that are compatible with the observed data.

$$p(\theta|\mathbf{y}) = \frac{p(\mathbf{y}|\theta)p(\theta)}{p(\mathbf{y})}$$

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

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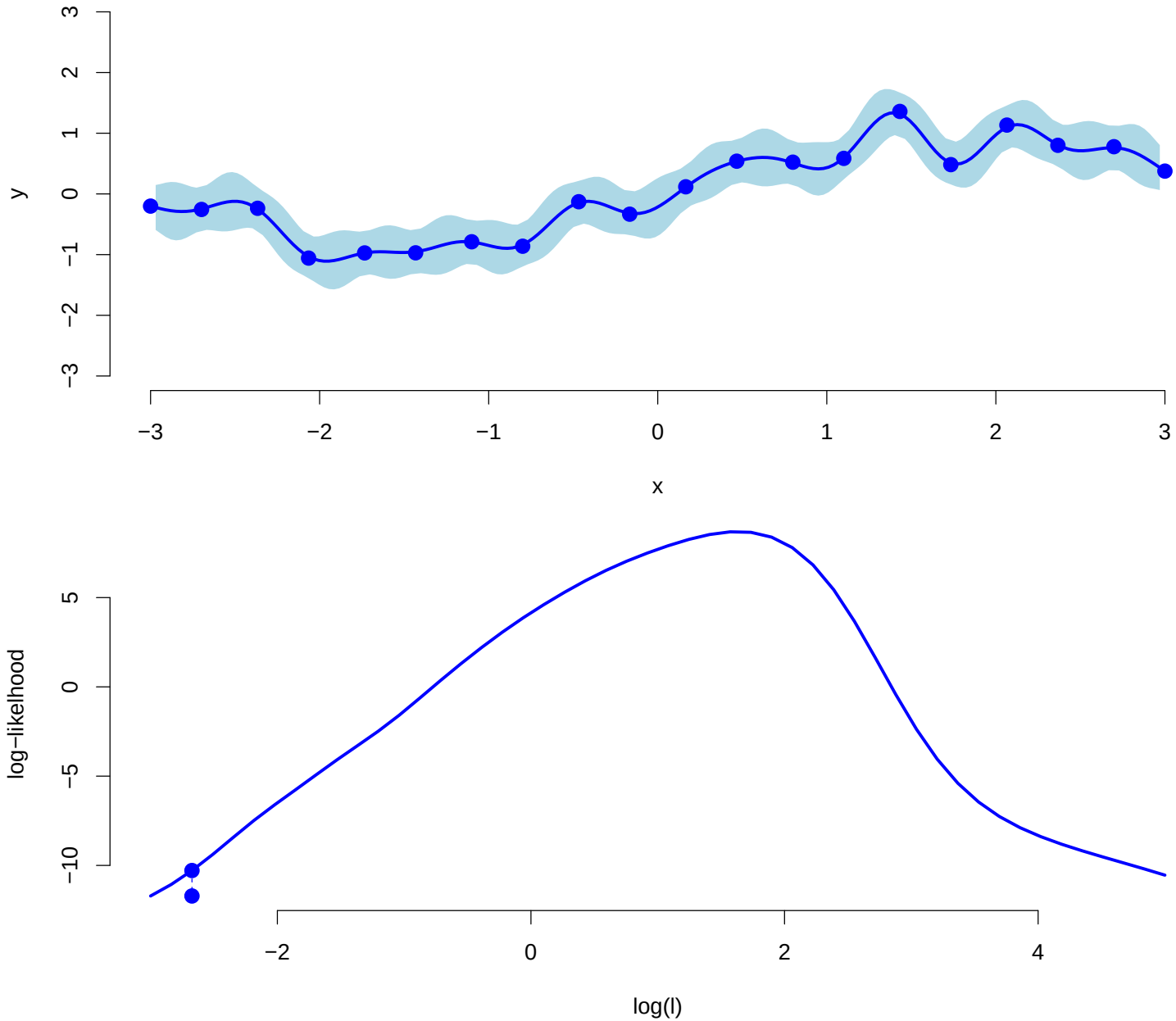

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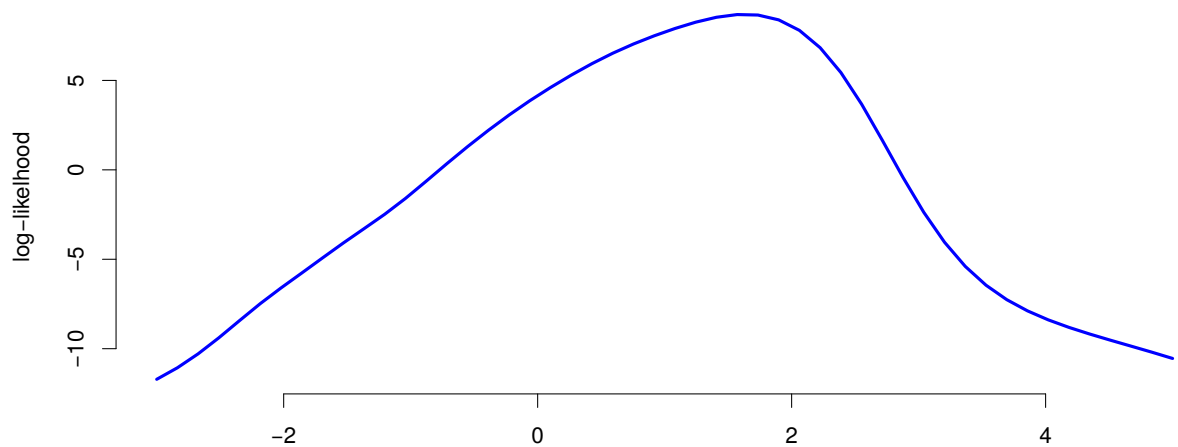

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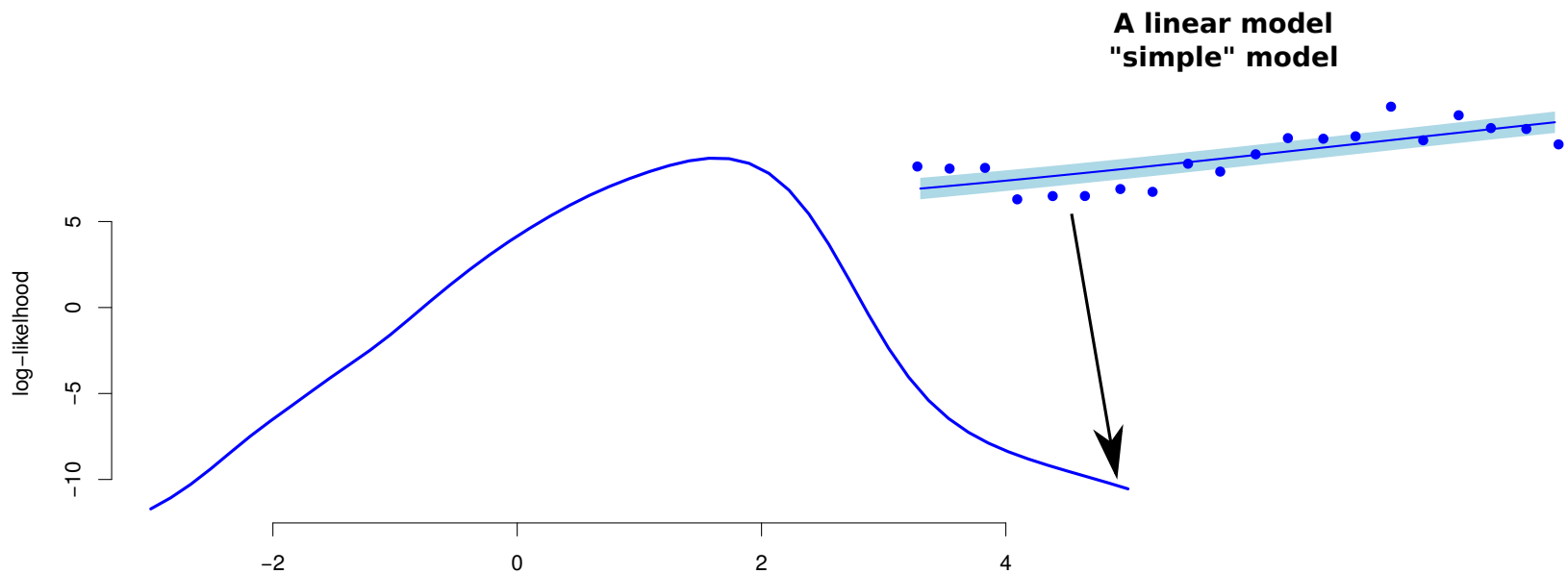

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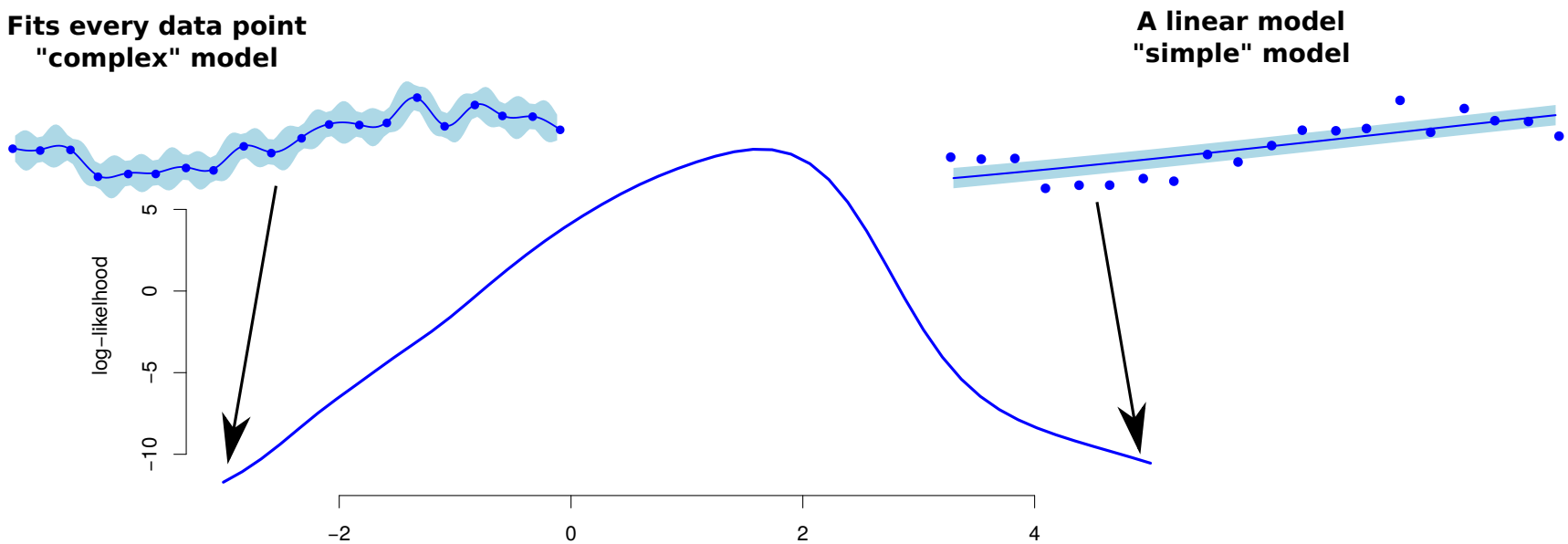

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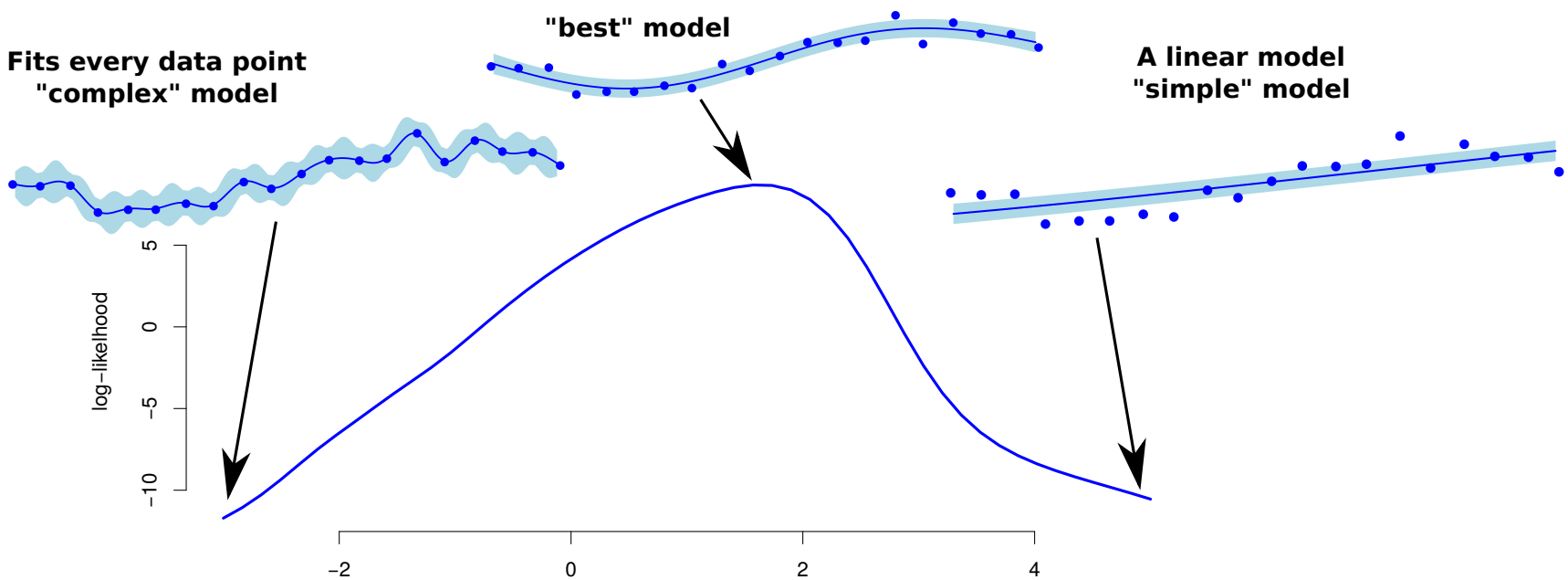

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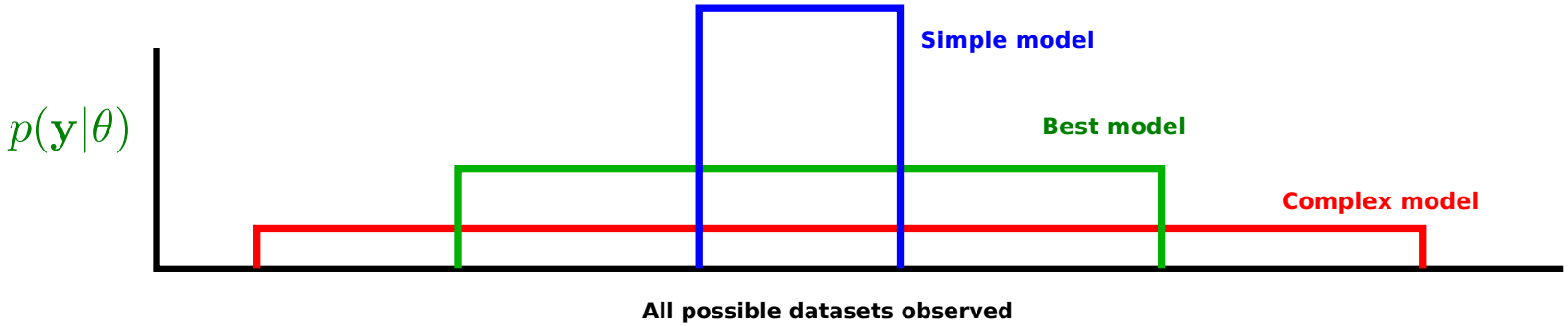


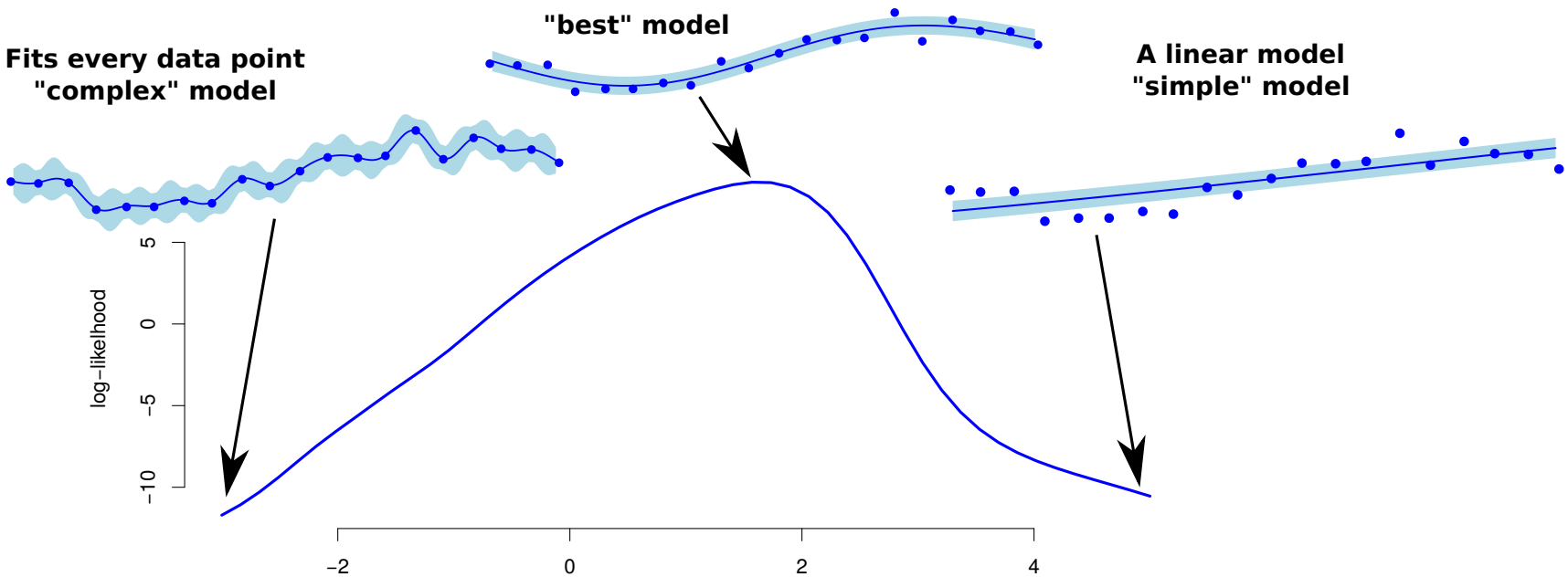

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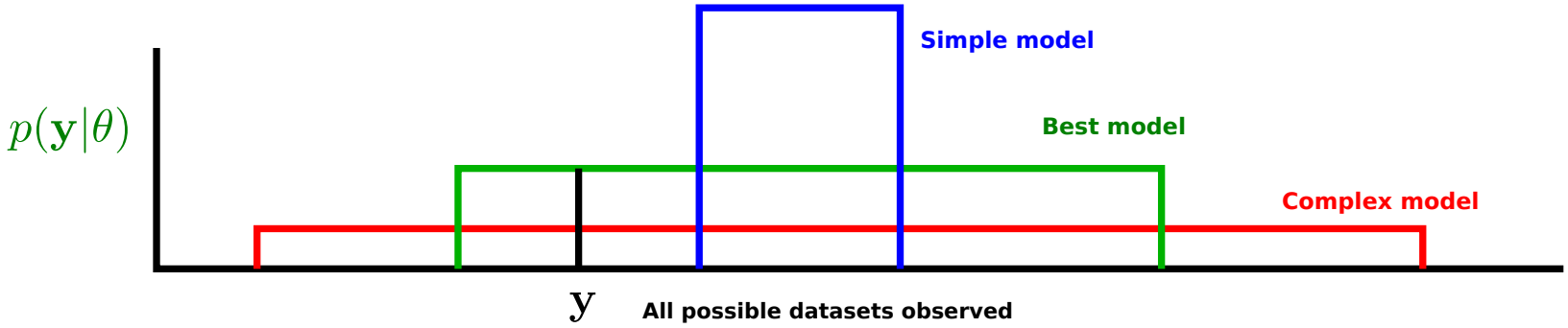


