An introduction to Gaussian processes for probabilistic inference

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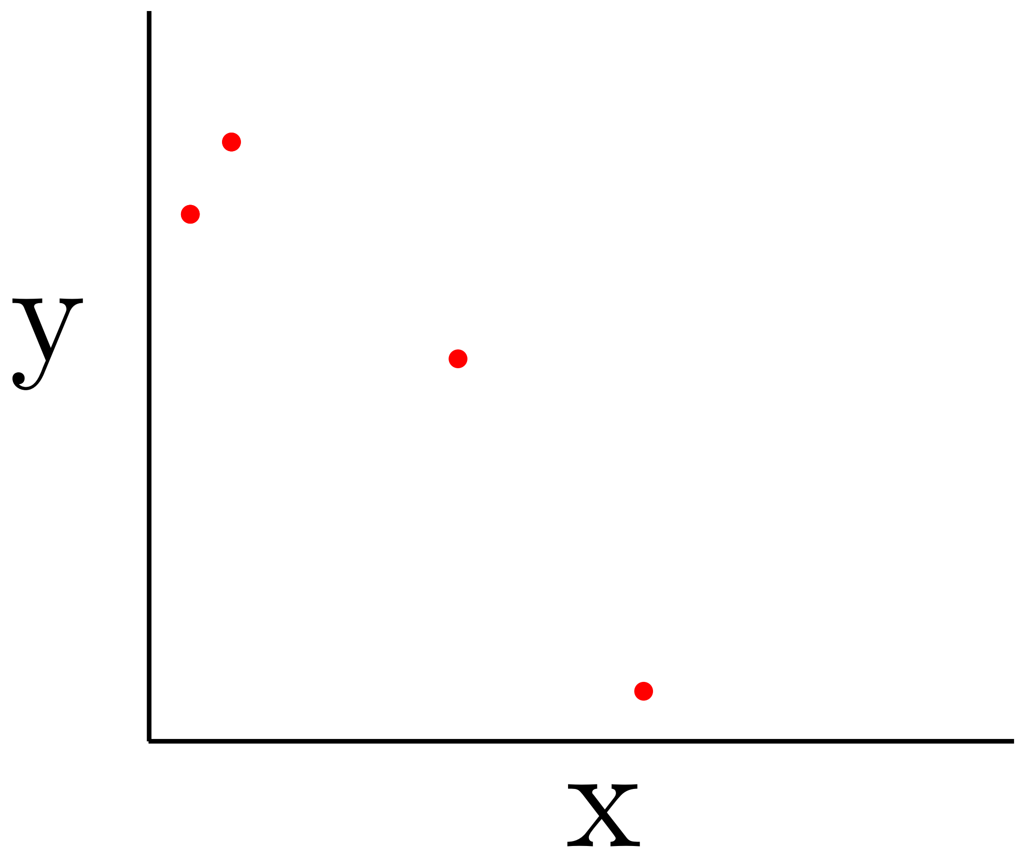
Computational and Biological Learning Lab, Department of Engineering,
University of Cambridge

Motivation: non-linear regression



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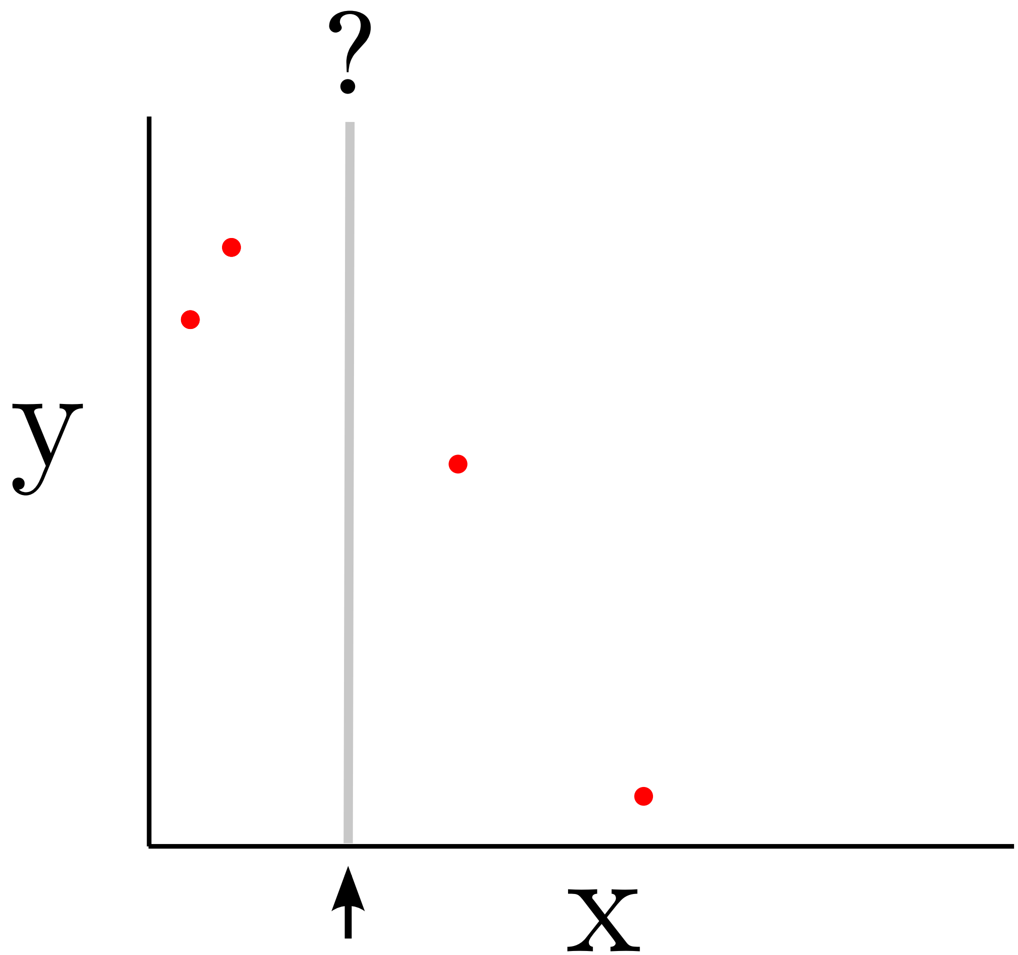

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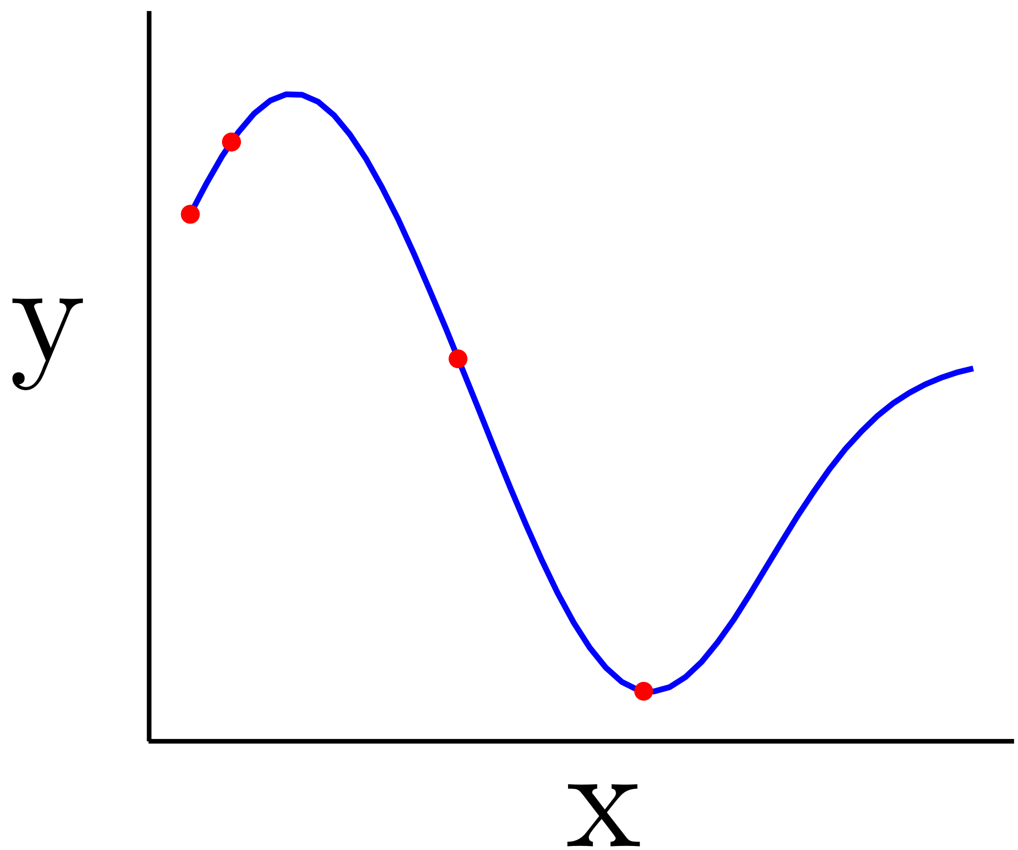

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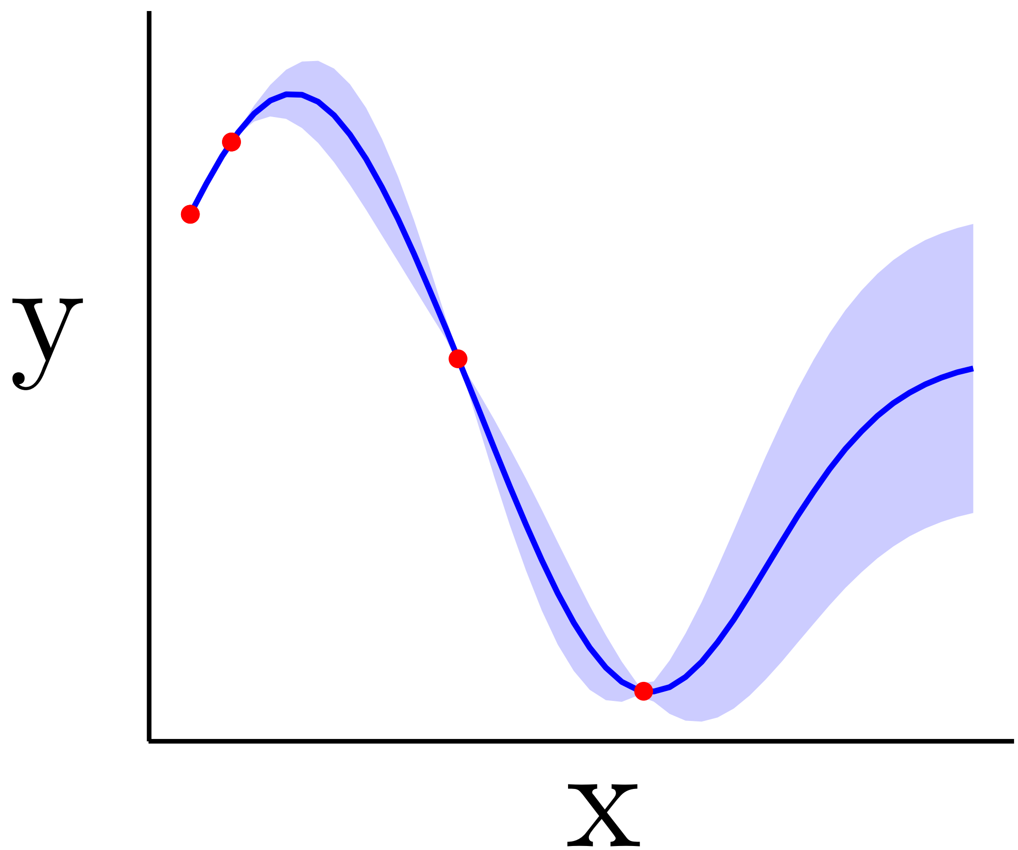
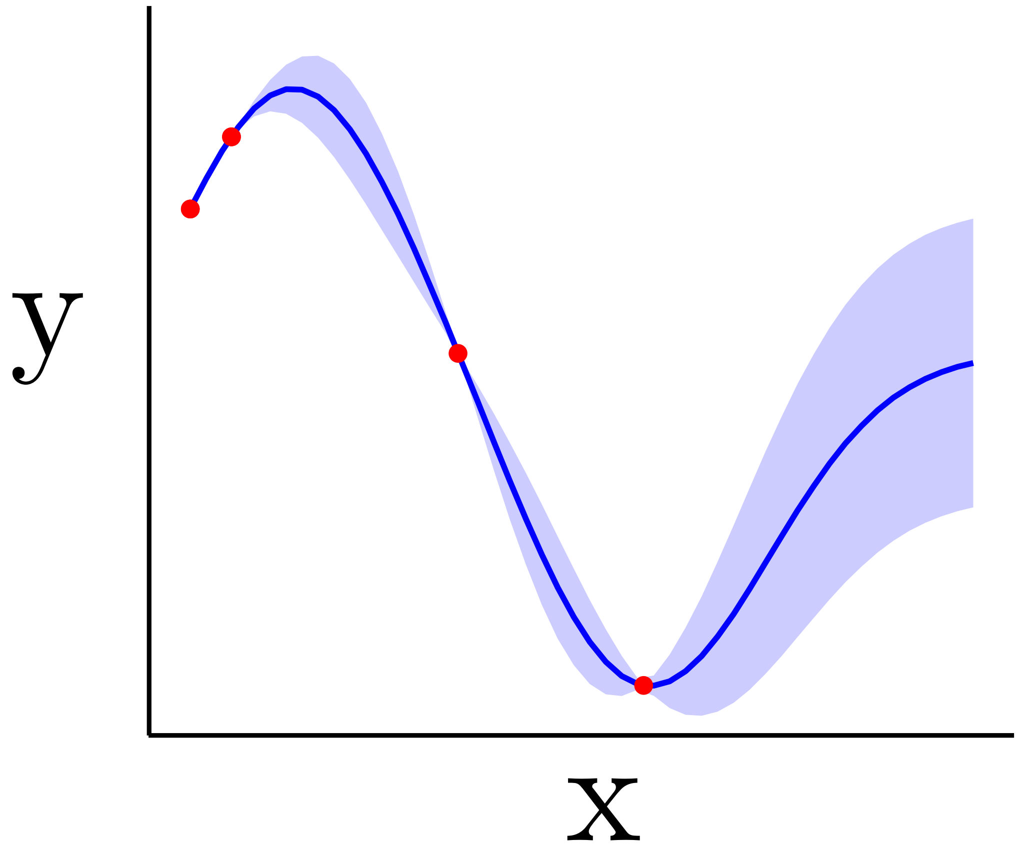


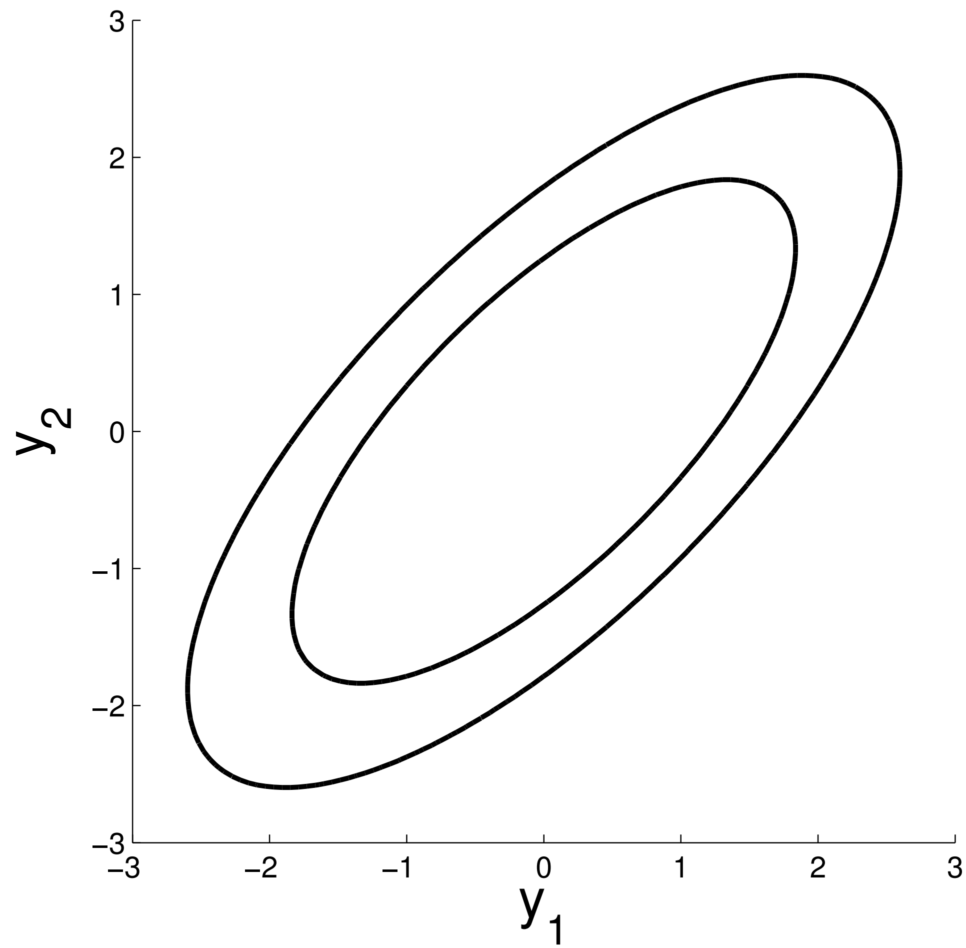
Motivation: non-linear regression

Can we do this with a plain old Gaussian?



Gaussian distribution

$$p(\mathbf{y}|\Sigma) \propto \exp\left(-\tfrac{1}{2}\mathbf{y}^\intercal\Sigma^{-1}\mathbf{y}\right) \qquad \Sigma = \begin{bmatrix} 1 & .7 \\ .7 & 1 \end{bmatrix}$$



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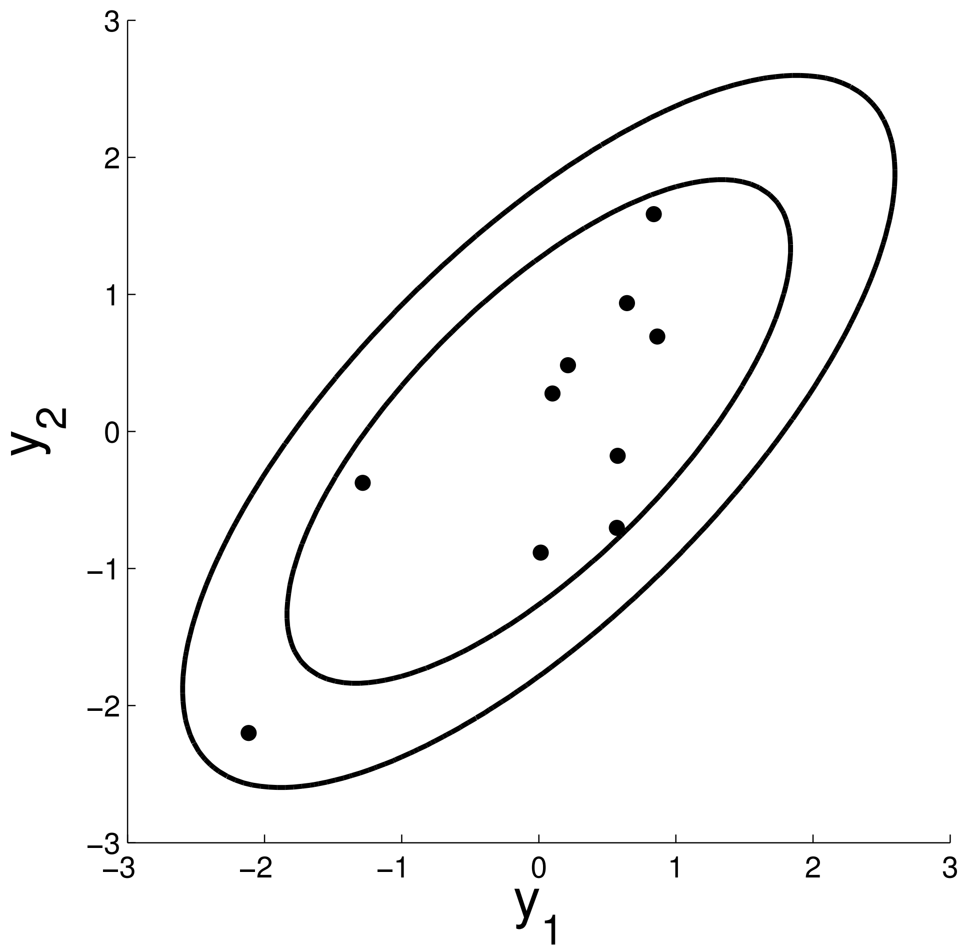
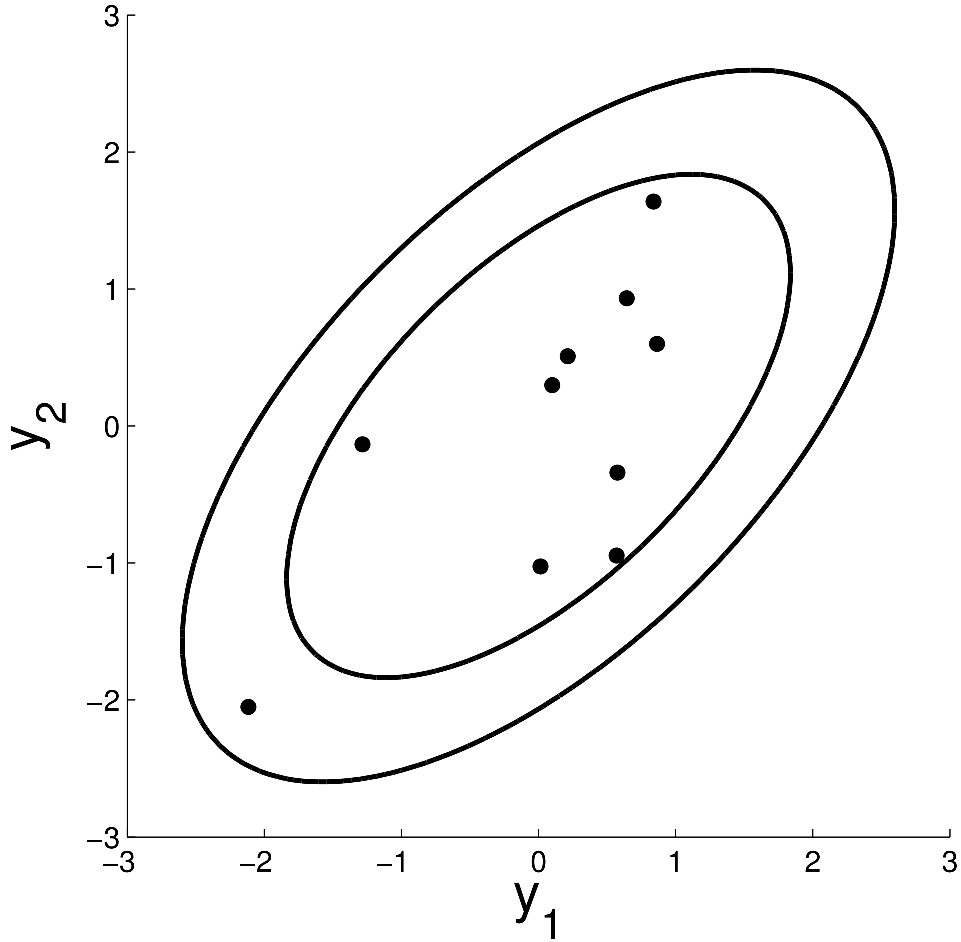


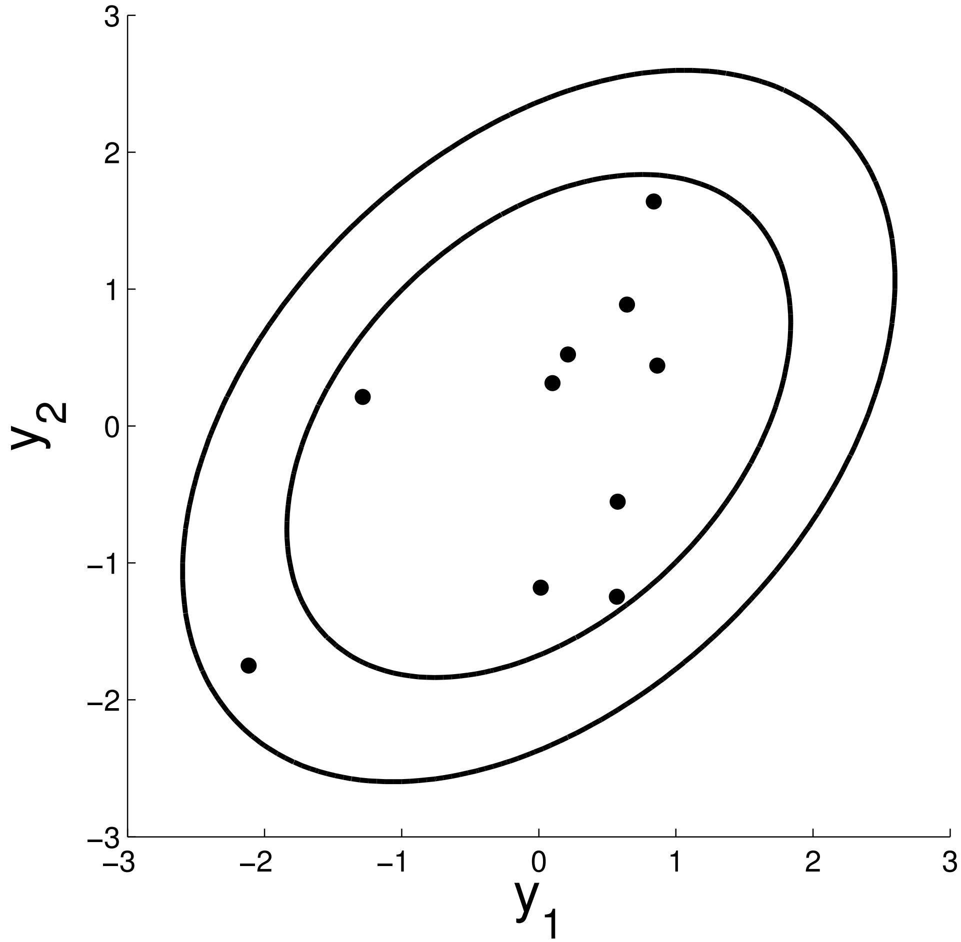
Gaussian distribution

$$p(\mathbf{y}|\Sigma) \propto \exp\left(-\tfrac{1}{2}\mathbf{y}^\mathsf{T}\Sigma^{-1}\mathbf{y}\right) \qquad \Sigma = \begin{bmatrix} 1 & .6 \\ .6 & 1 \end{bmatrix}$$



Gaussian distribution

$$p(\mathbf{y}|\Sigma) \propto \exp\left(-\tfrac{1}{2}\mathbf{y}^\top \Sigma^{-1}\mathbf{y}\right) \qquad \Sigma = \begin{bmatrix} 1 & .4 \\ .4 & 1 \end{bmatrix}$$



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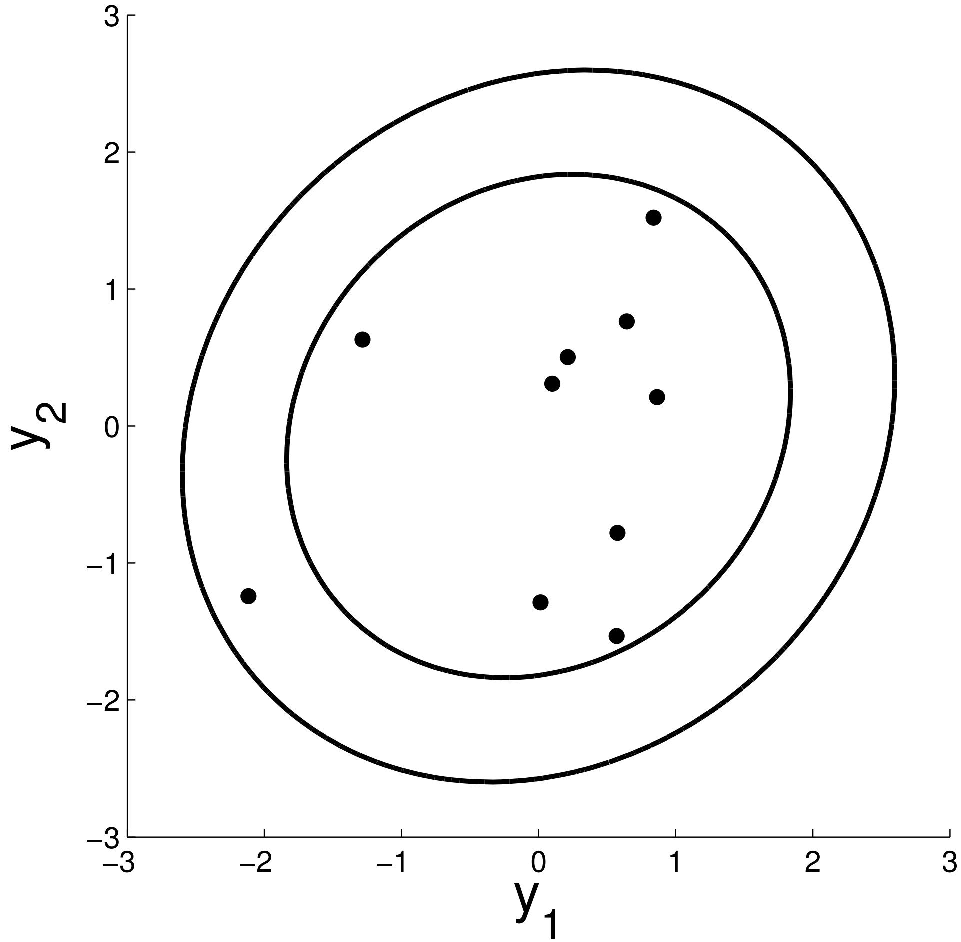

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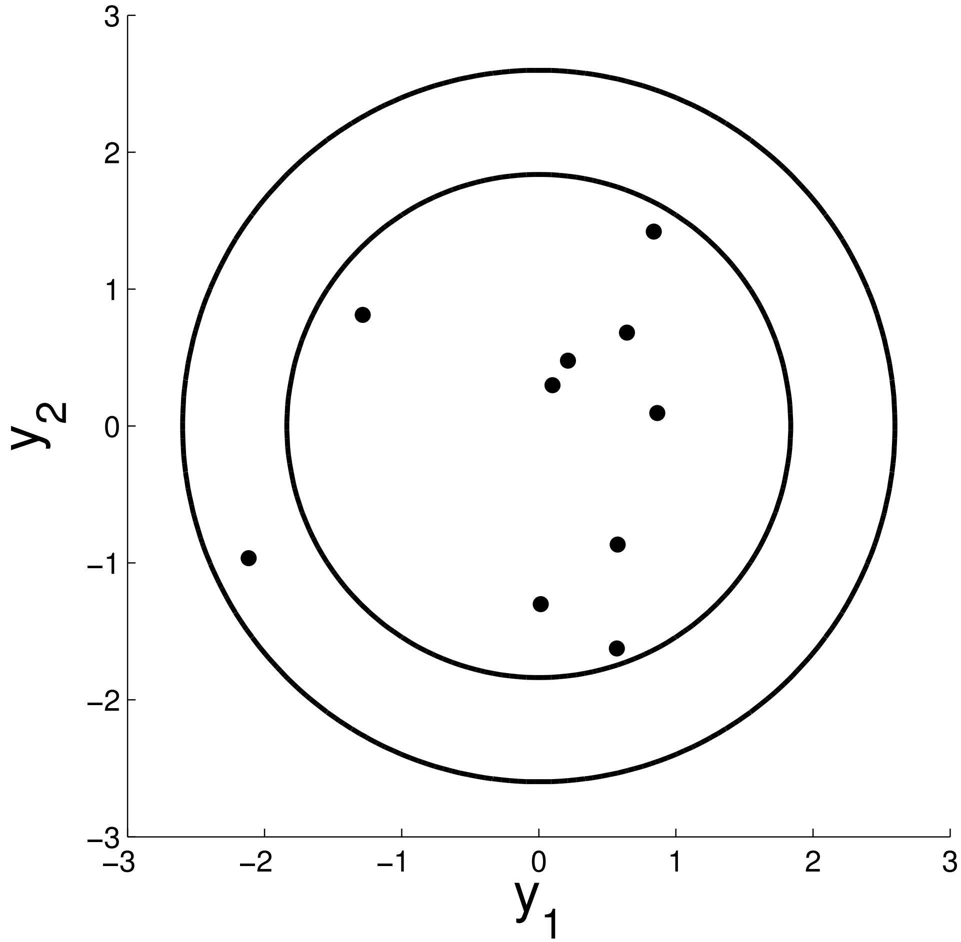

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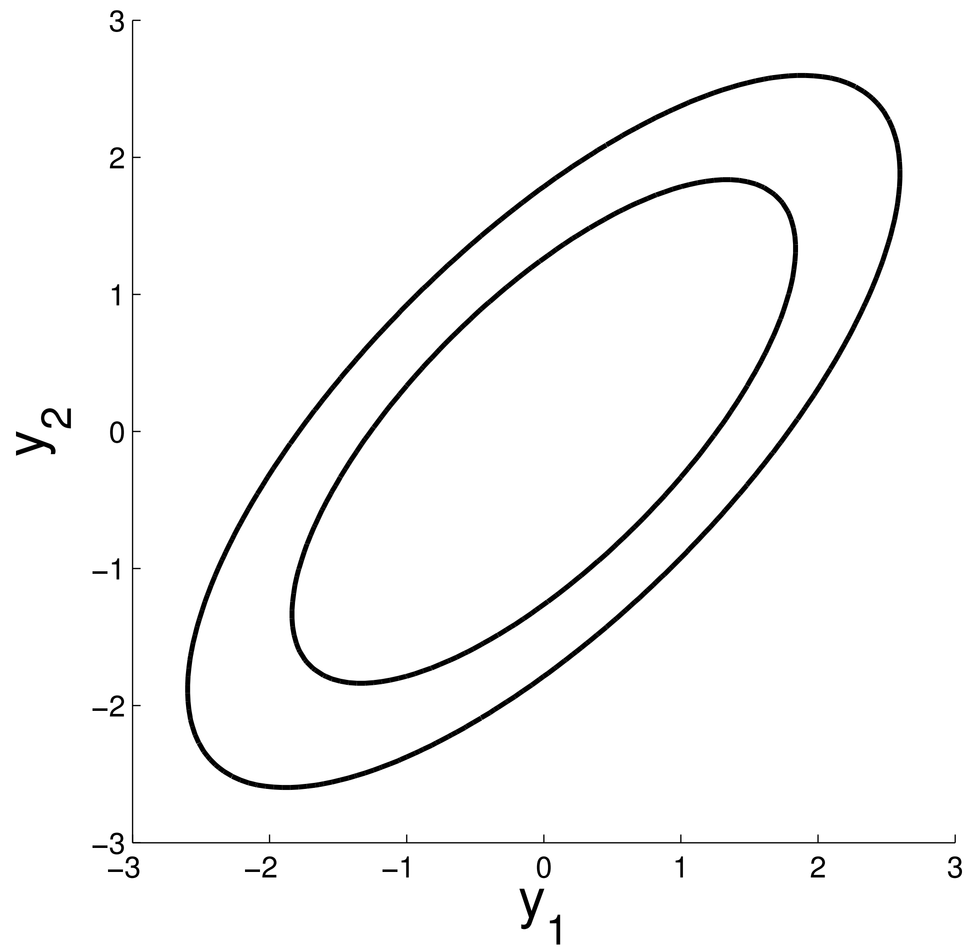

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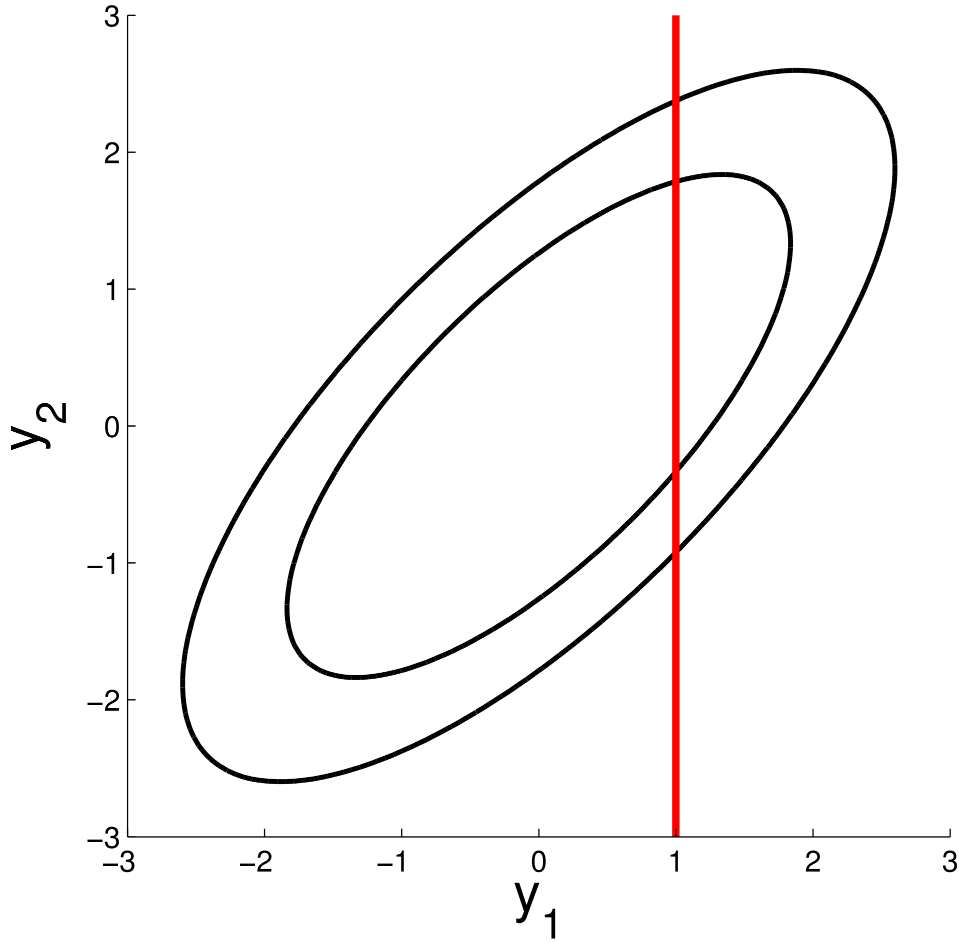
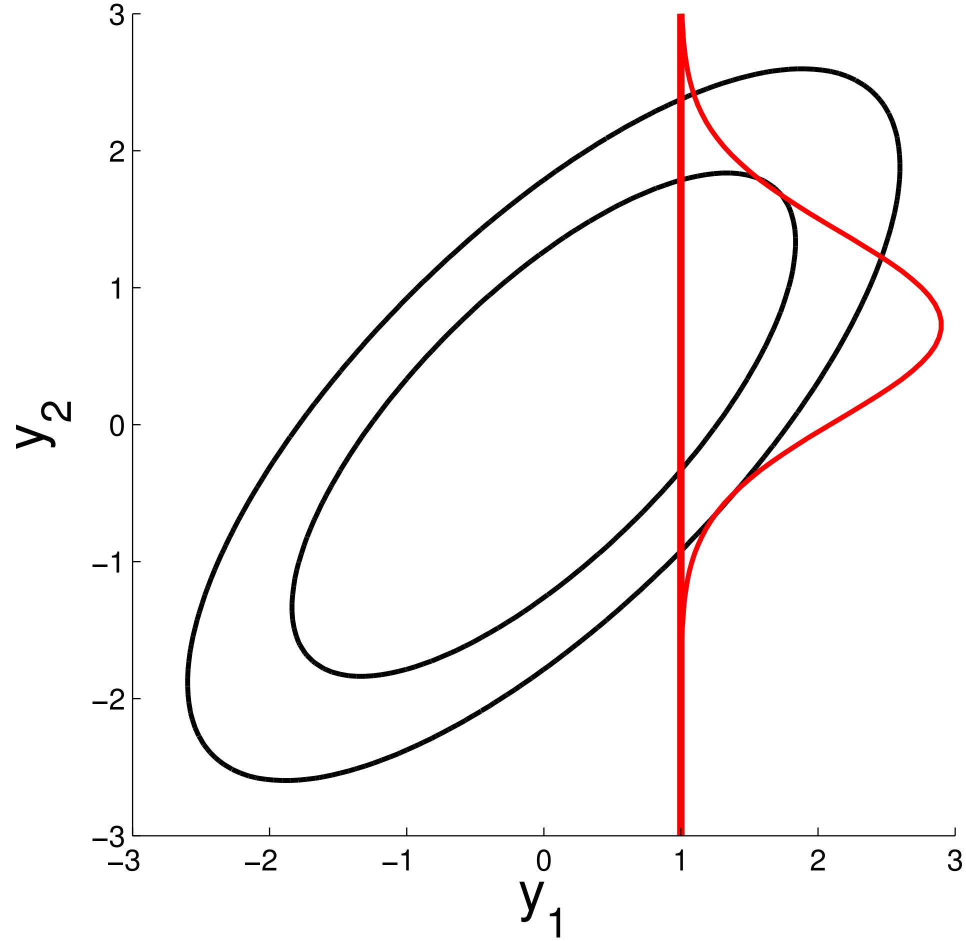


Gaussian distribution

$$p(\mathsf{y}_2|\mathsf{y}_1, \Sigma) \propto \exp\left(-\frac{1}{2}(\mathsf{y}_2 - \mu_*)\Sigma_*{}^{-1}(\mathsf{y}_2 - \mu_*)\right)$$



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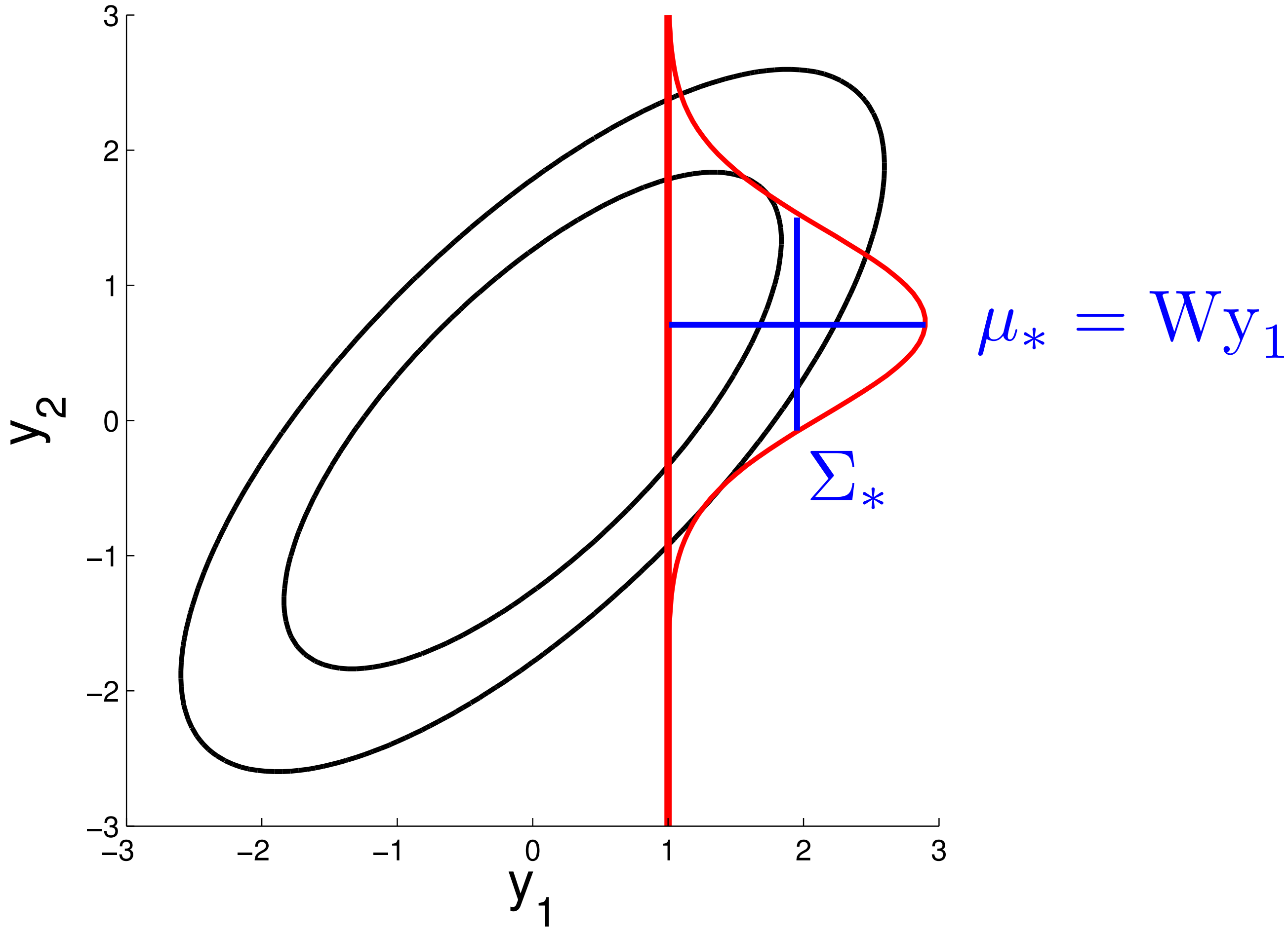

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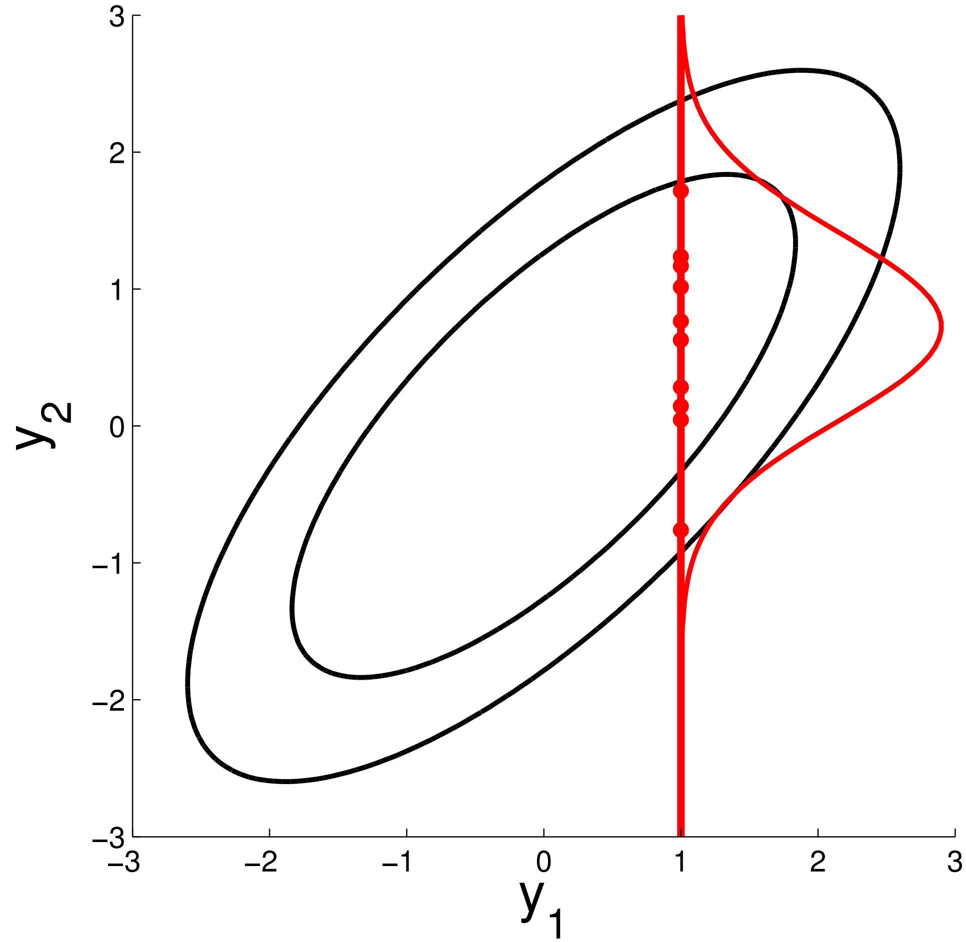

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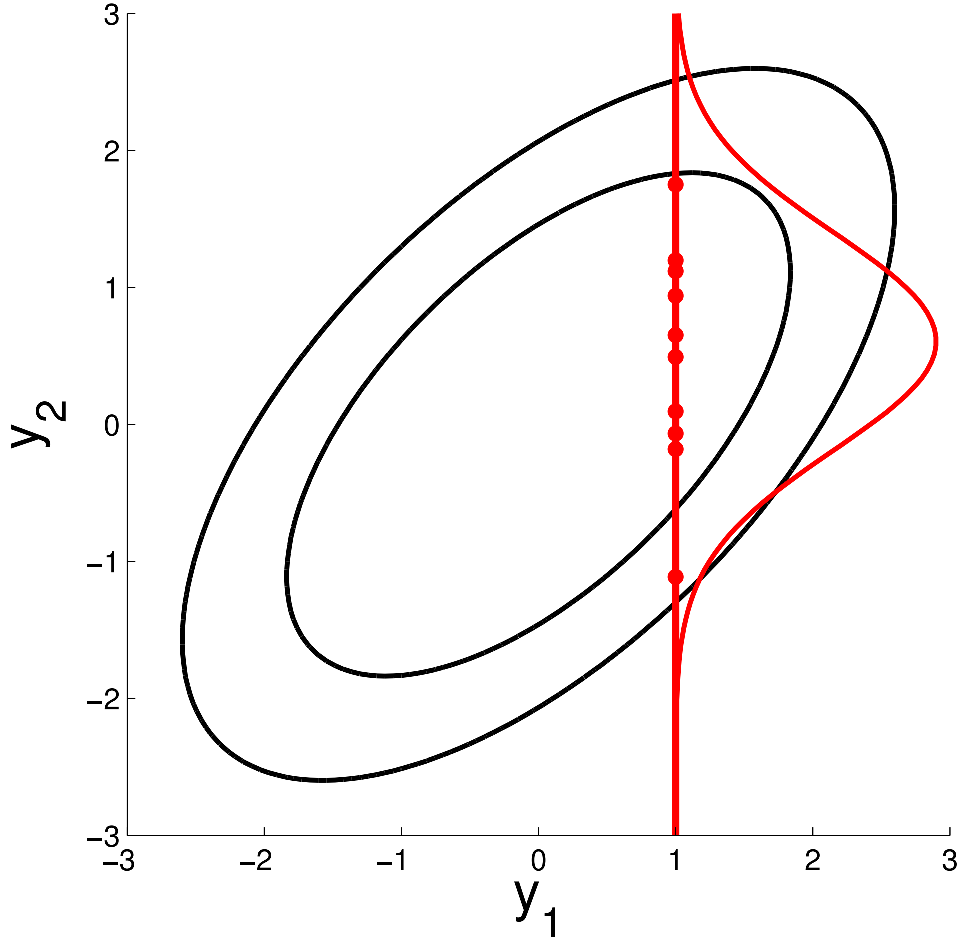

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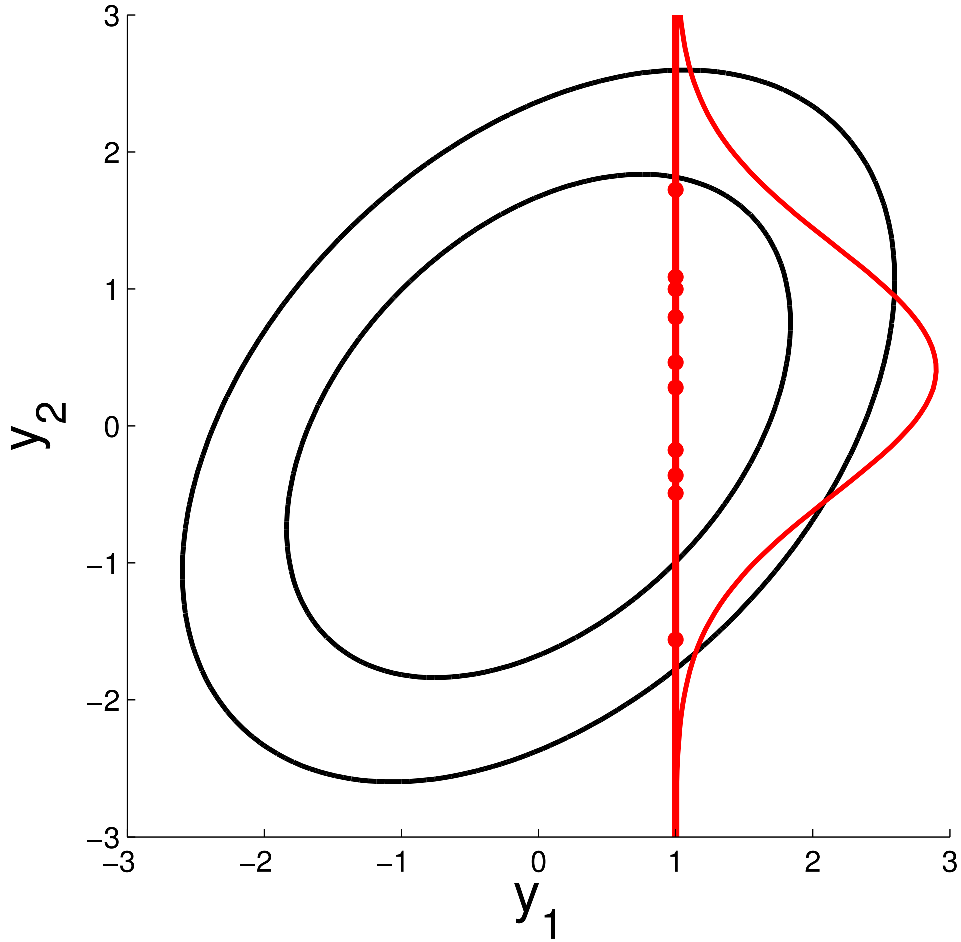

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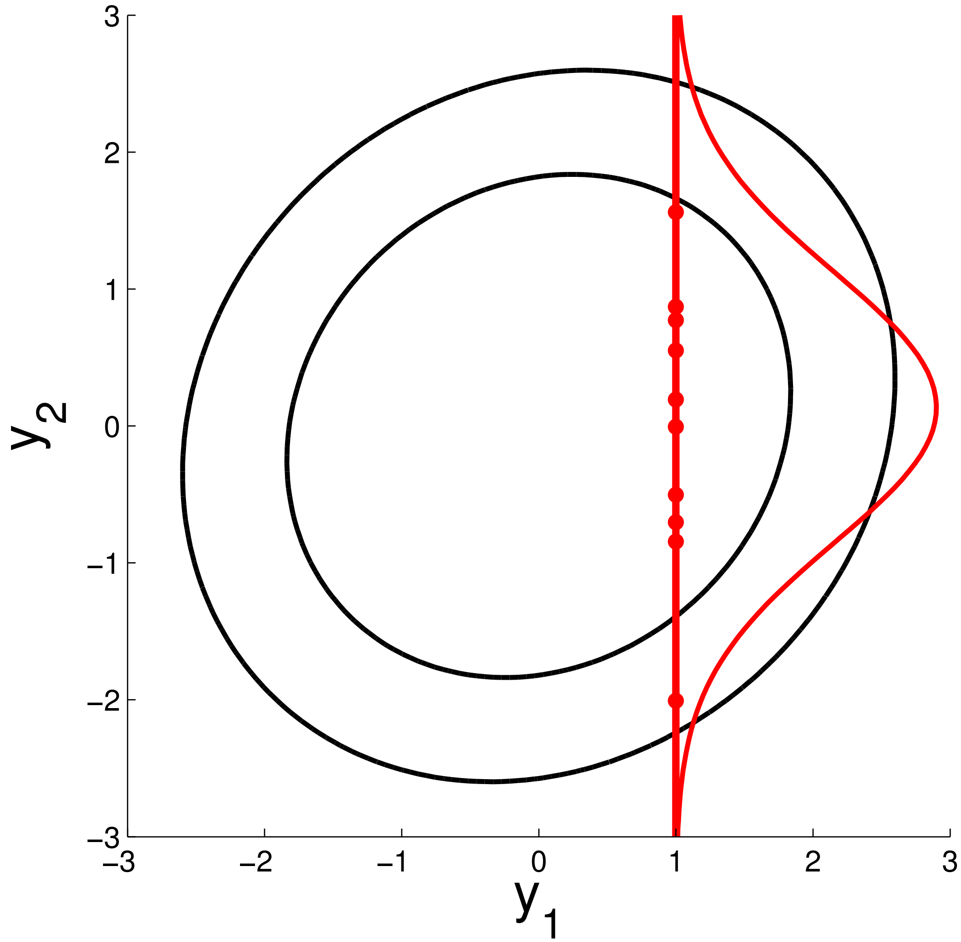

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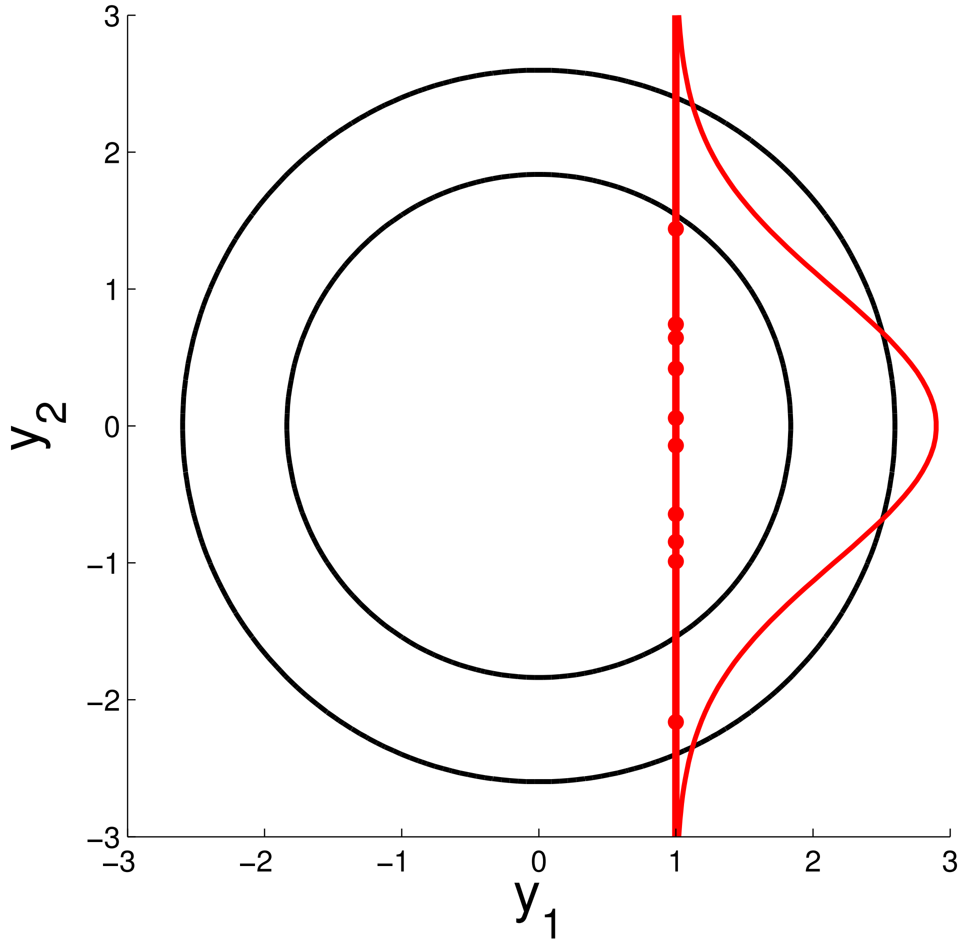
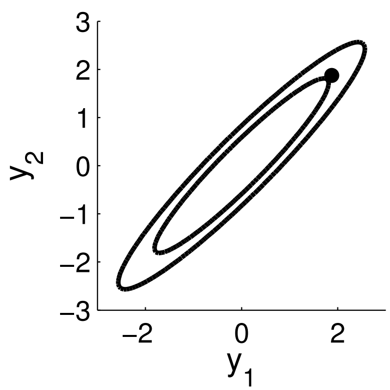


New visualisation



$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$

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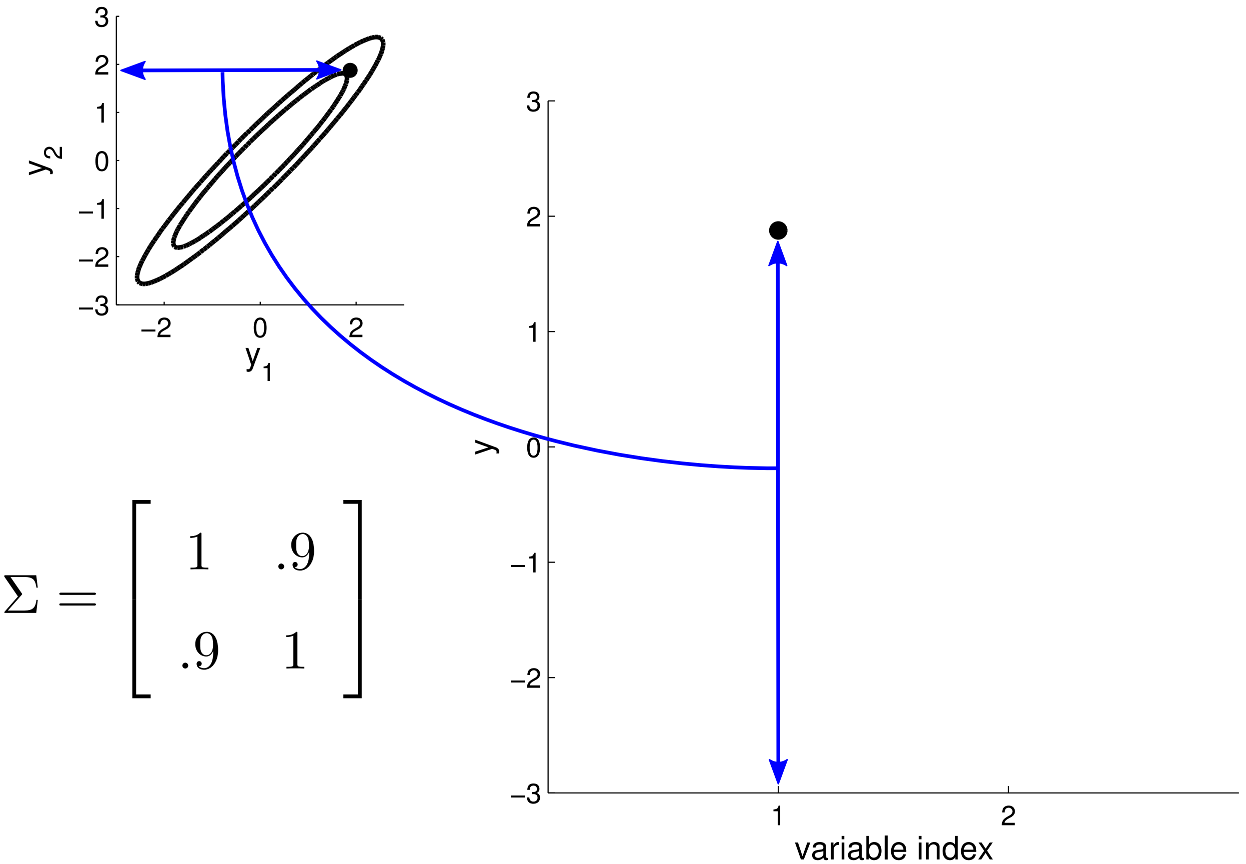

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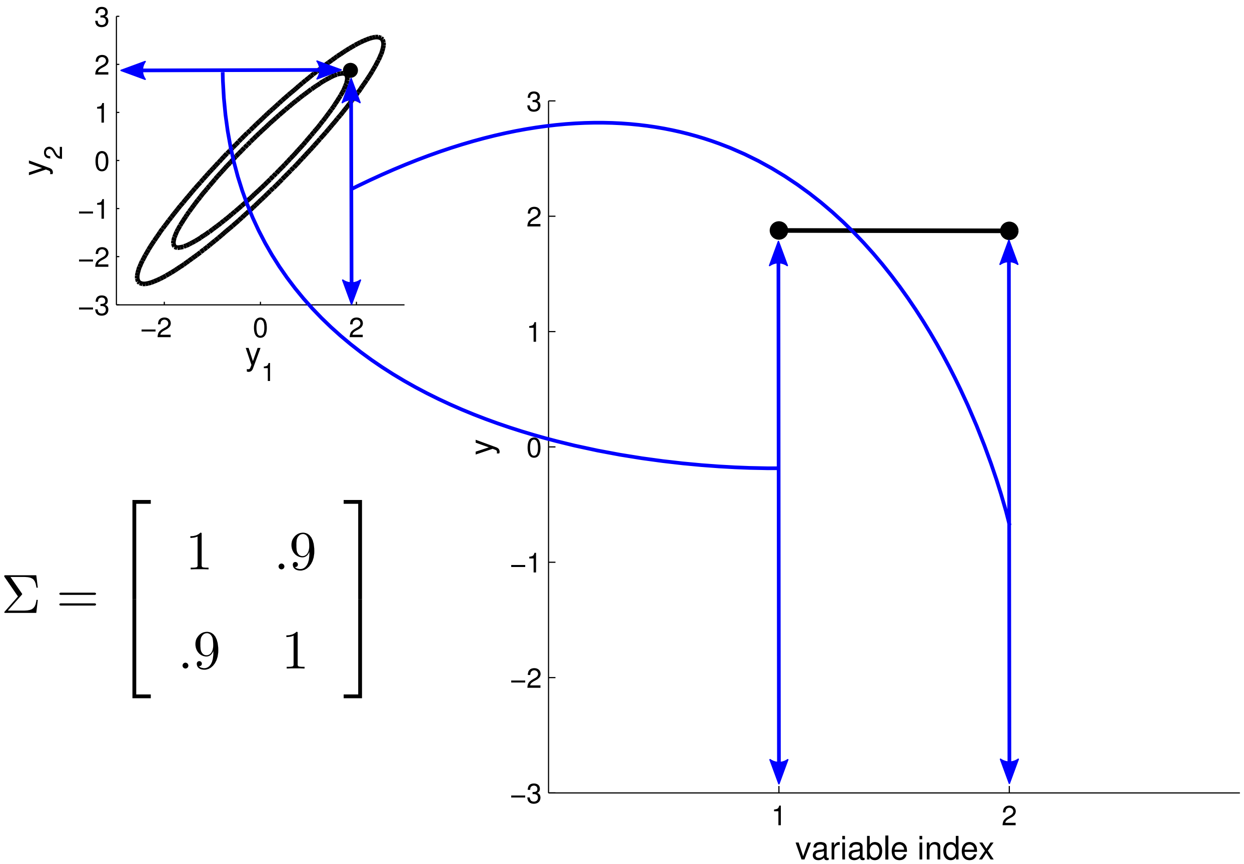

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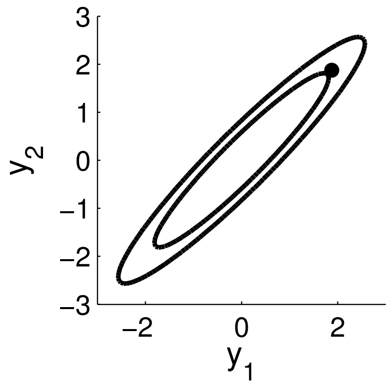

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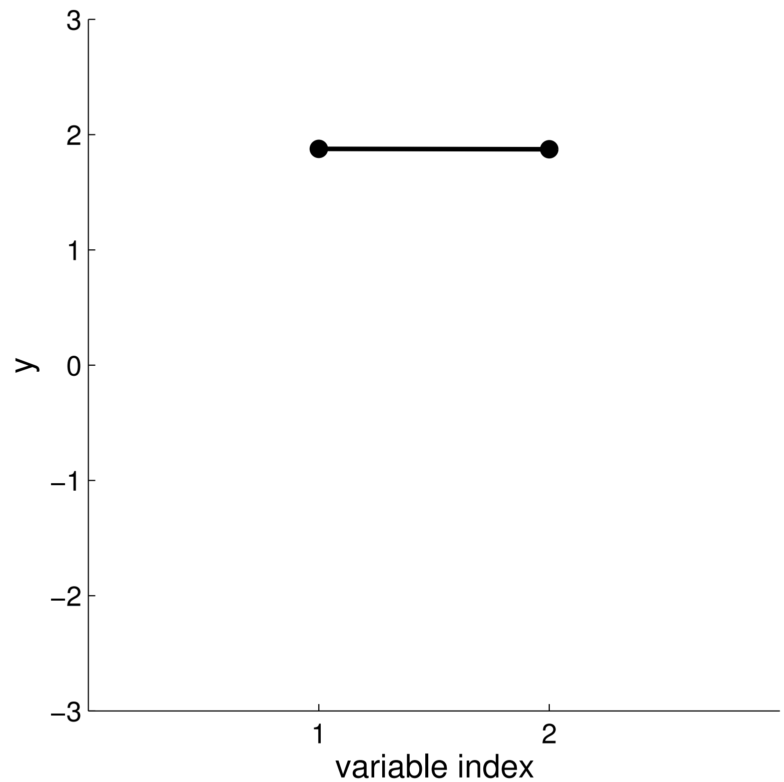

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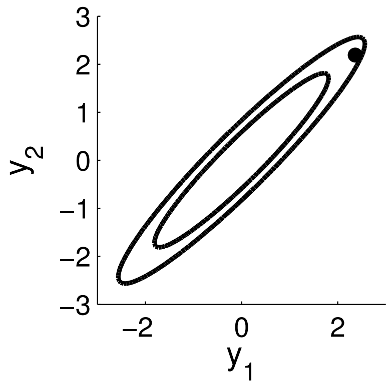

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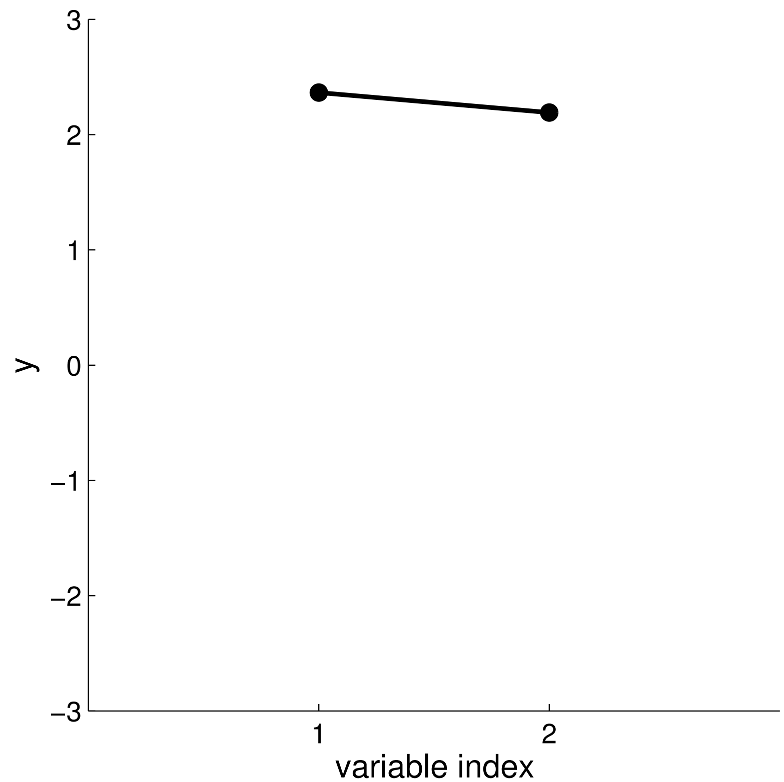

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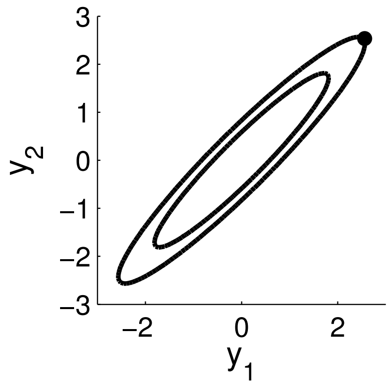

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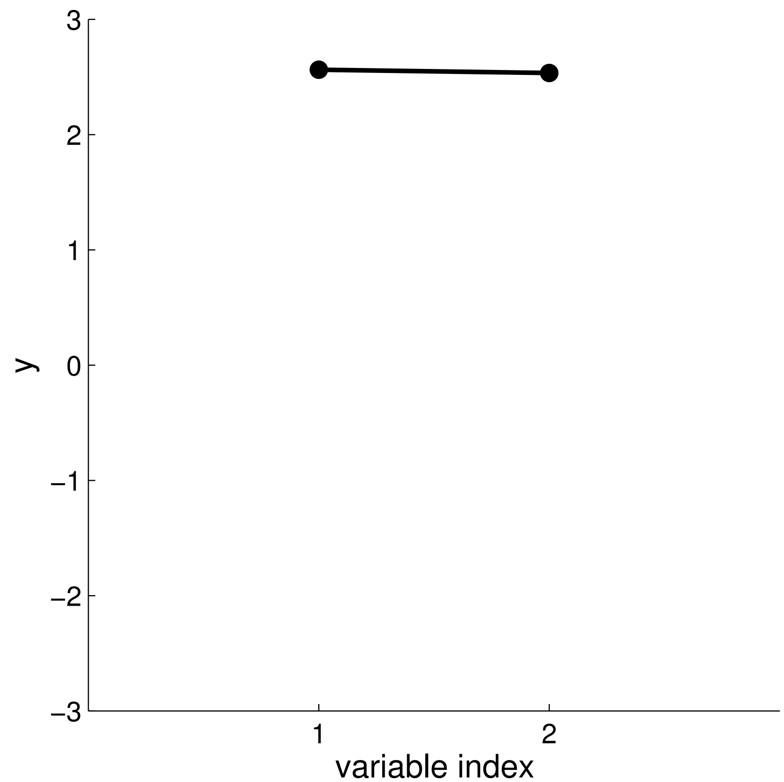

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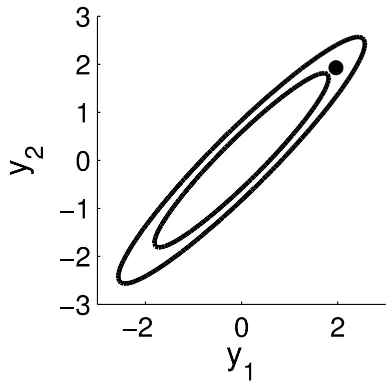

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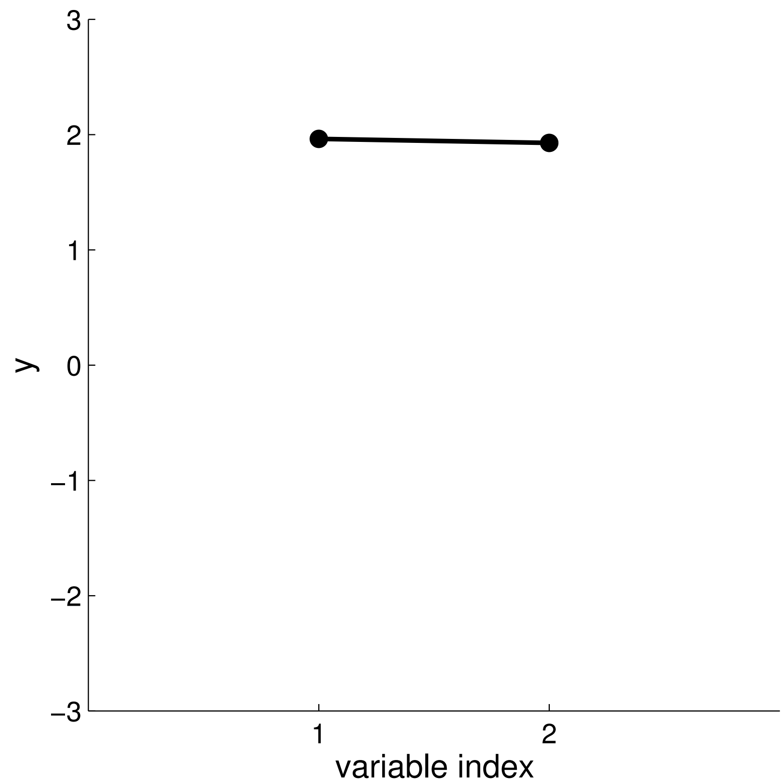

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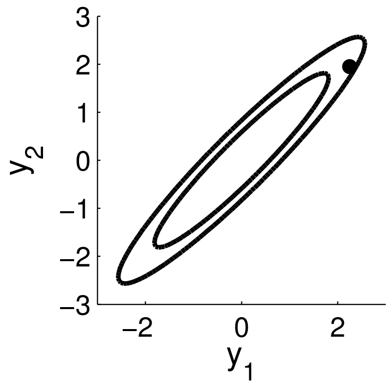

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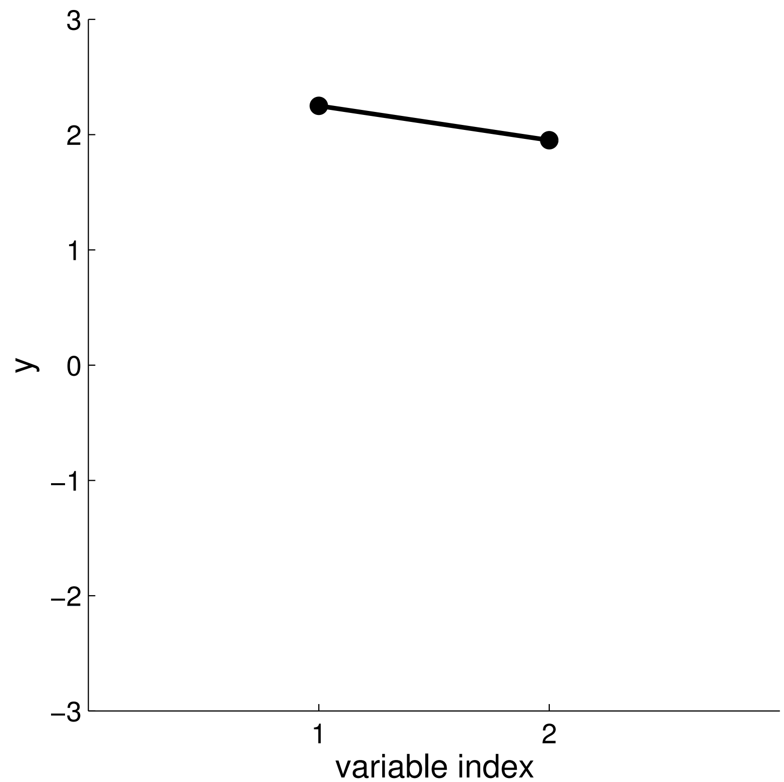