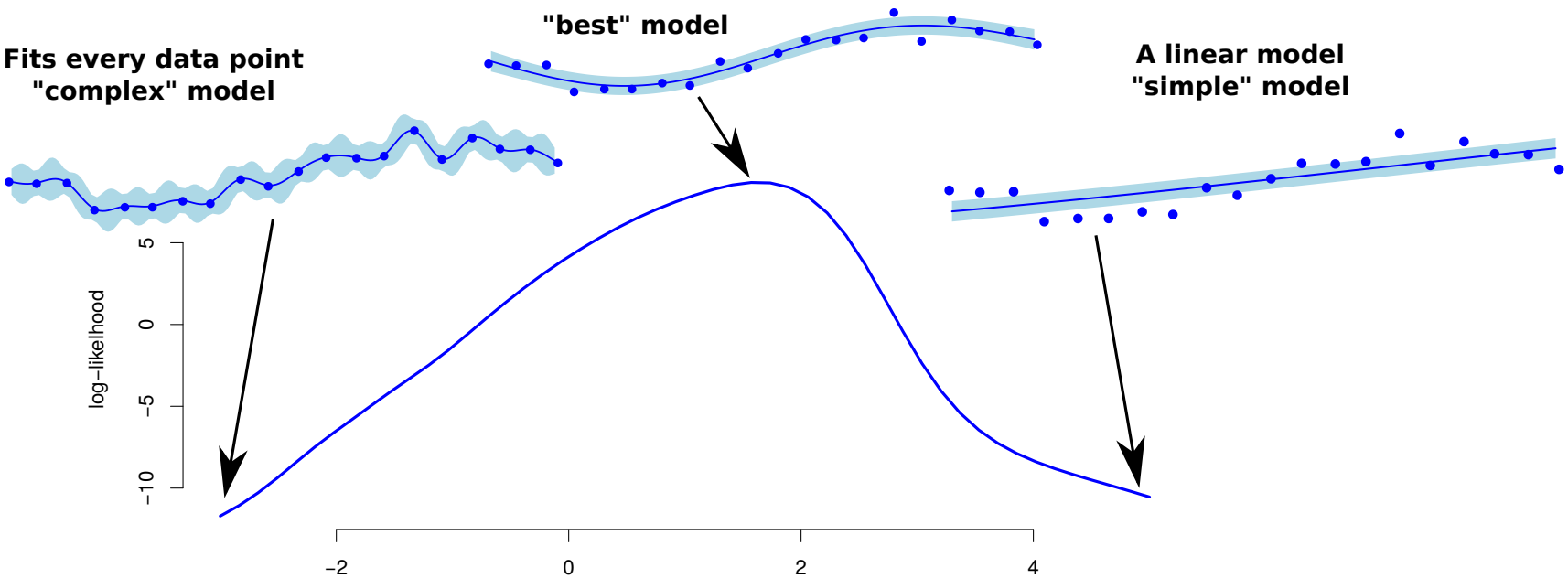

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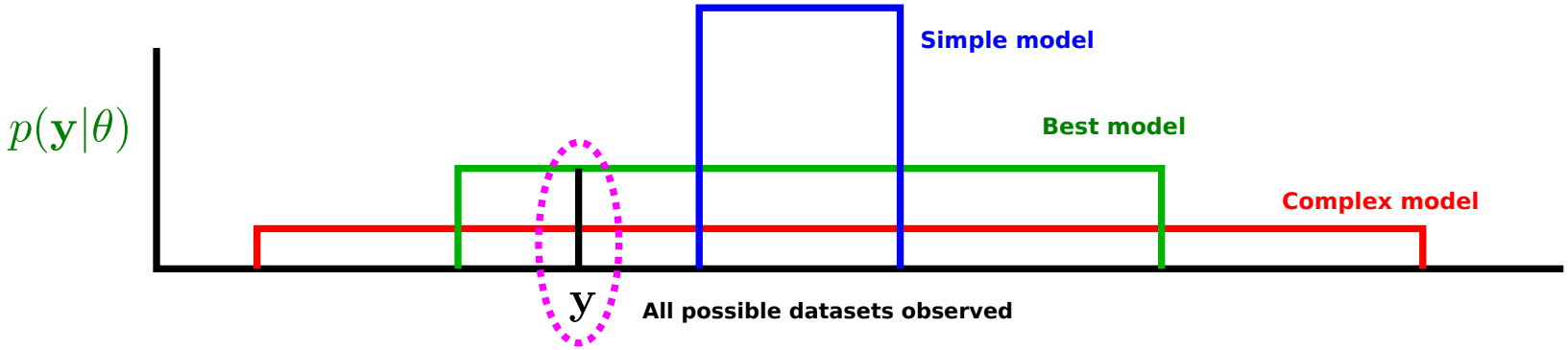


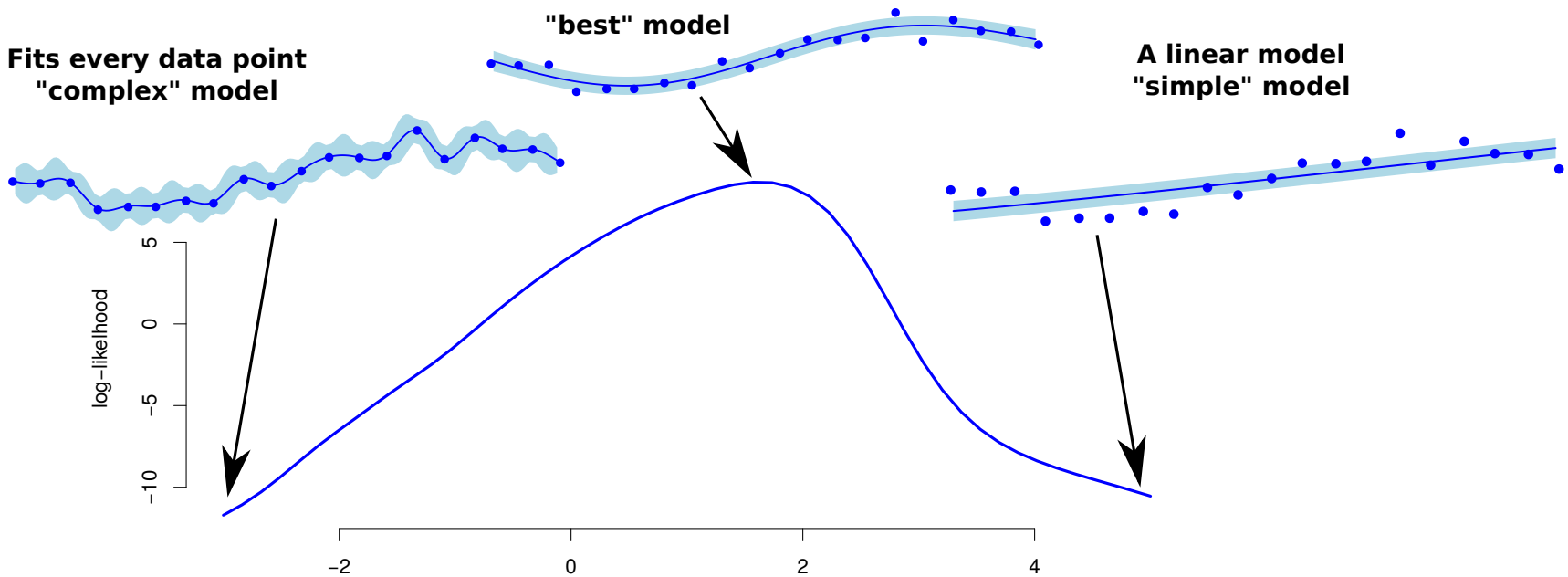

**Run the cells of the provided notebook to find good model hyper-parameters!**

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**Compare the predictive distribution with and with-out optimization of the hyper-parameters.**

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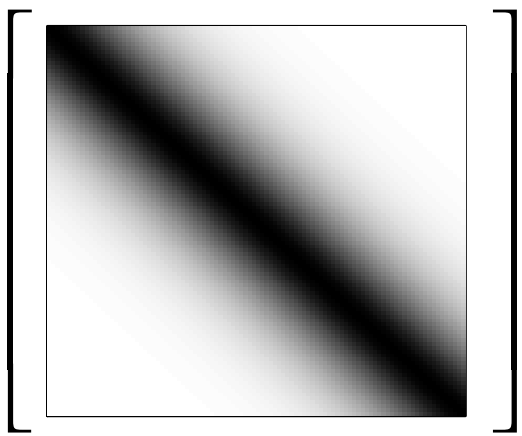
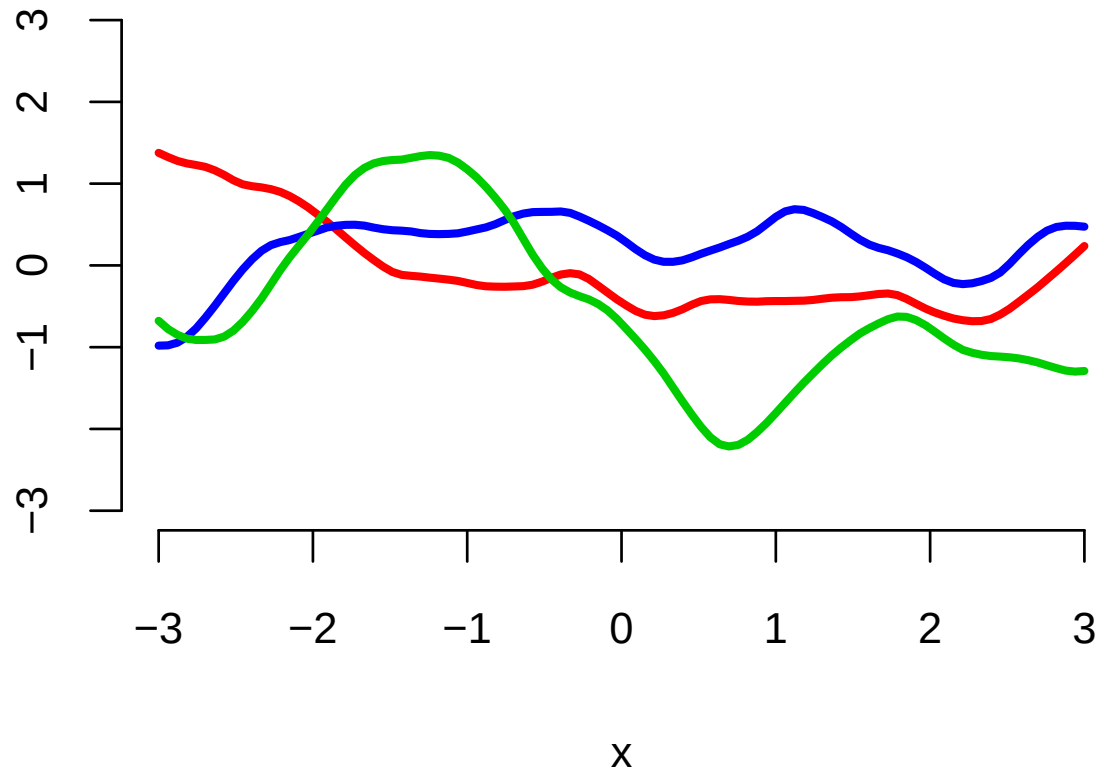
$\Sigma =$ 



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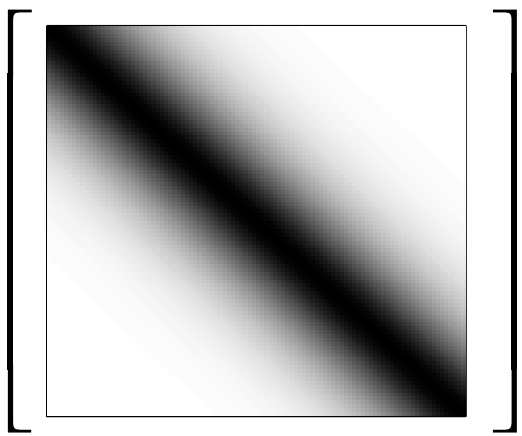
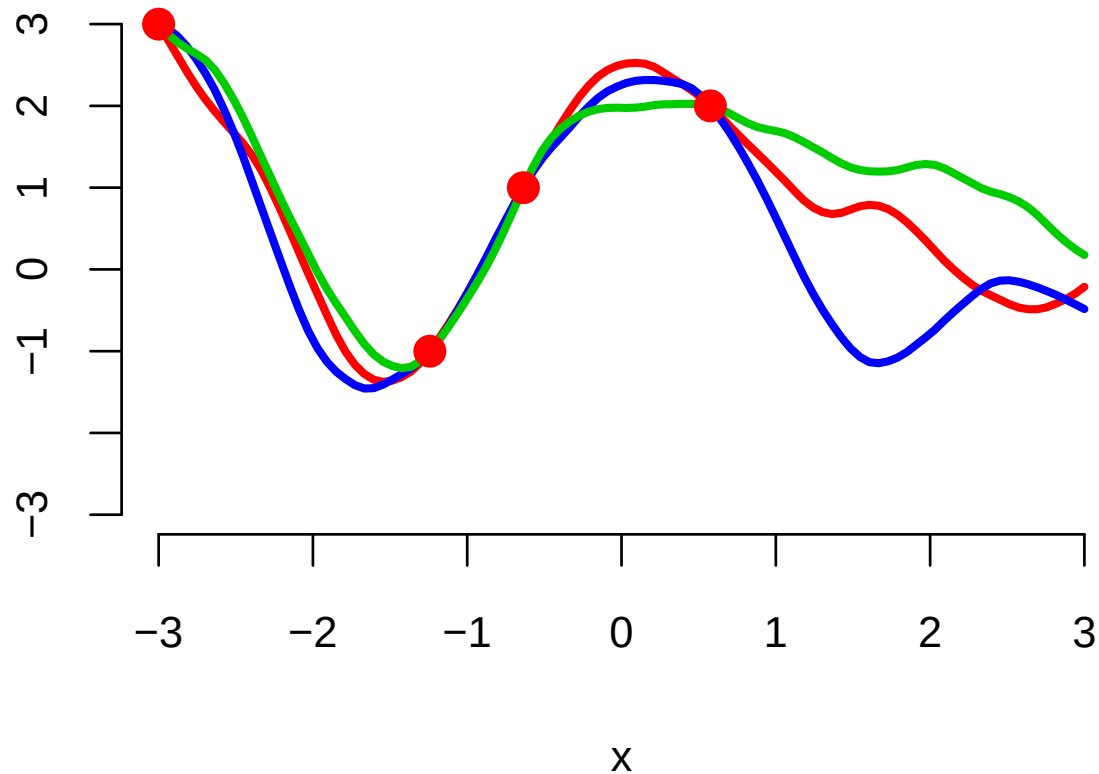
$\Sigma =$ 



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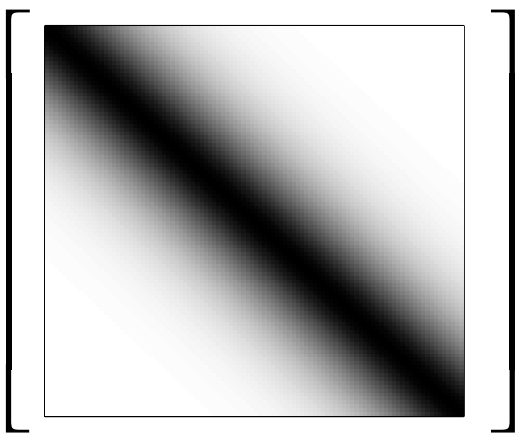
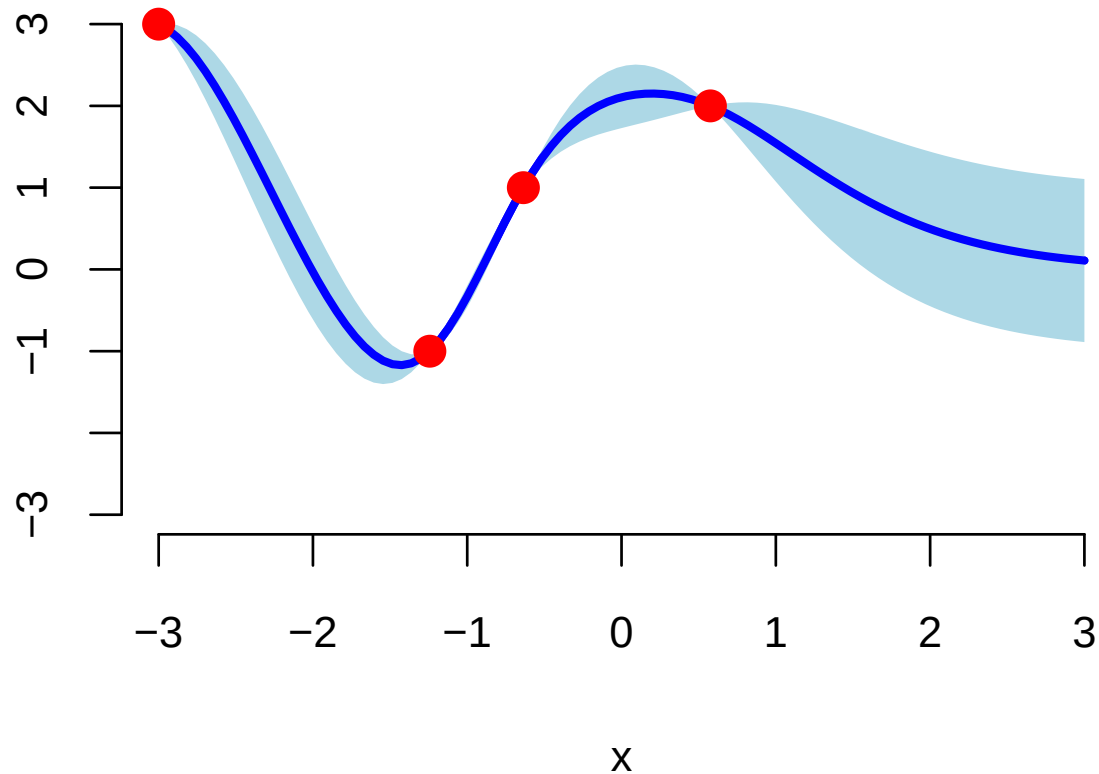
$\Sigma =$ 