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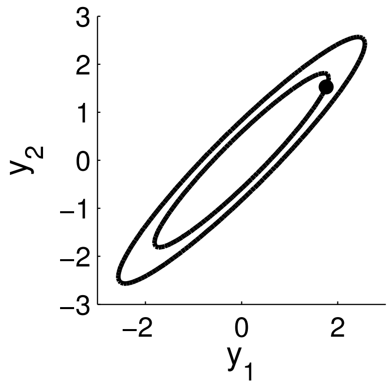

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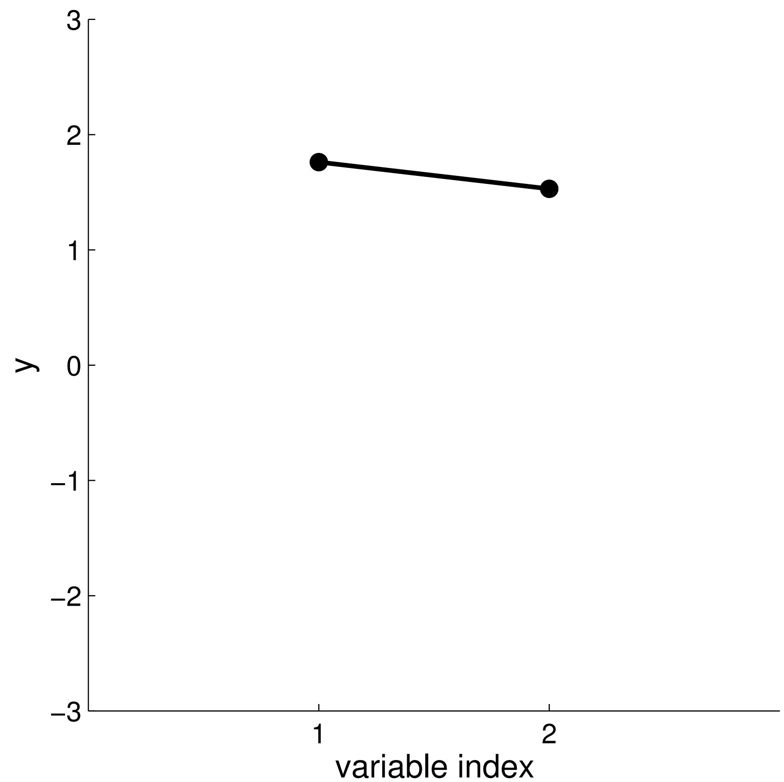

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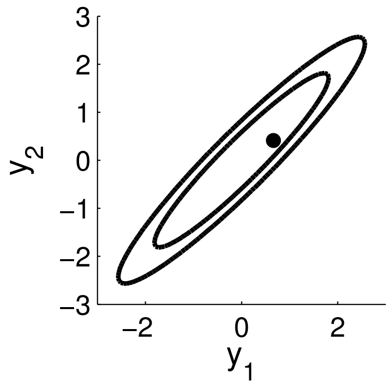

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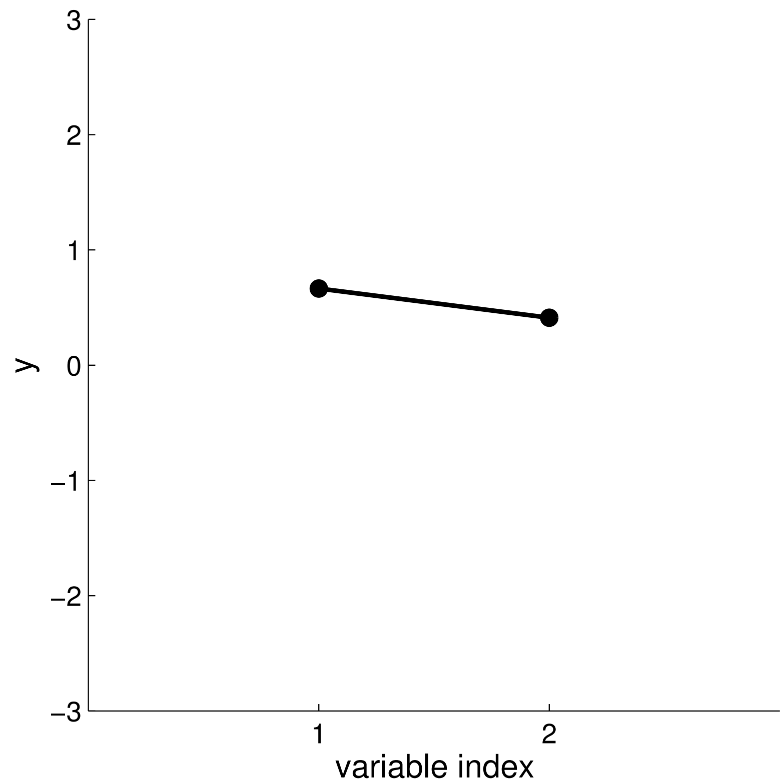

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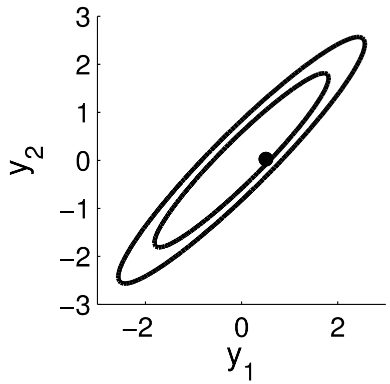

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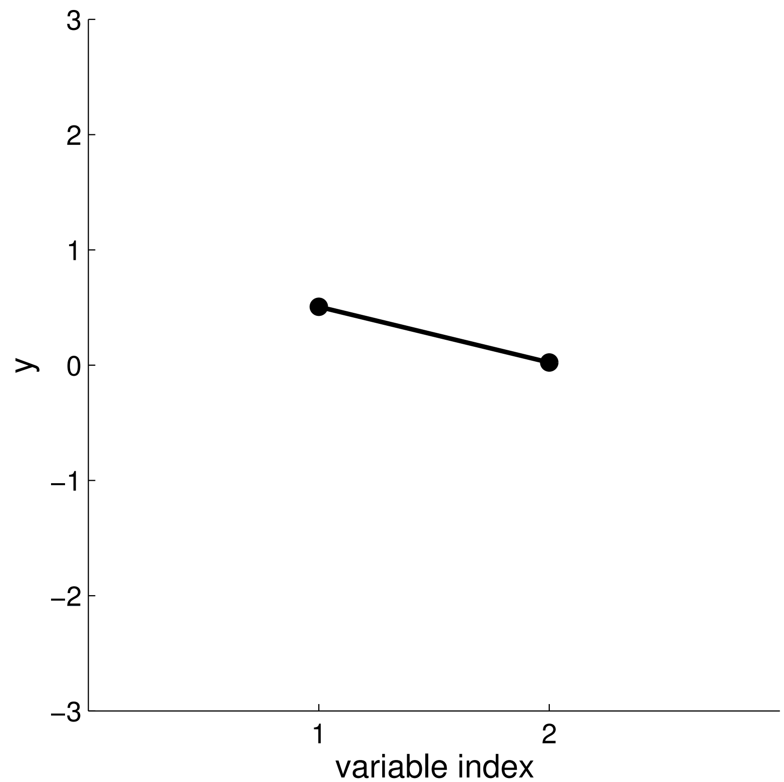

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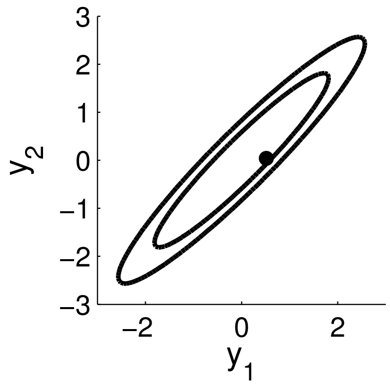

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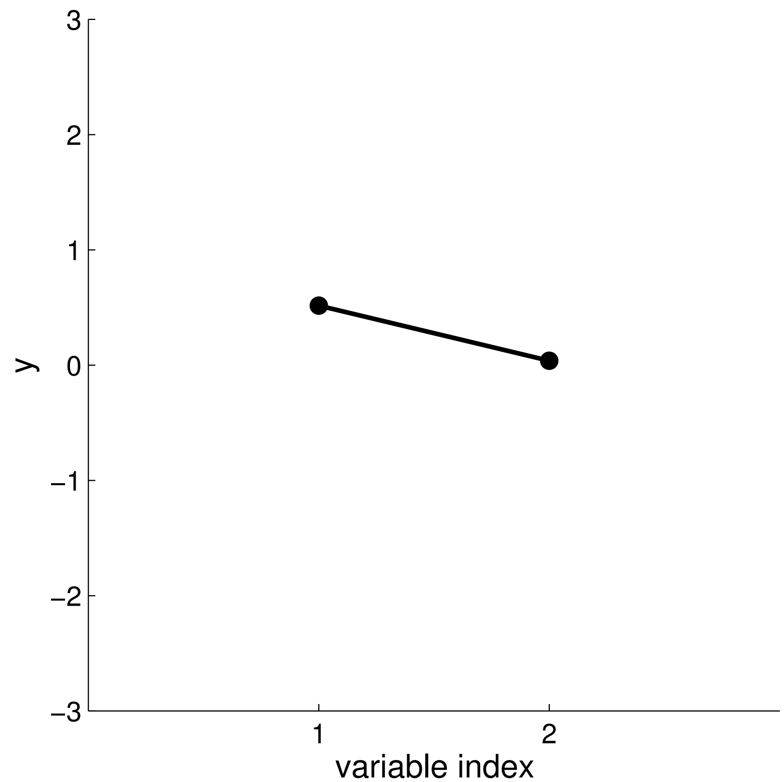

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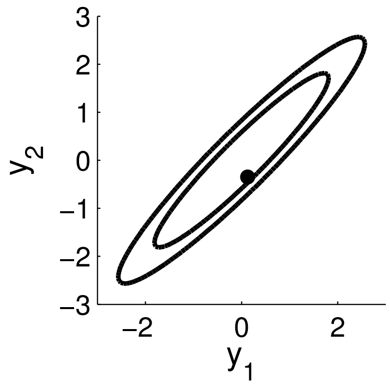

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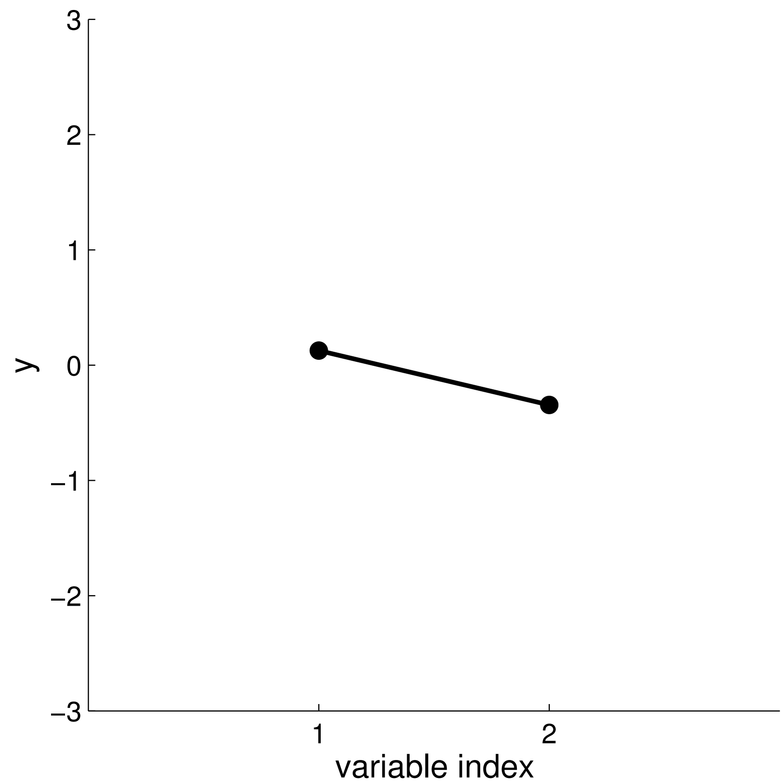

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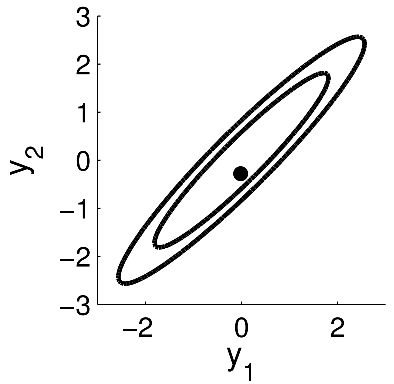

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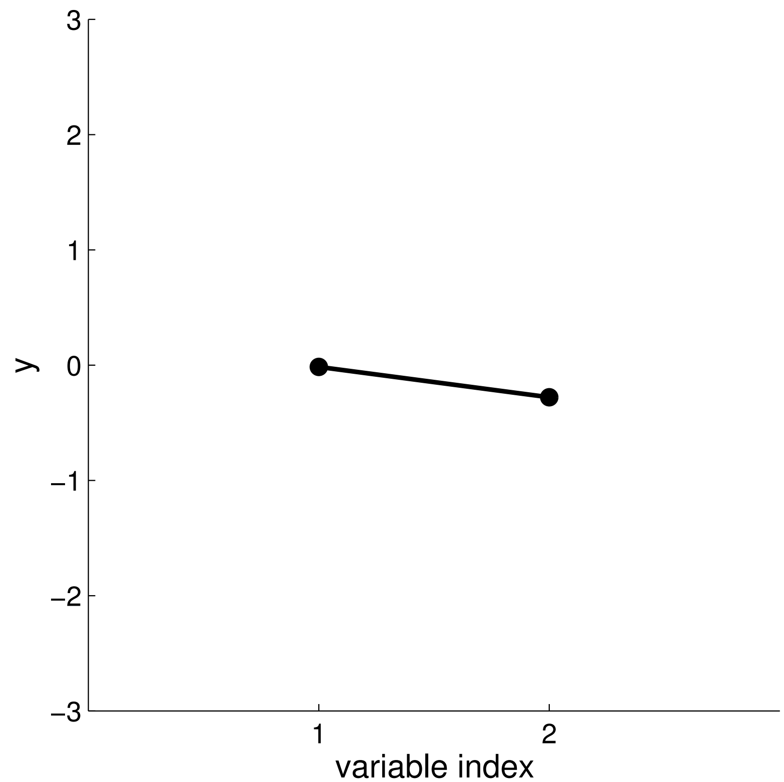

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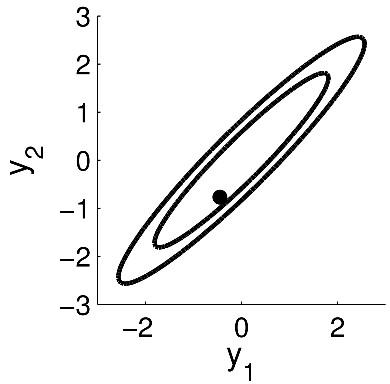

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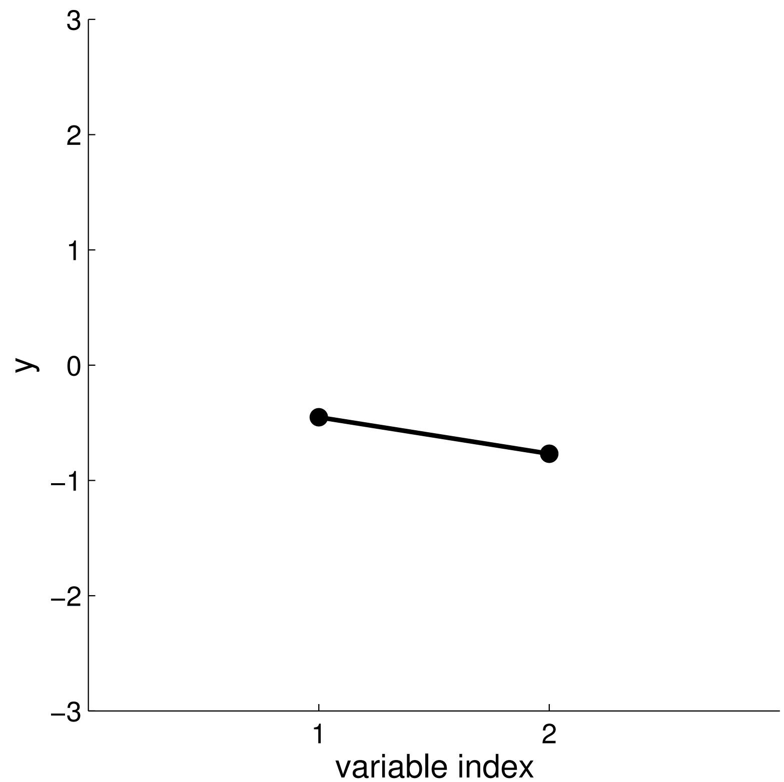

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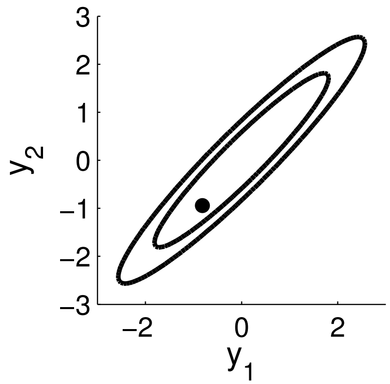

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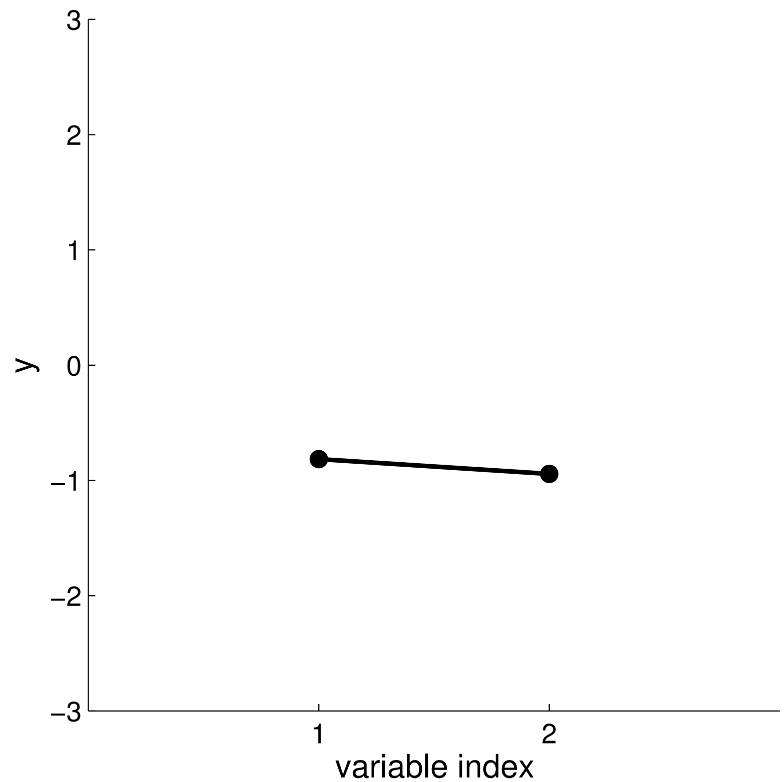

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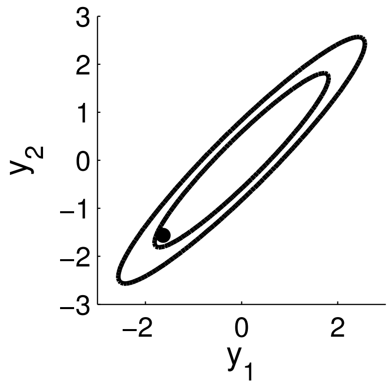

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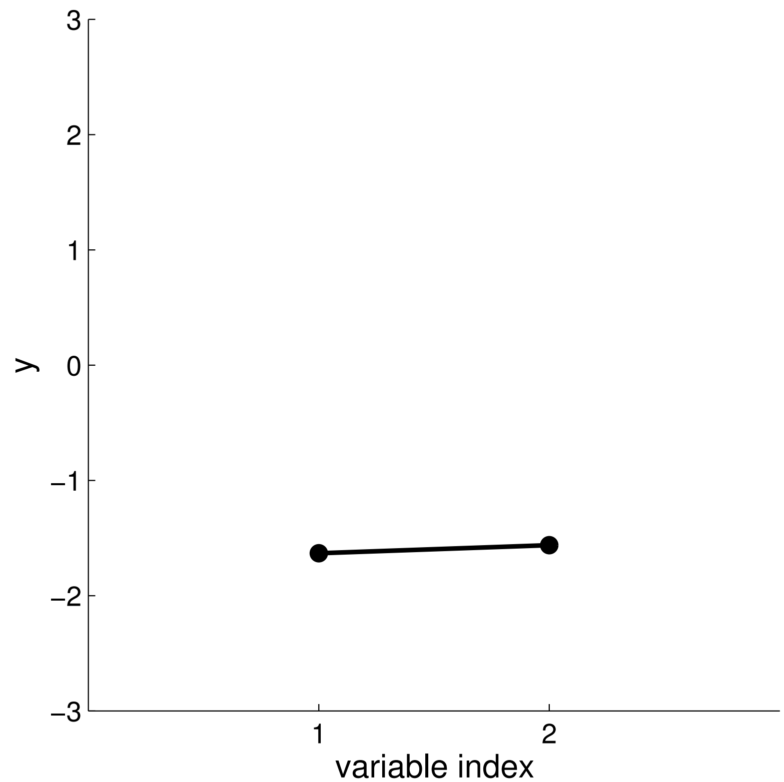

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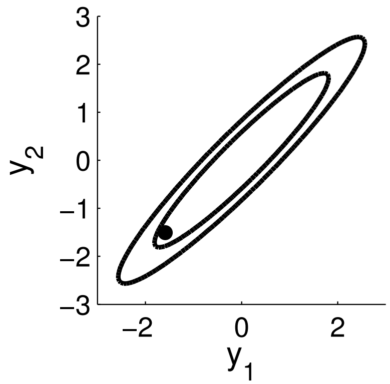

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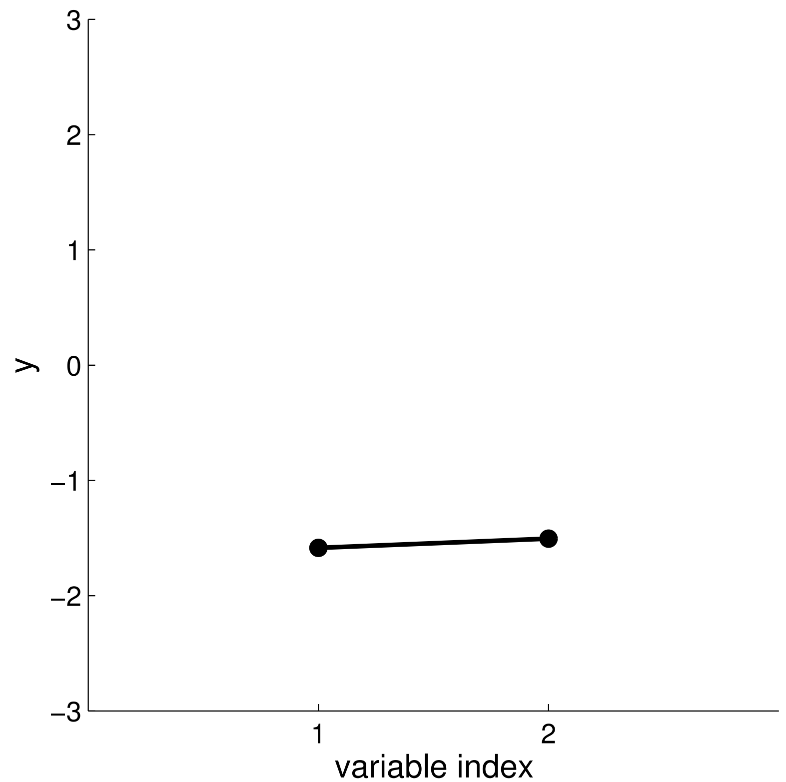

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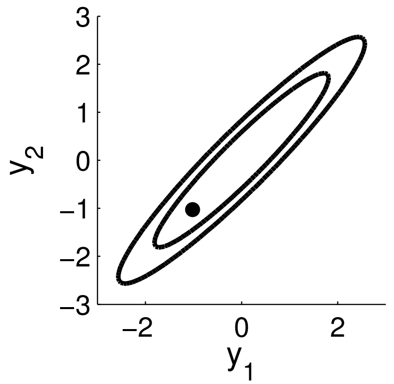

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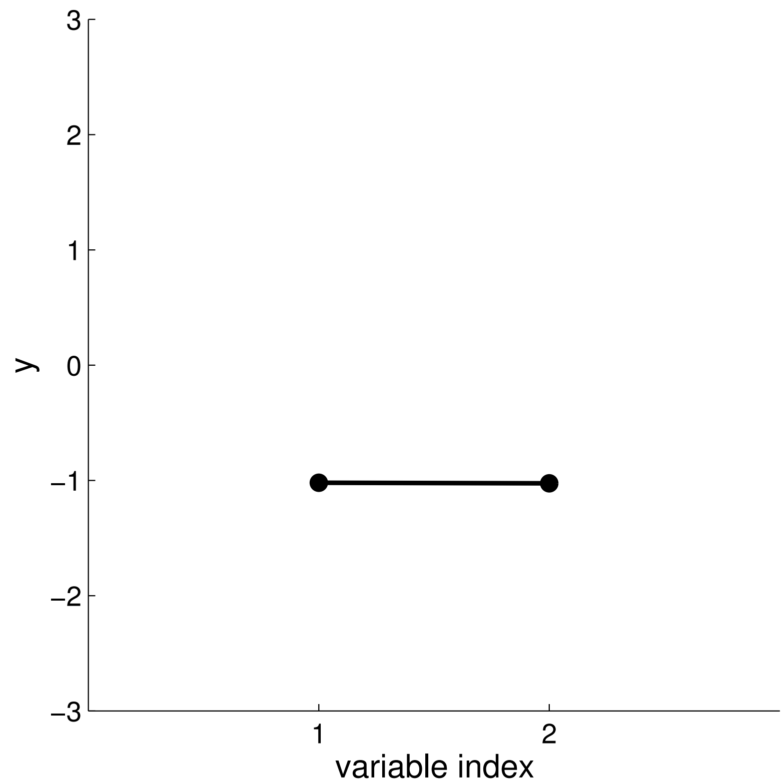

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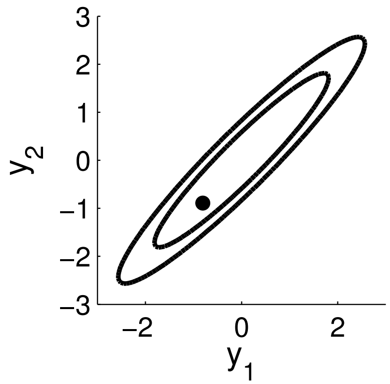

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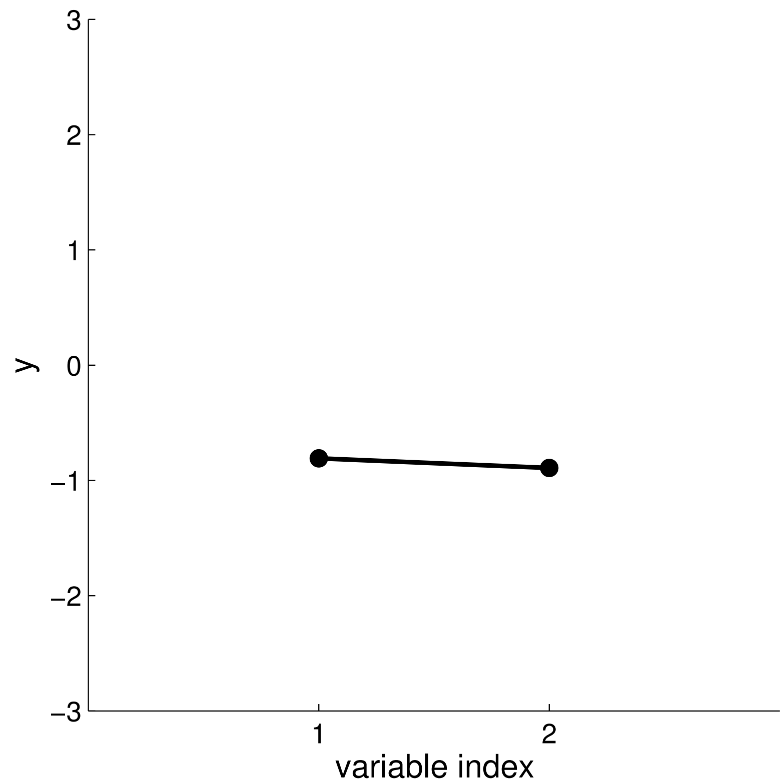

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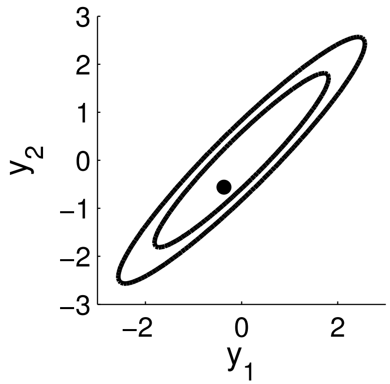

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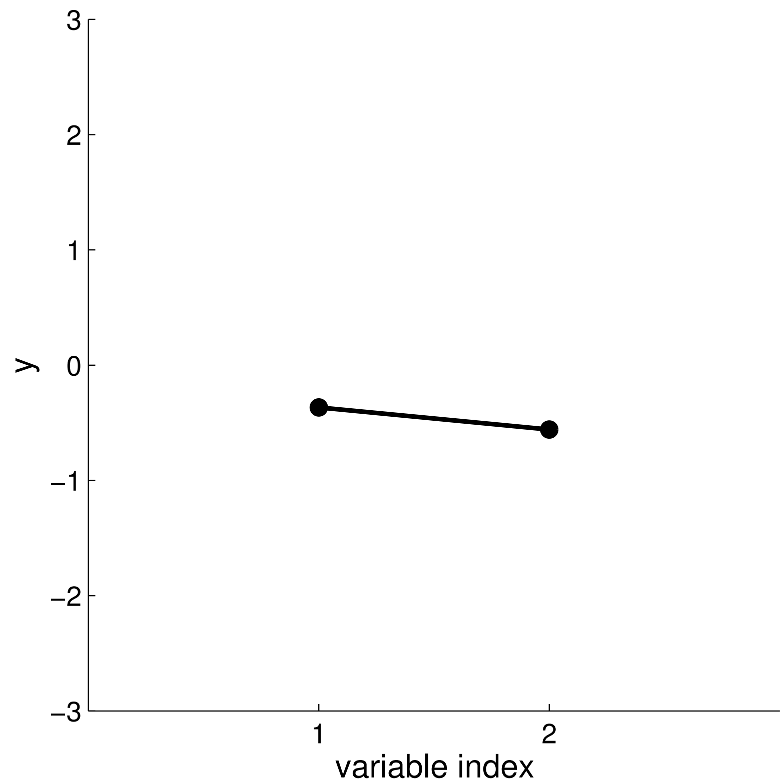

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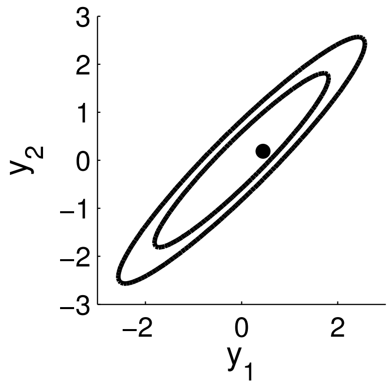

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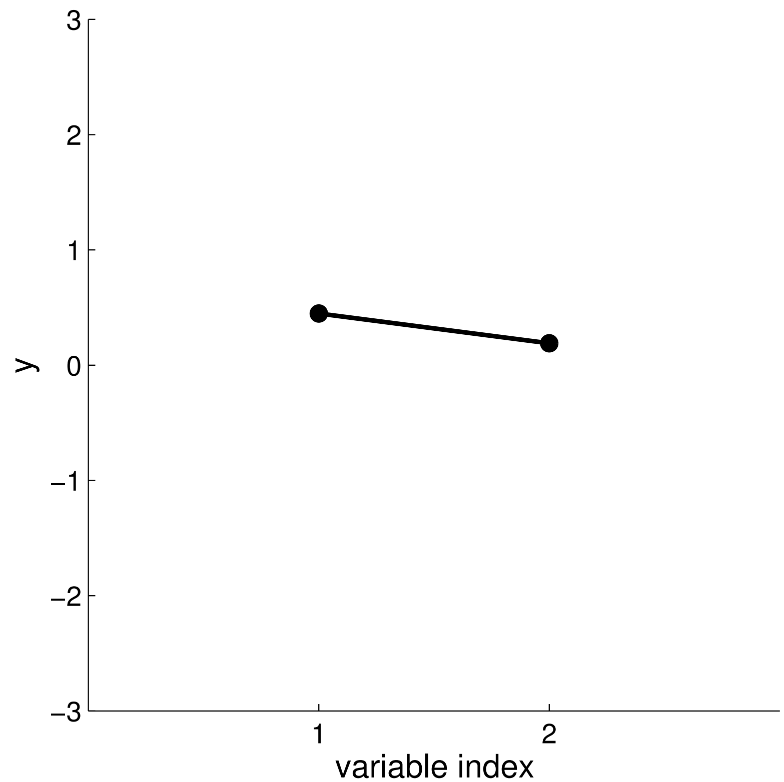

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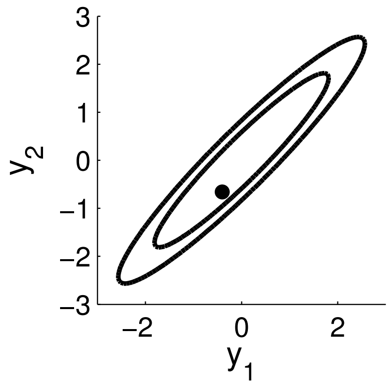
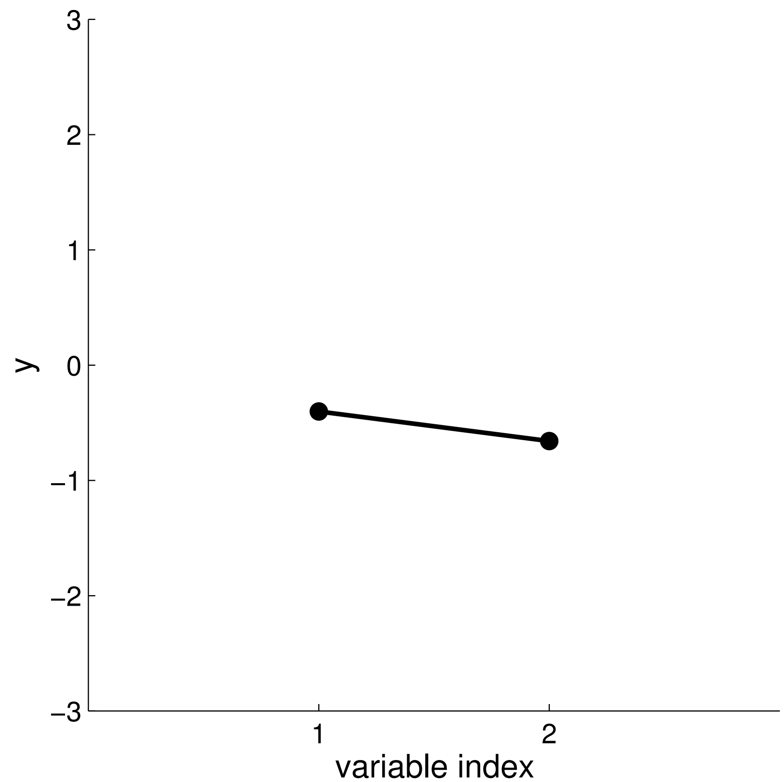


$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



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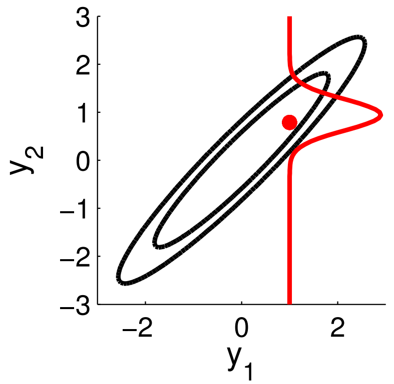

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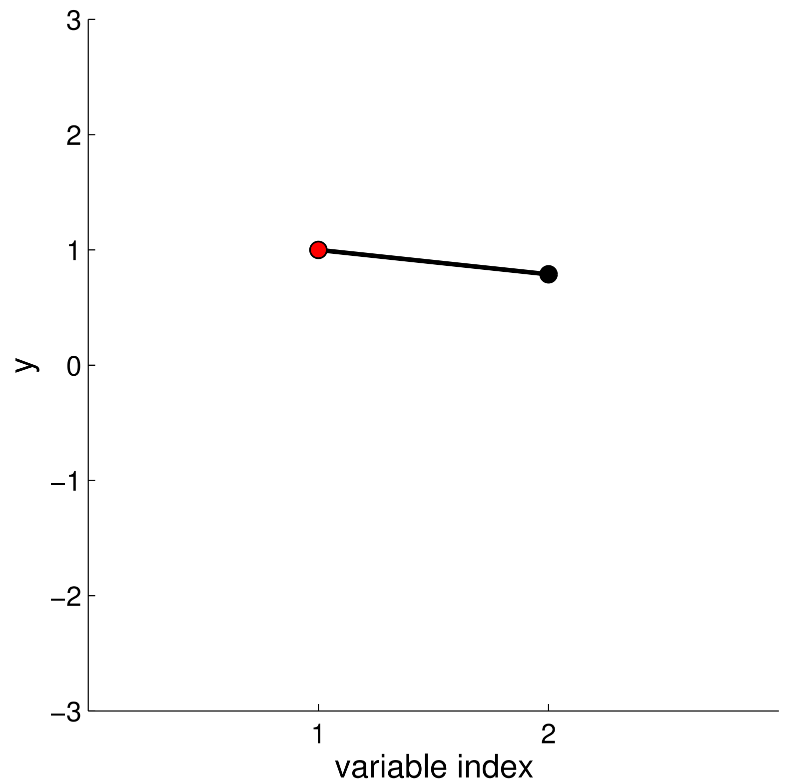

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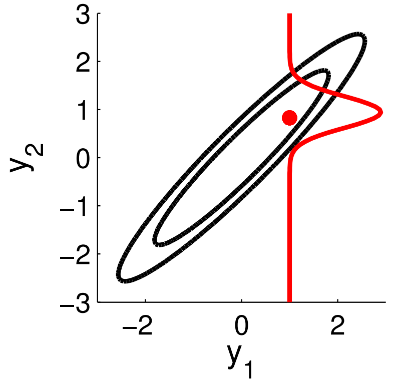

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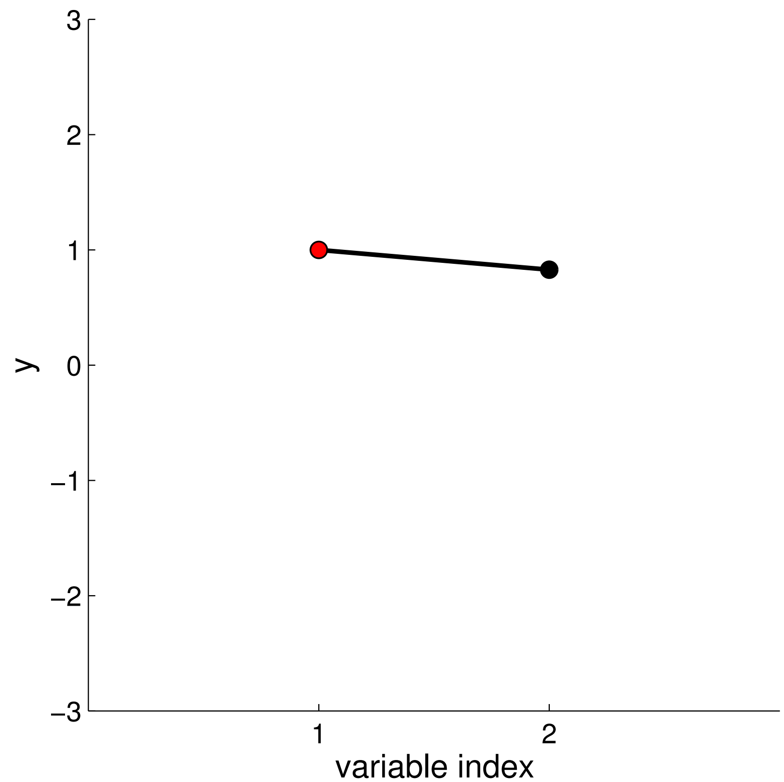

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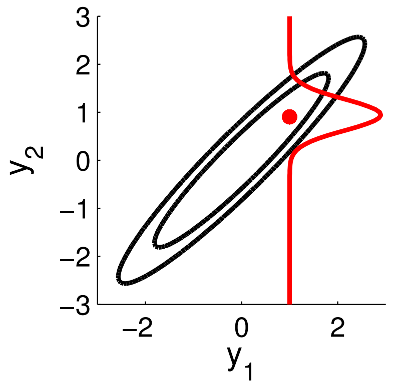

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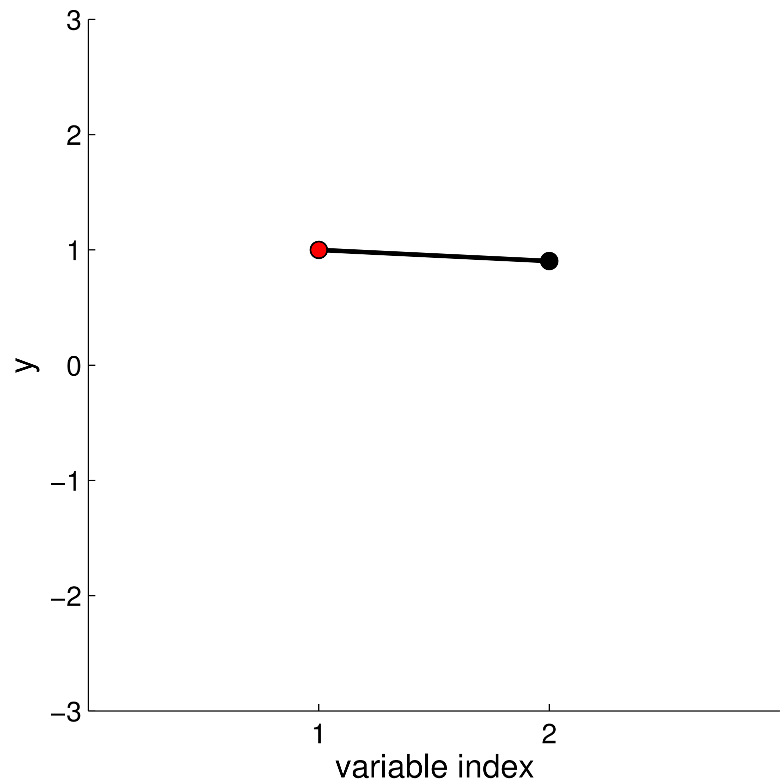

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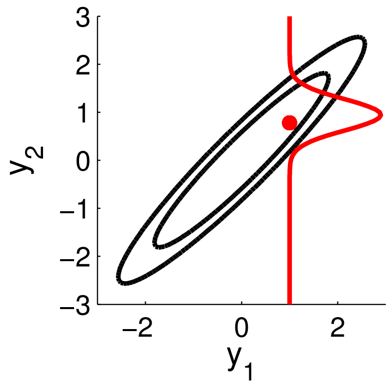

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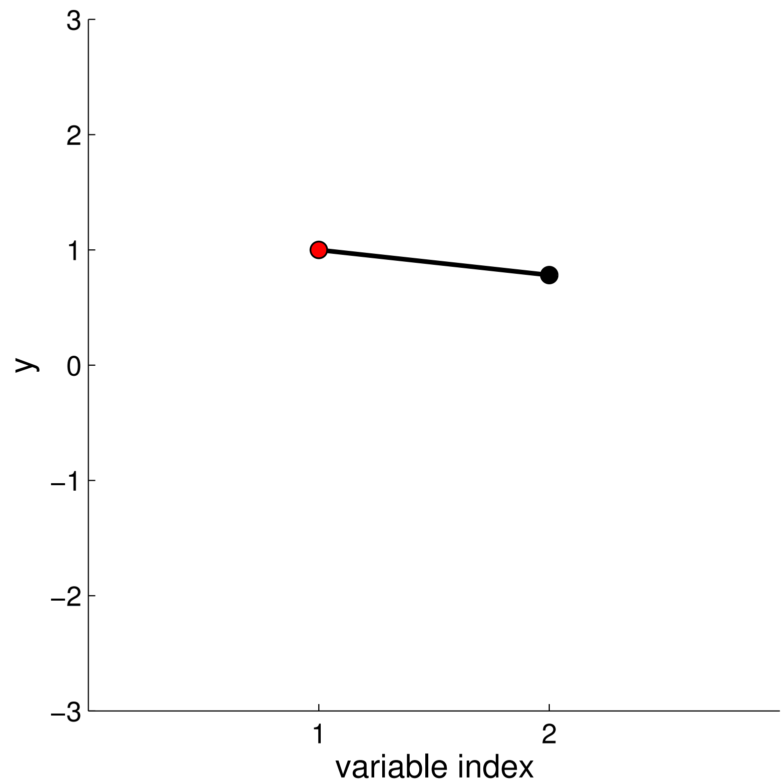

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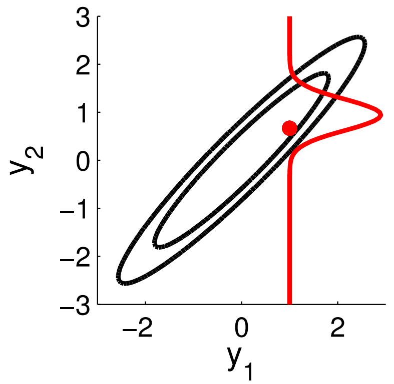

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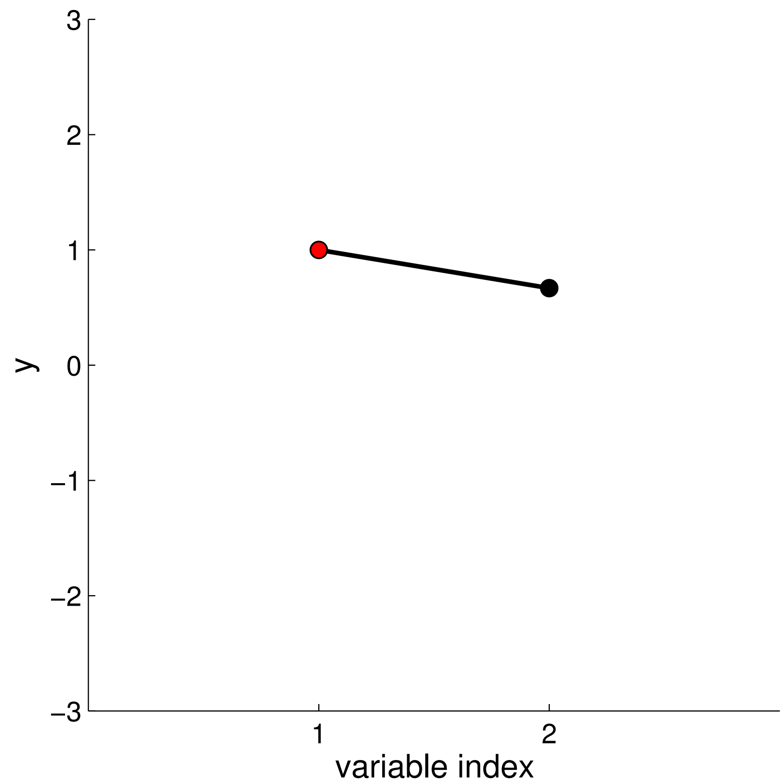

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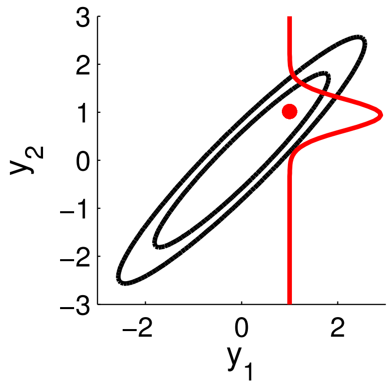

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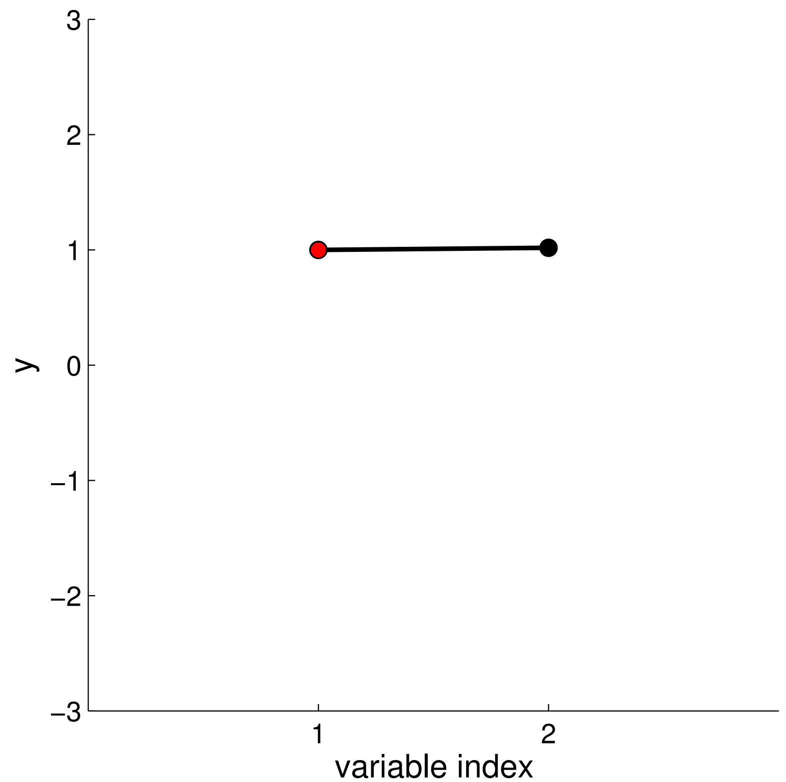

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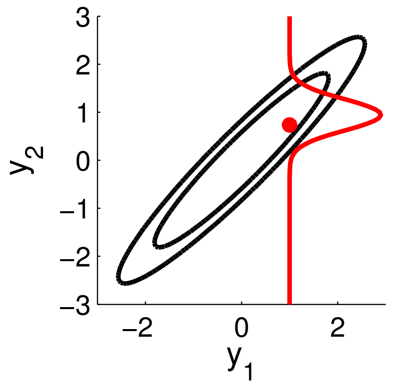

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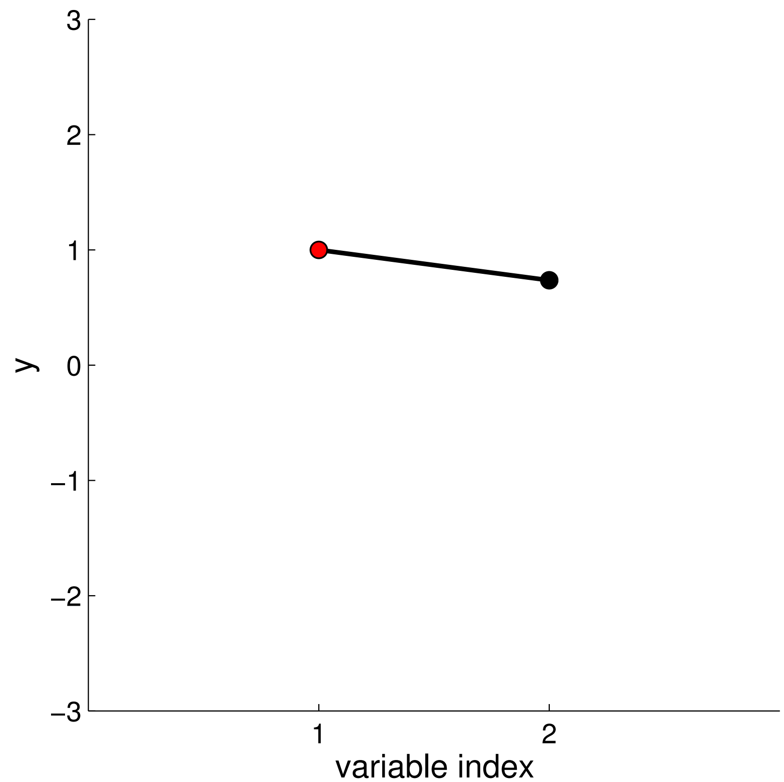

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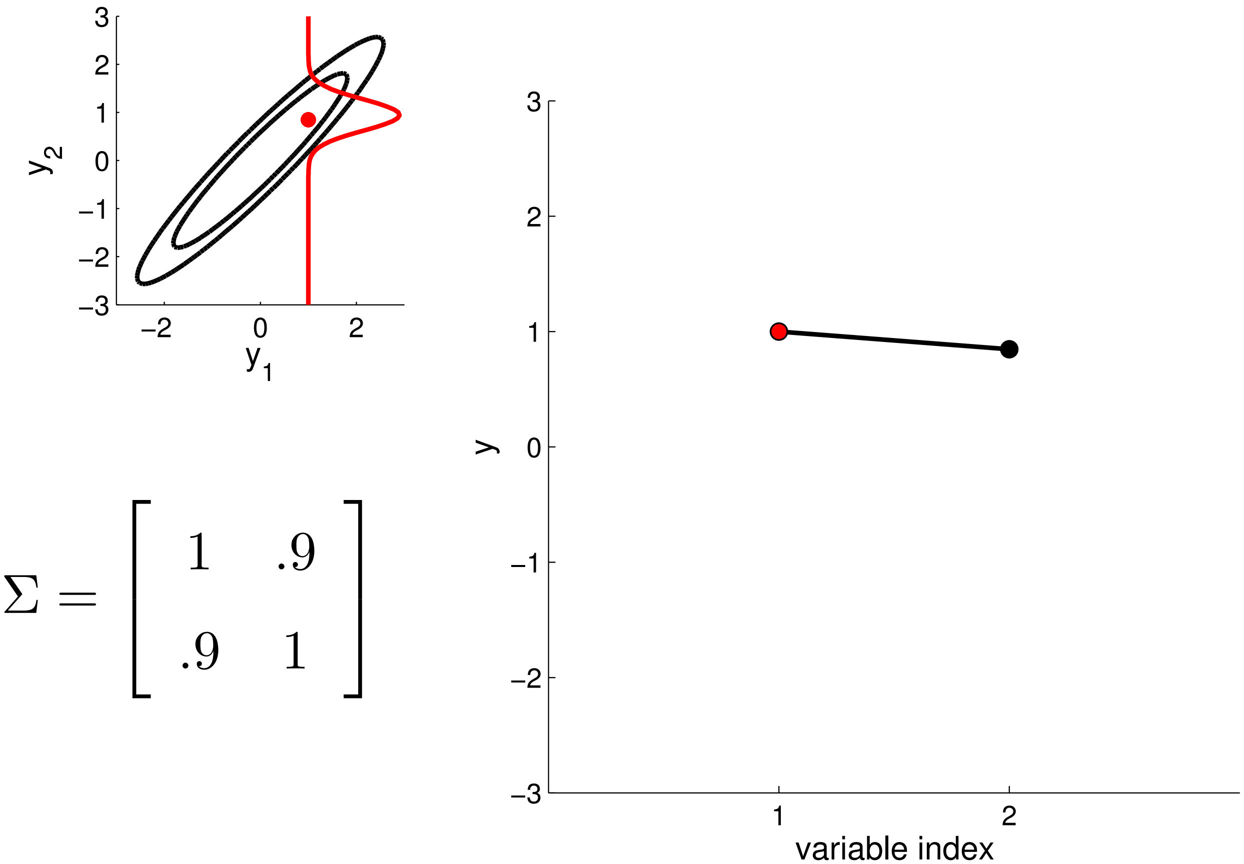

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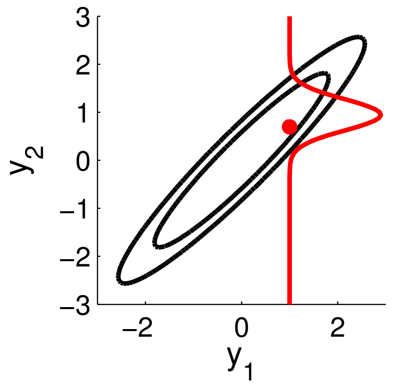

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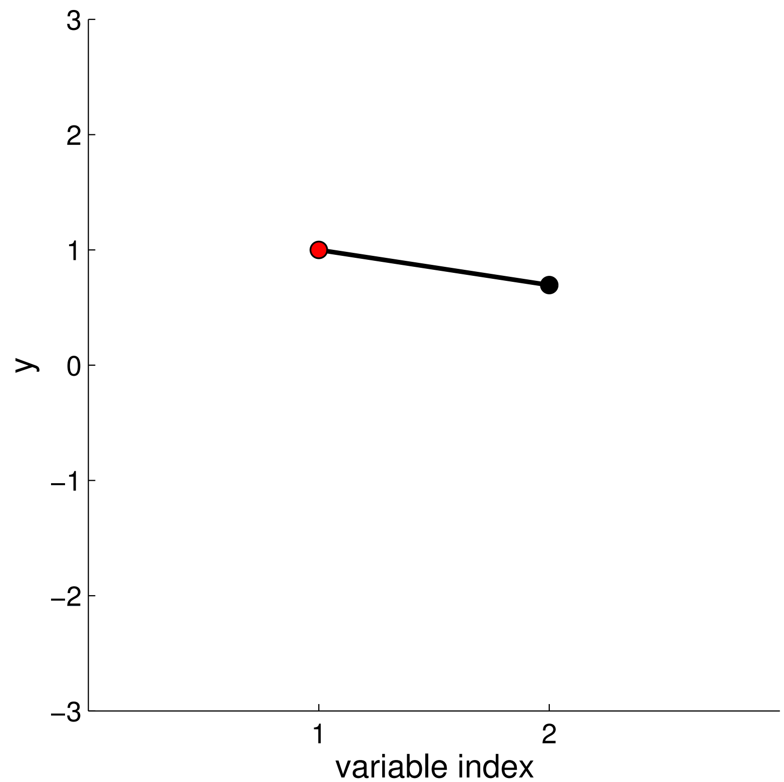

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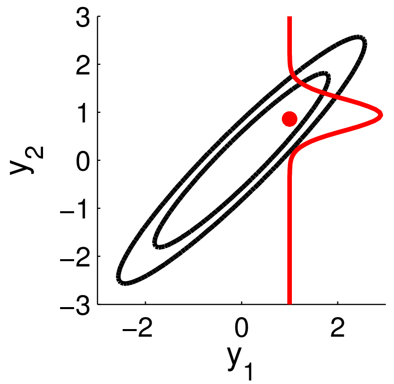

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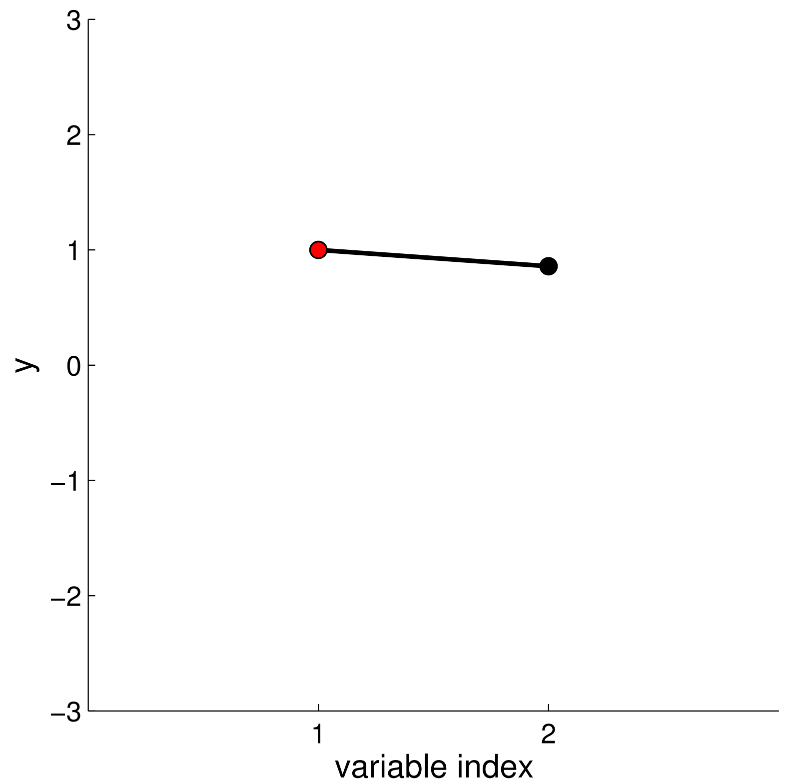

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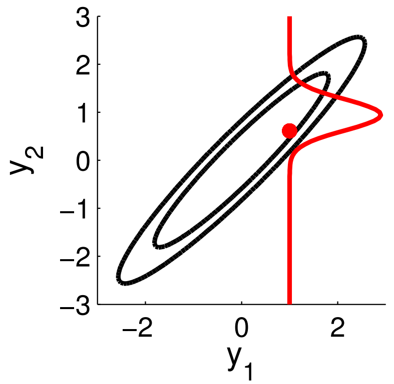

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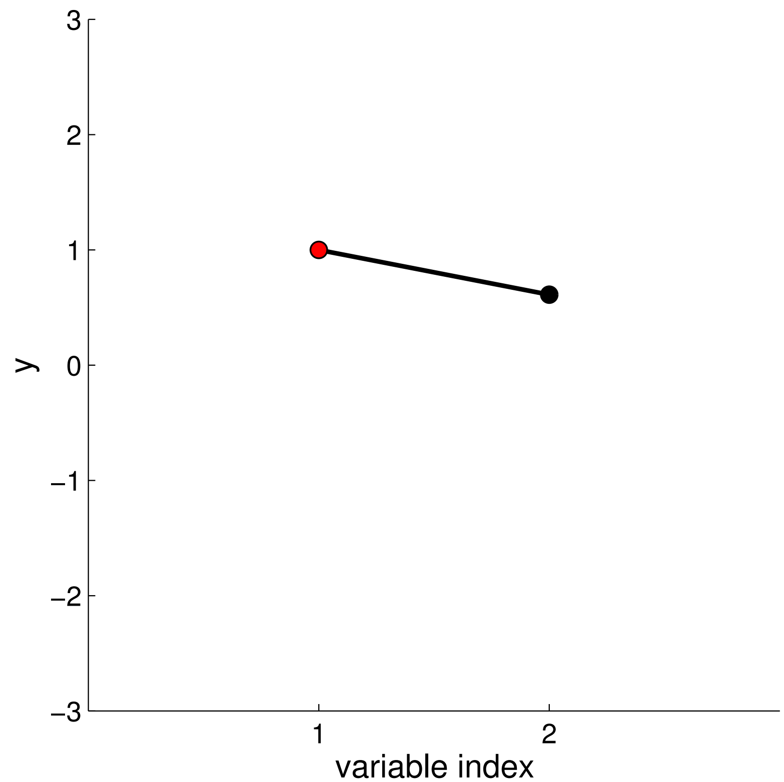

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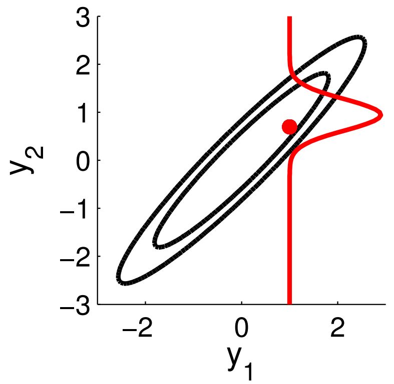

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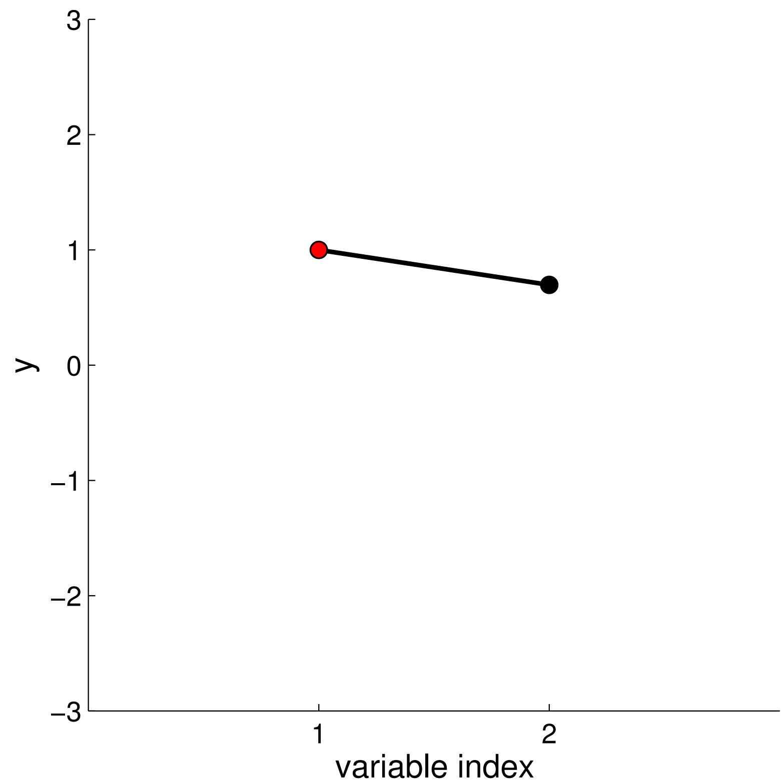

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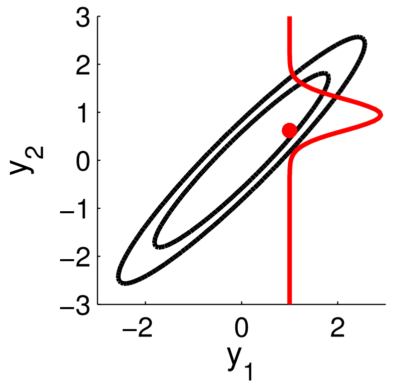

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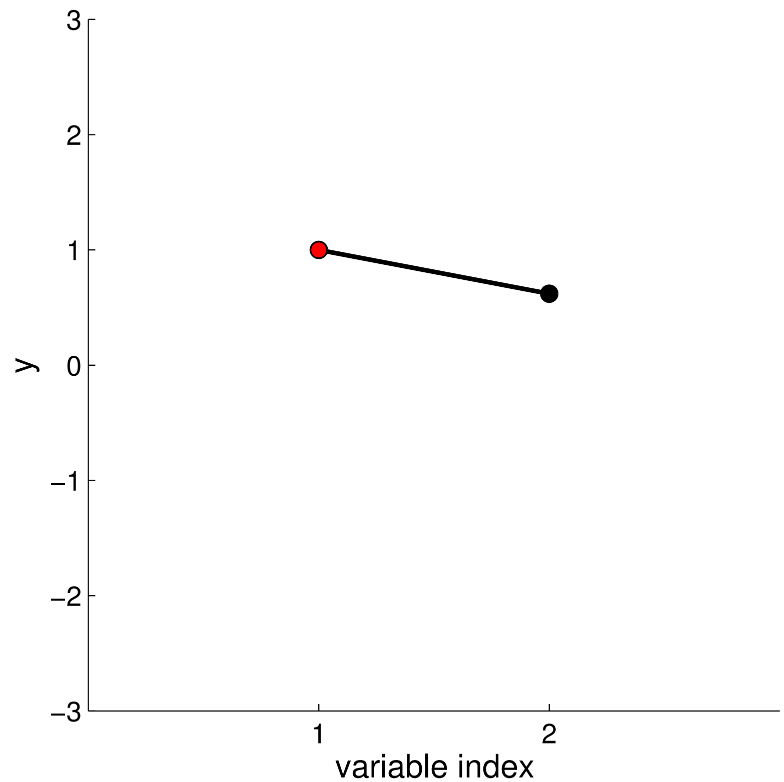

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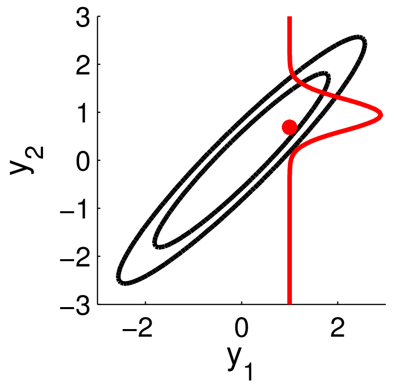

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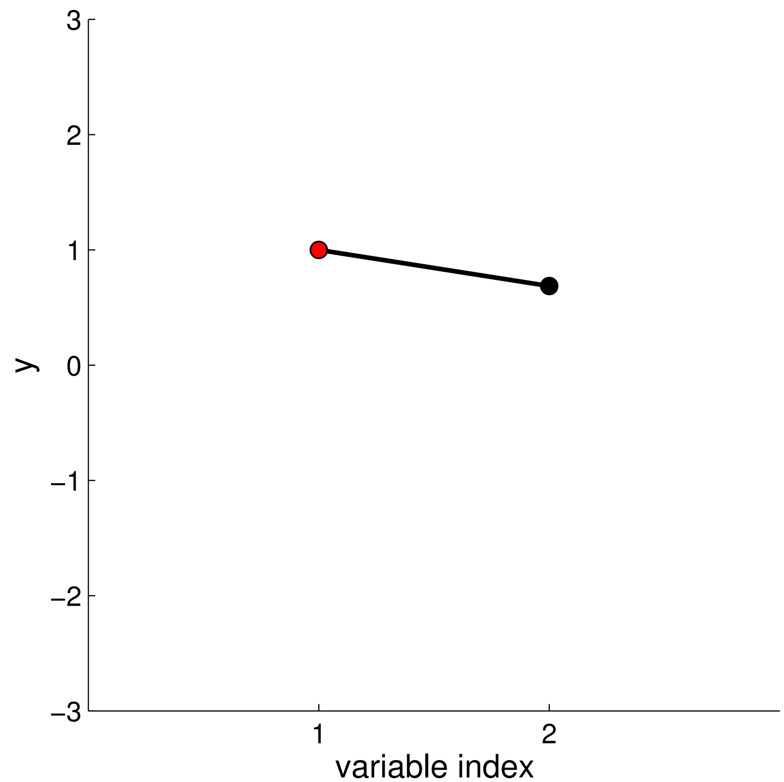

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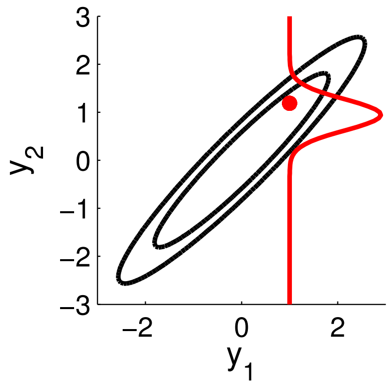

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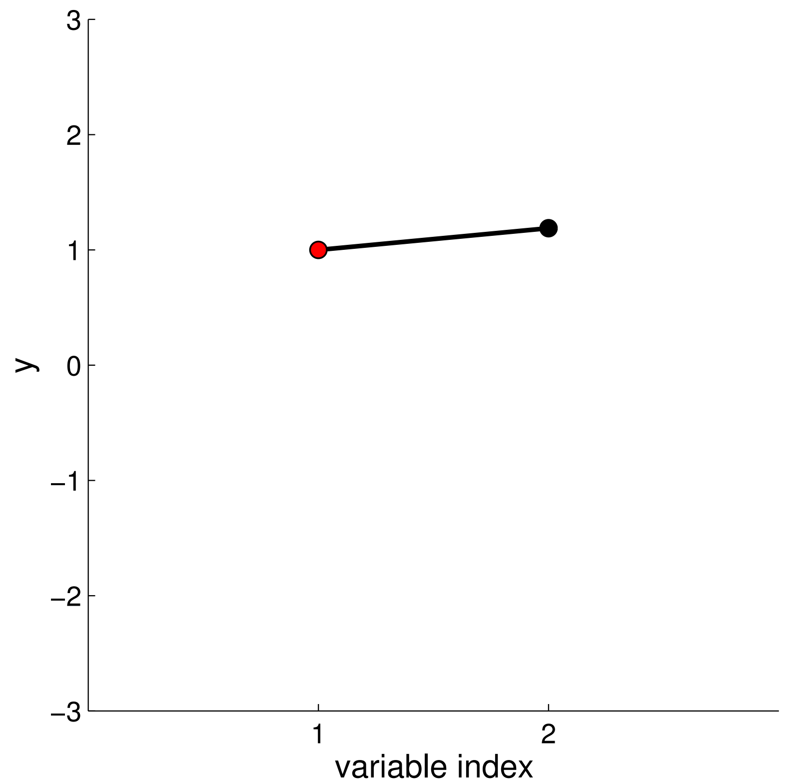

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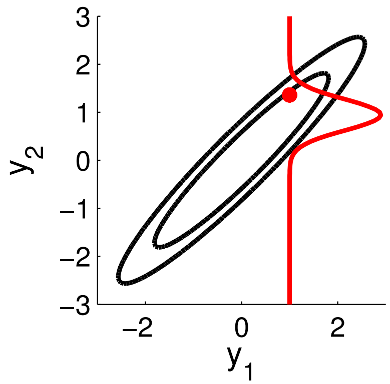

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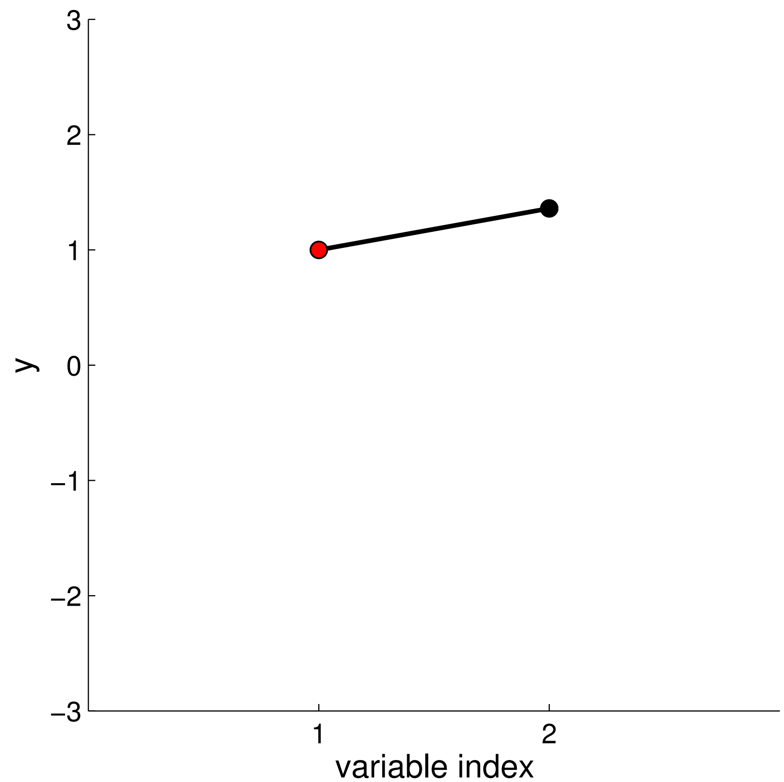

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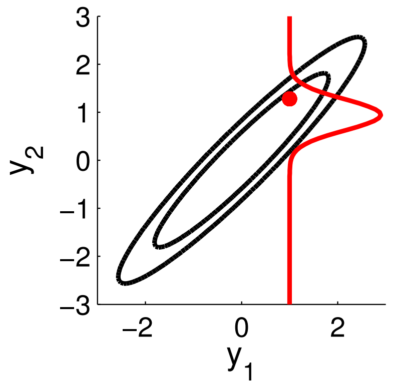

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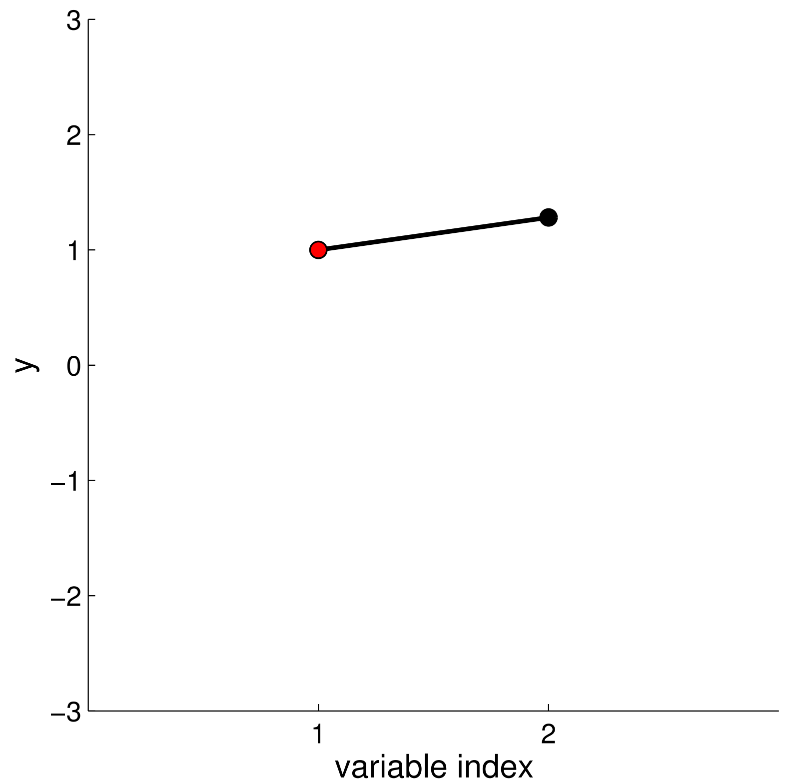

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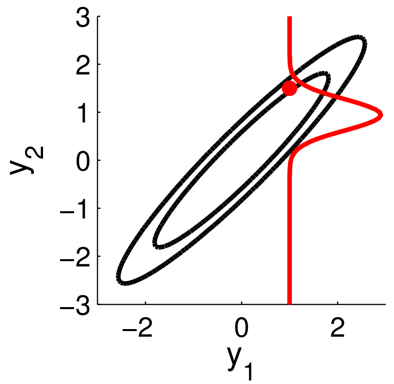