# Covariance Functions: Neural Network

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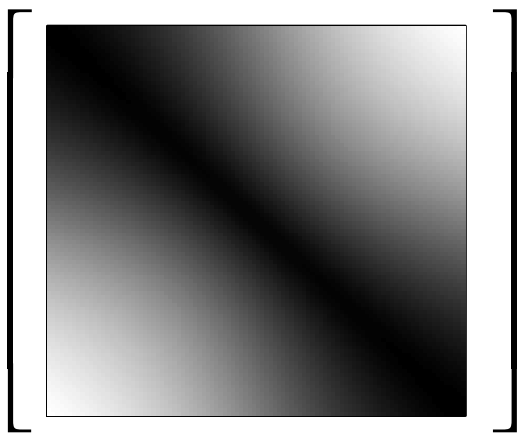
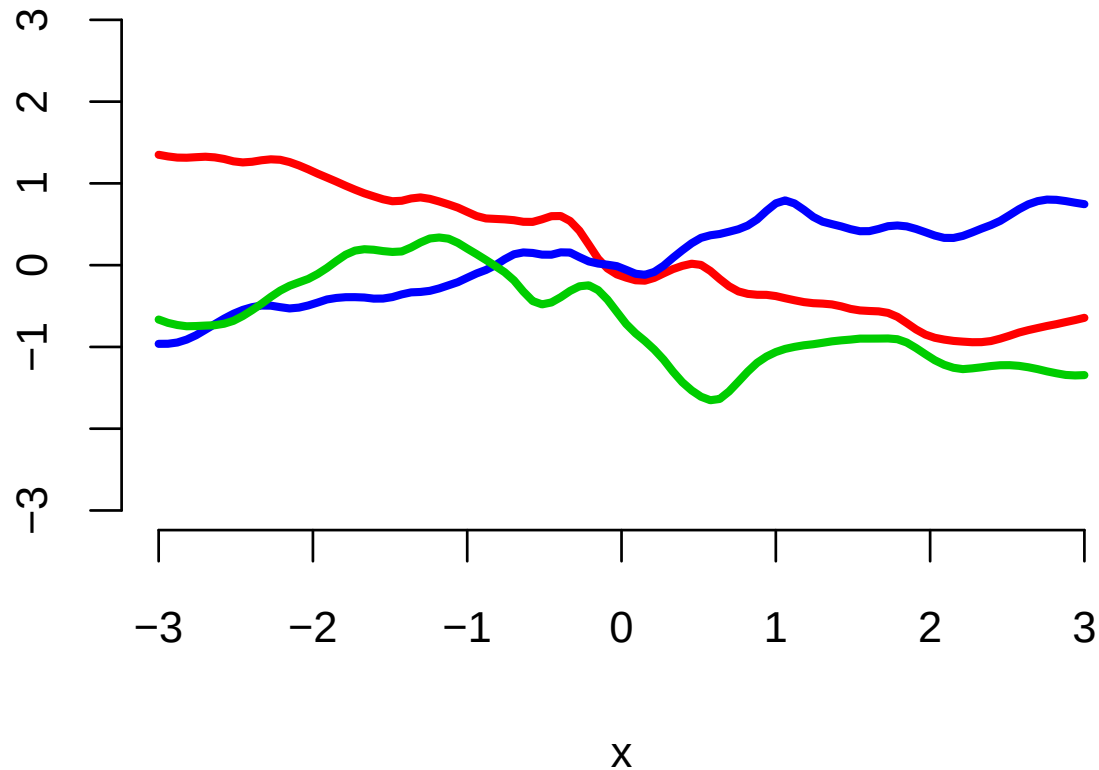
$\Sigma =$ 



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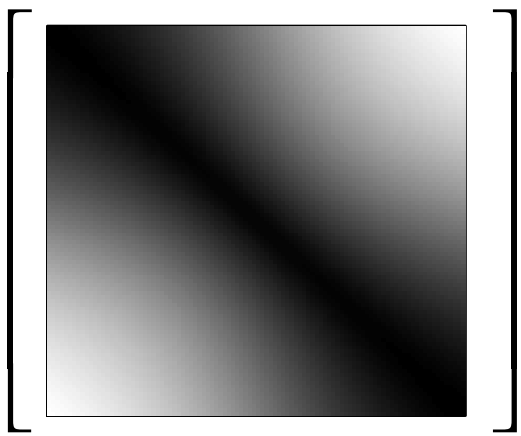
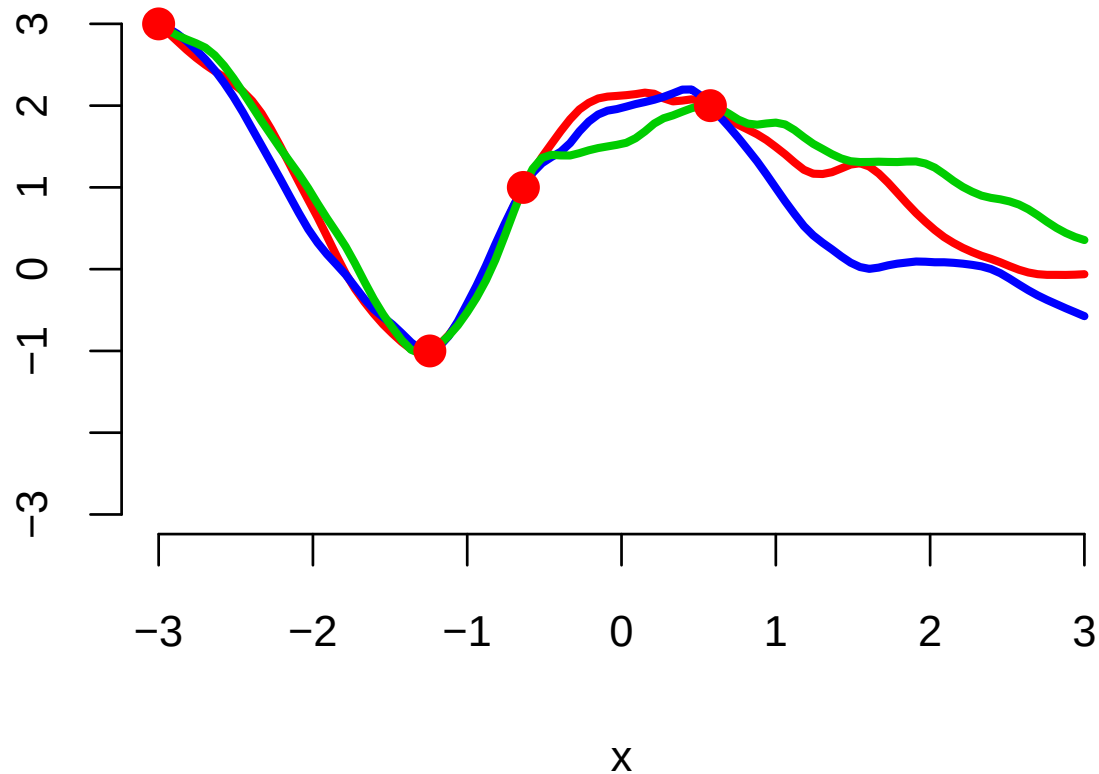
$\Sigma =$ 



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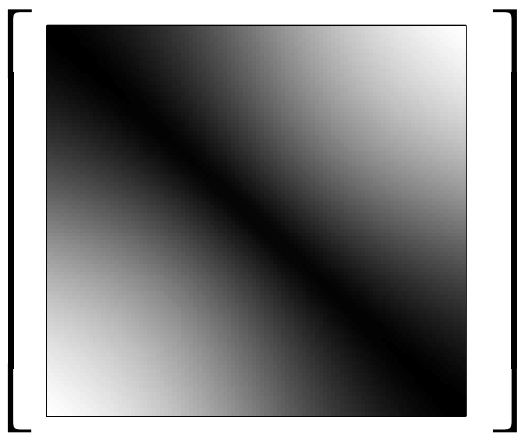
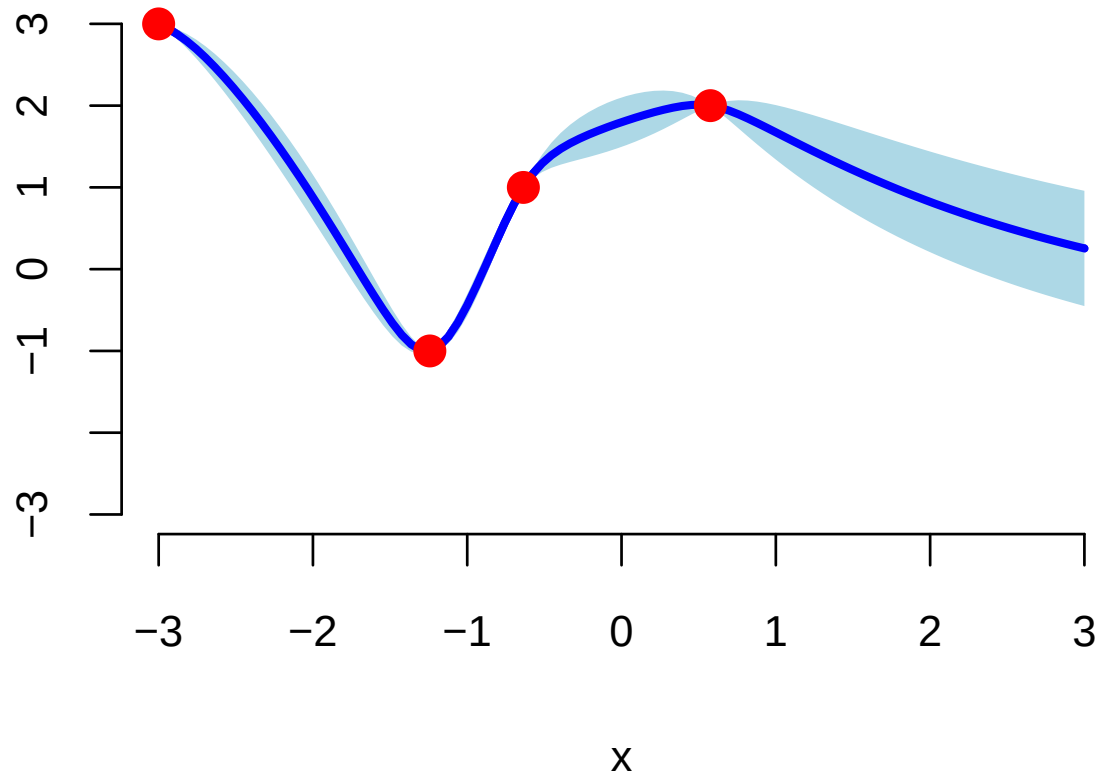
$\Sigma =$ 



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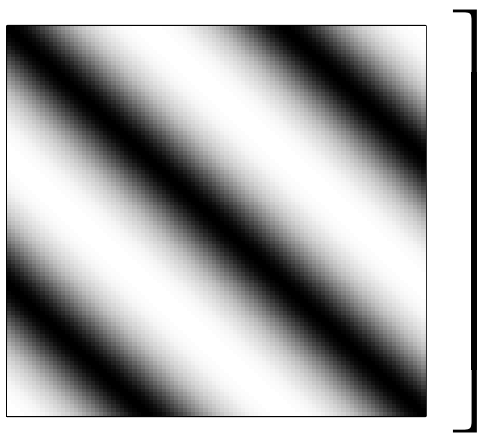

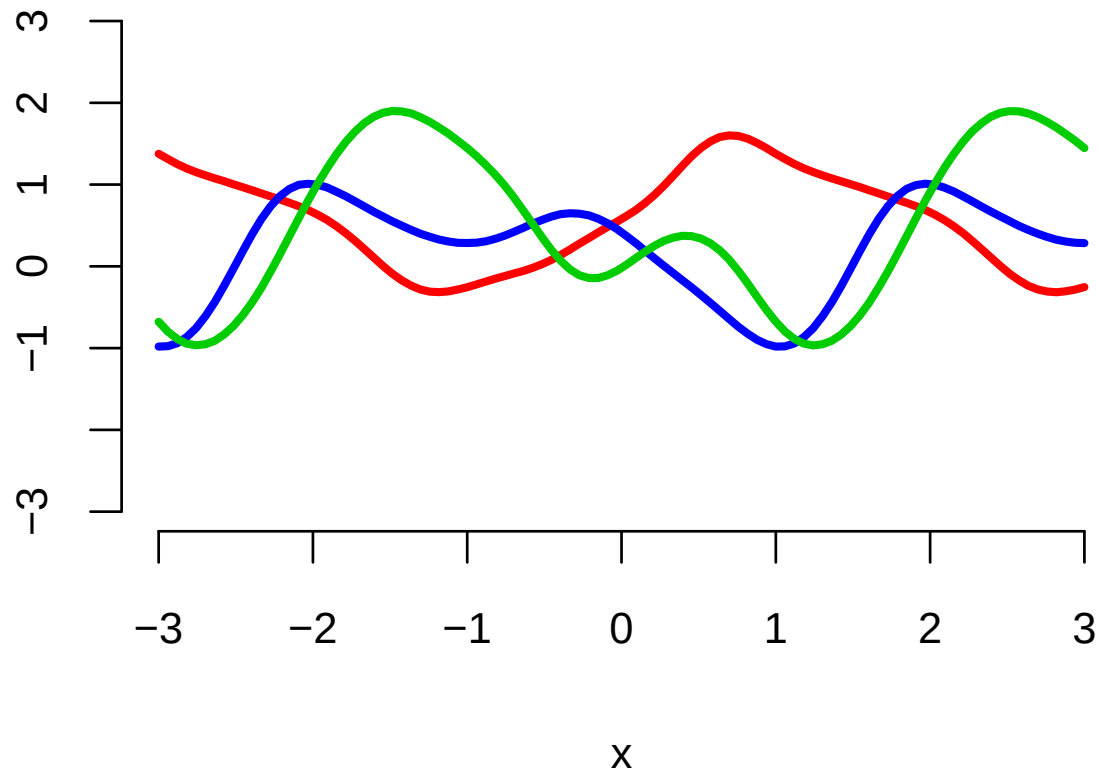

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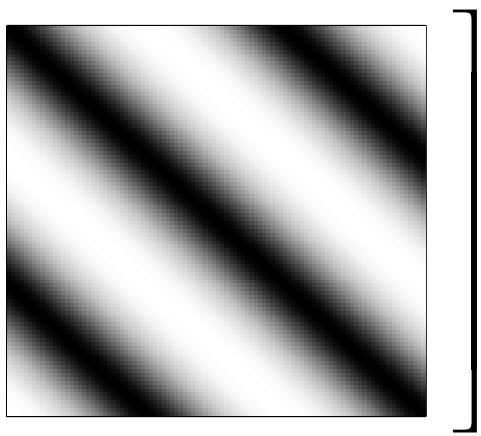

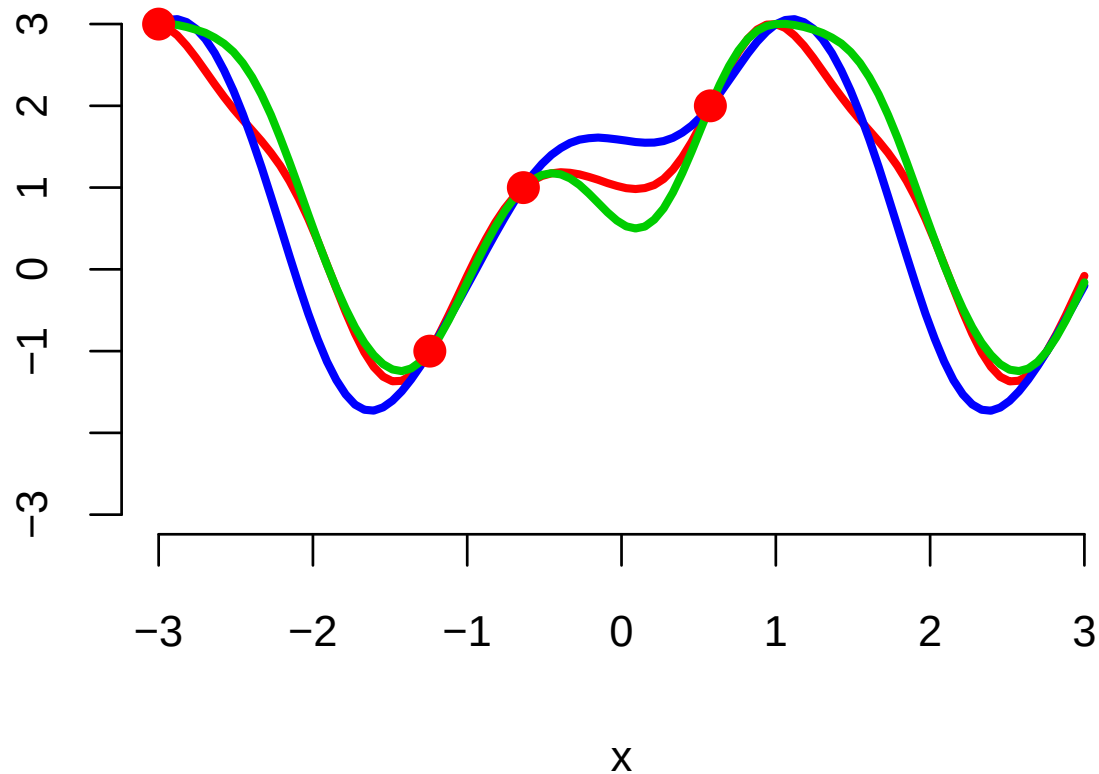

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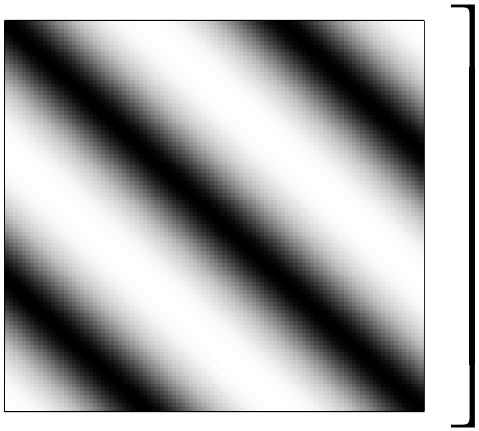

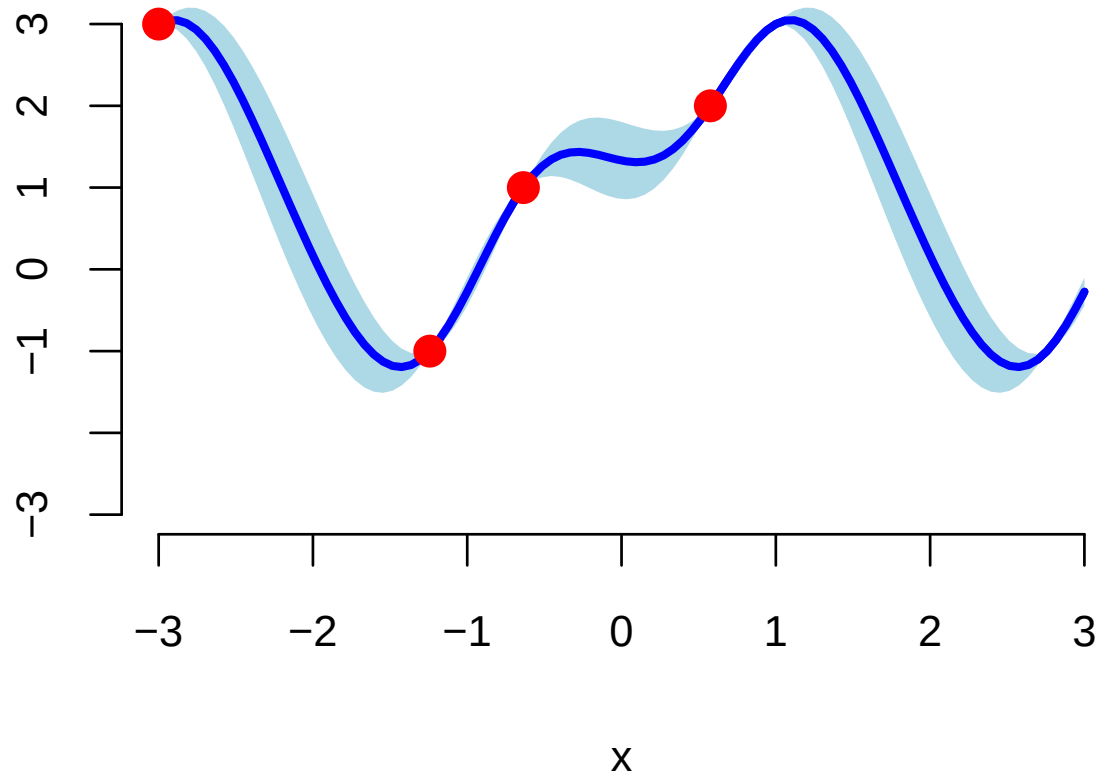

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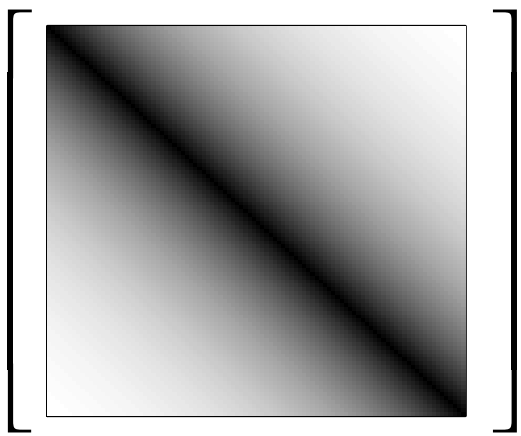
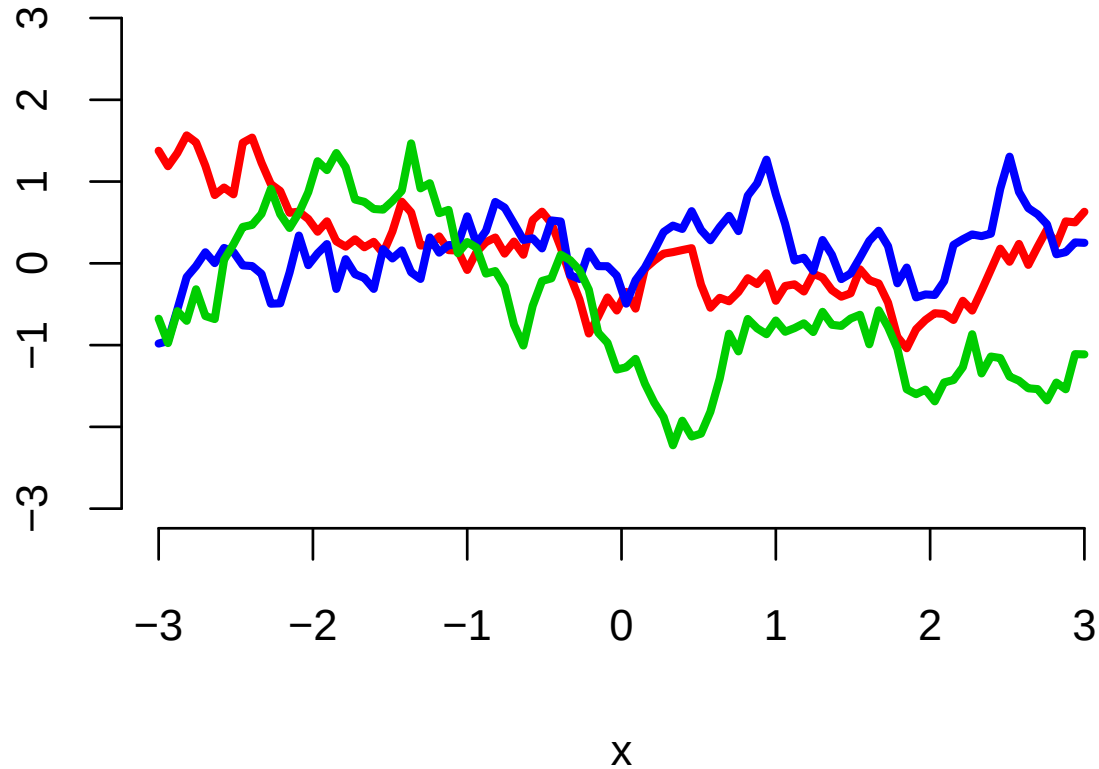
$\Sigma =$ 



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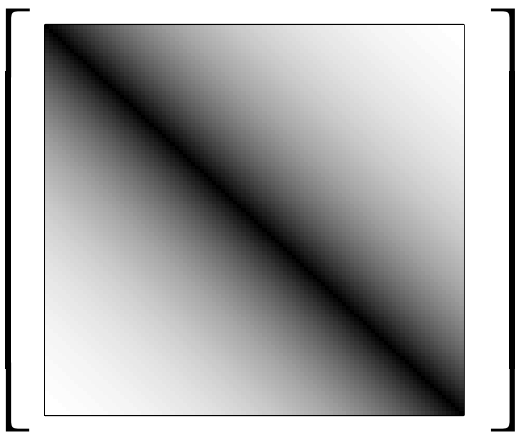
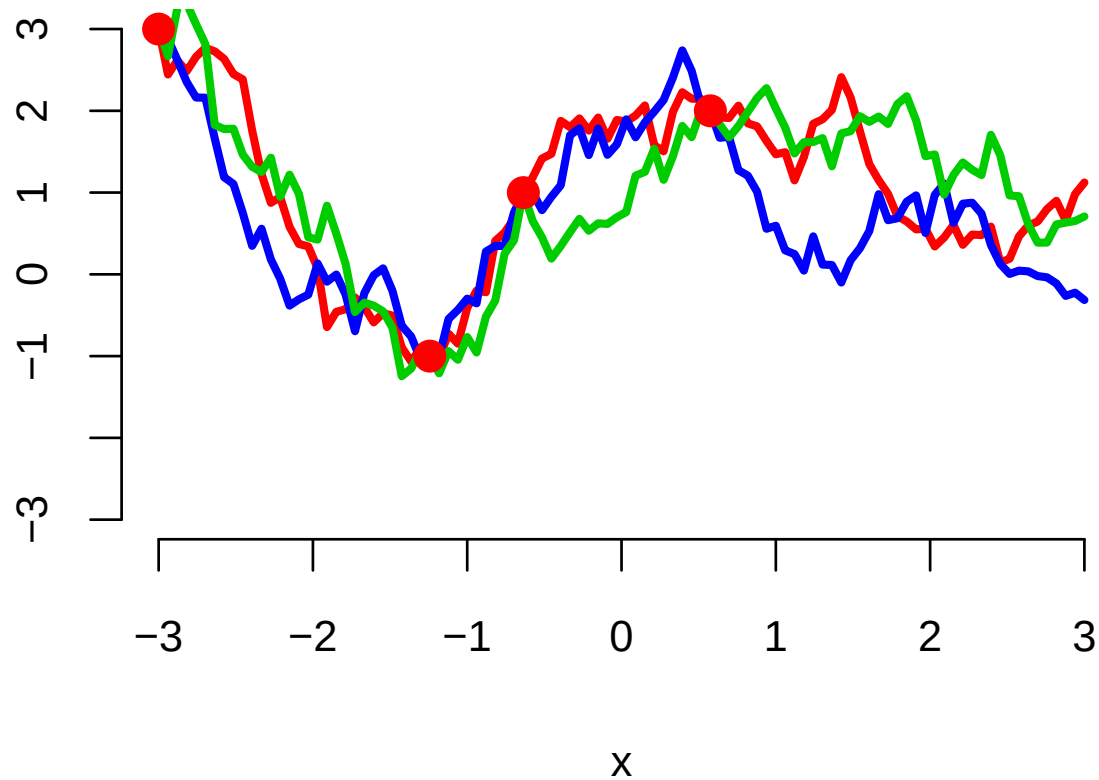
$\Sigma =$ 



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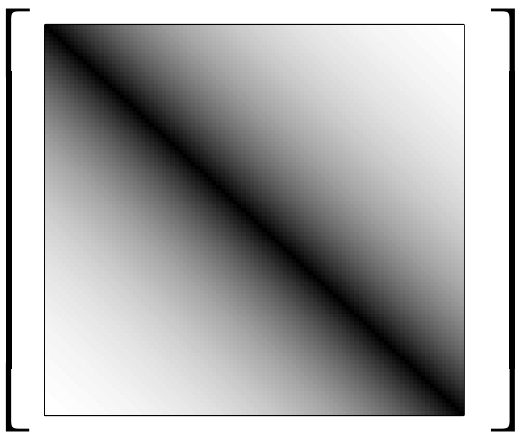
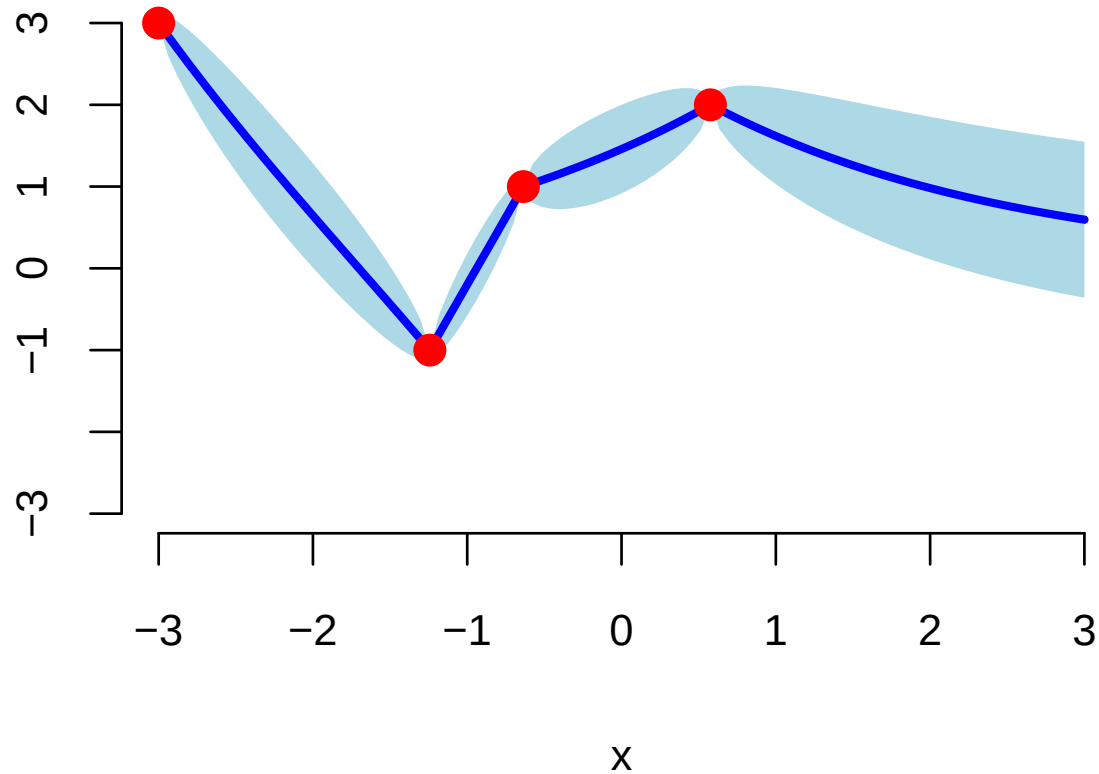
$\Sigma =$ 



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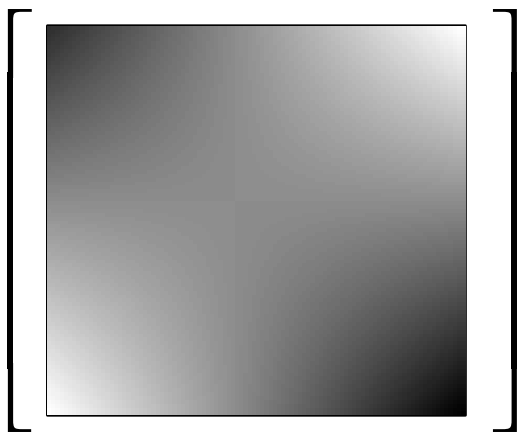
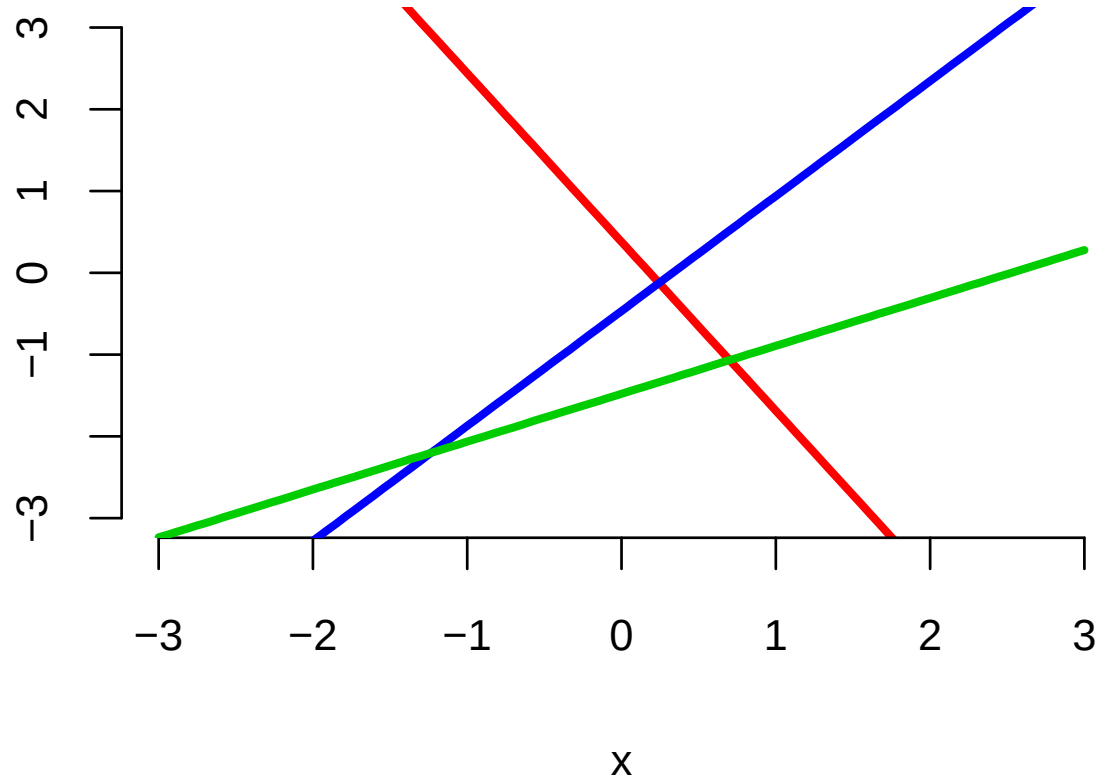
$\Sigma =$ 



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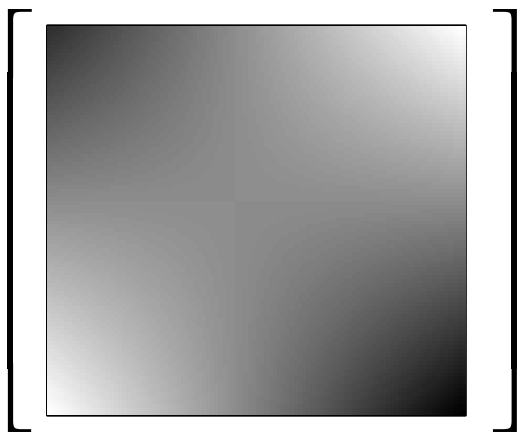
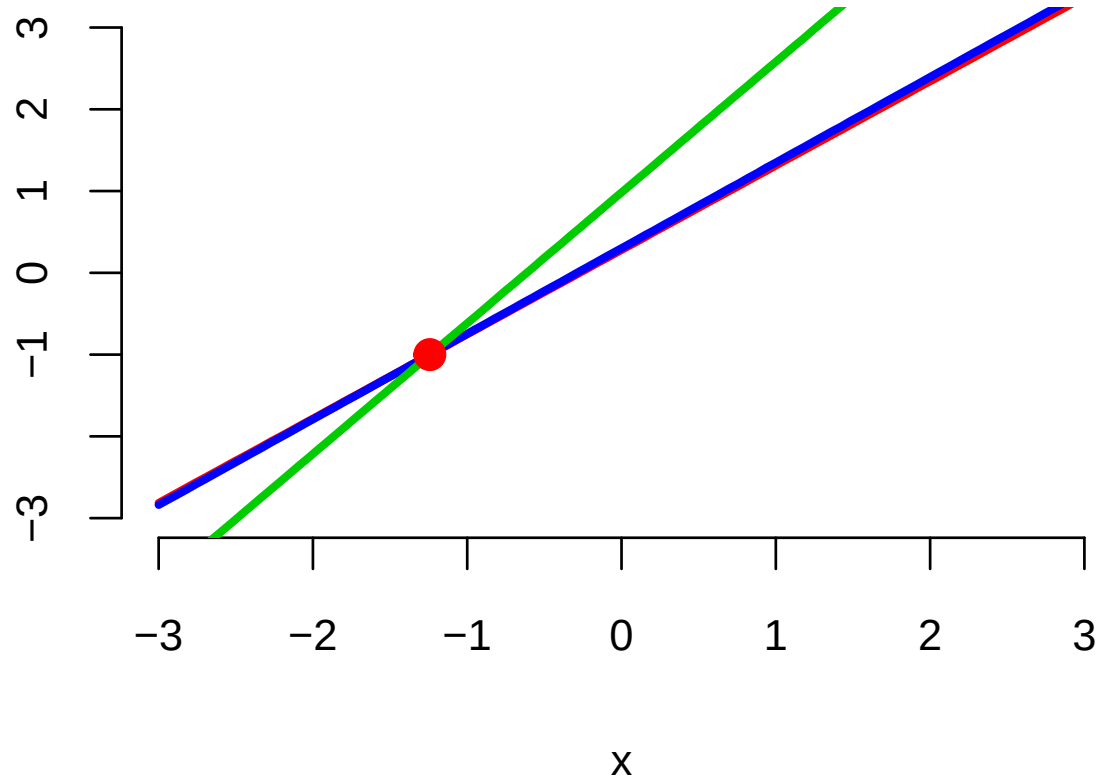
$\Sigma =$ 