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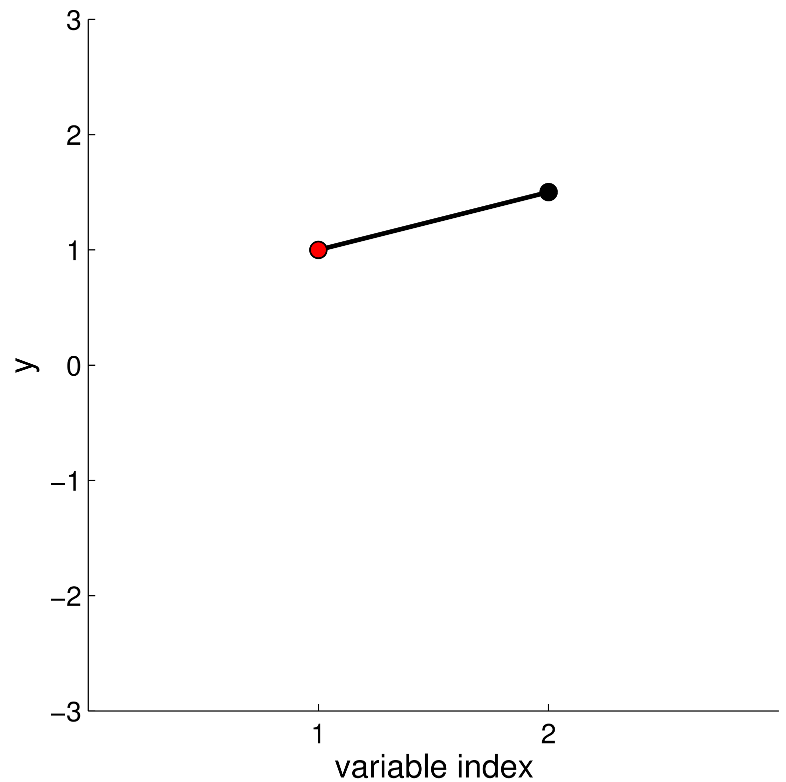

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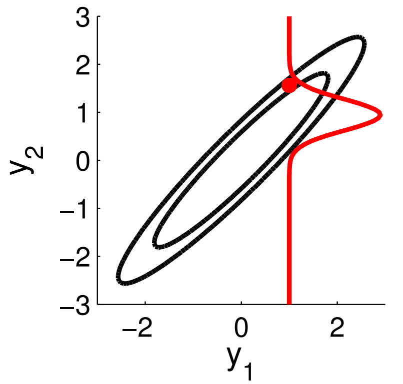

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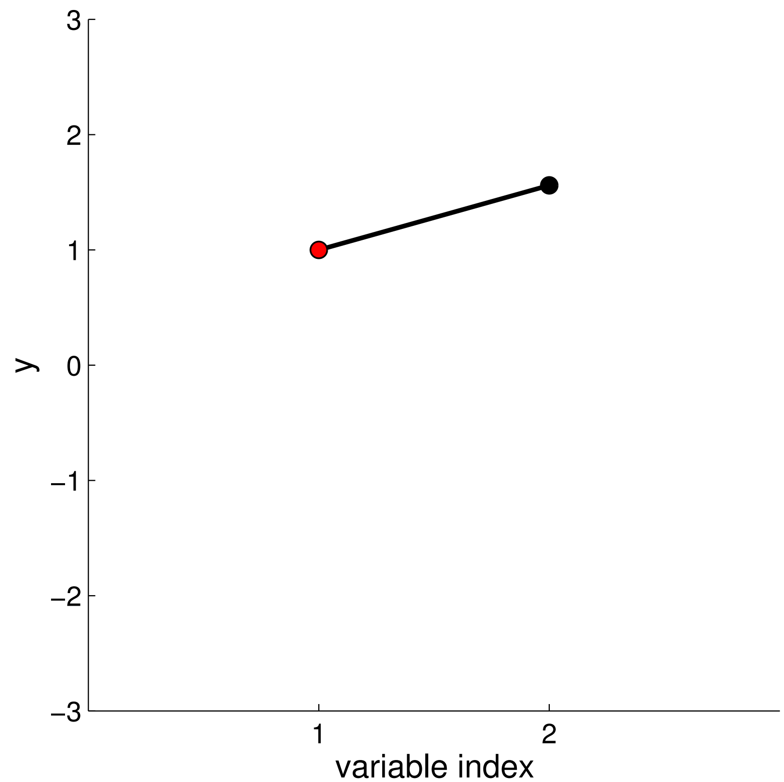

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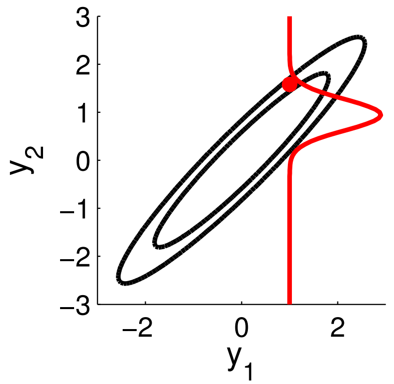
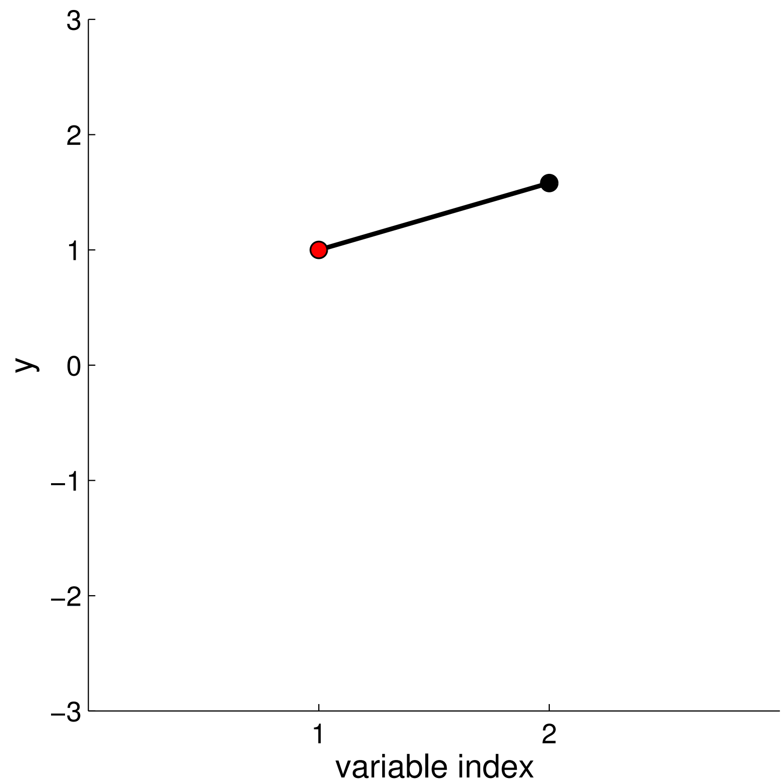


$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



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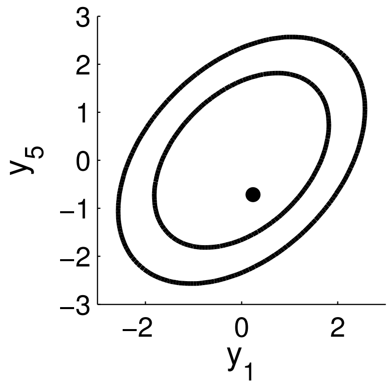

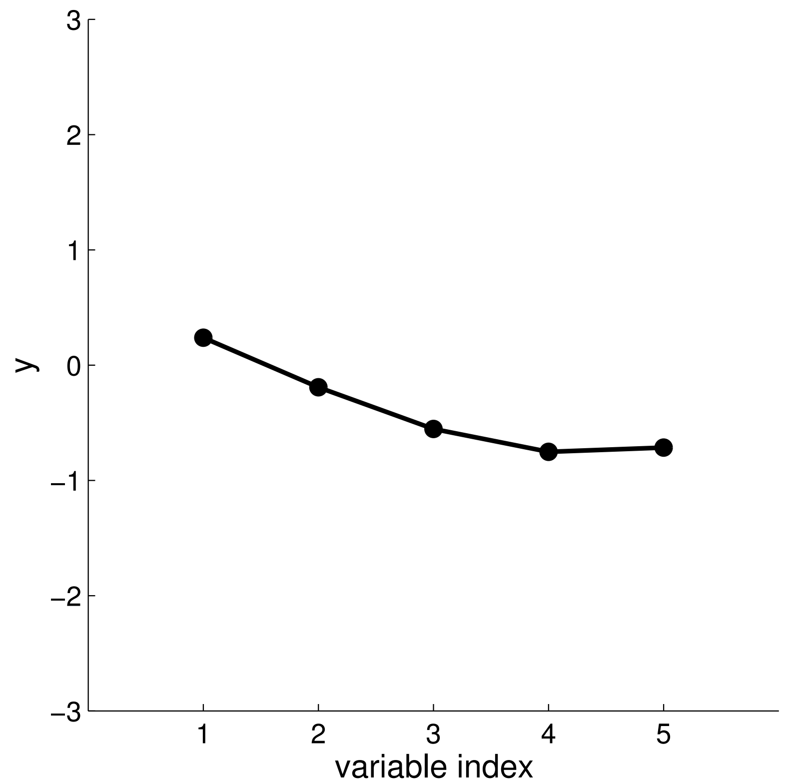

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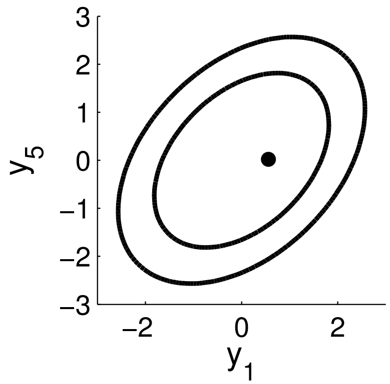
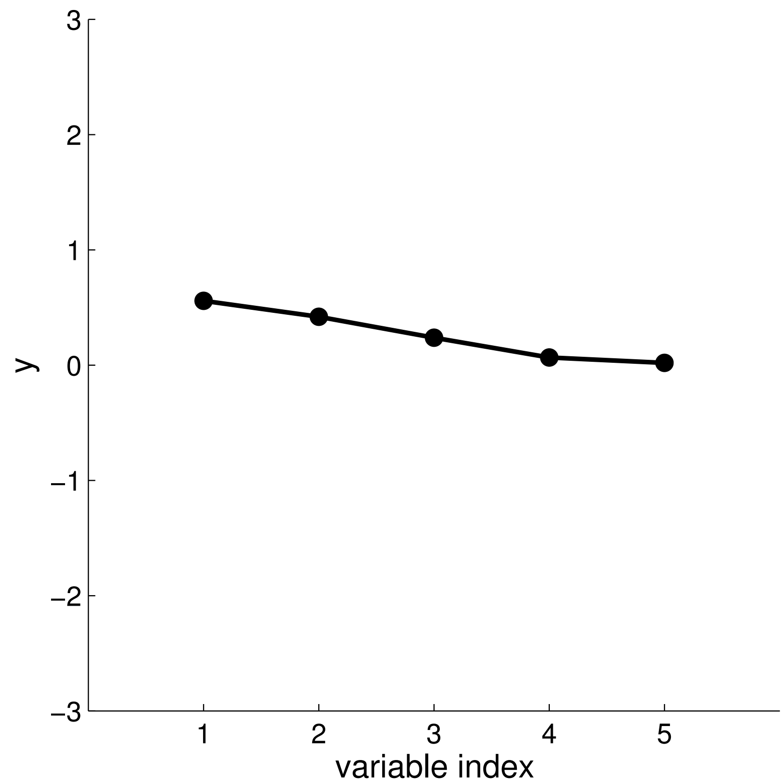
New visualisation





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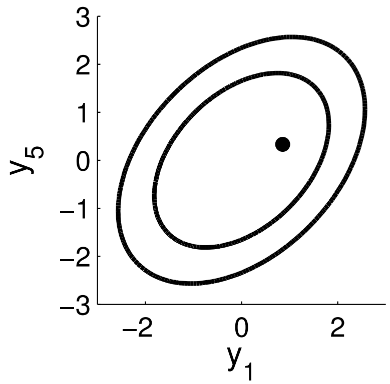
New visualisation



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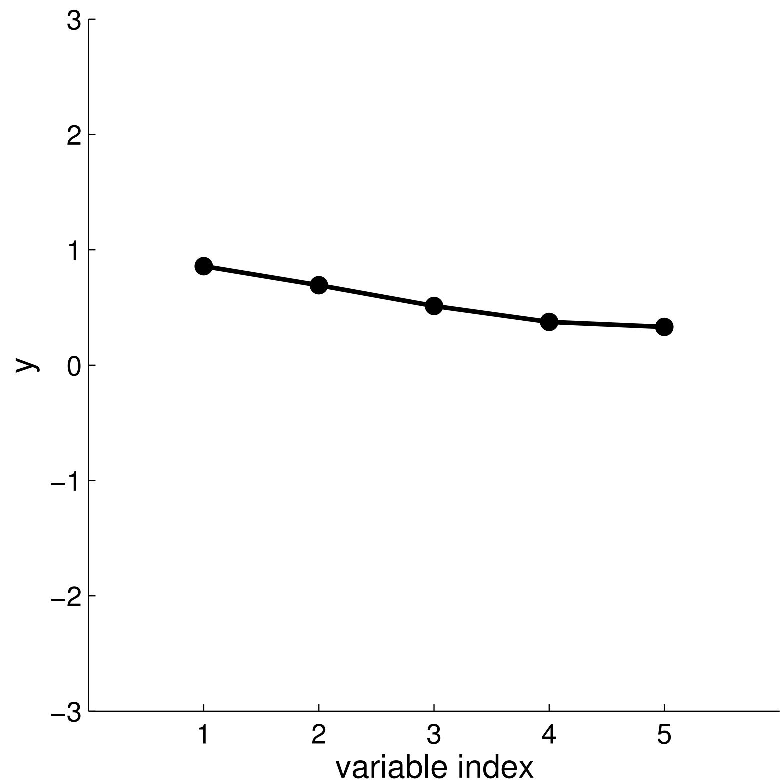

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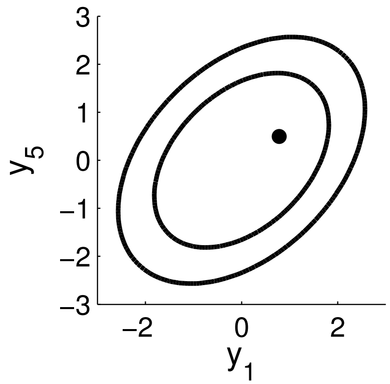

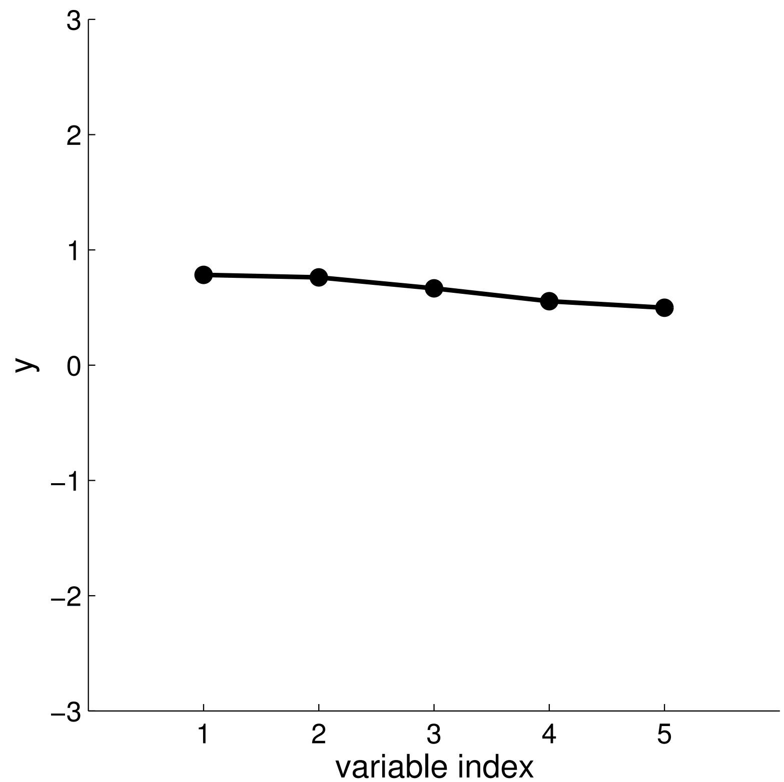

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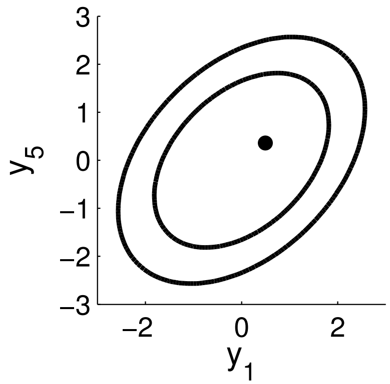
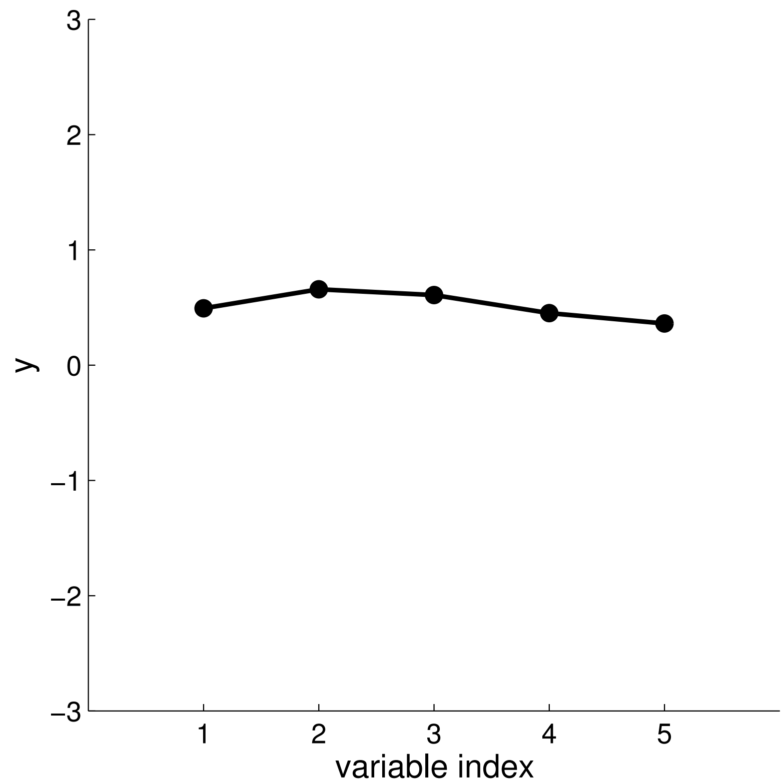
New visualisation





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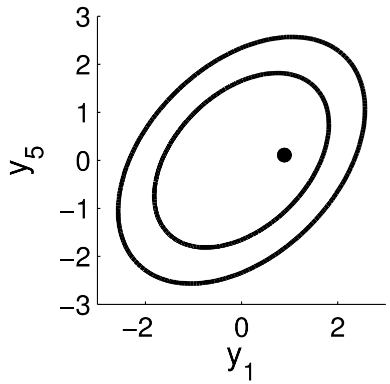
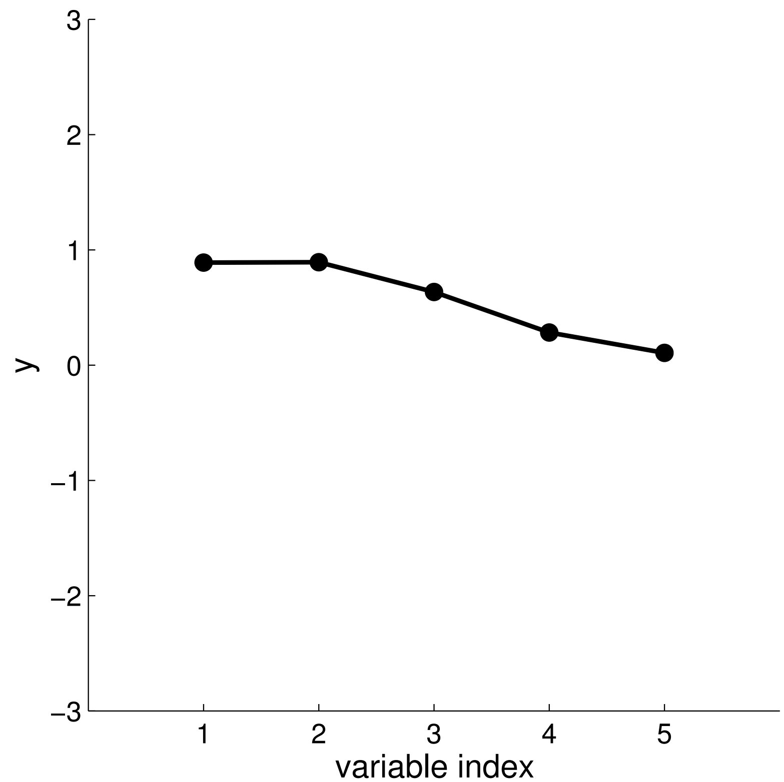
New visualisation





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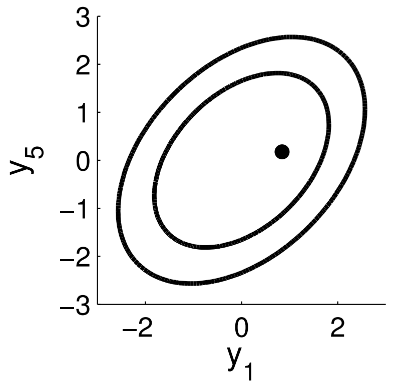
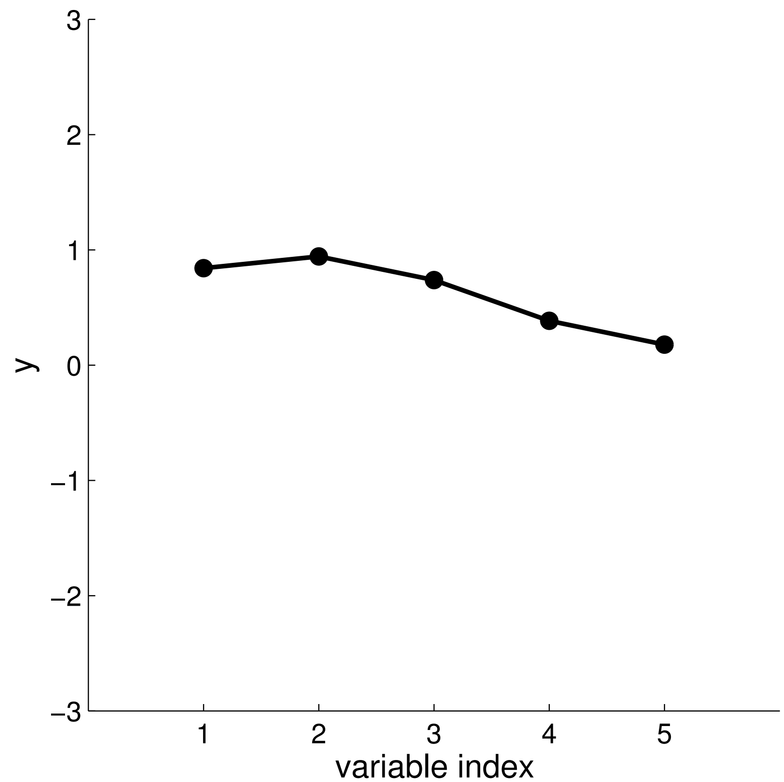
New visualisation





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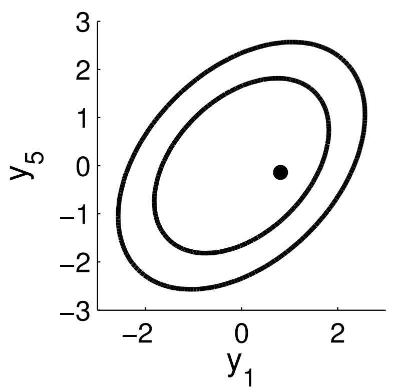
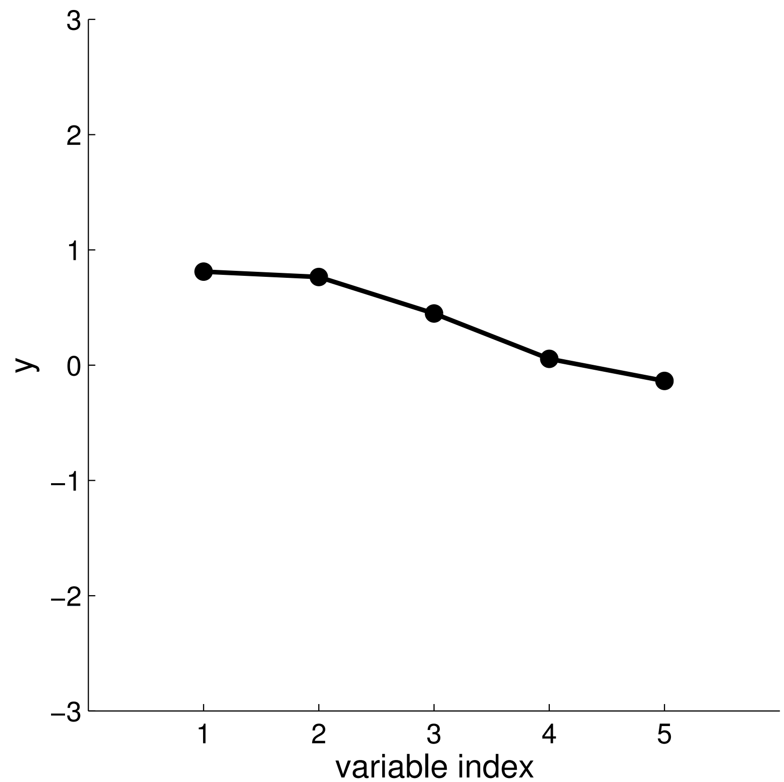
New visualisation





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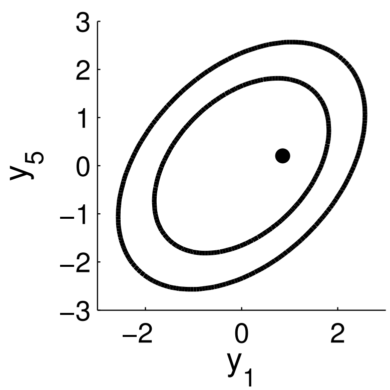
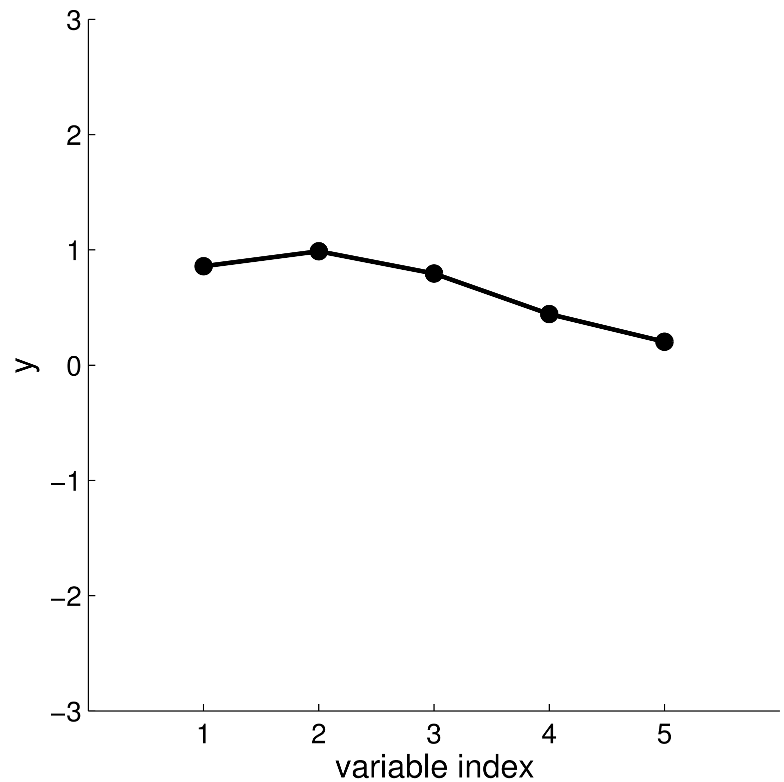
New visualisation





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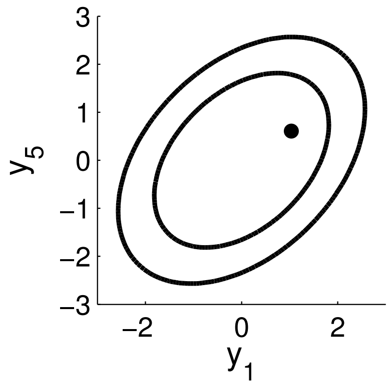
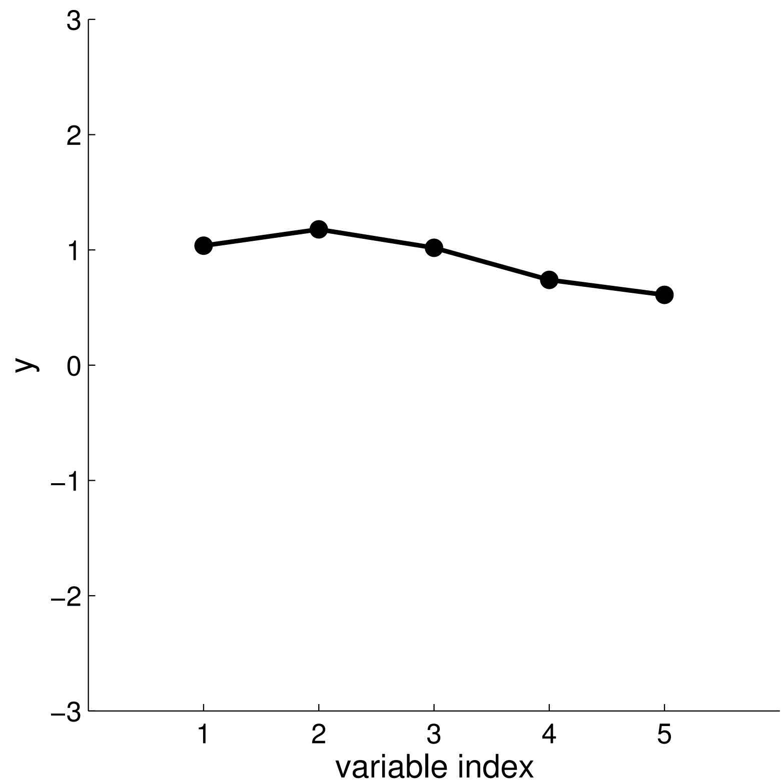
New visualisation





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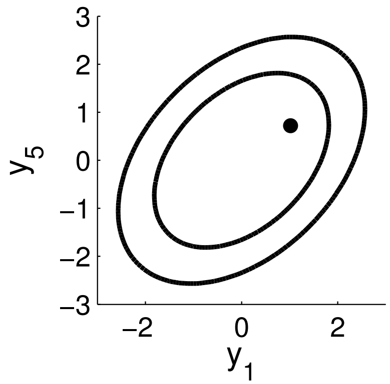
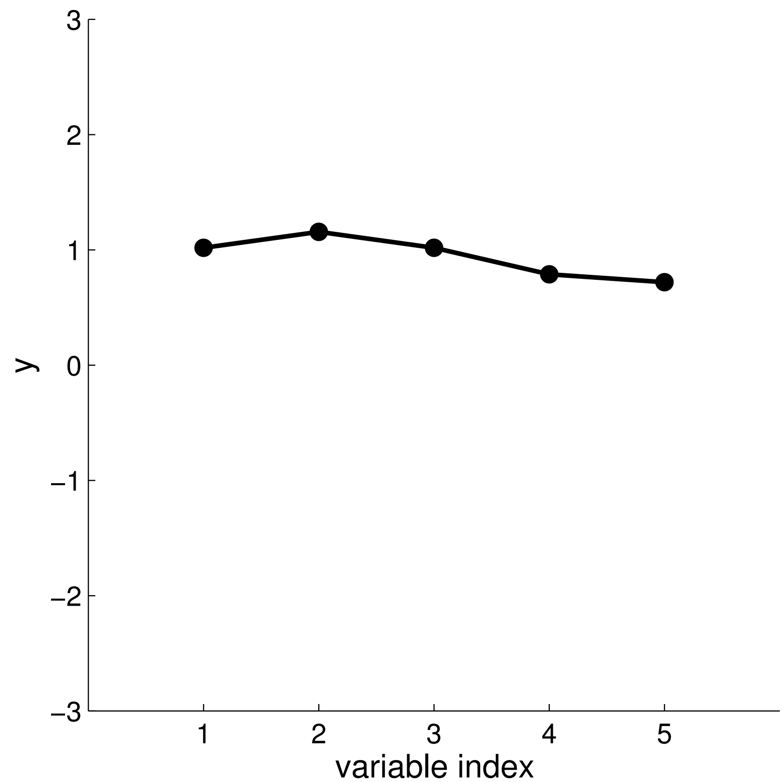
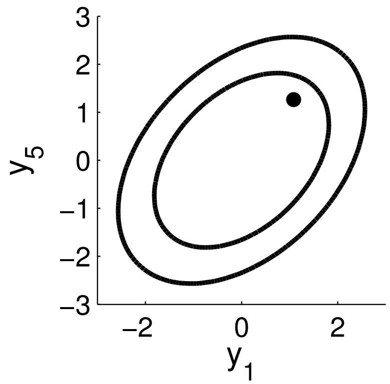
New visualisation

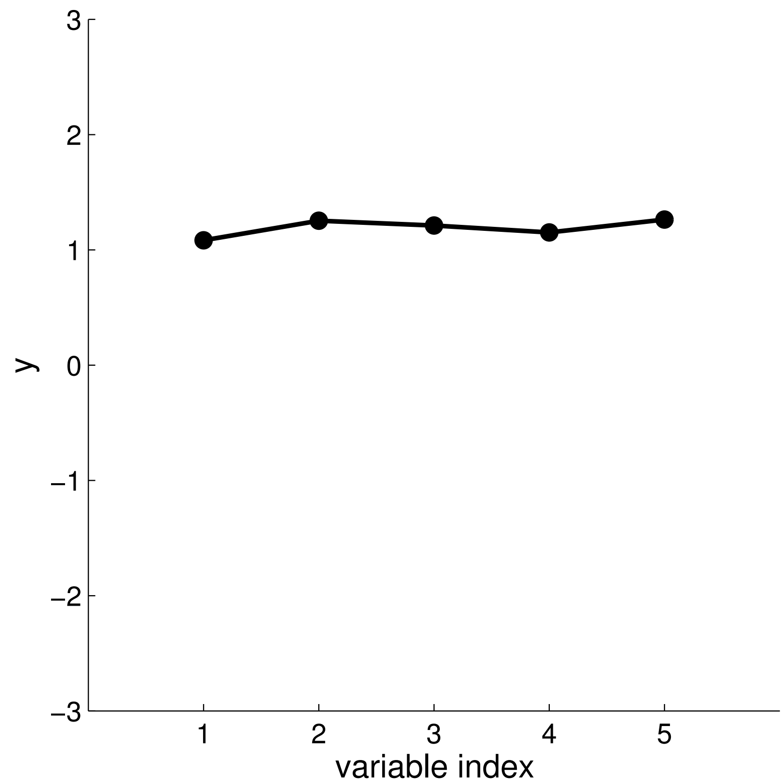




$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

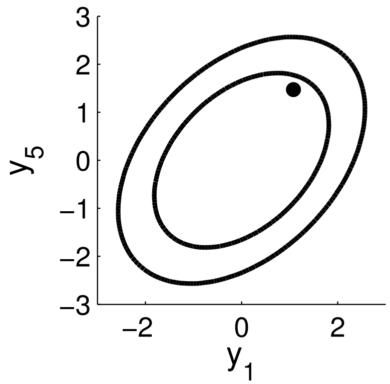
New visualisation

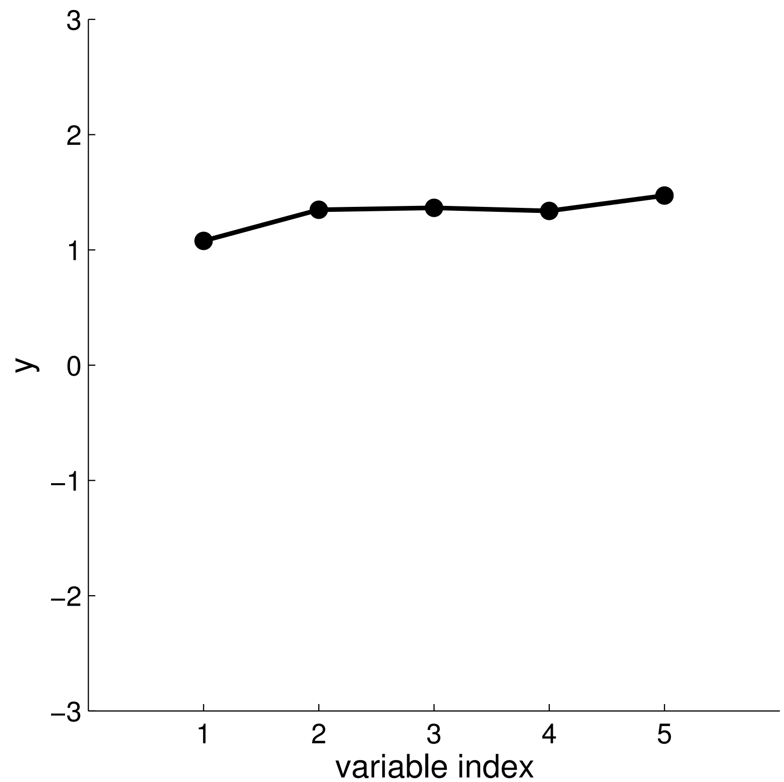




$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

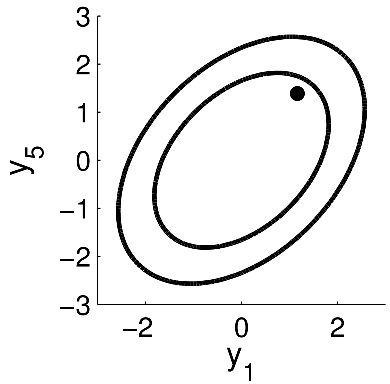
New visualisation

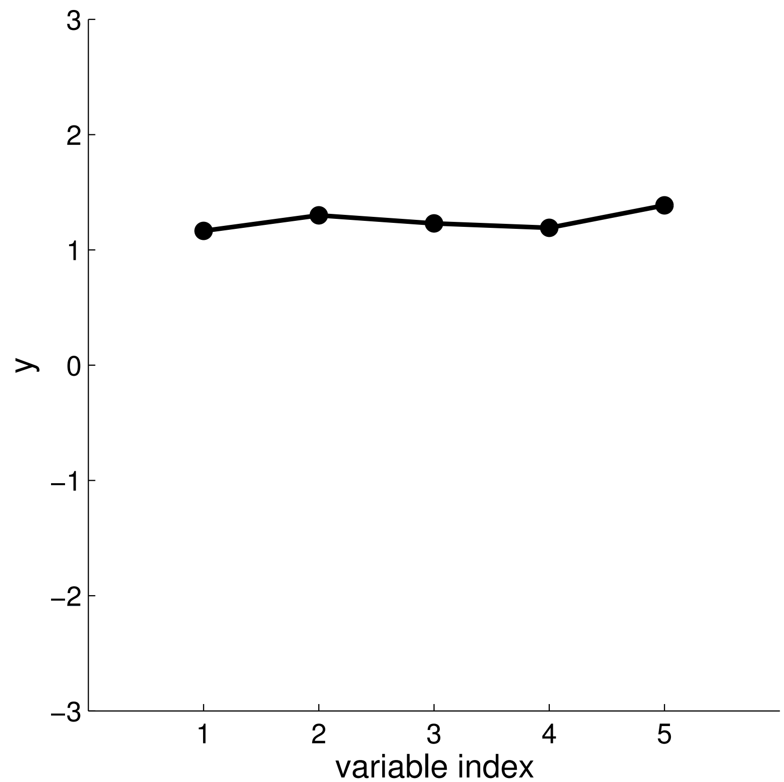




$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation





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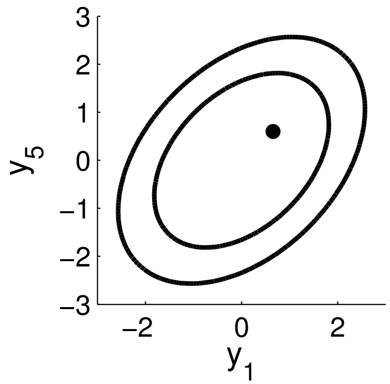
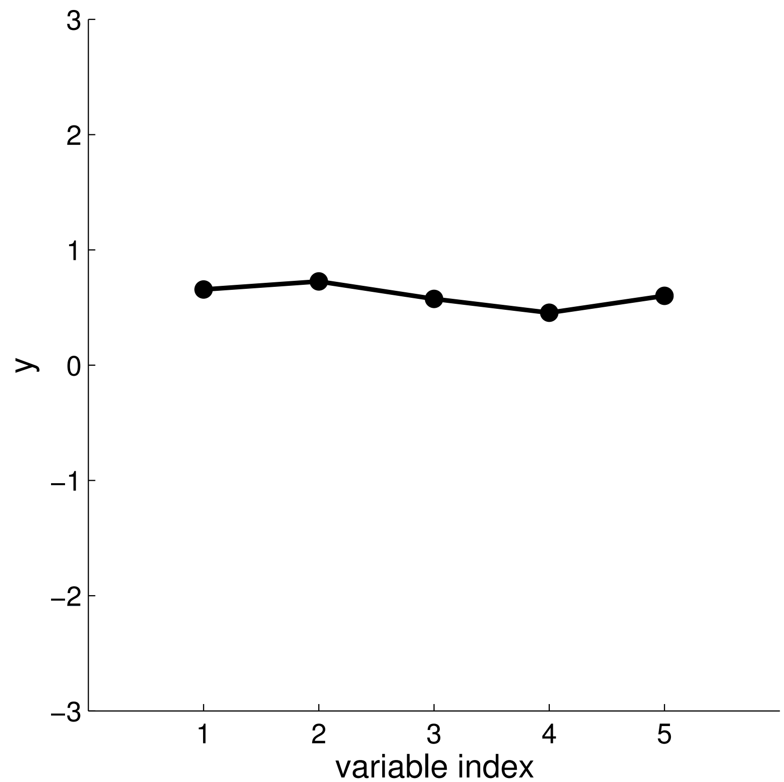
New visualisation