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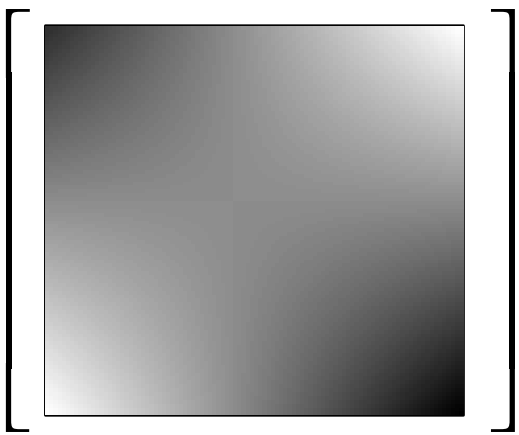
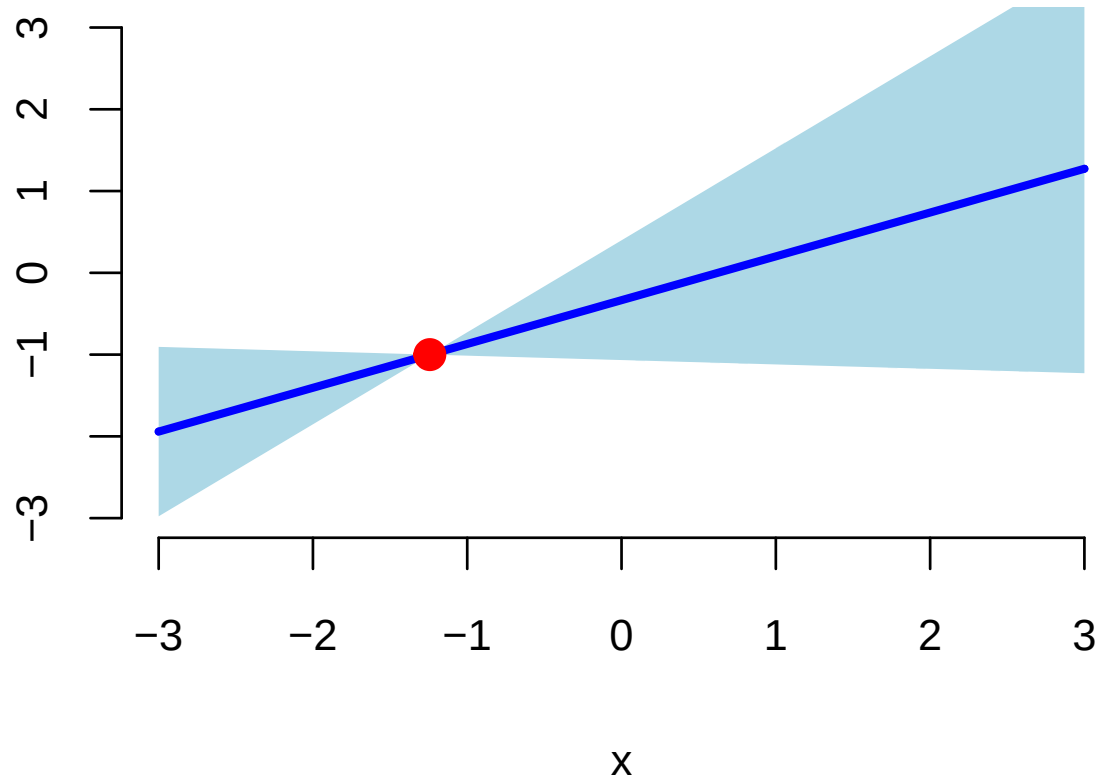
$\Sigma =$ 



**Complete task 2 of the notebook to see the influence of the prior mean and the covariance function on the prior samples and the predictive distribution!**

# Combining Covariance Functions: Multiplication

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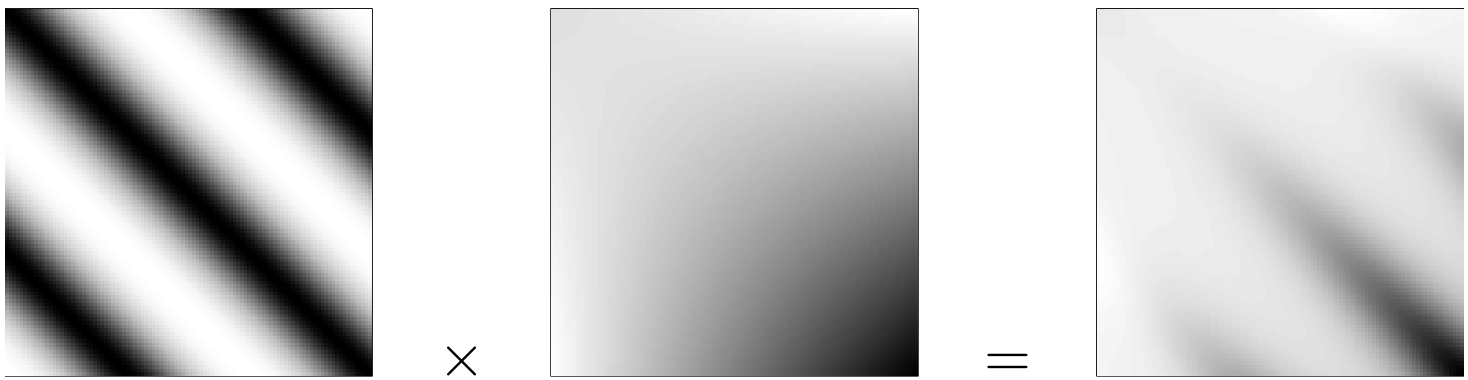

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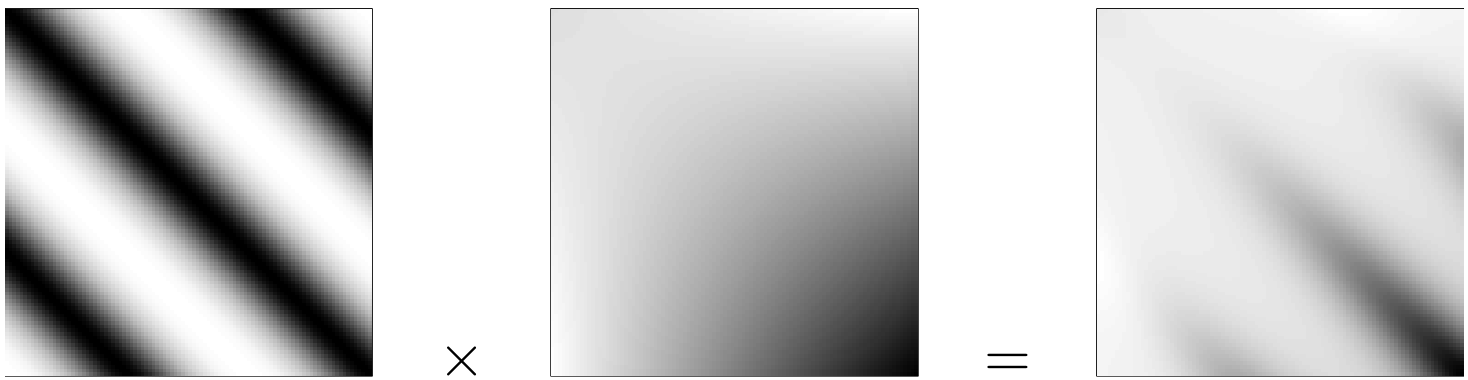

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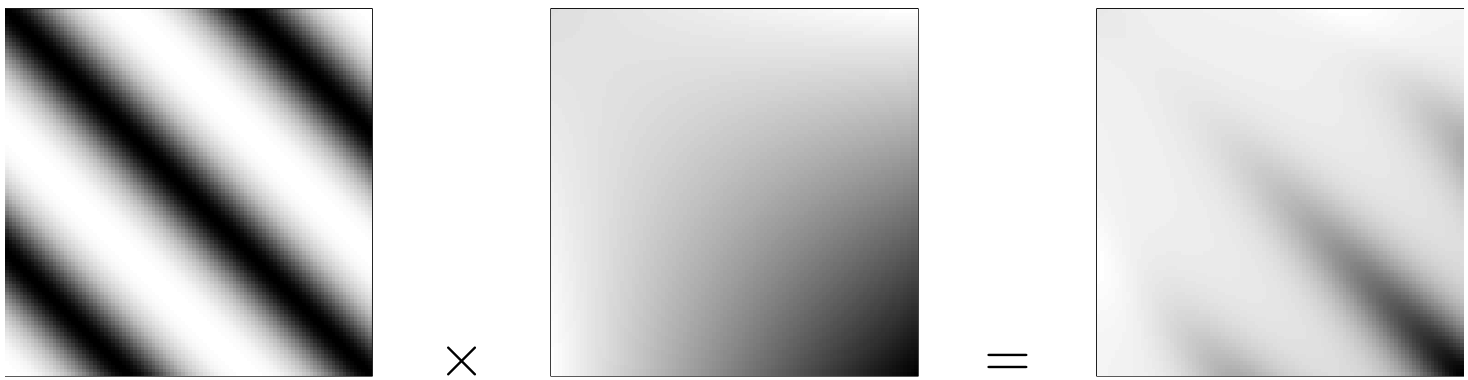

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**Equivalent to computing the product of latent functions!**

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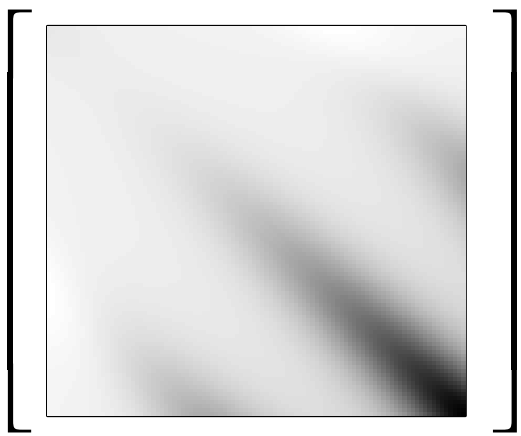
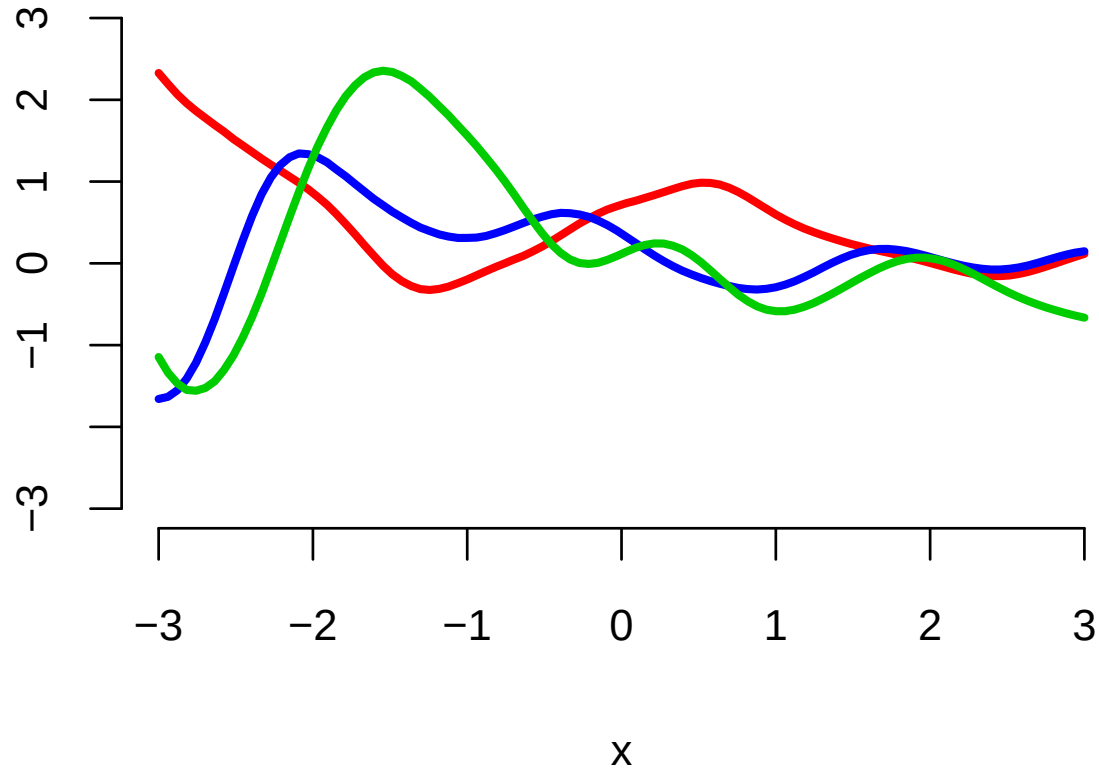
$\Sigma =$ 



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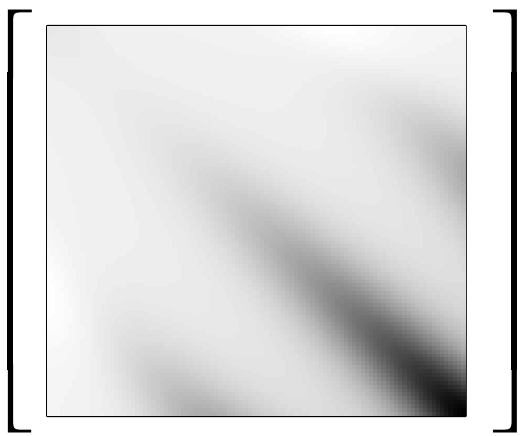
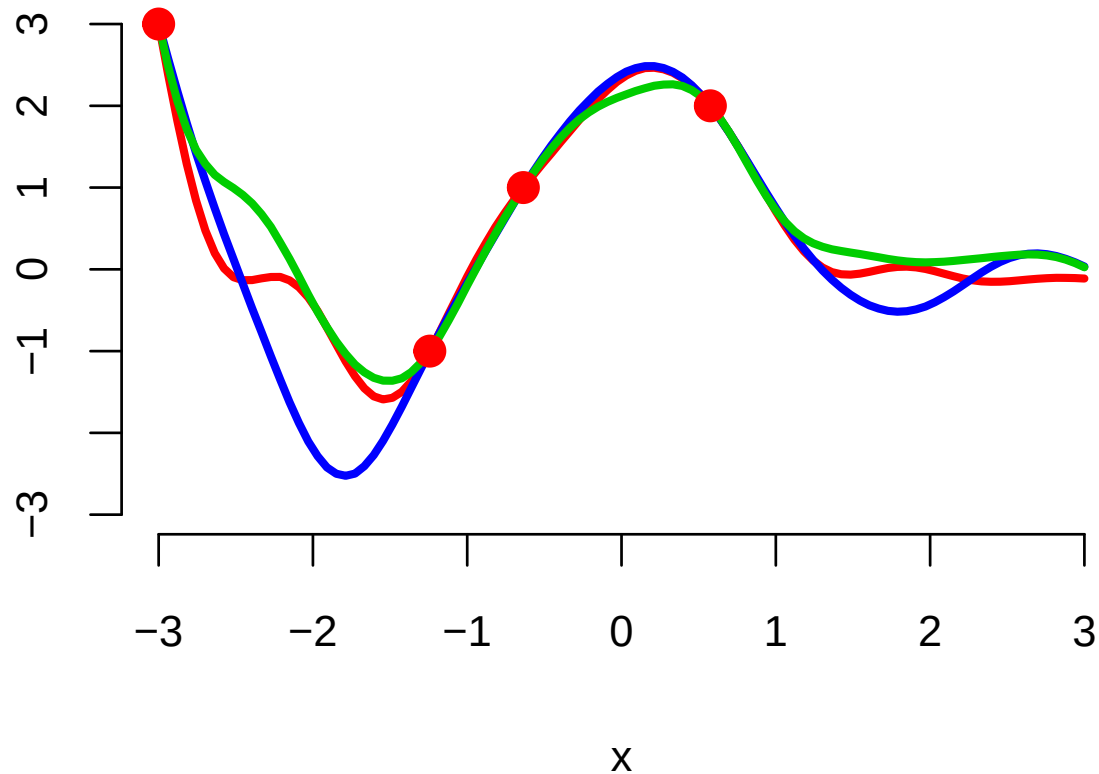
$\Sigma =$ 



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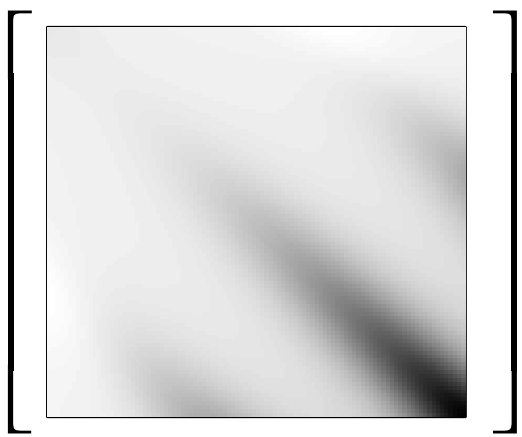
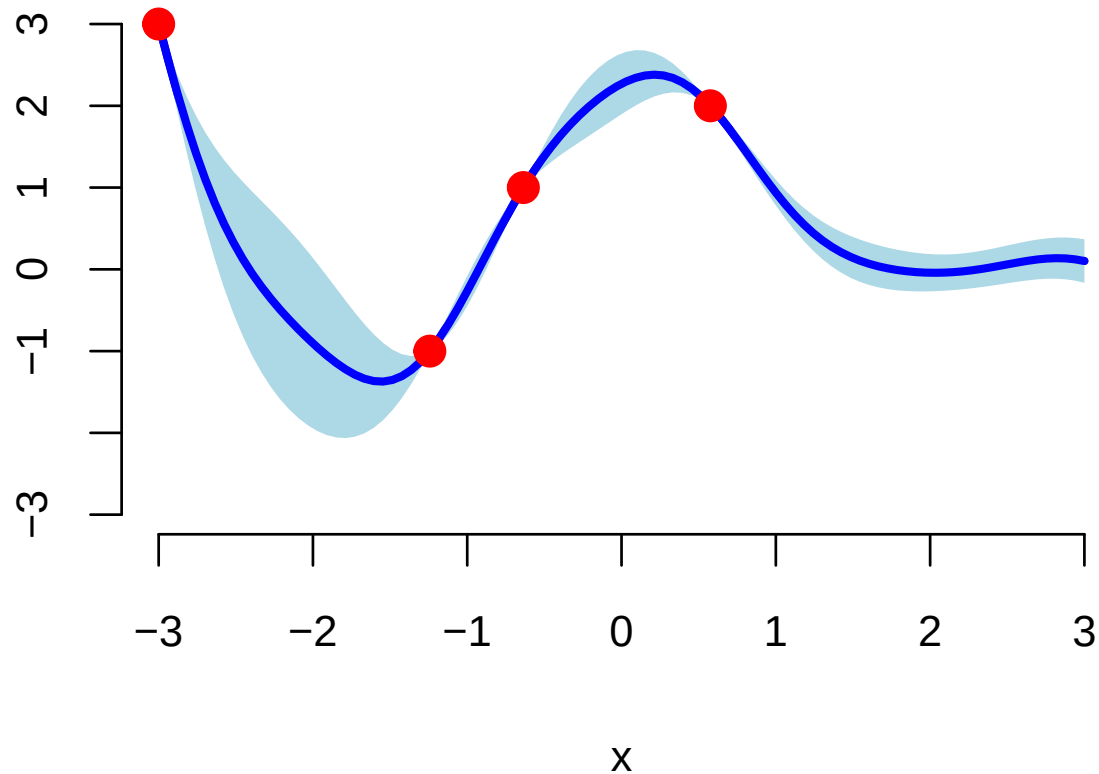
$\Sigma =$ 



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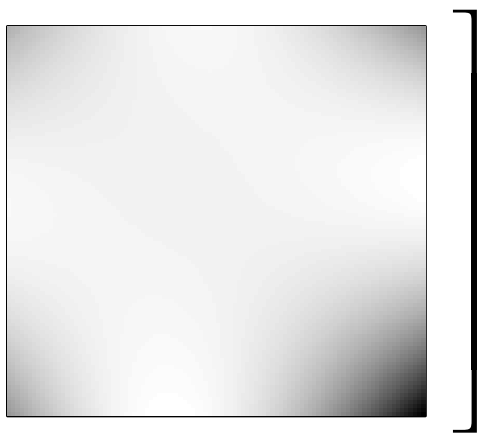

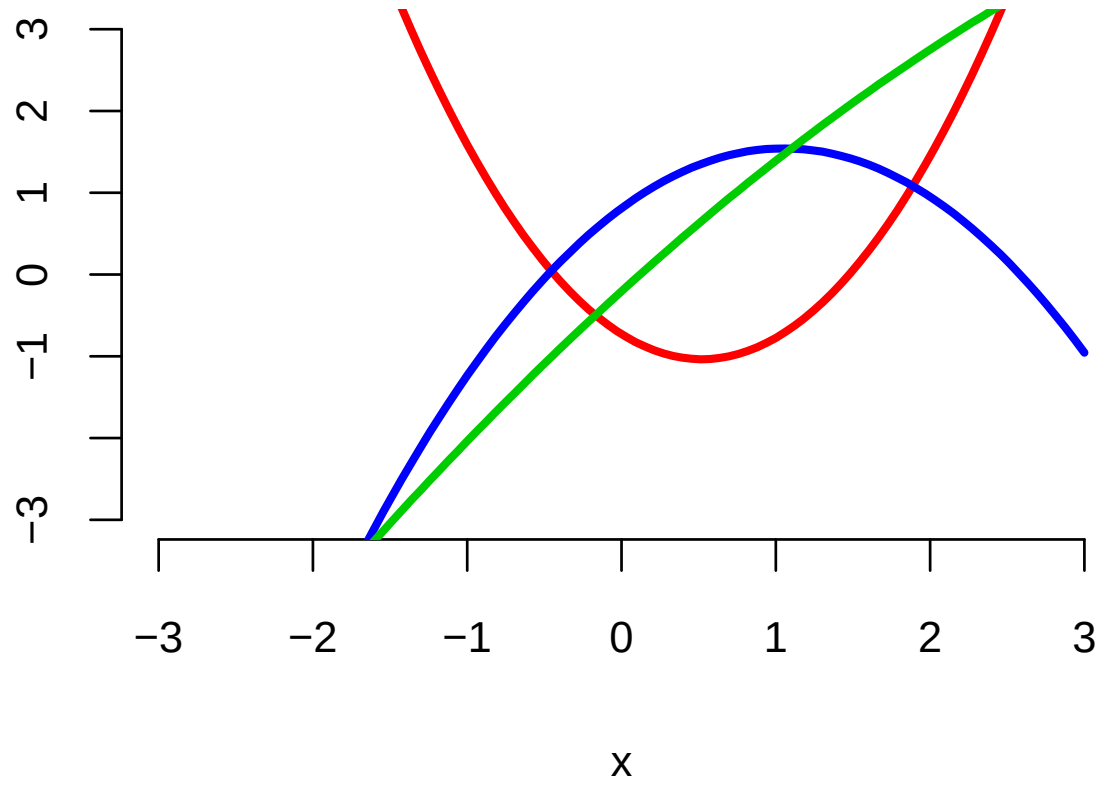

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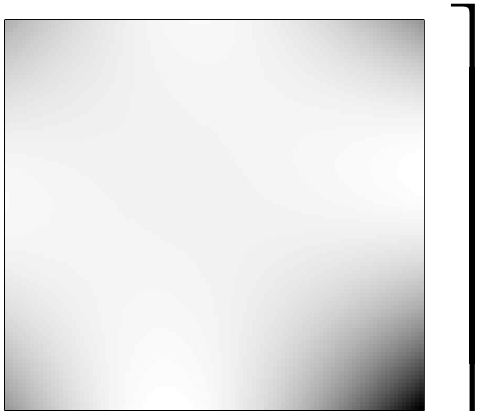

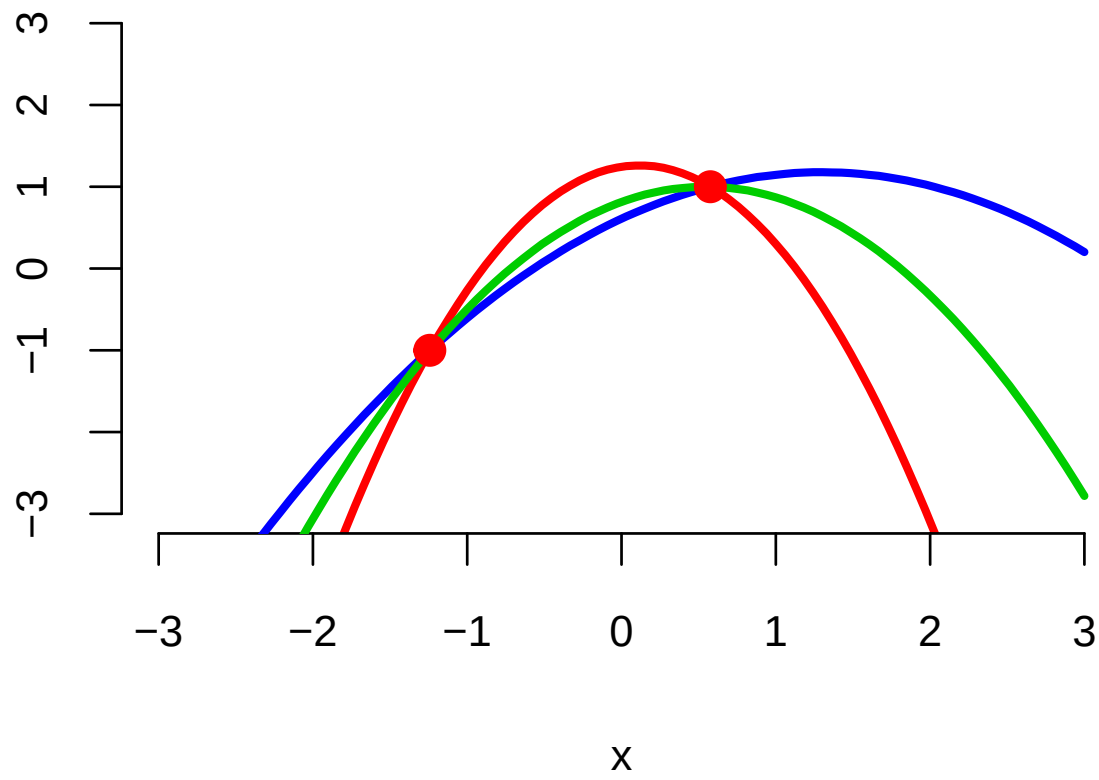

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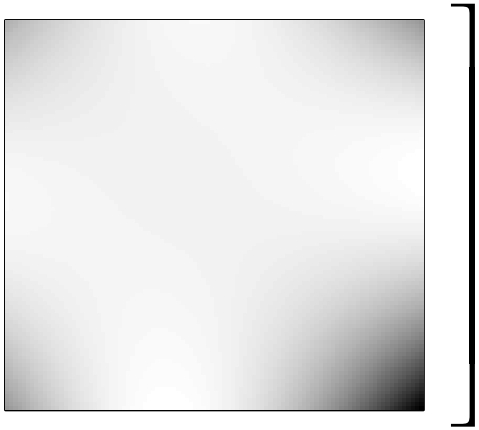

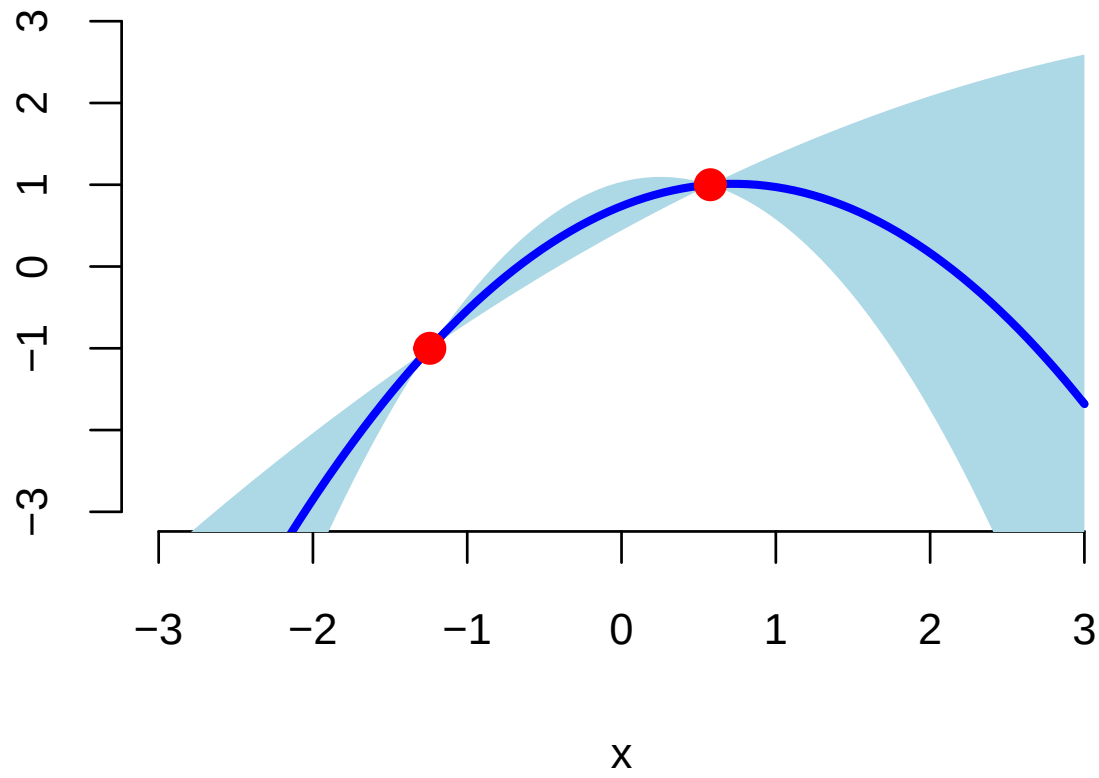

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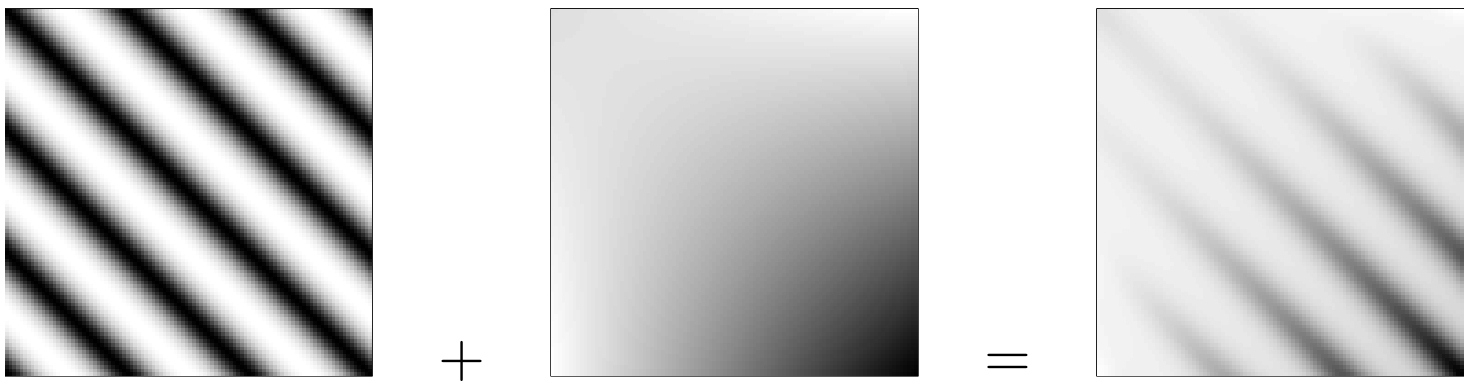

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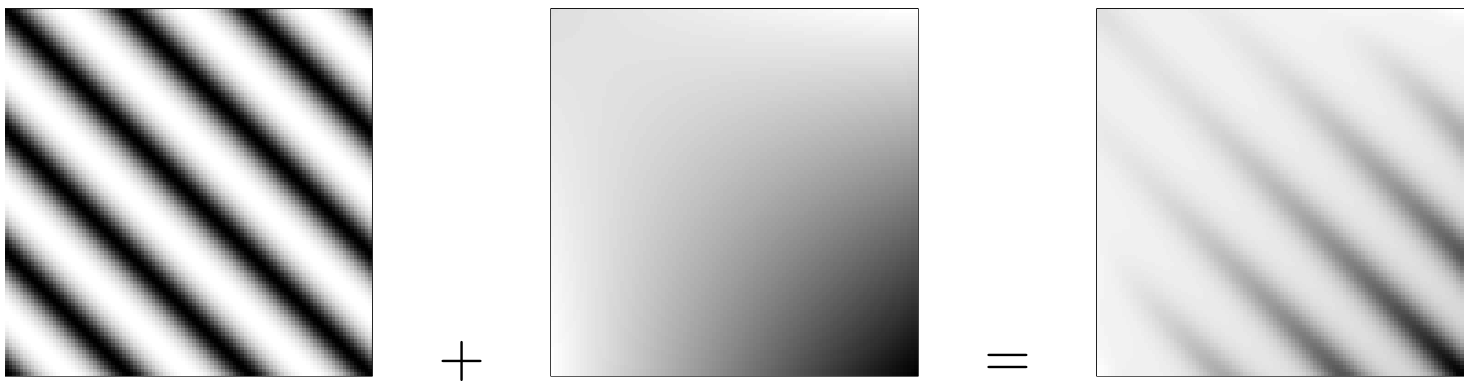

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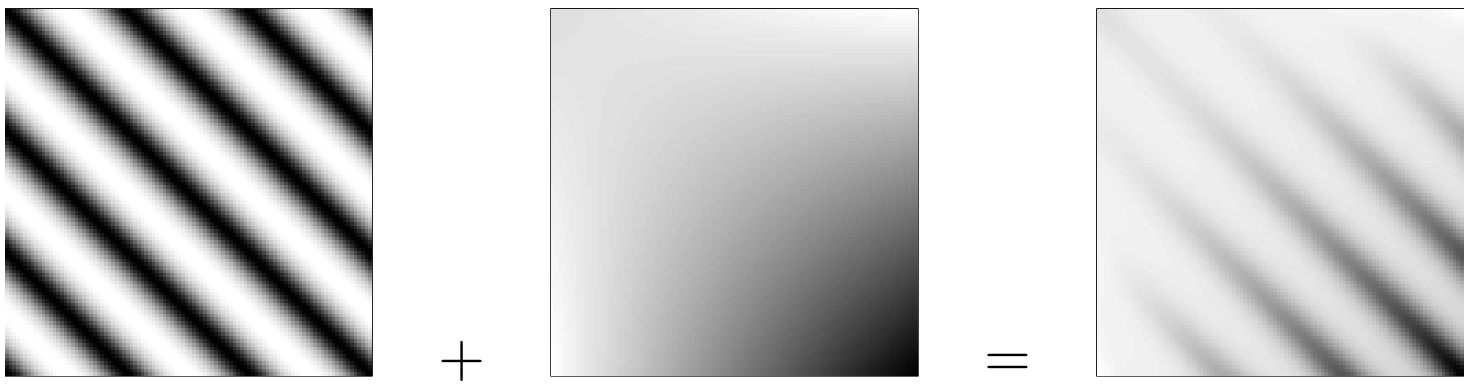

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**Equivalent to summing latent functions!**

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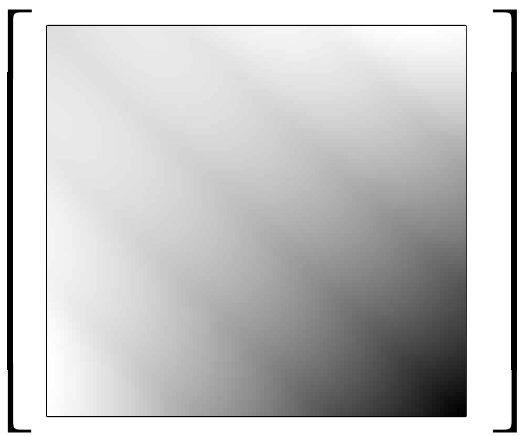
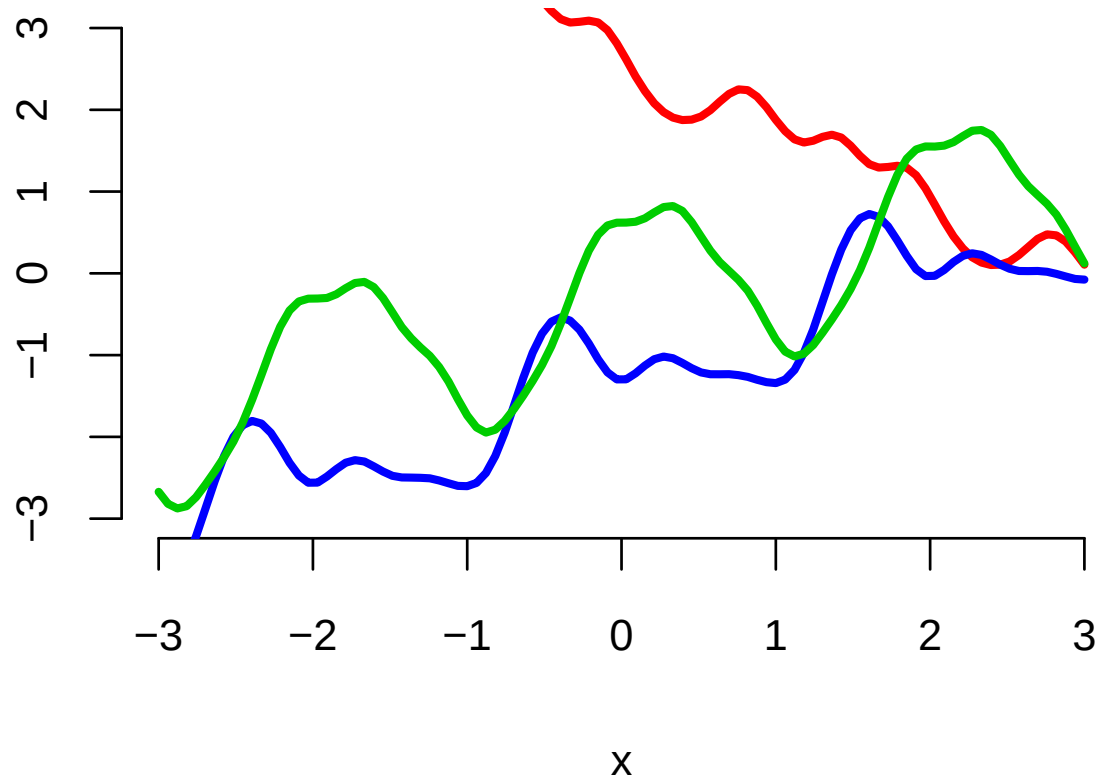
$\Sigma =$ 