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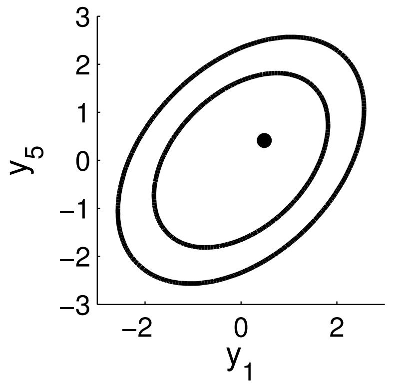
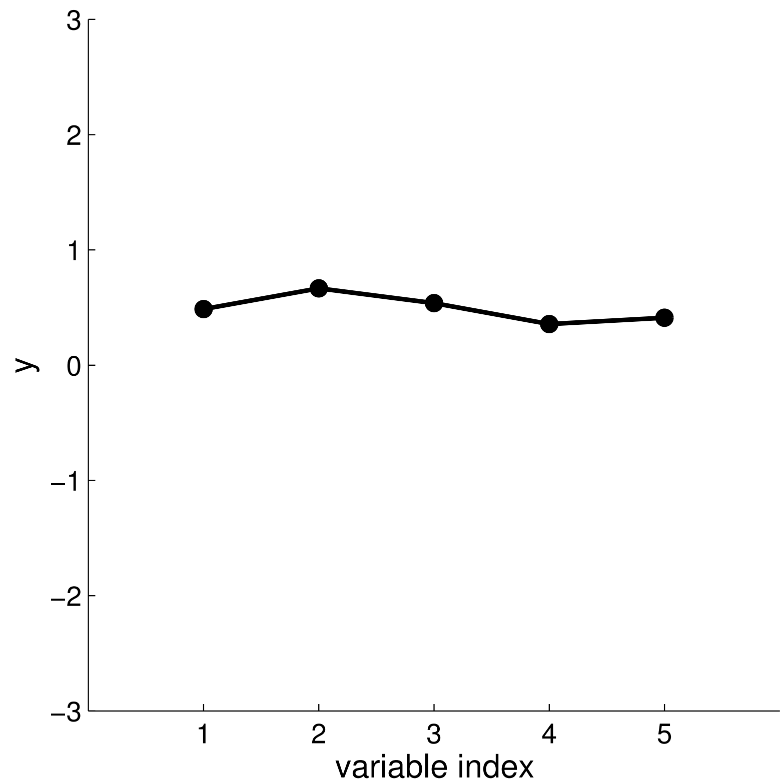
New visualisation





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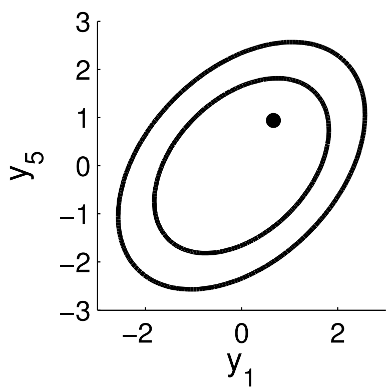
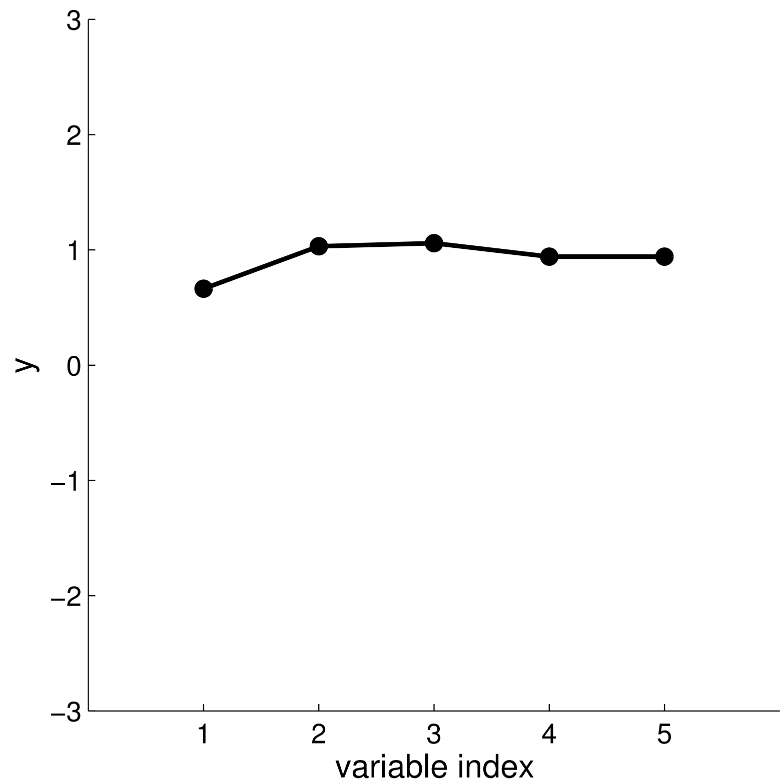
New visualisation





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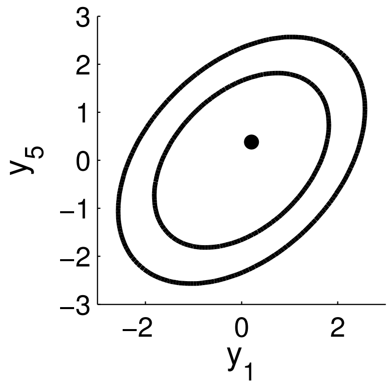
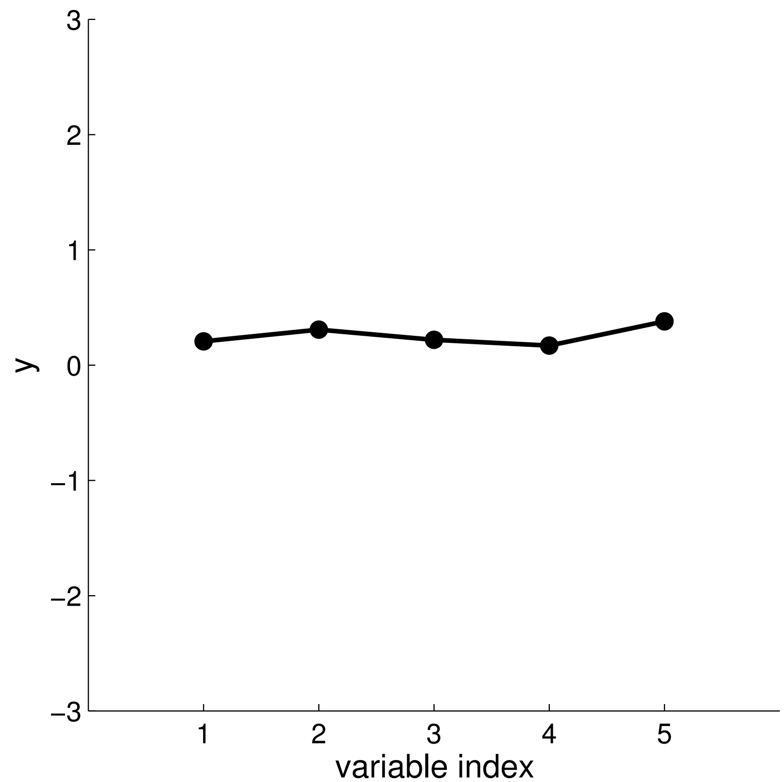
New visualisation





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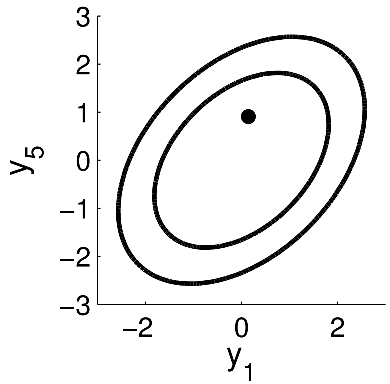
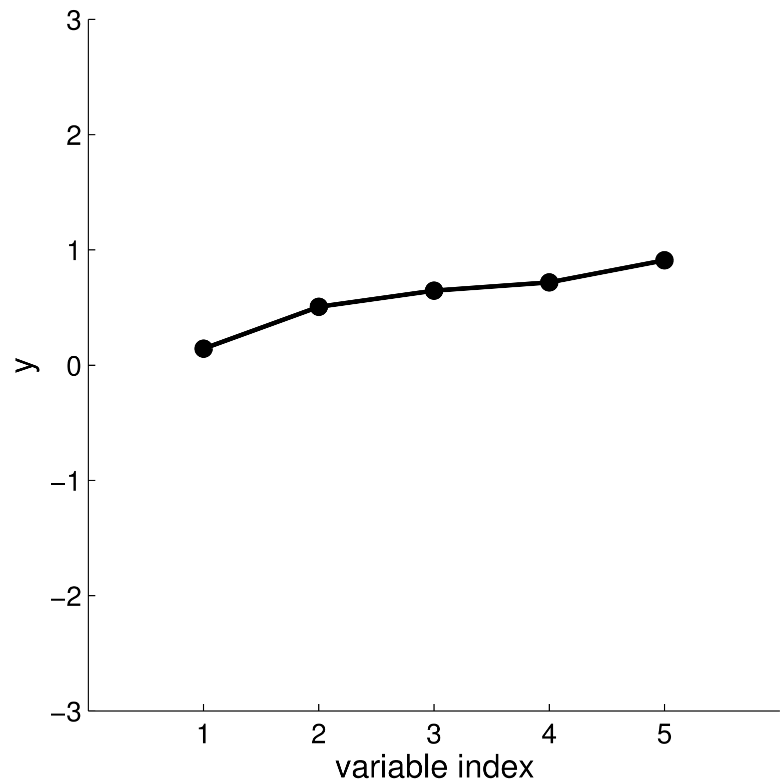
New visualisation





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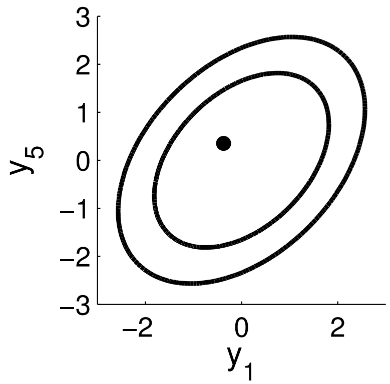
New visualisation



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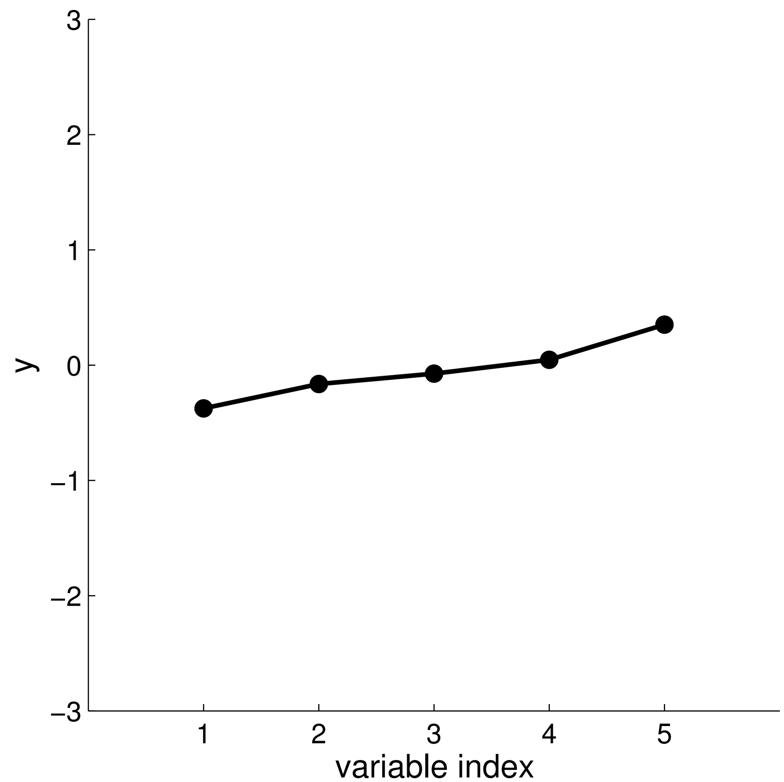
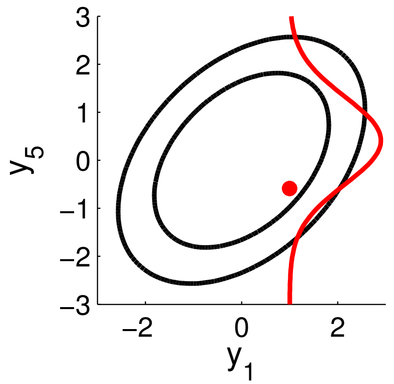
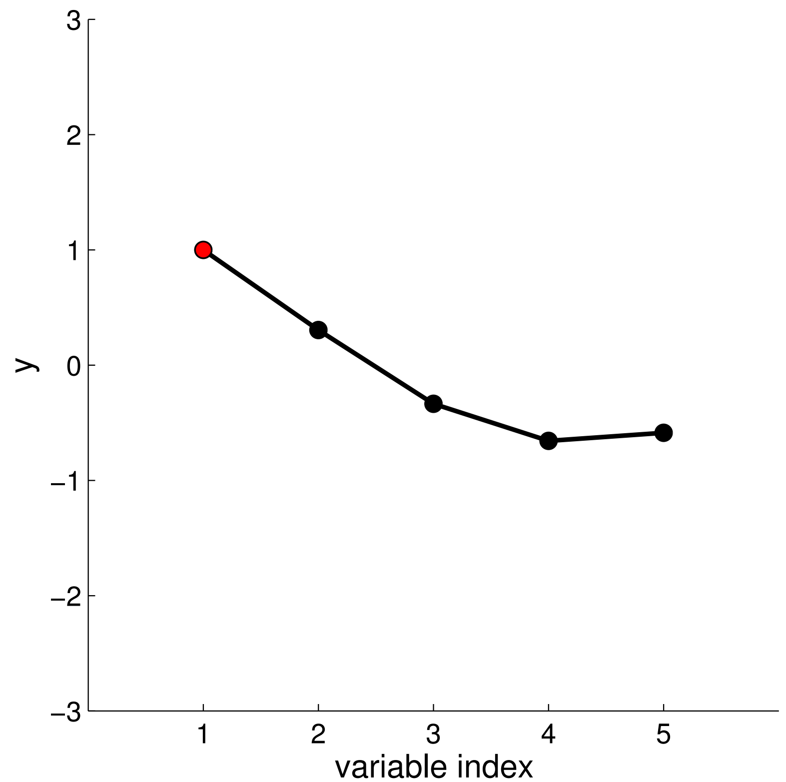


New visualisation





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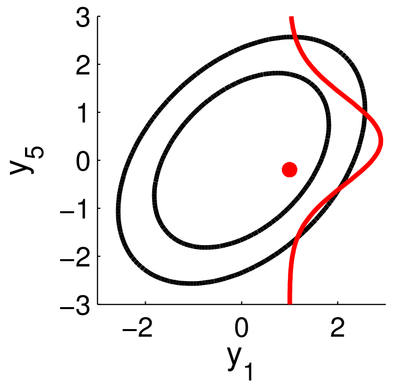
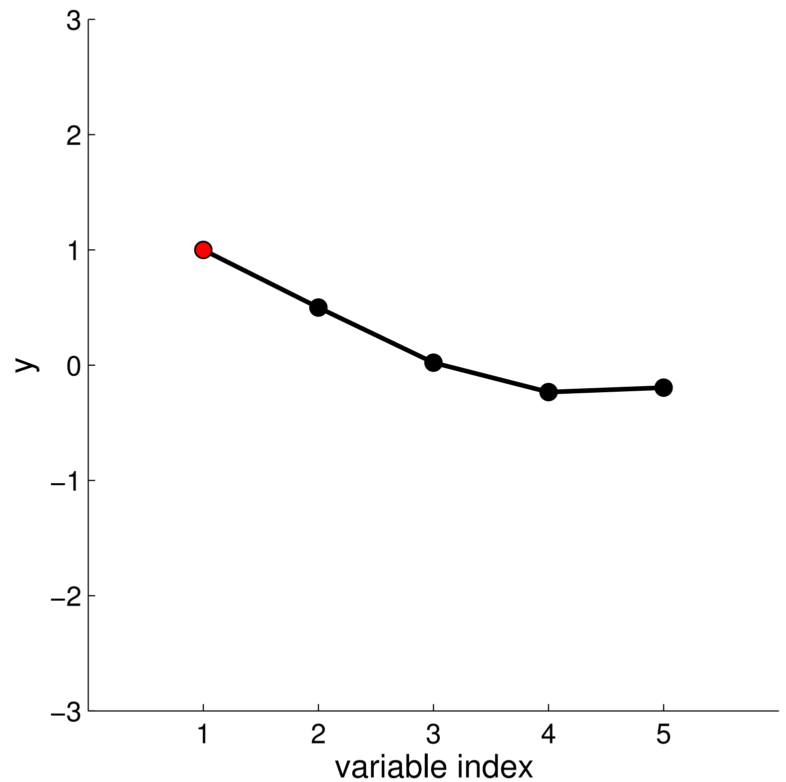
New visualisation





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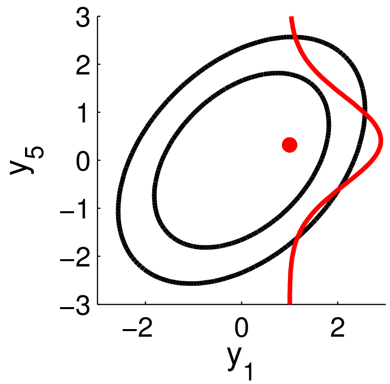
New visualisation



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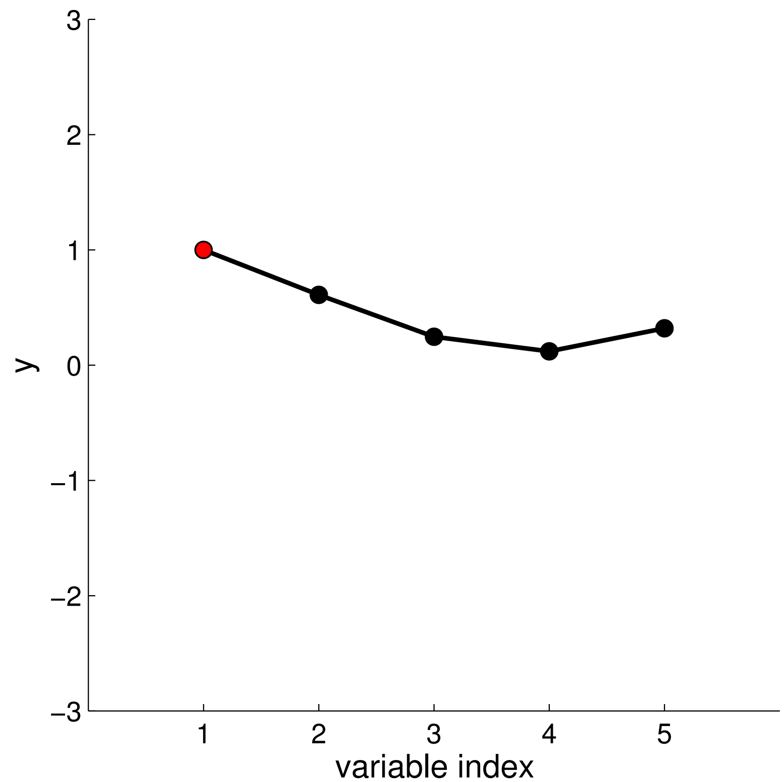

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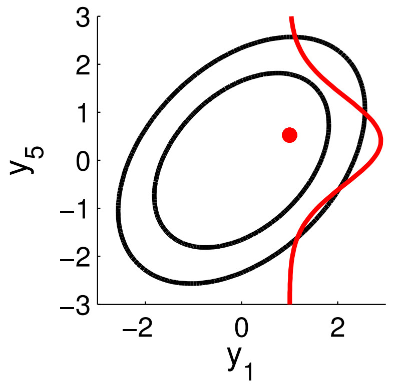

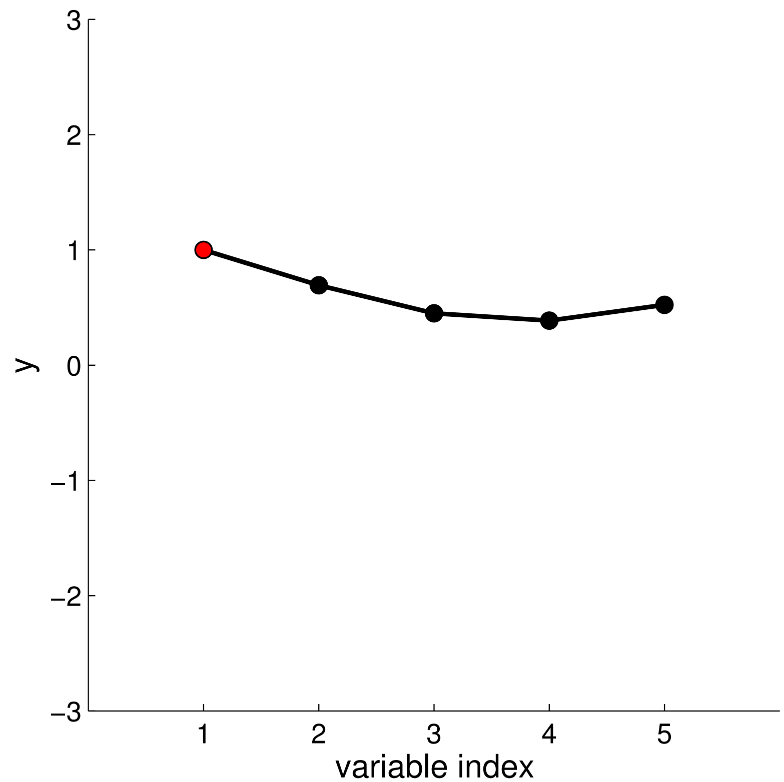

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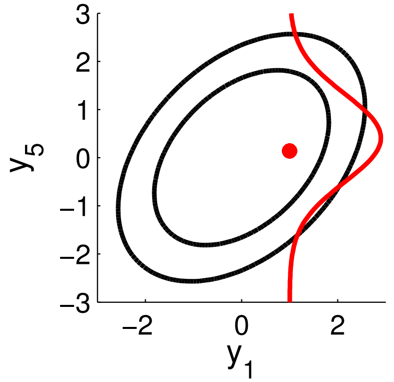
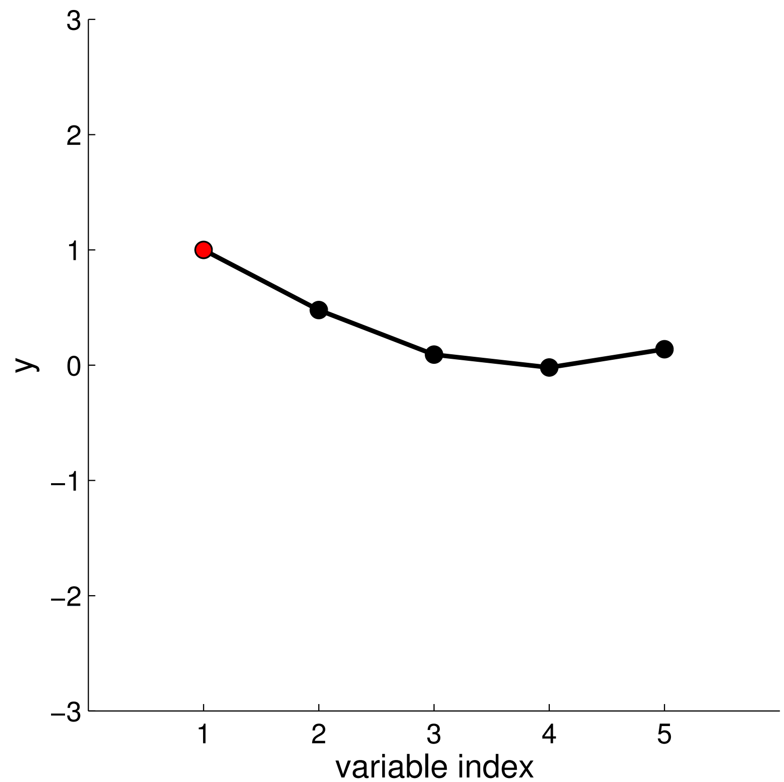
New visualisation





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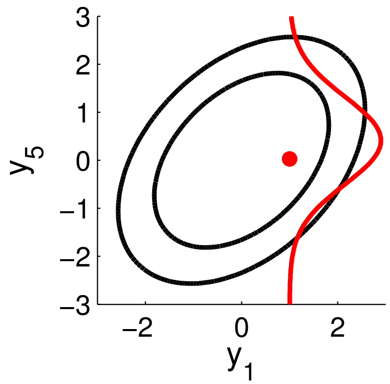
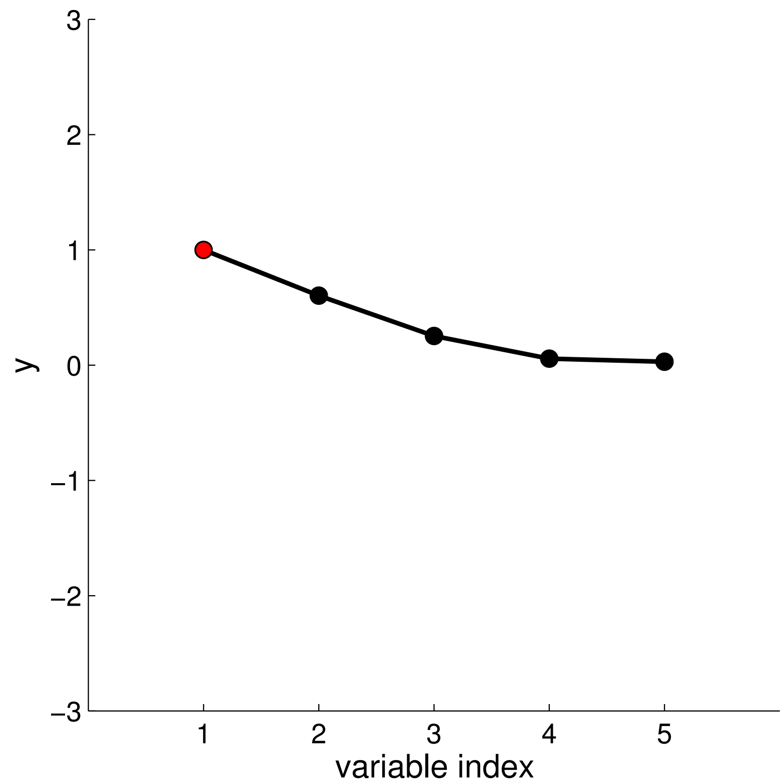
New visualisation





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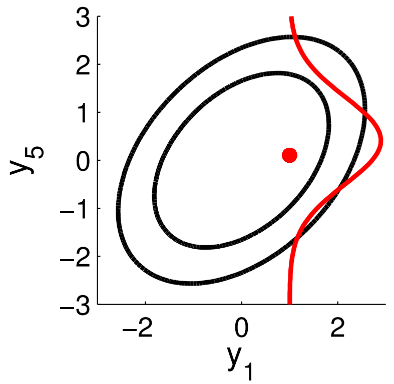
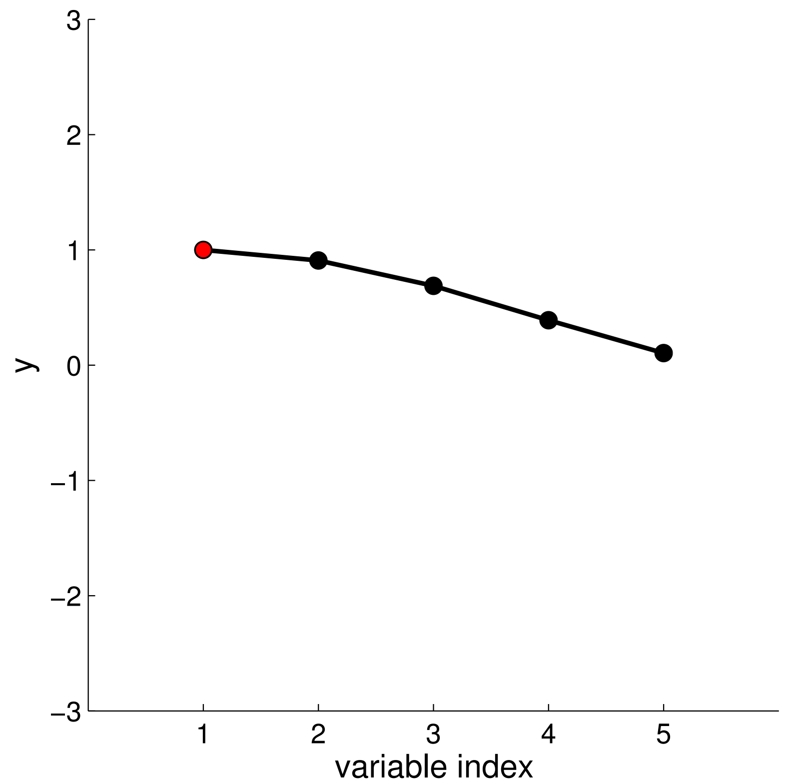
New visualisation





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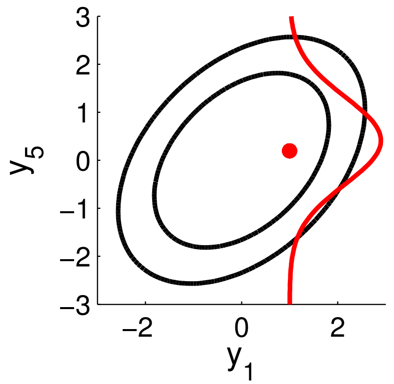
New visualisation



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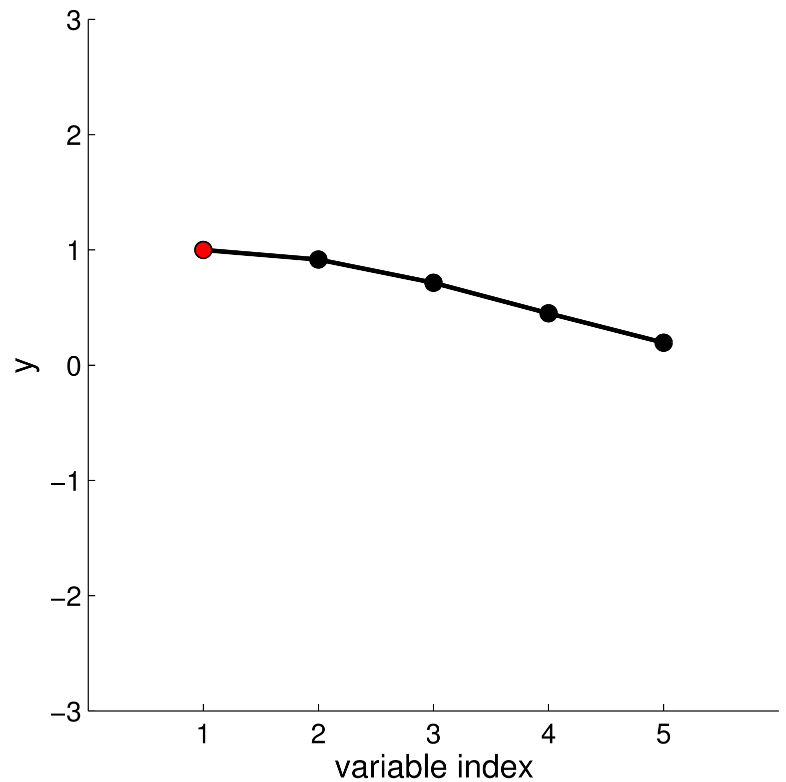
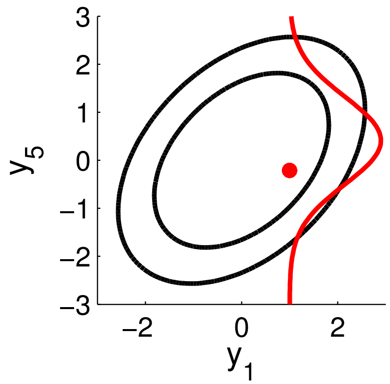
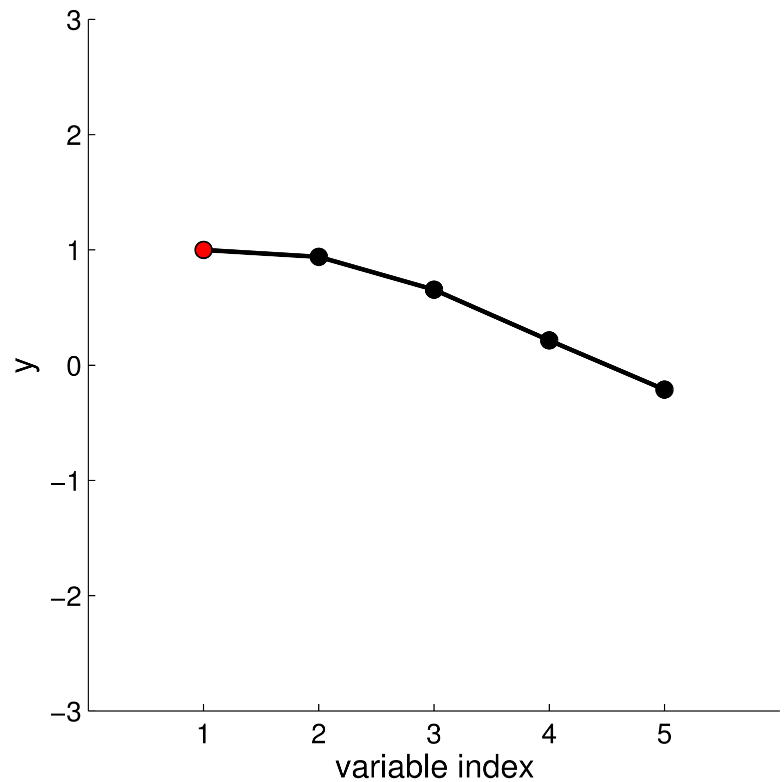


New visualisation





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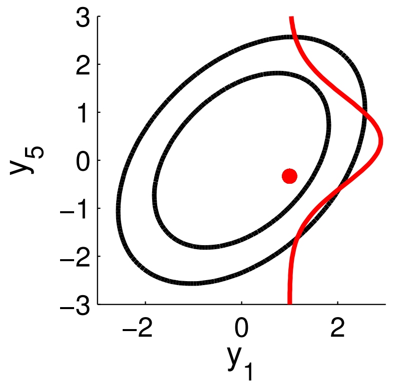
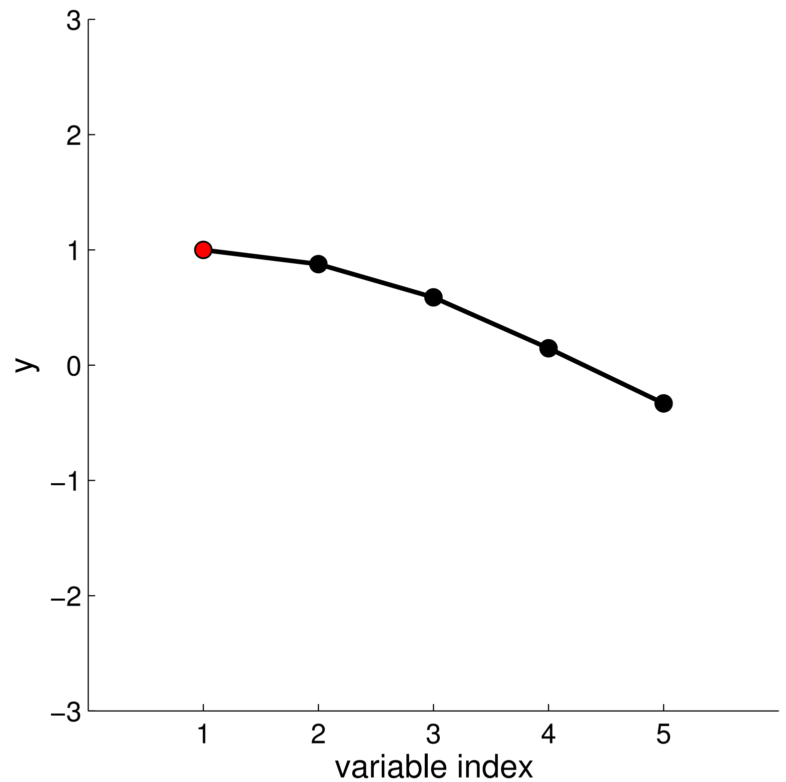
New visualisation