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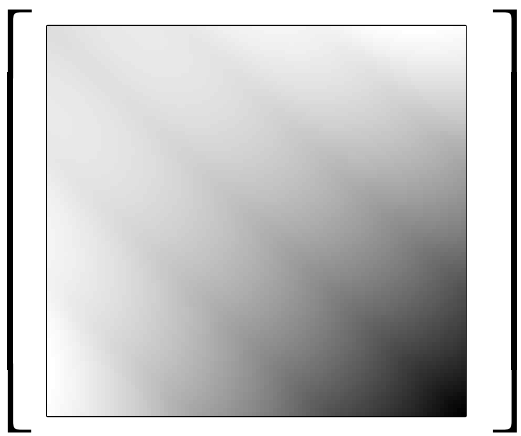
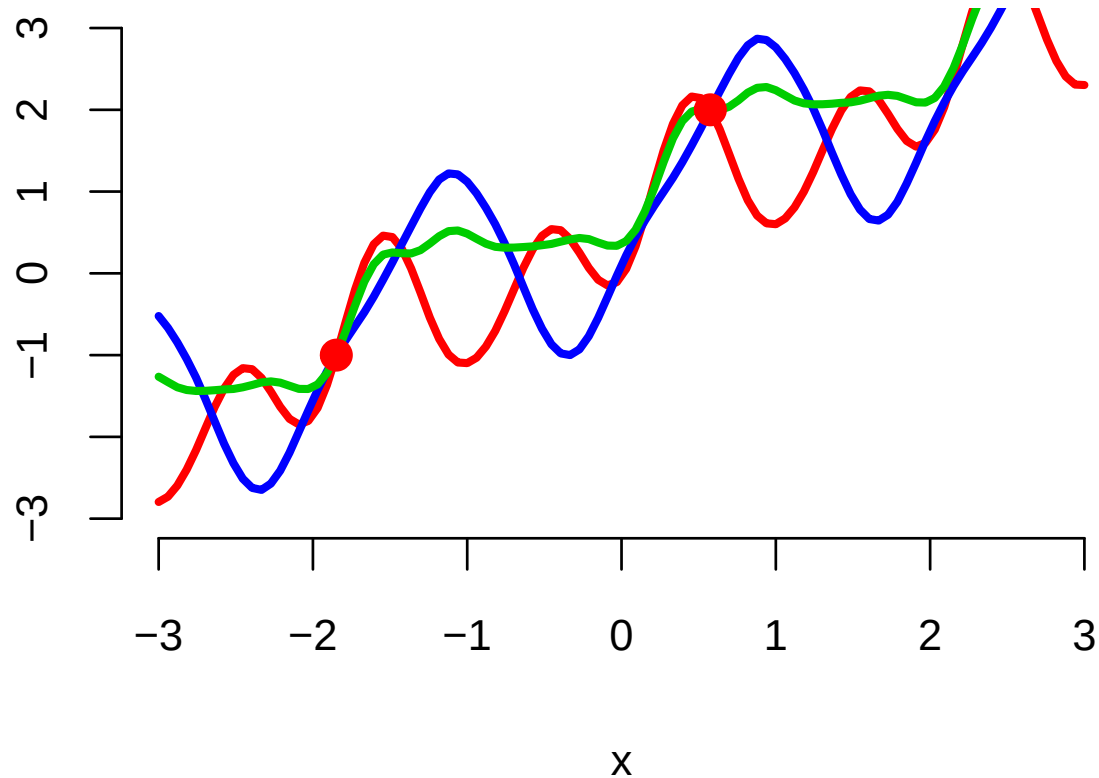
$\Sigma =$ 



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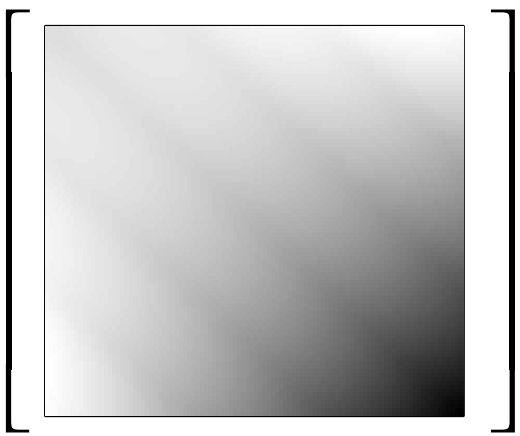
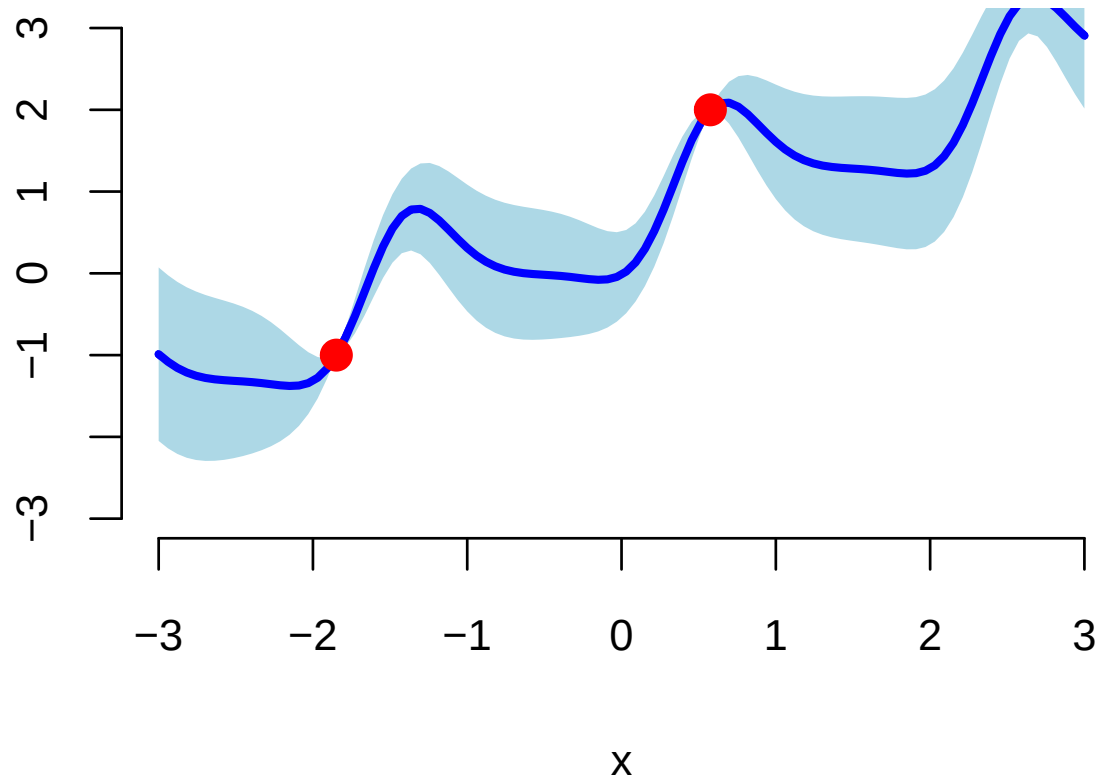
$\Sigma =$ 



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- The likelihood $p(\mathbf{y})$ can *discriminate* among them (use with care).

**Run the notebook code for extrapolation and interpretation and complete task 3!**

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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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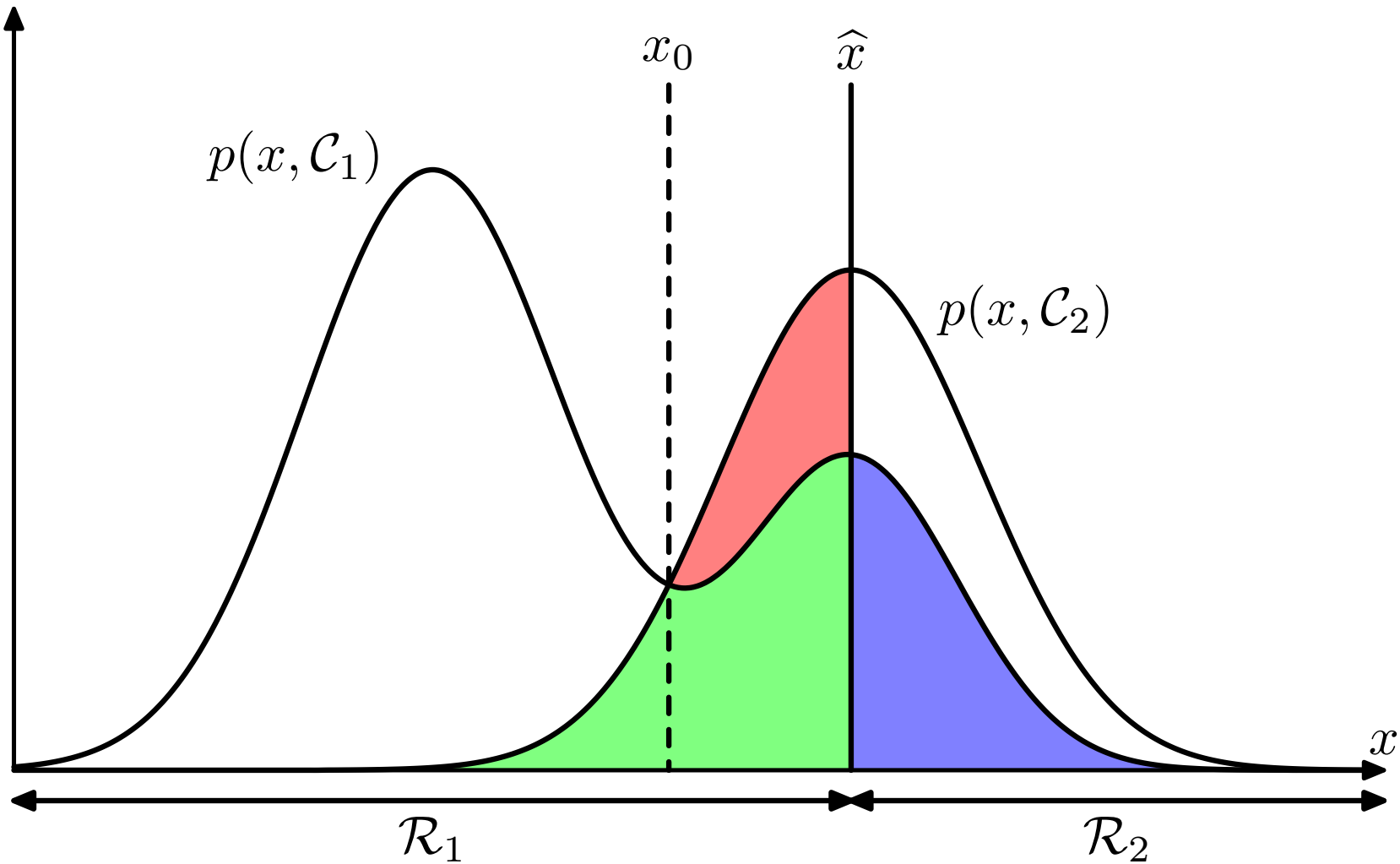


(Bishop, 2006)

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

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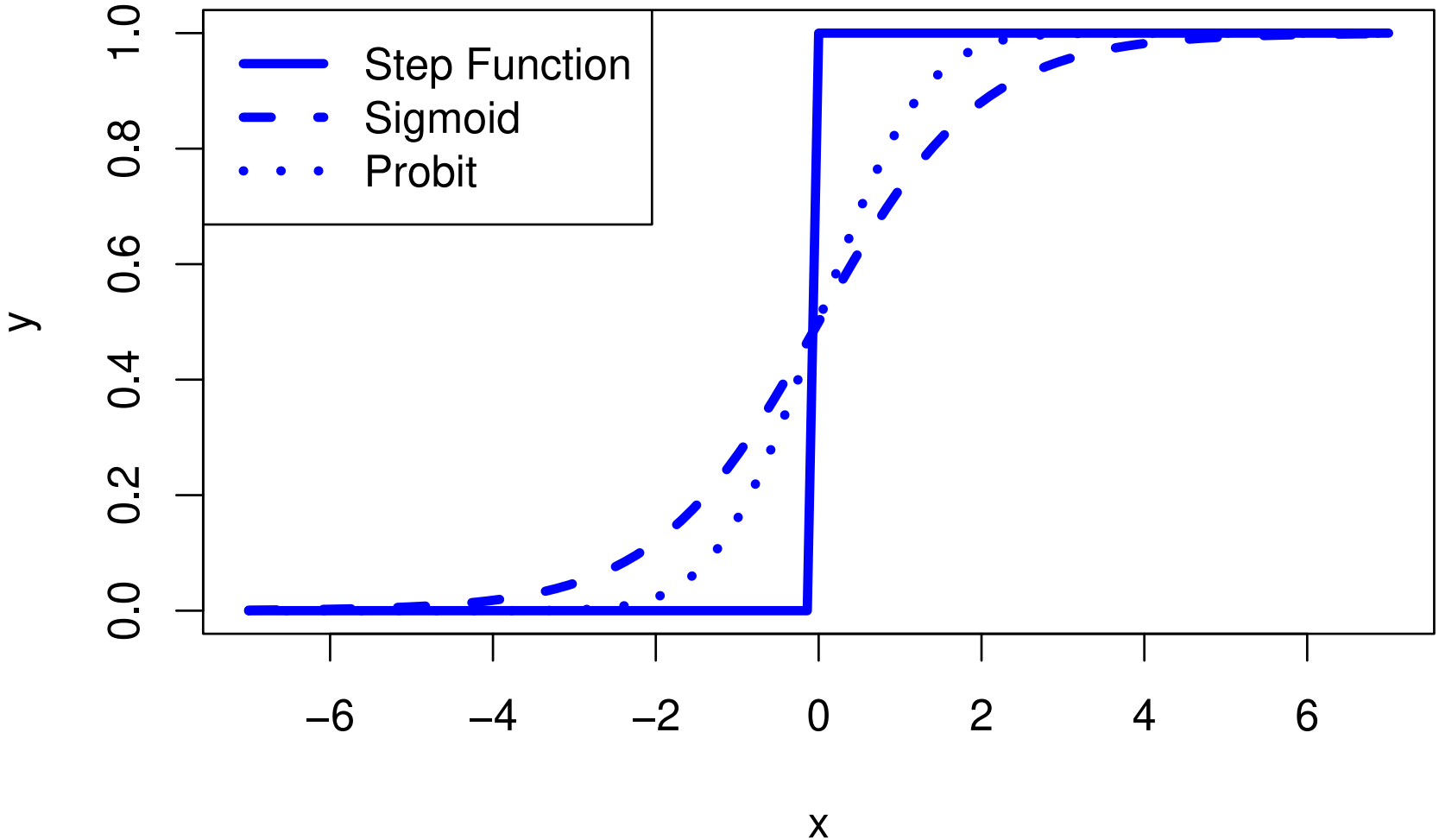

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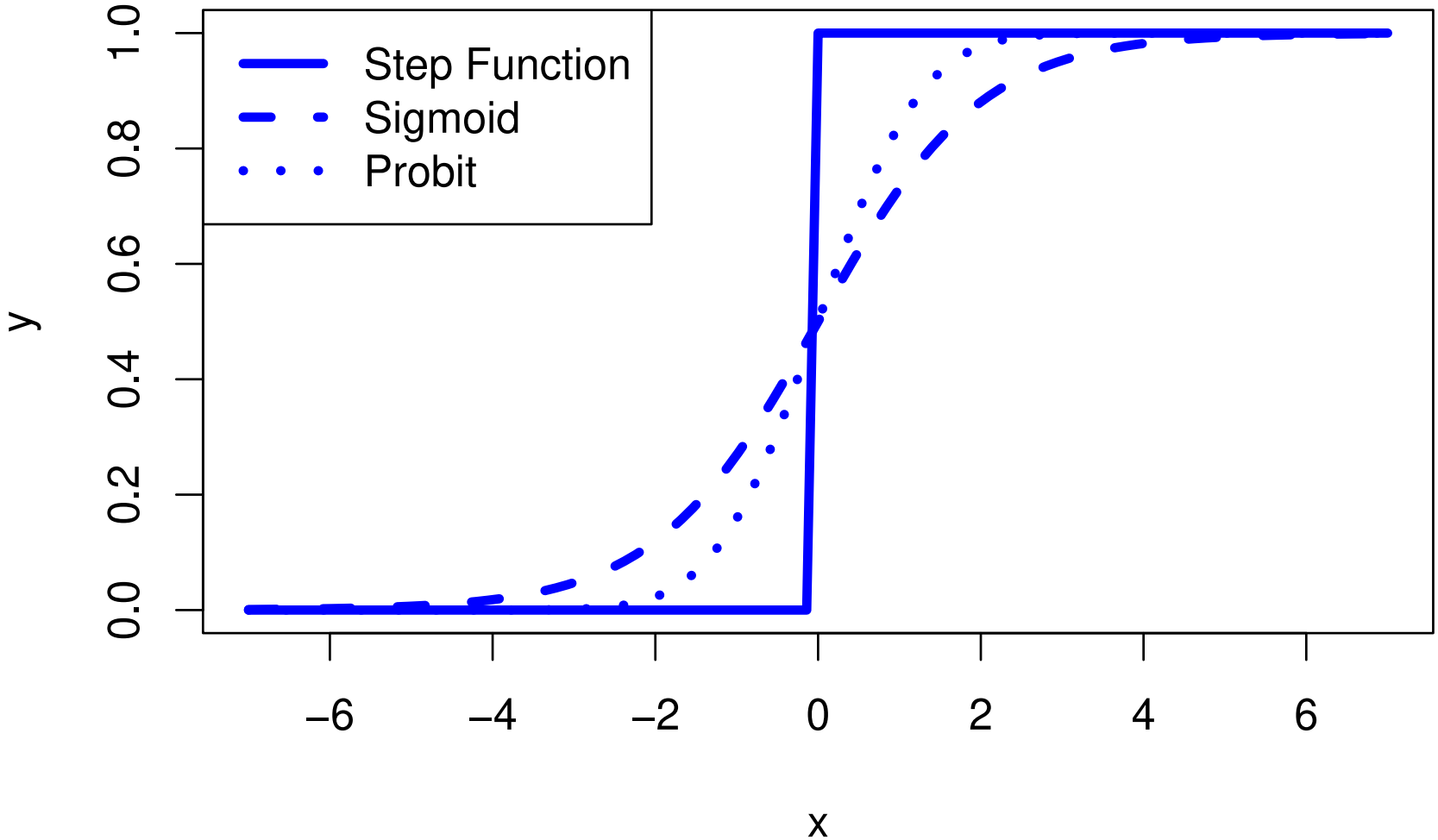


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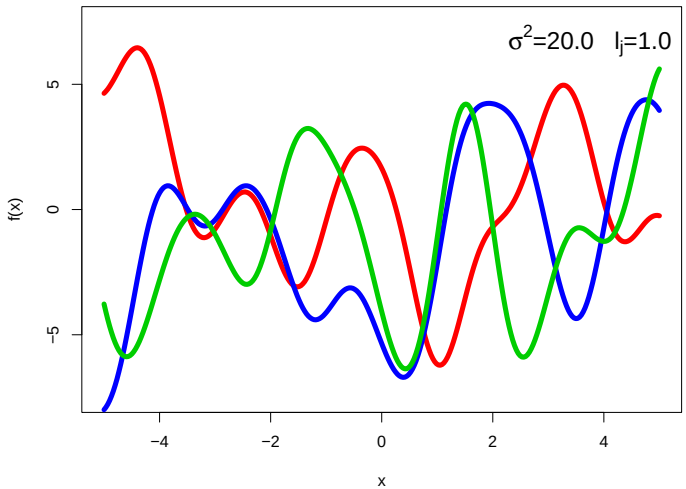
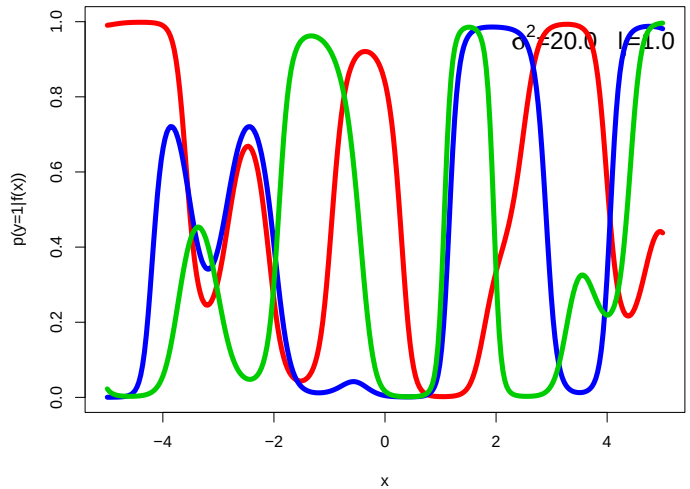
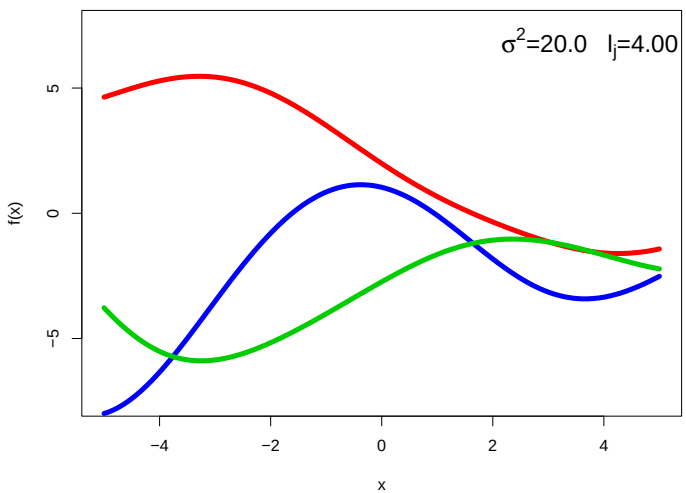
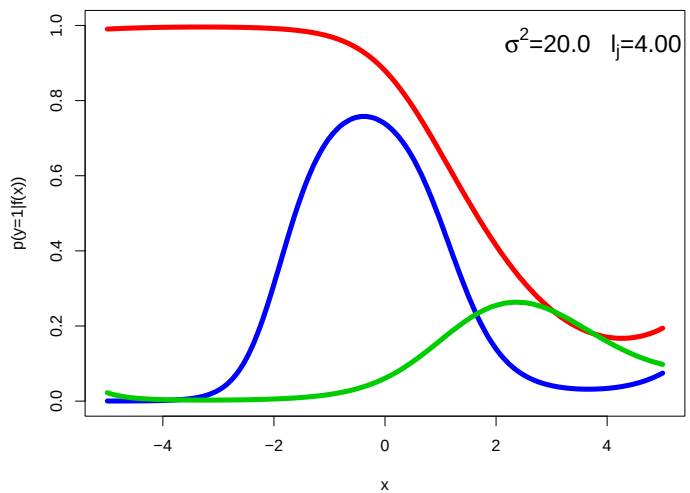
# Prior Samples Squashed via the Sigmoid Function



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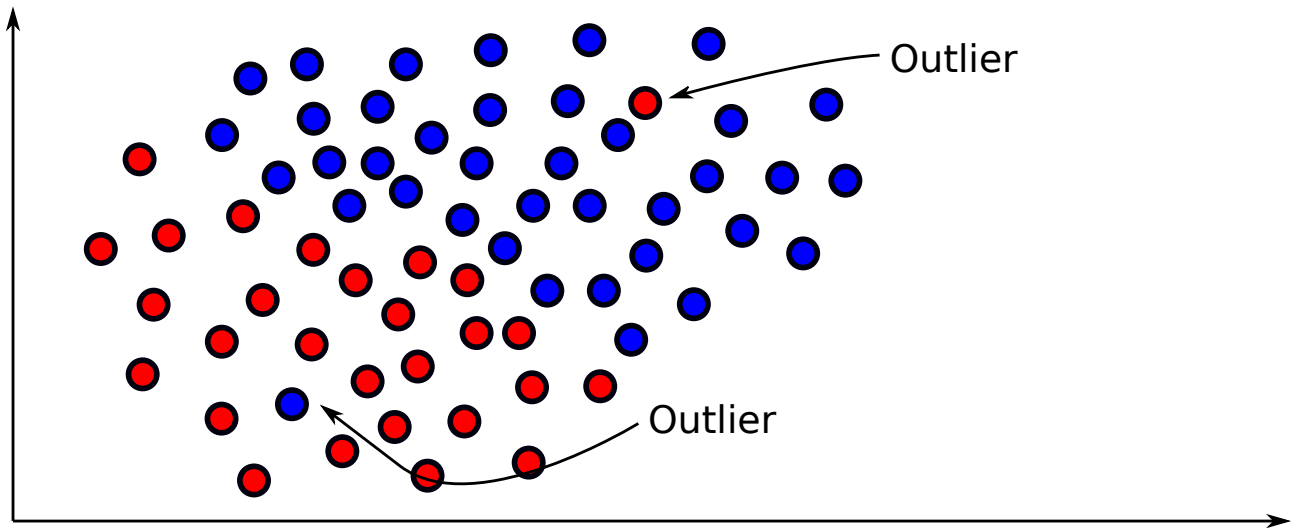

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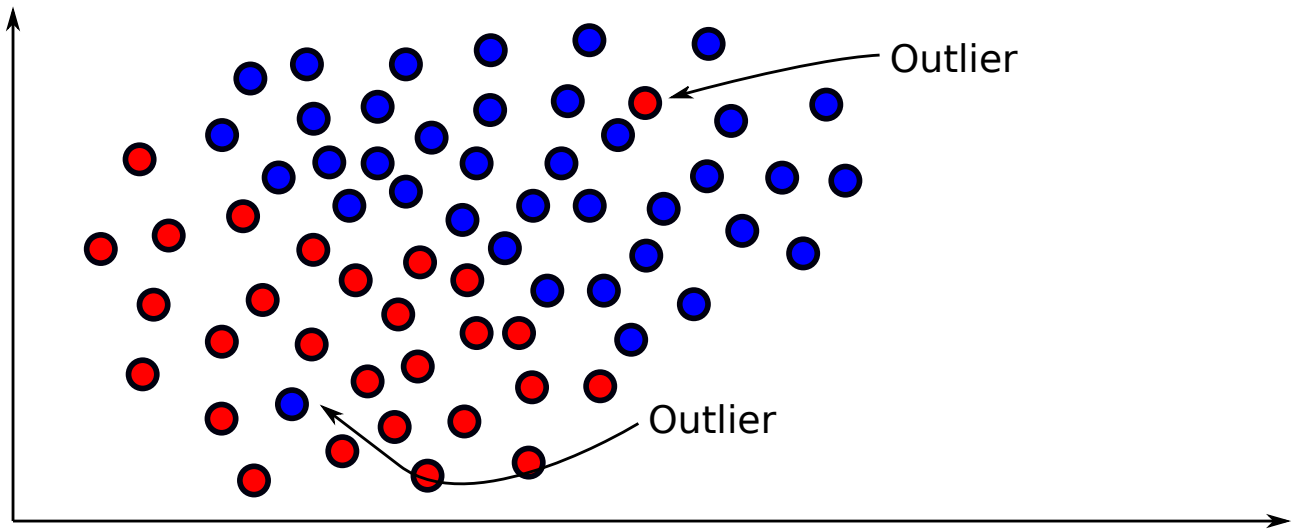


**Robust likelihood** with probability $\epsilon$ of label flip:

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

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The approximate **normalization constant** $Z_q$ is $f(z_0)\sqrt{\frac{2\pi}{A}}$.

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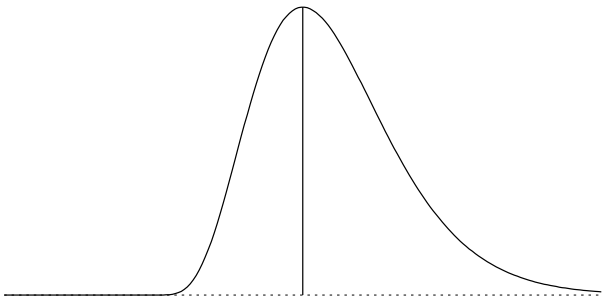

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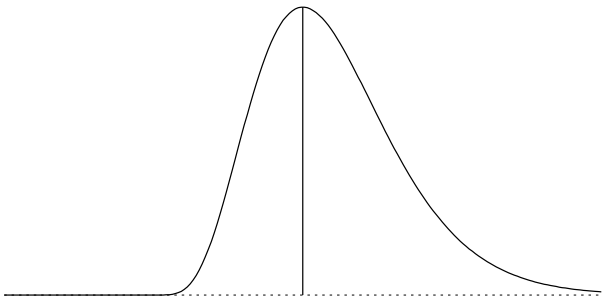

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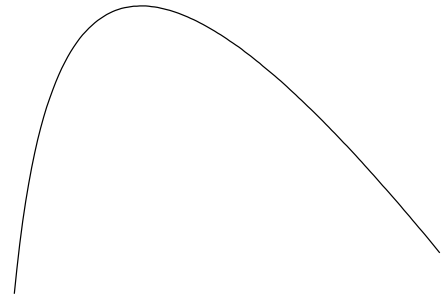

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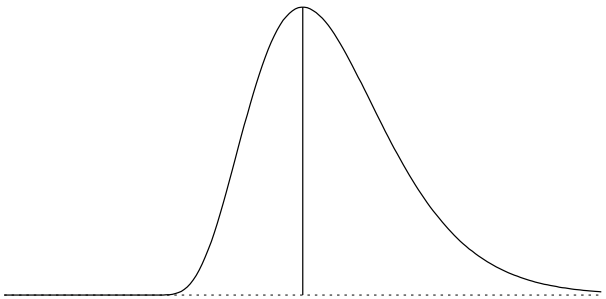

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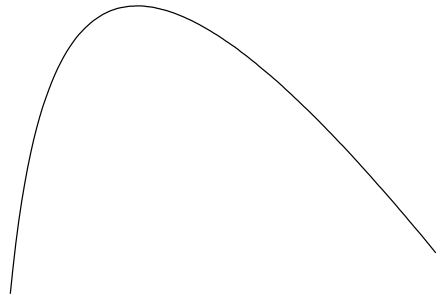

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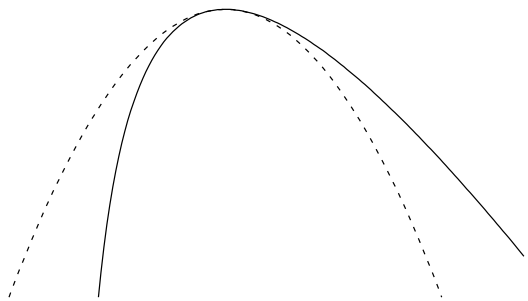

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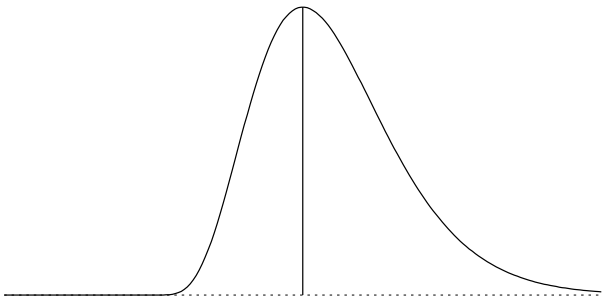

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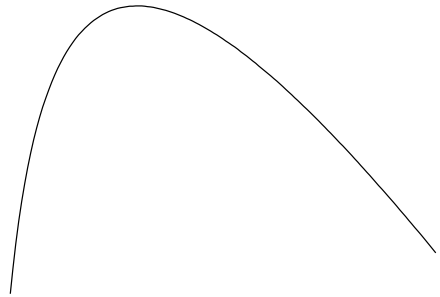

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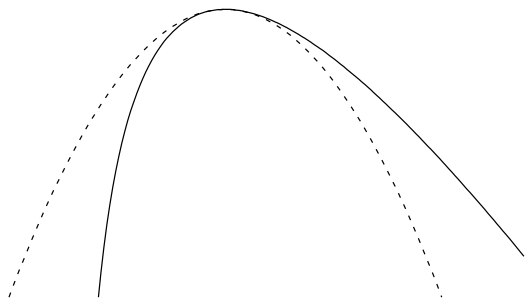

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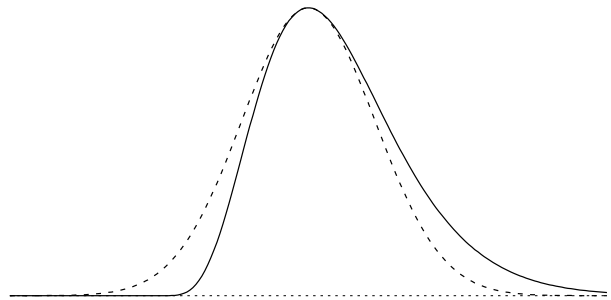

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The posterior is unimodal and hence $\mathbf{A}$ is positive semidefinite.

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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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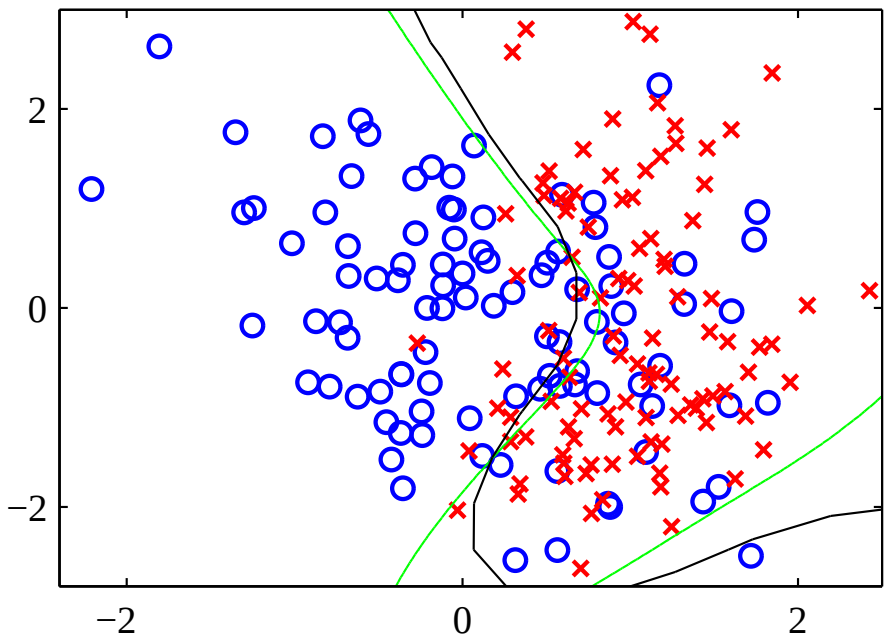
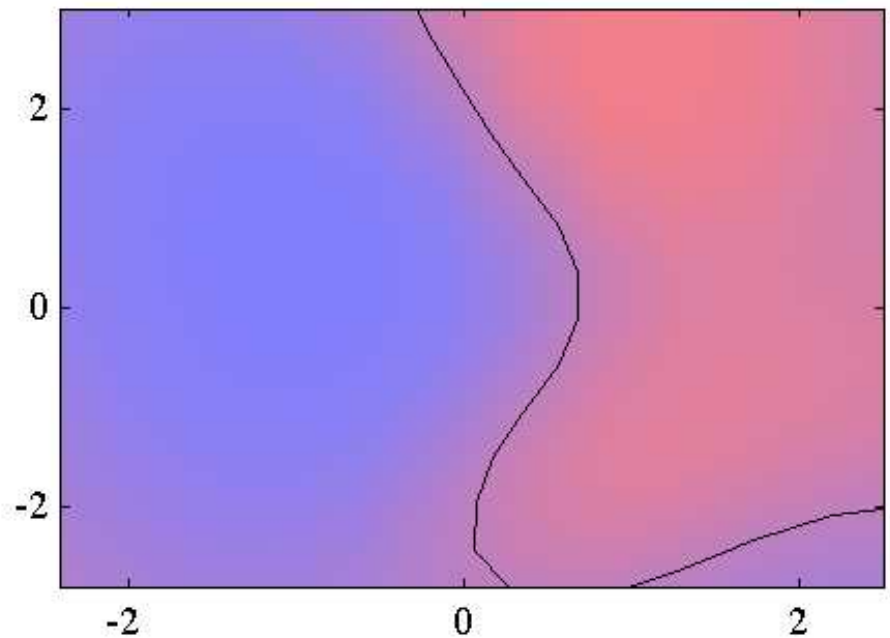
Decision boundary and prediction uncertainty:



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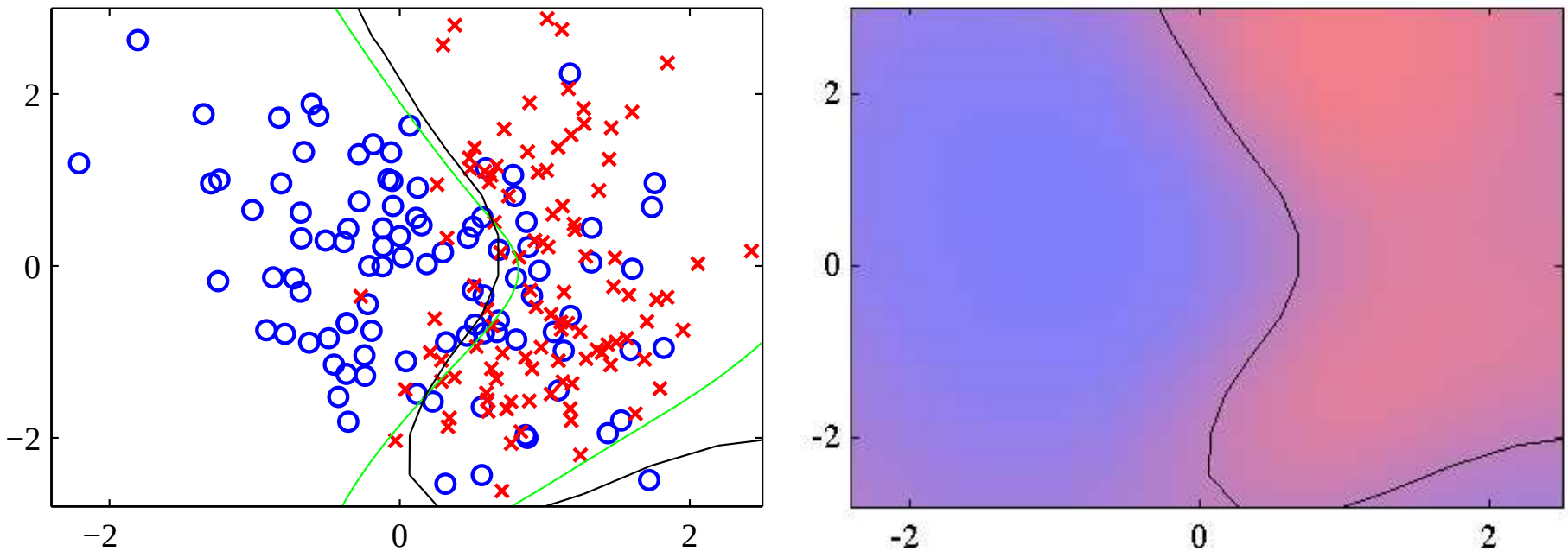


**Prediction uncertainty is higher in regions with no observed data.**

(Bishop, 2006)

**Run the notebook code for binary classification and complete task 4!**

# 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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**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.

# References


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