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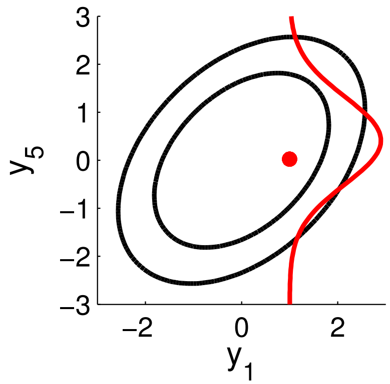
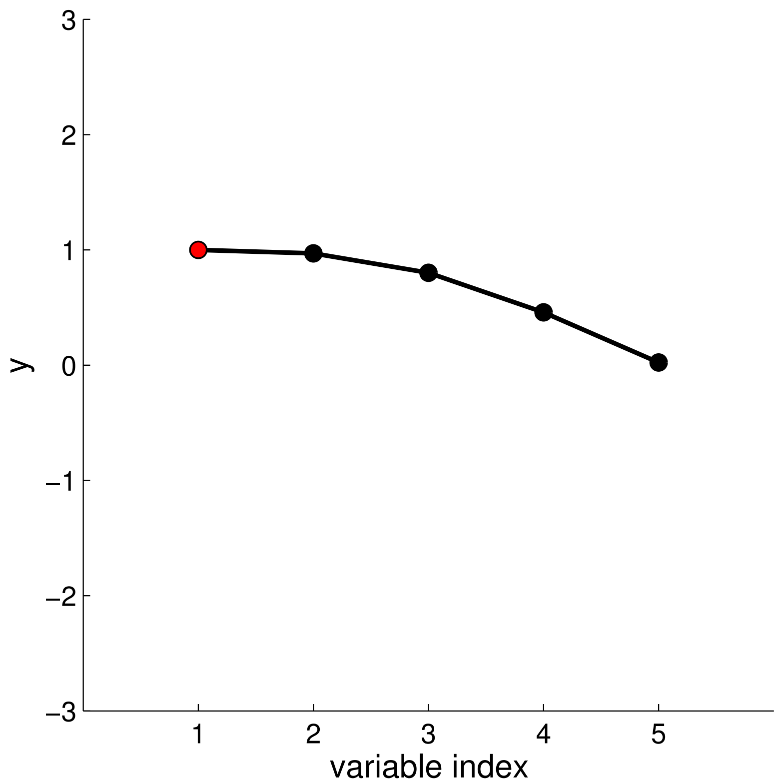
New visualisation





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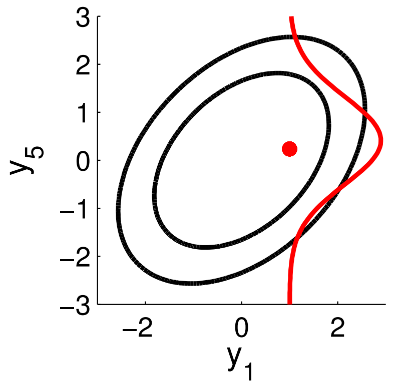
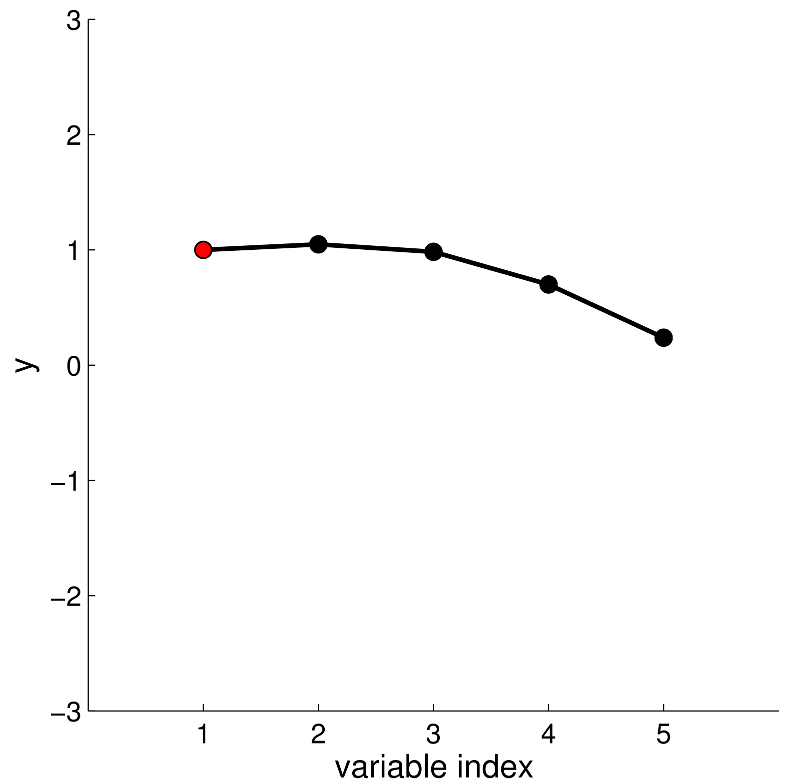
New visualisation





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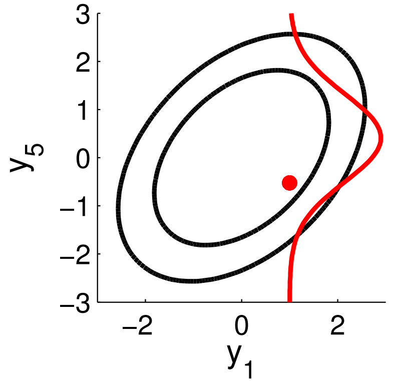
New visualisation



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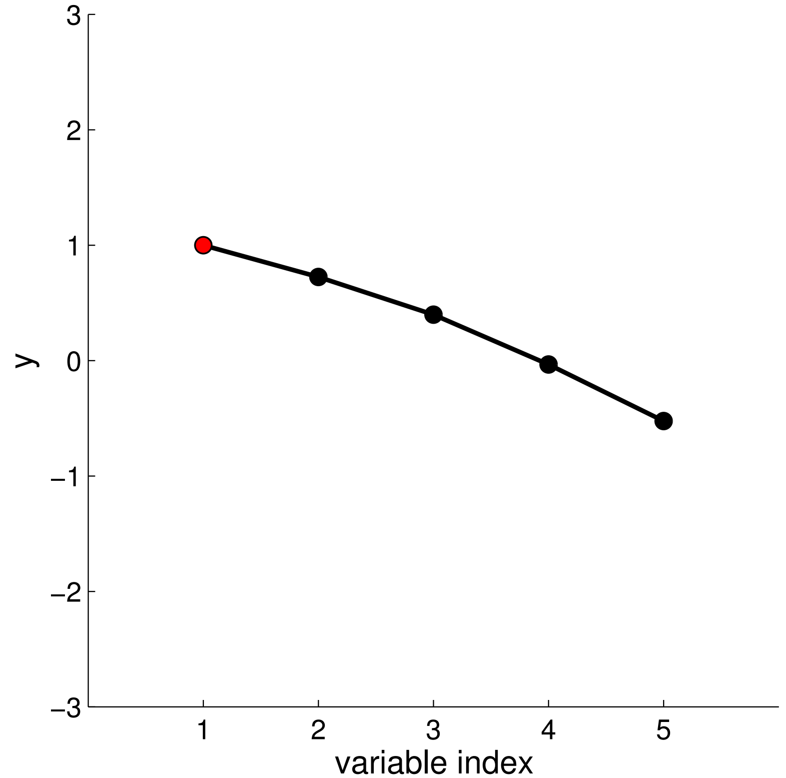
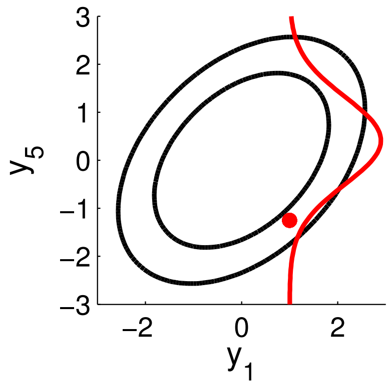
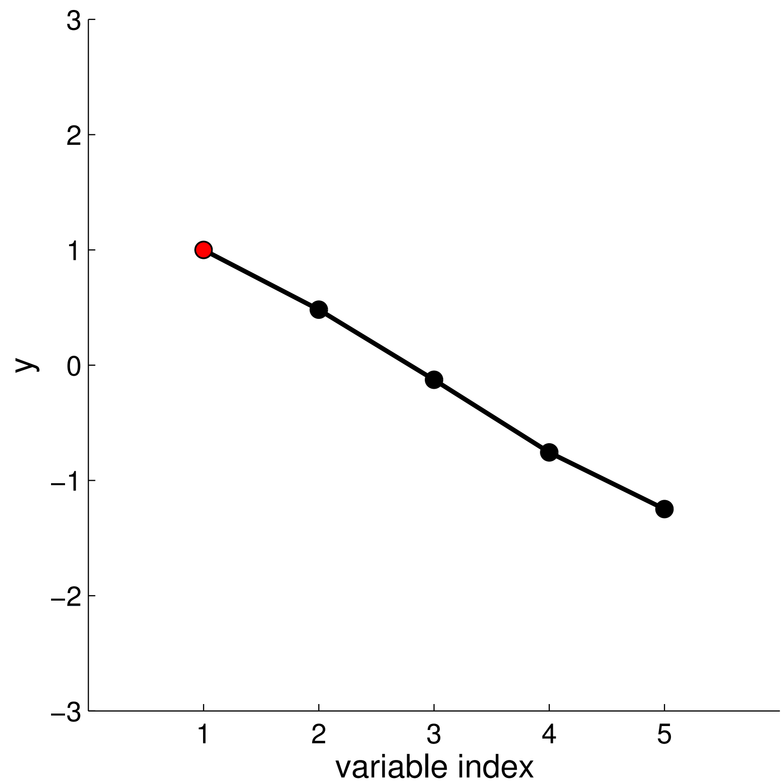


New visualisation





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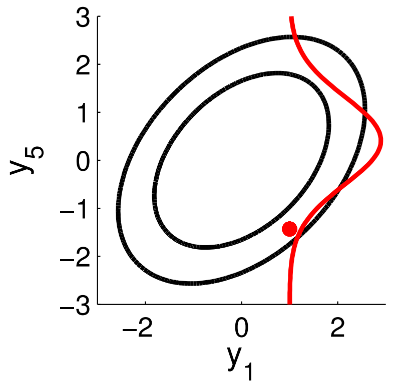
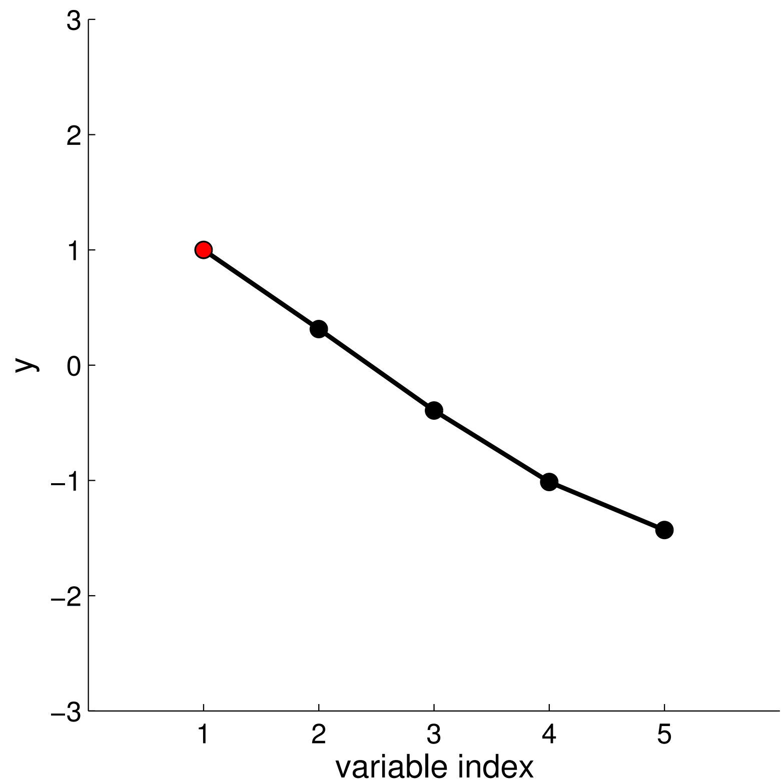
New visualisation





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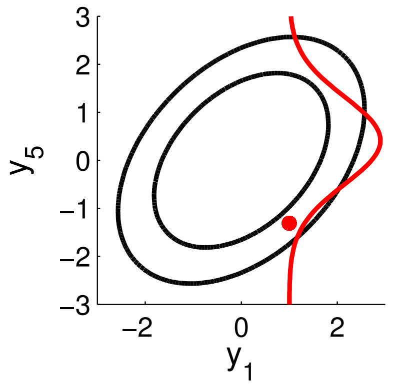
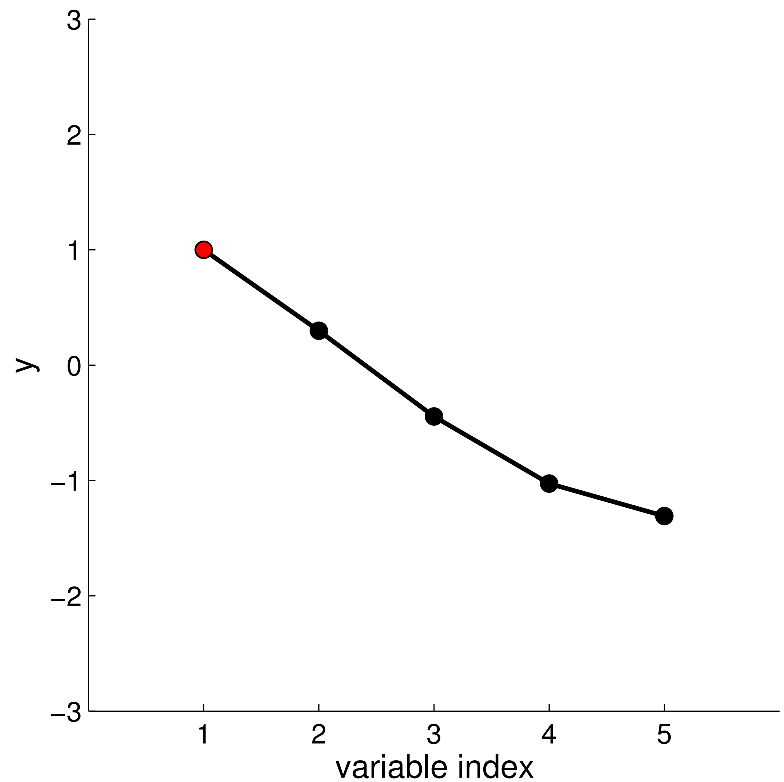
New visualisation





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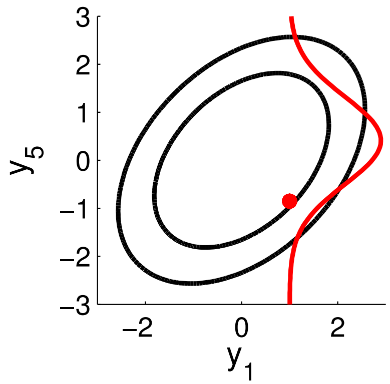
New visualisation



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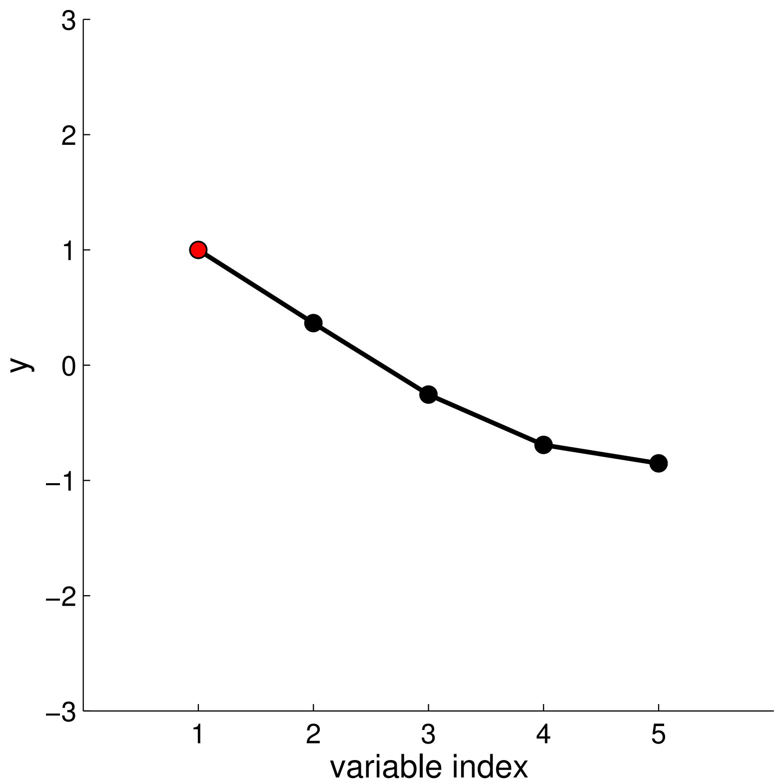
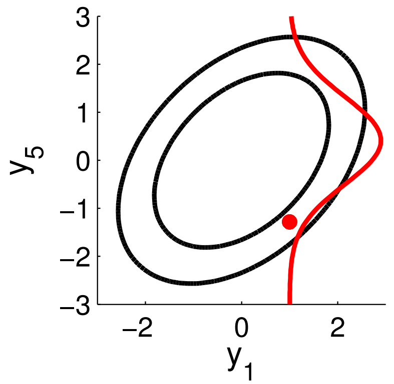
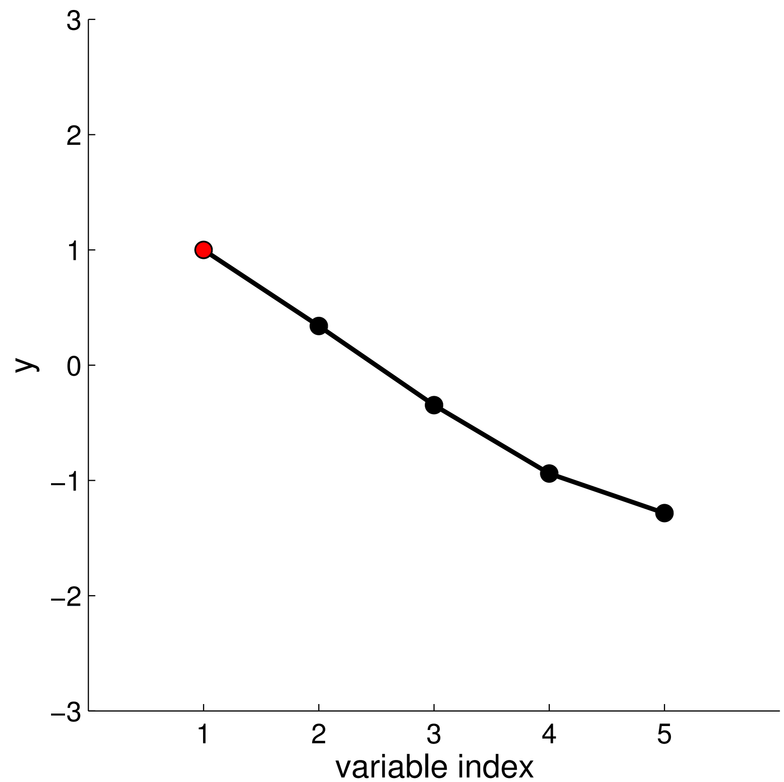


New visualisation





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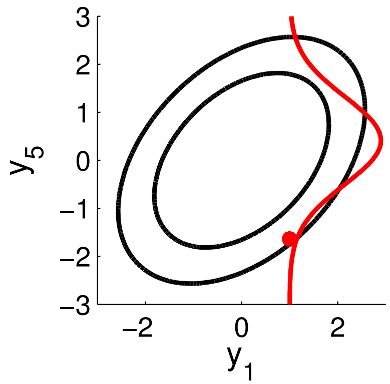
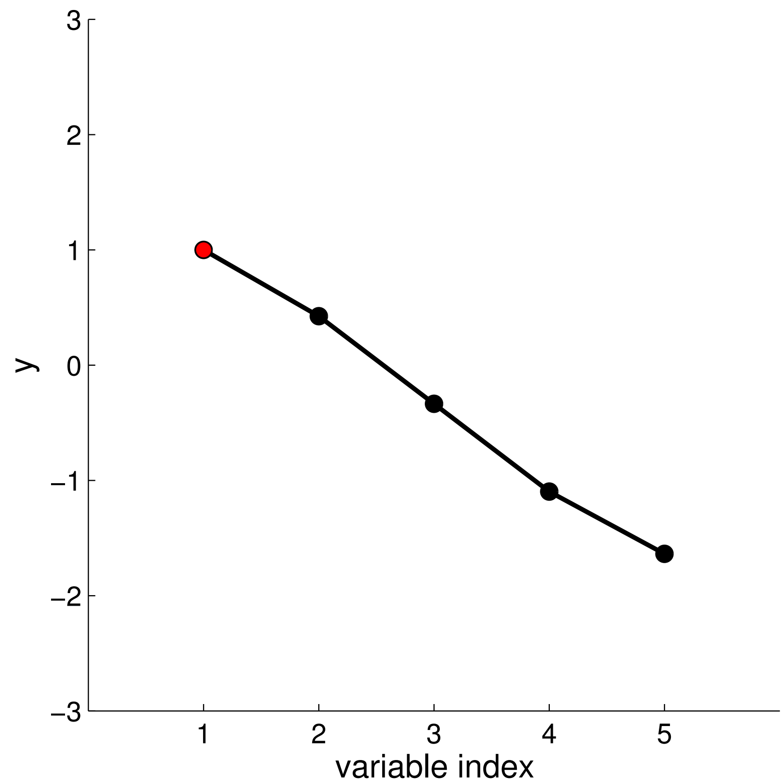
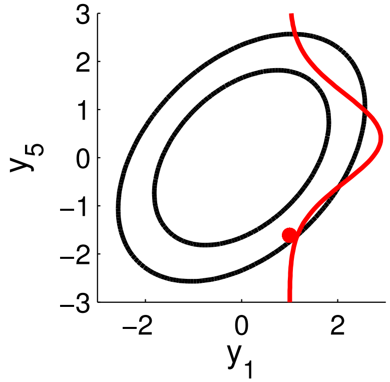
New visualisation

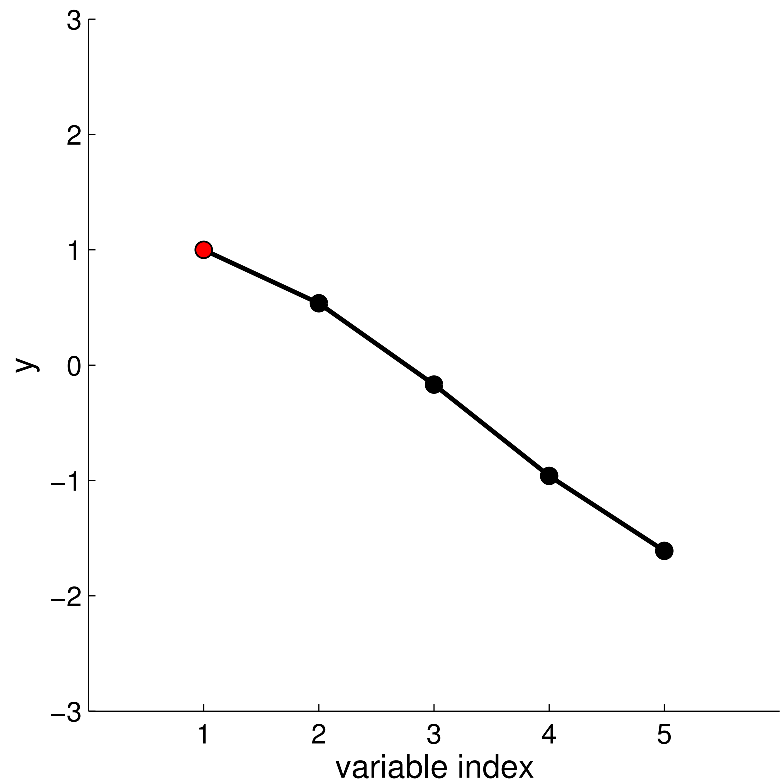




$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

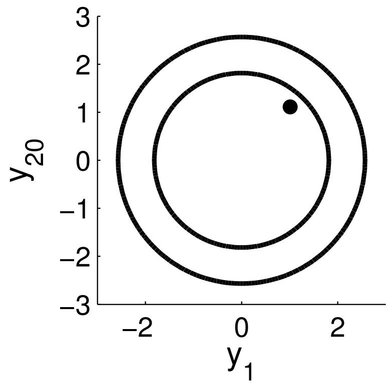
New visualisation

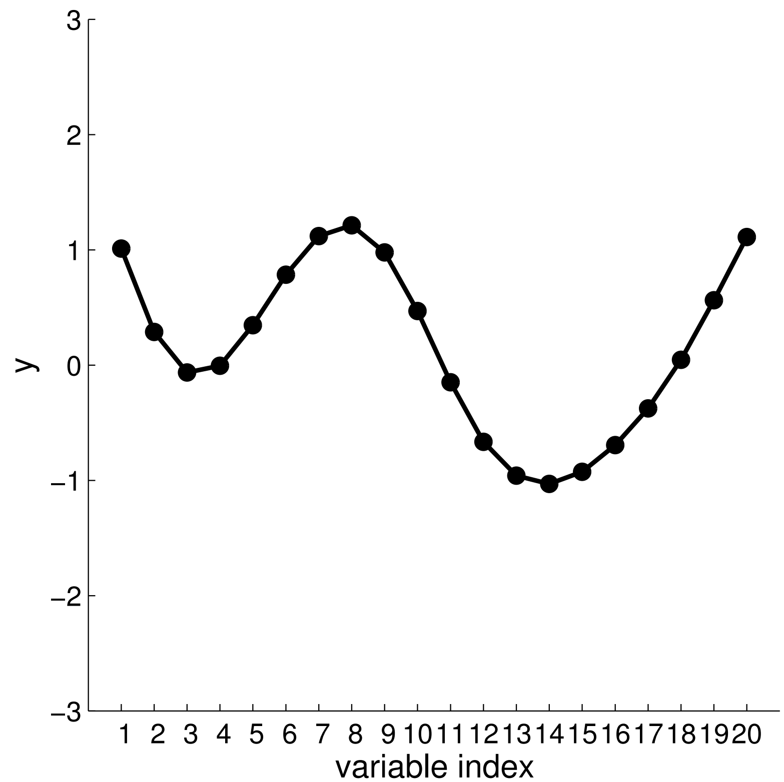




$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation





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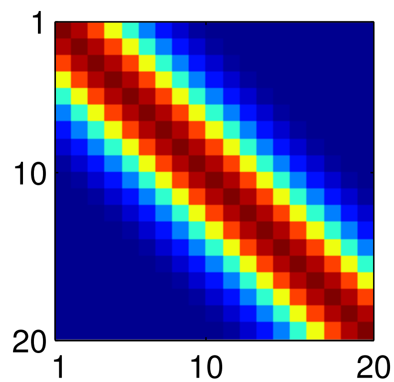

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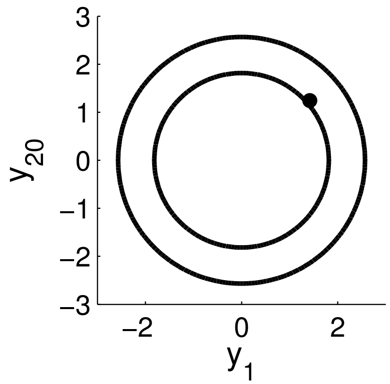

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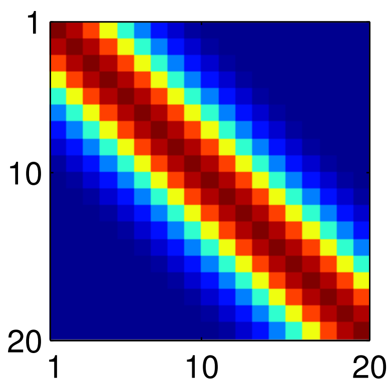

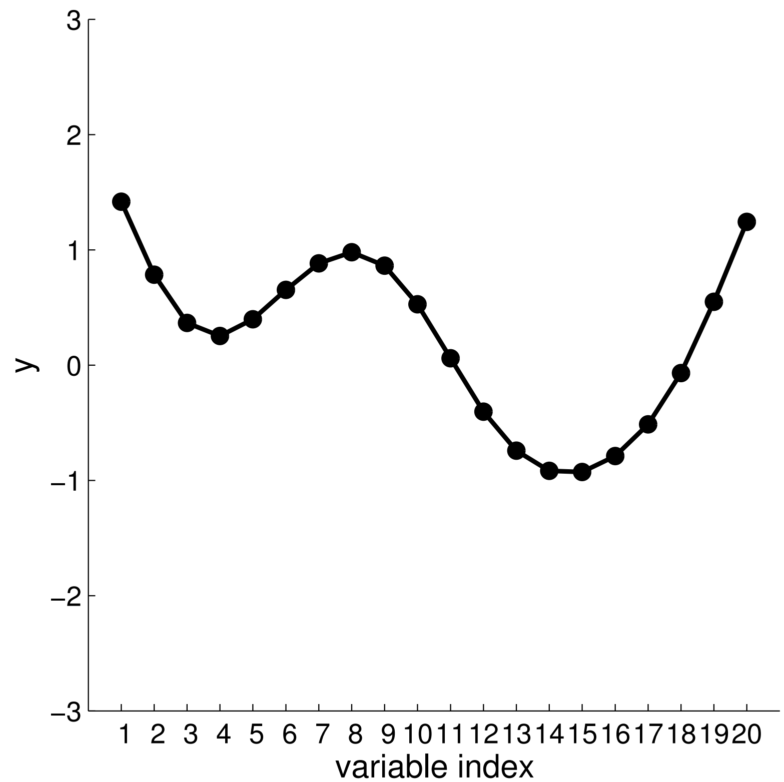

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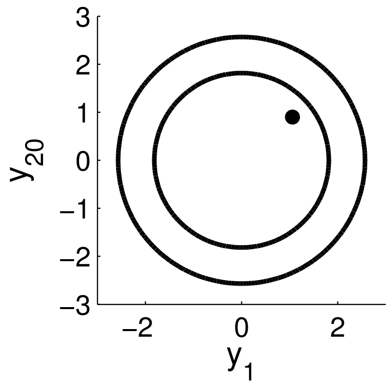

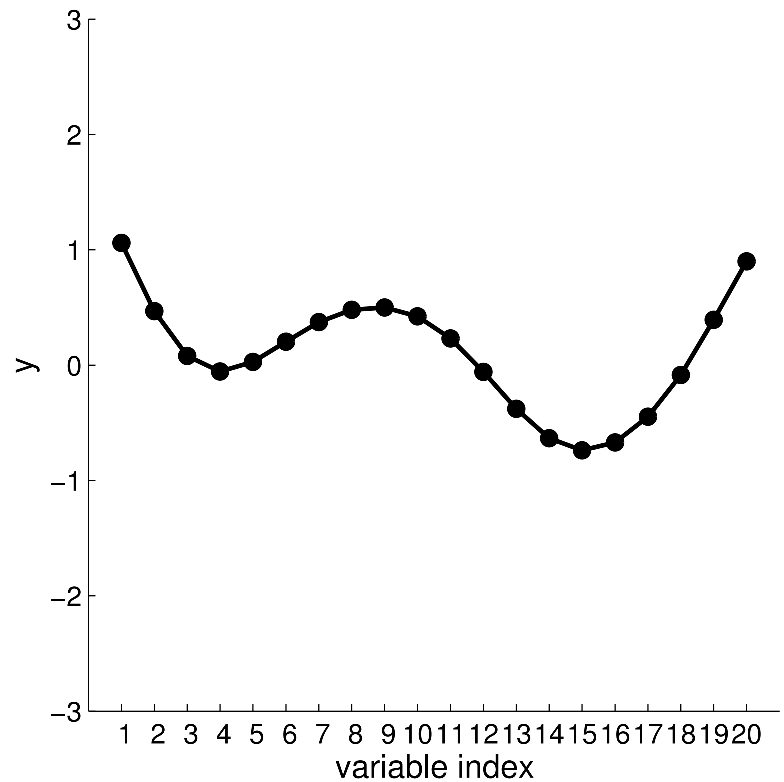

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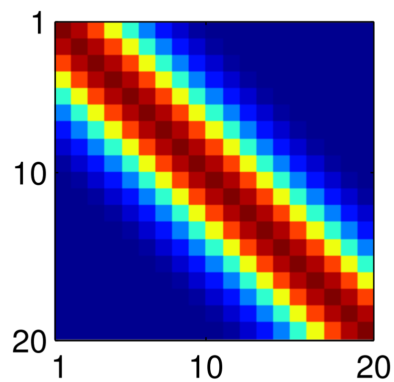

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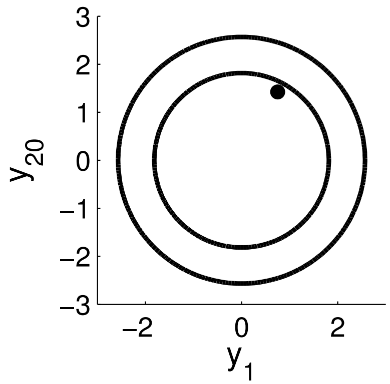
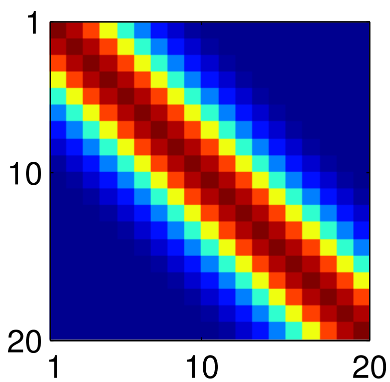
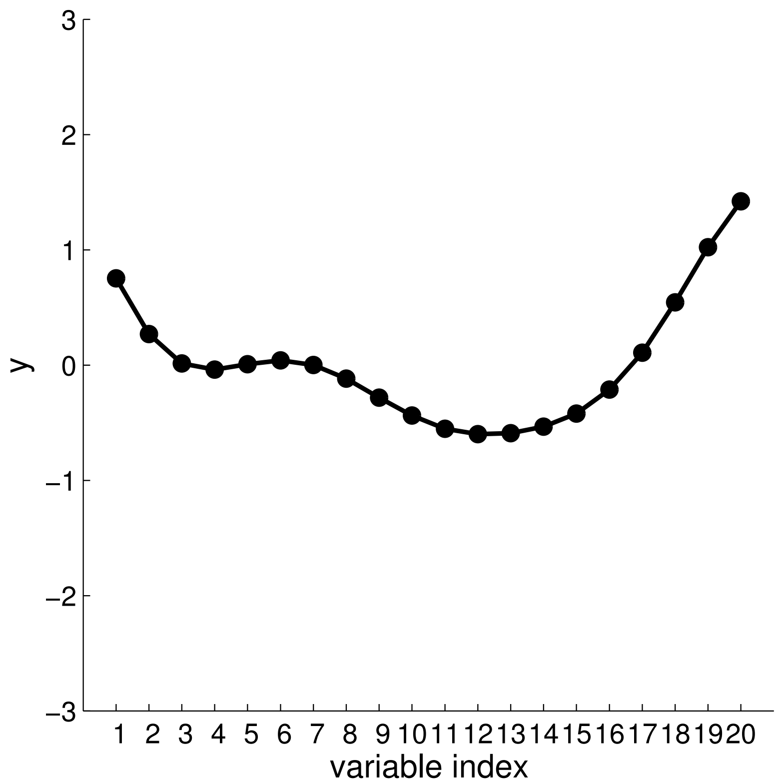


$\Sigma =$ 



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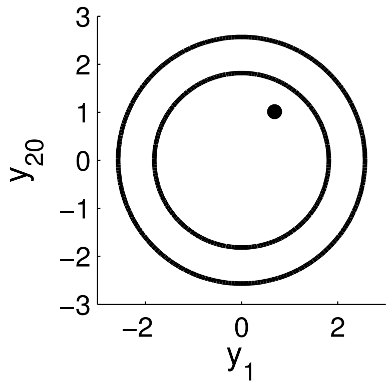

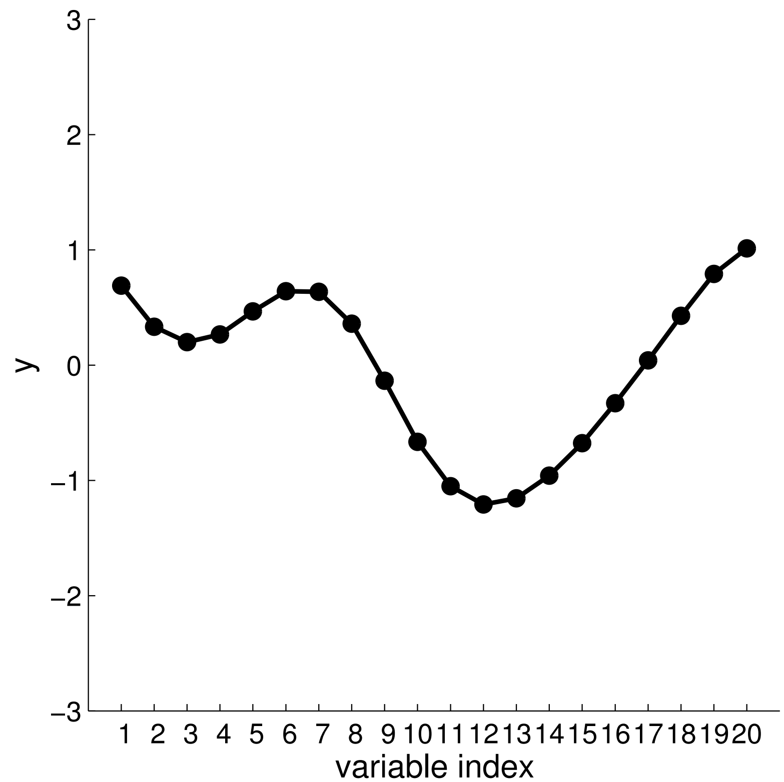

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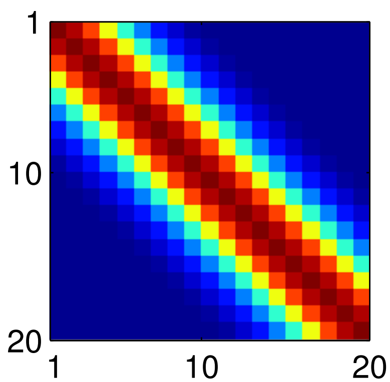

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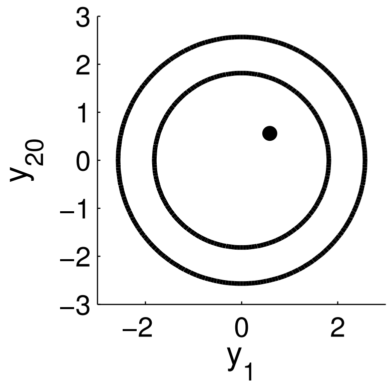

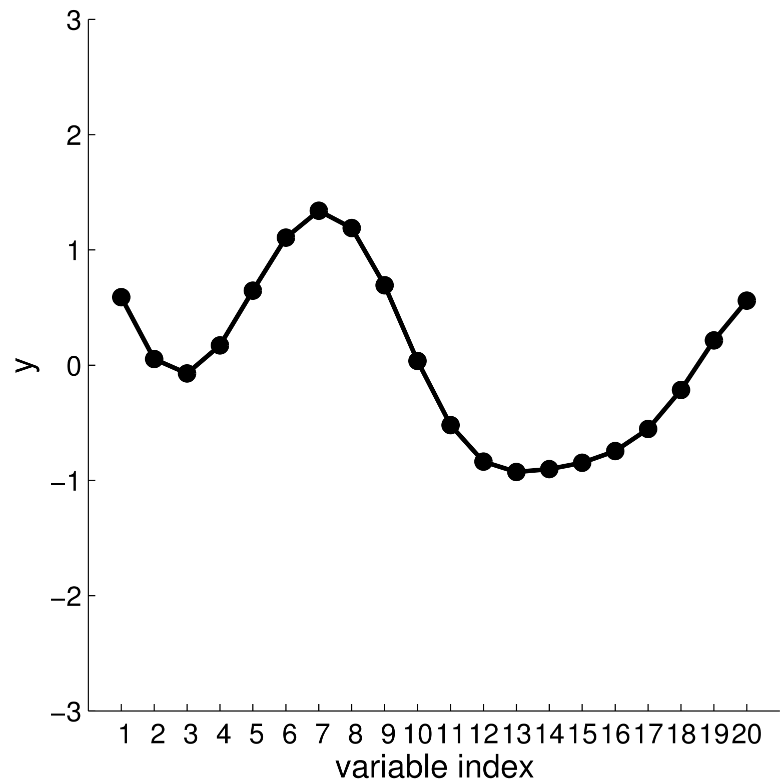

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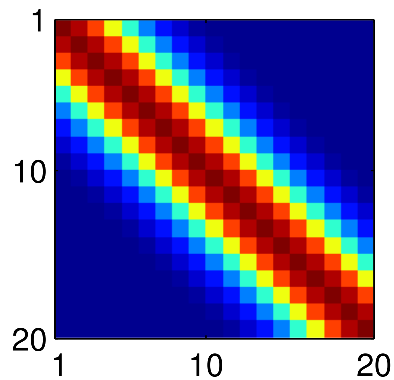

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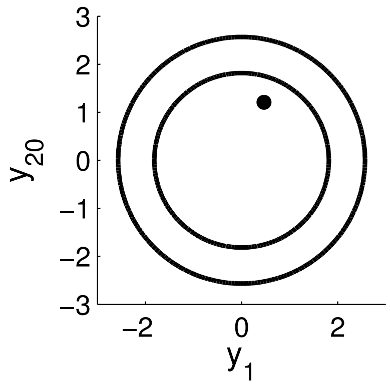

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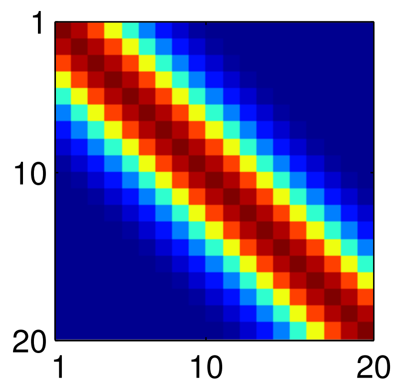

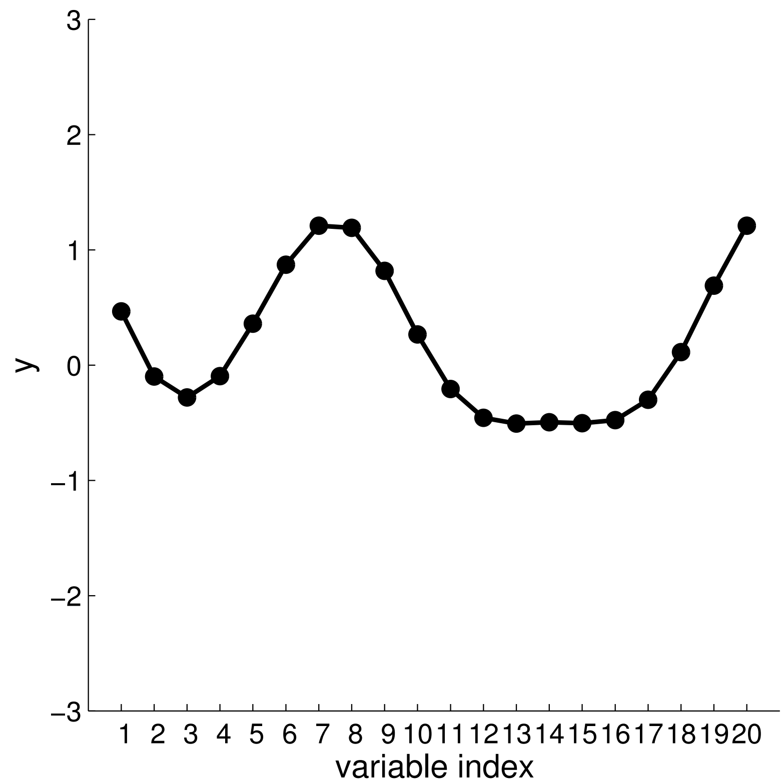

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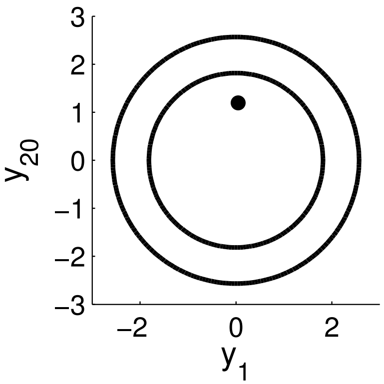

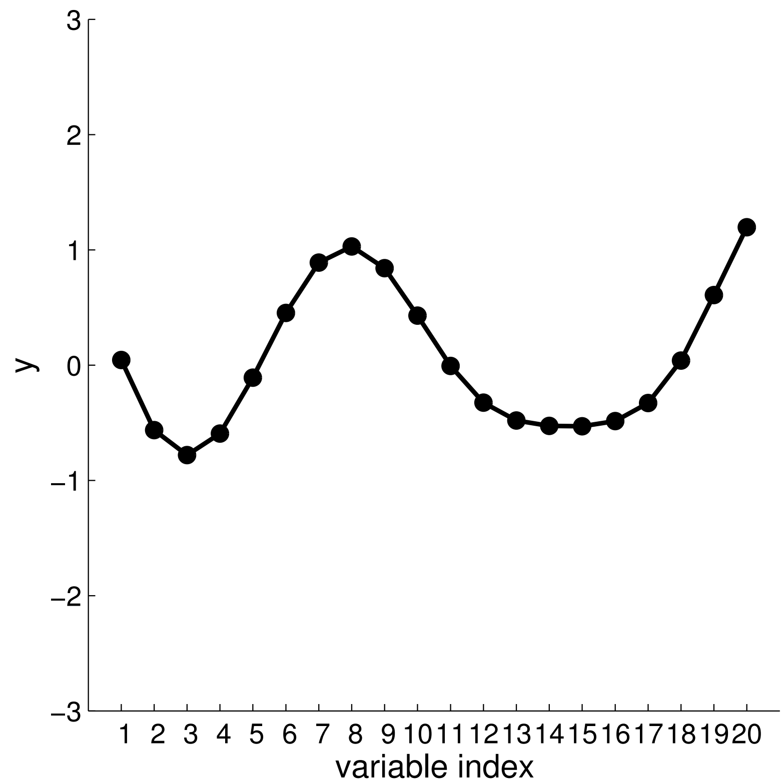

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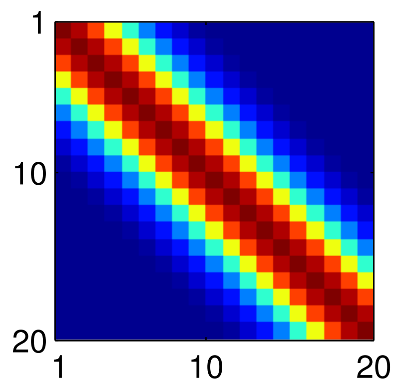

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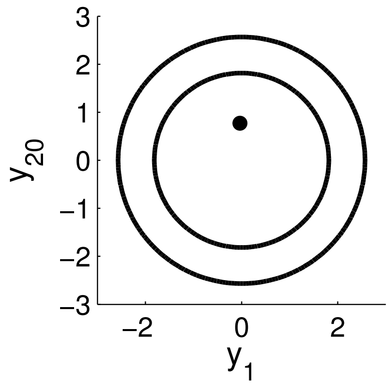

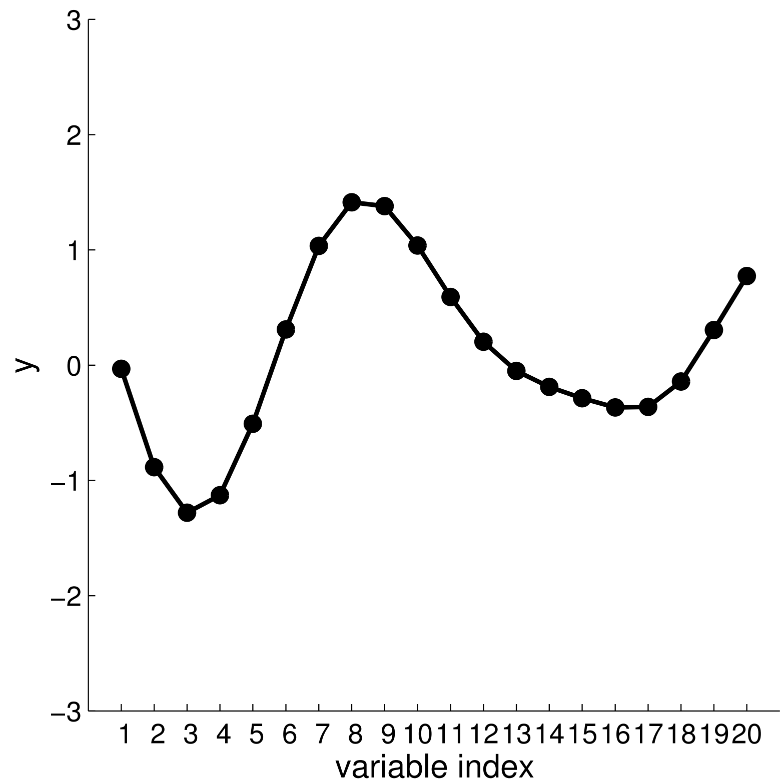

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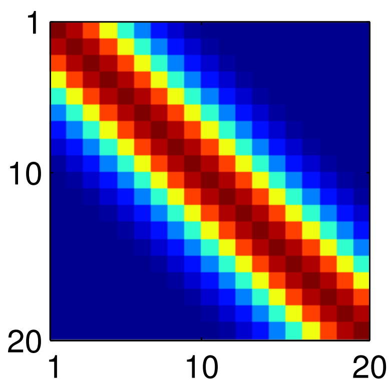

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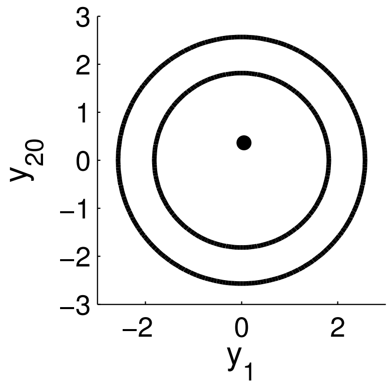

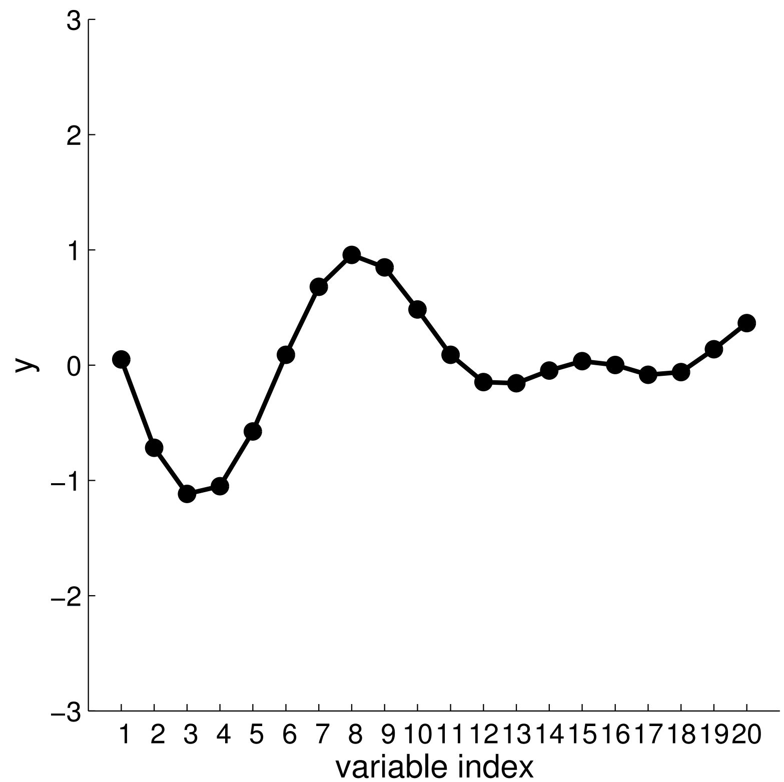

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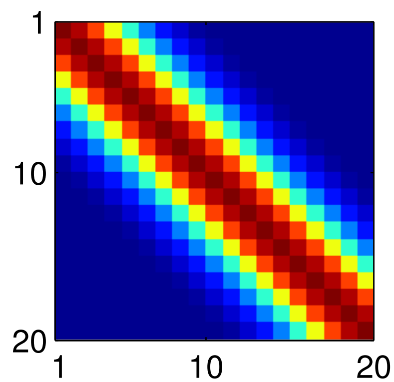

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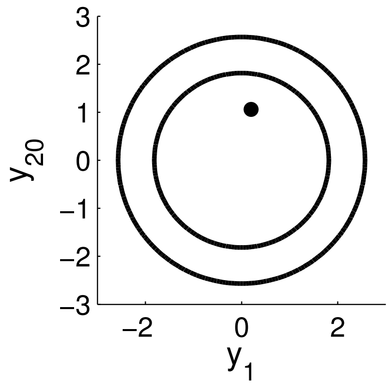

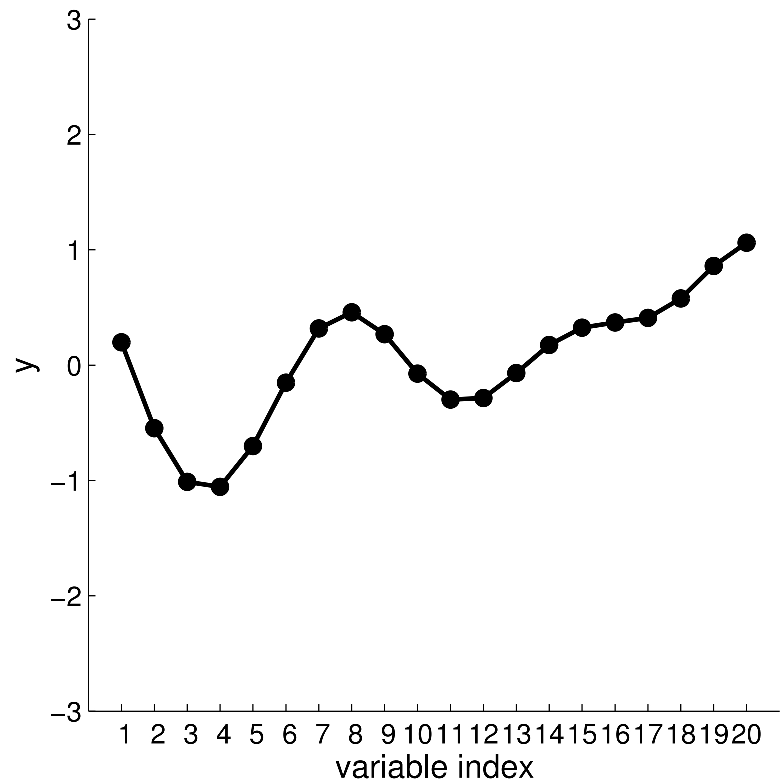

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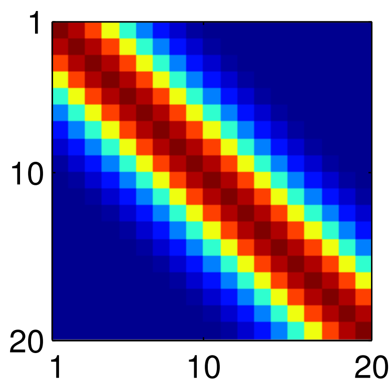

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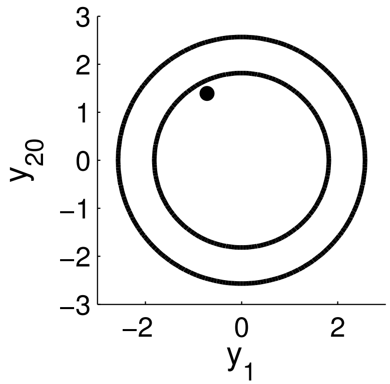

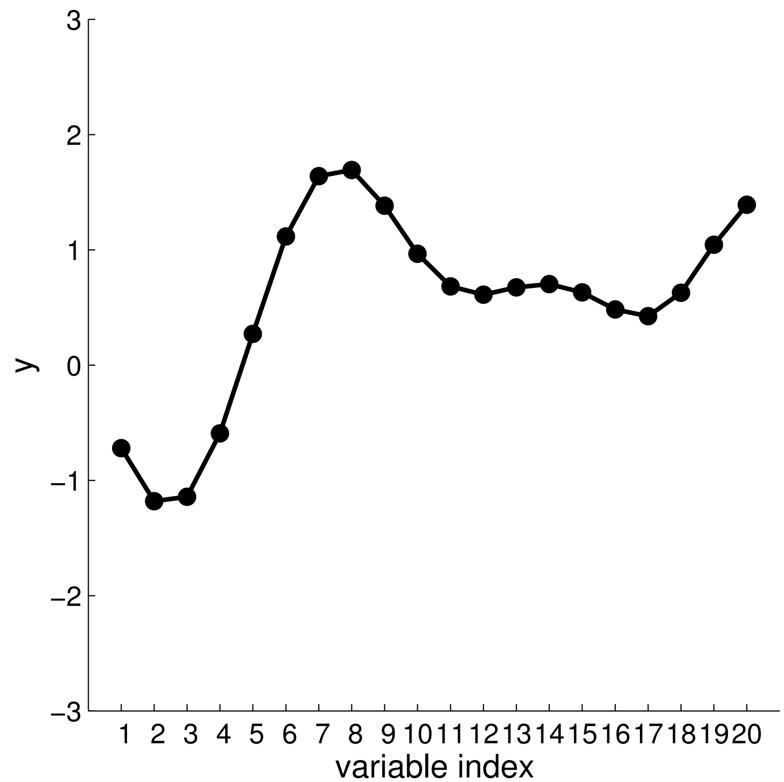

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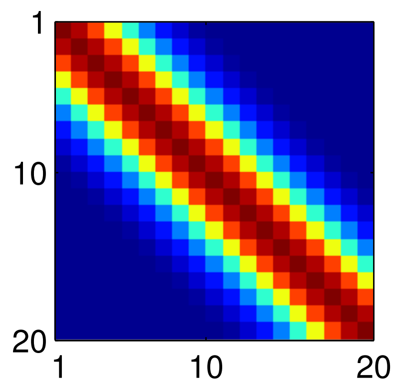

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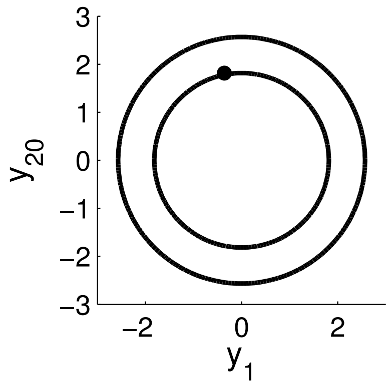

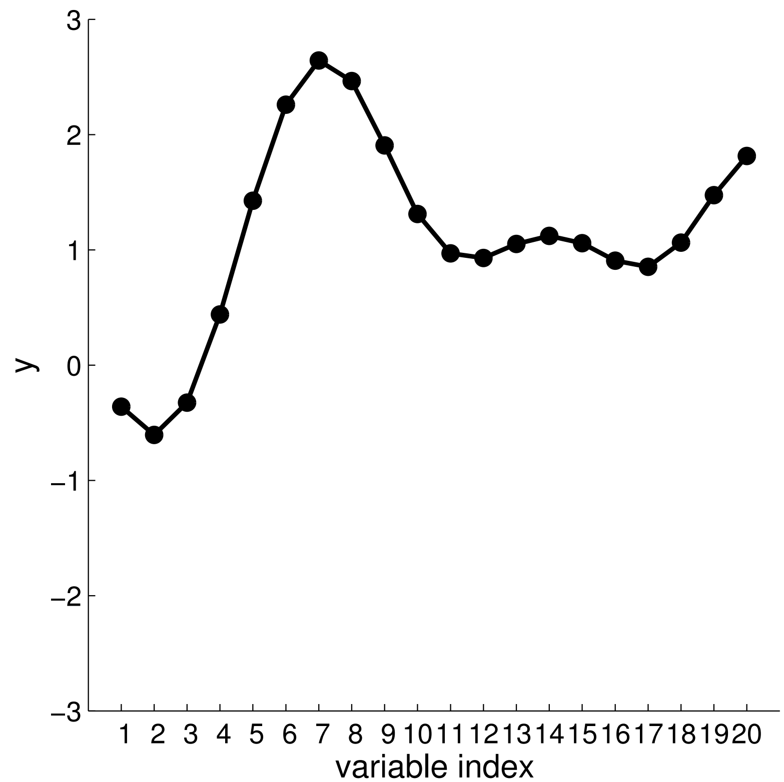

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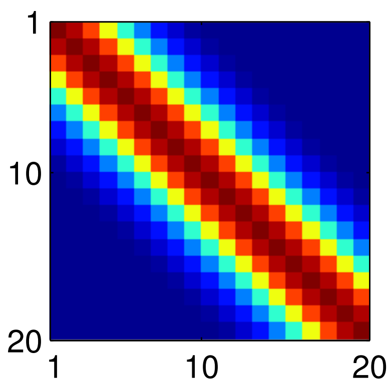

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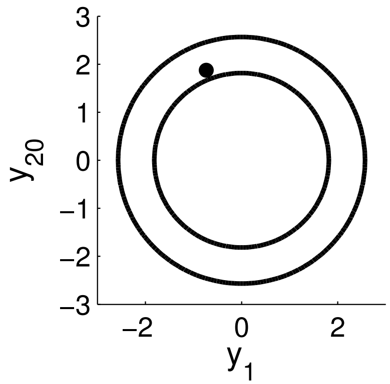

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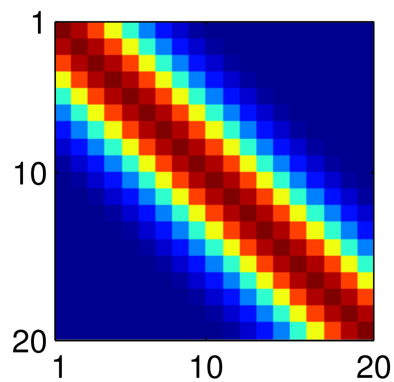

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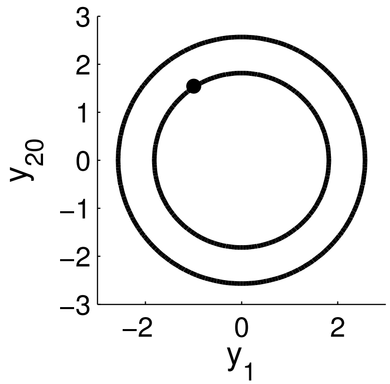

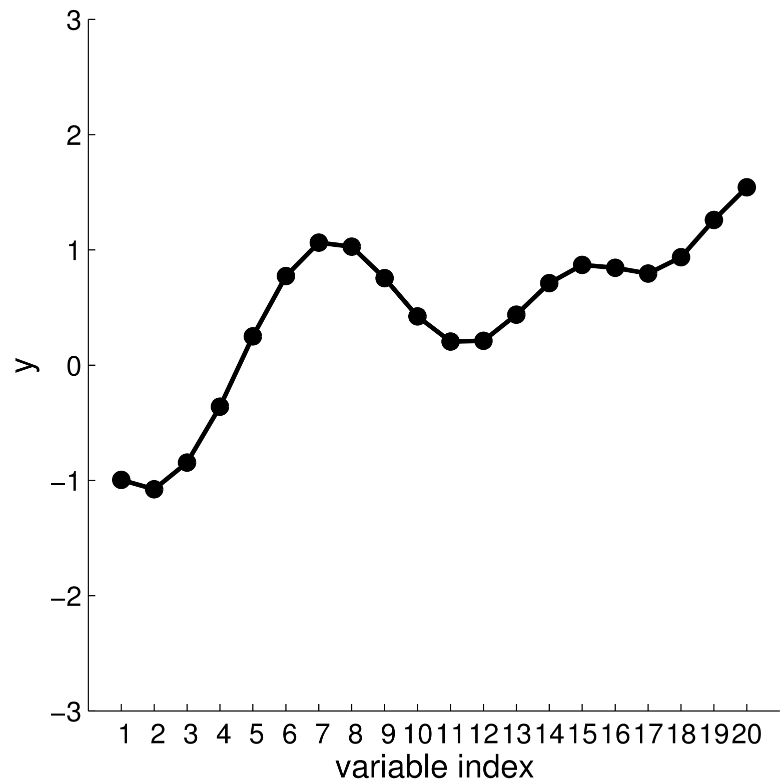

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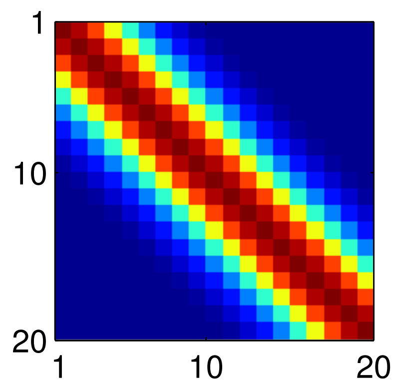

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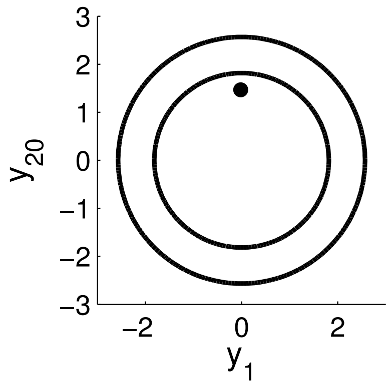

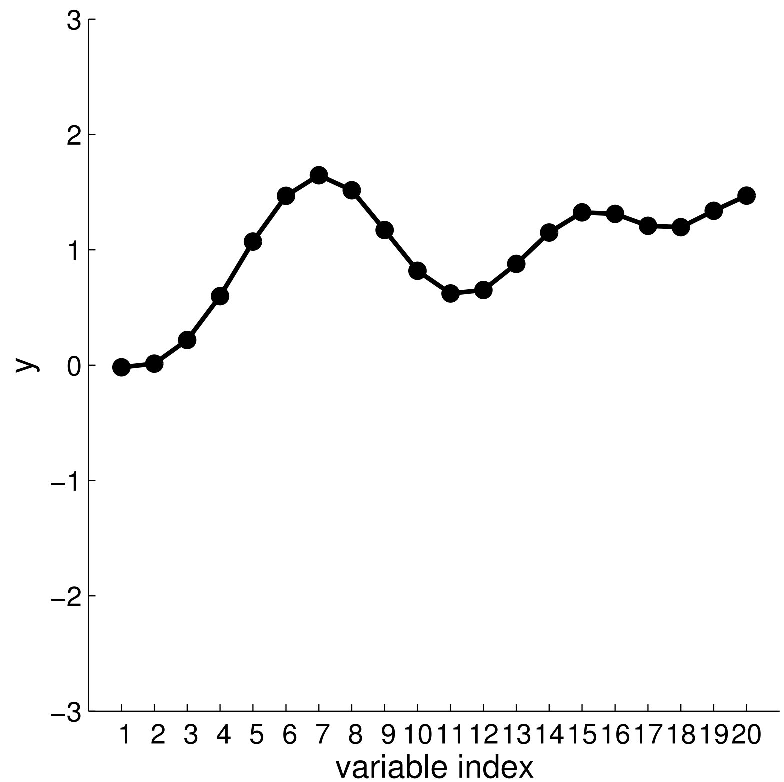

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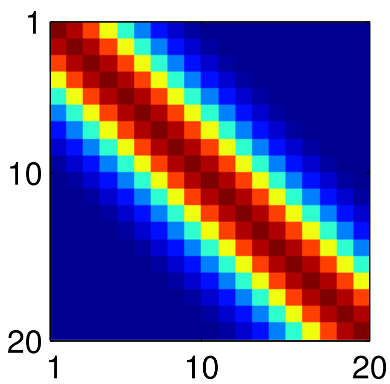

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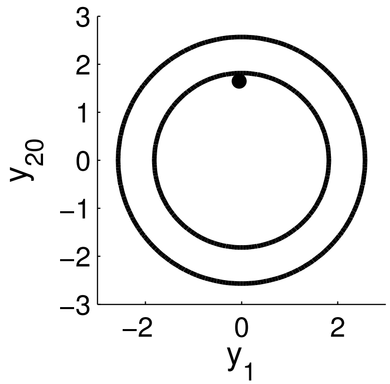

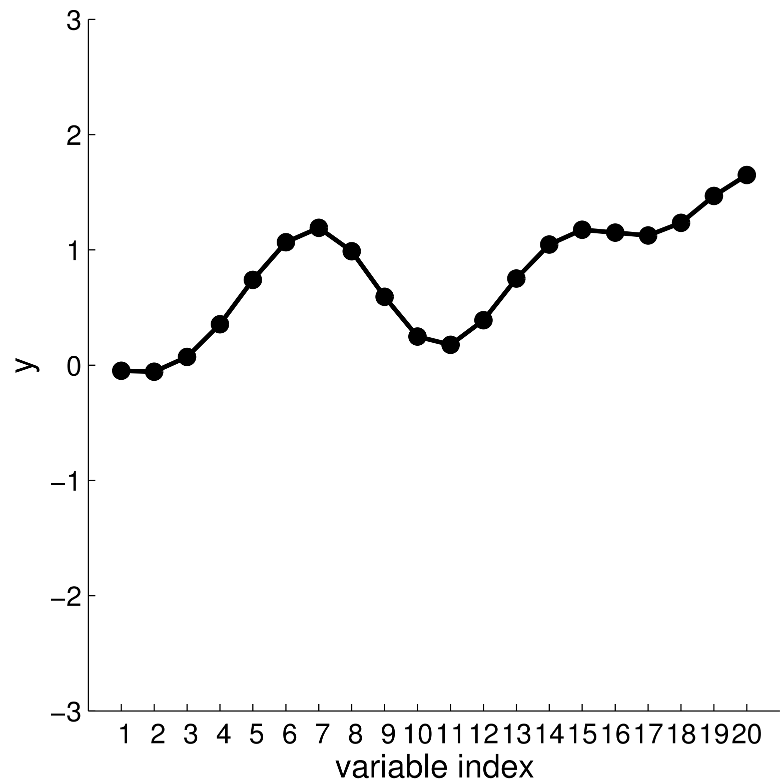

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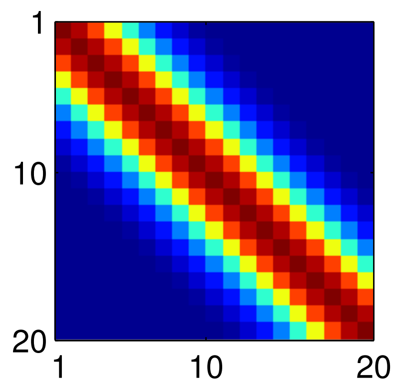

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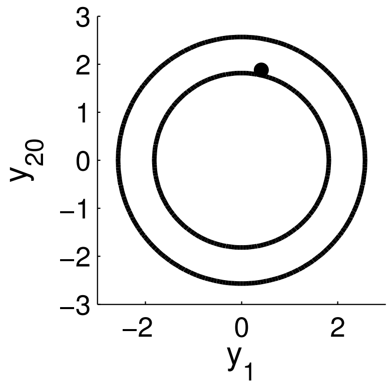

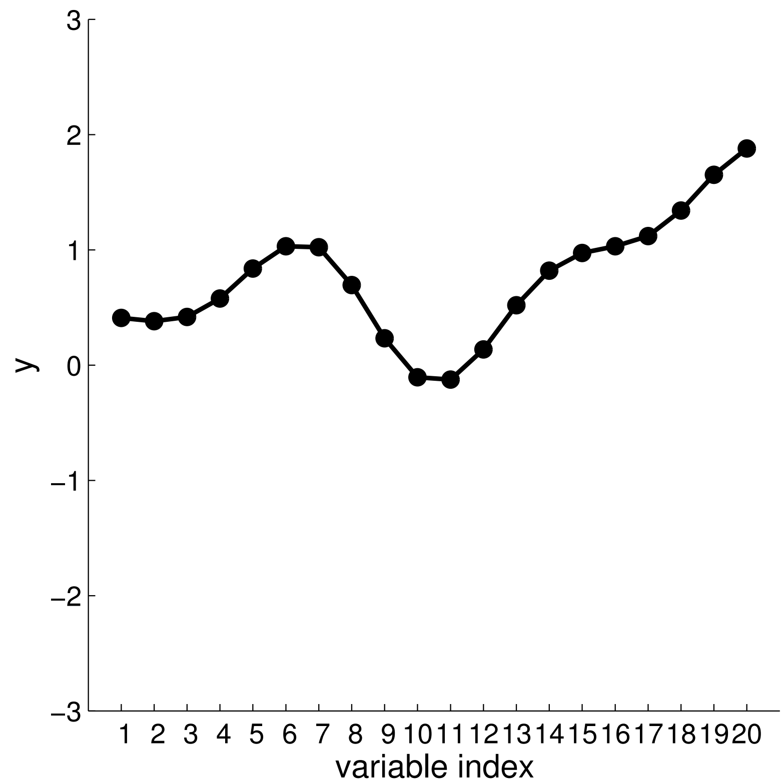

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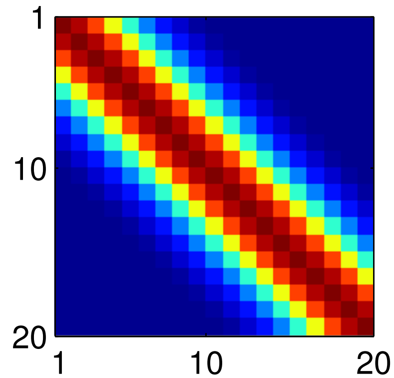

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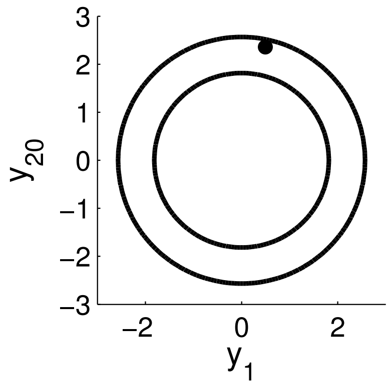

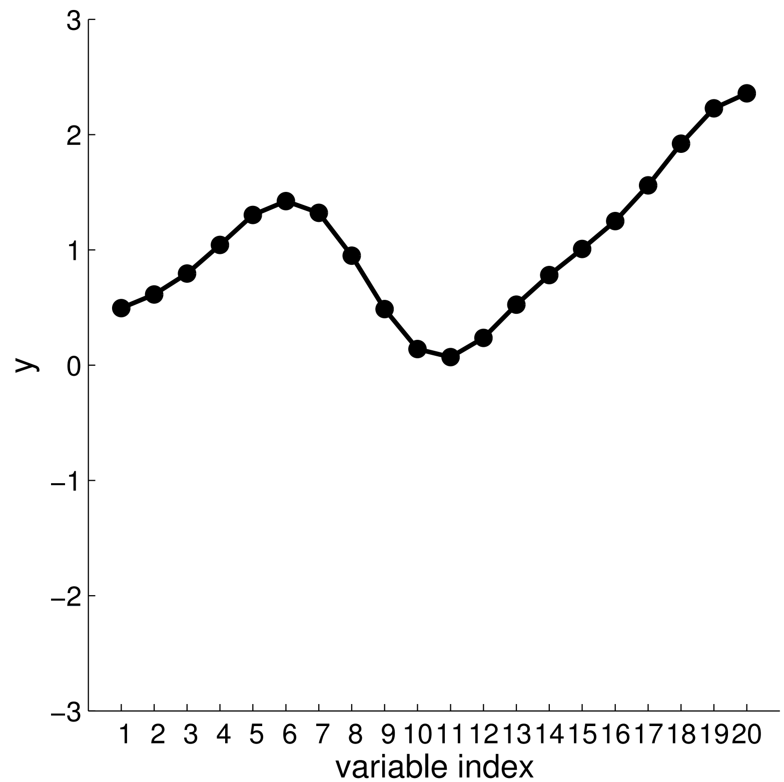

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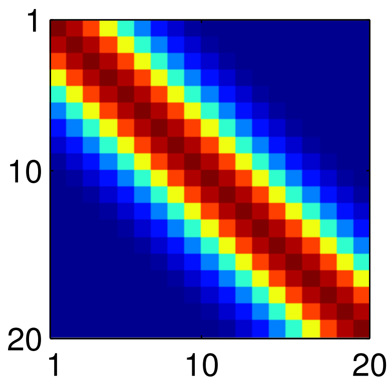

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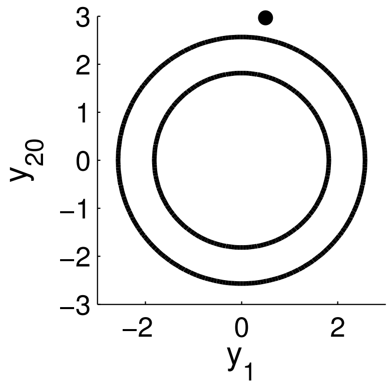

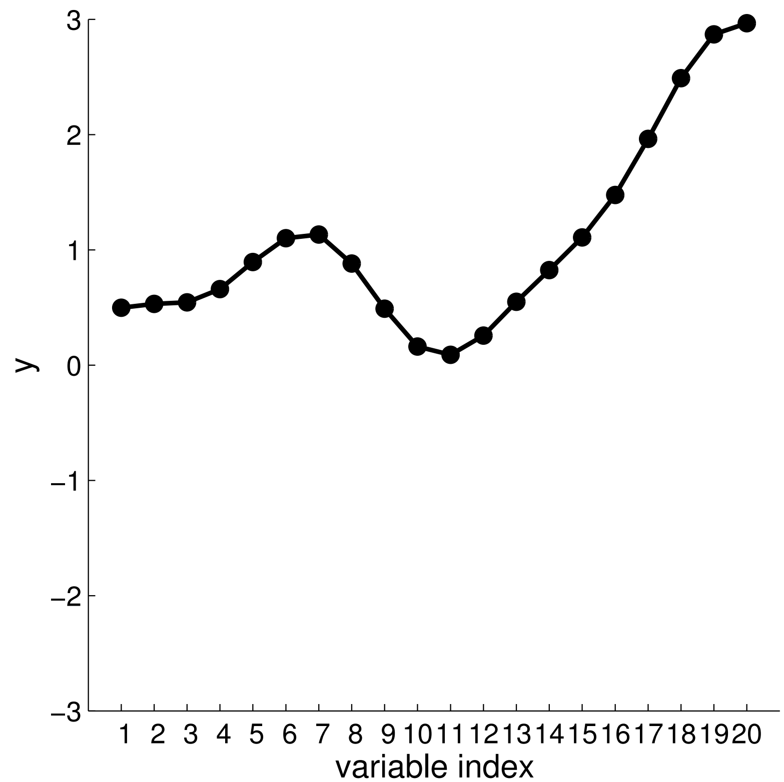

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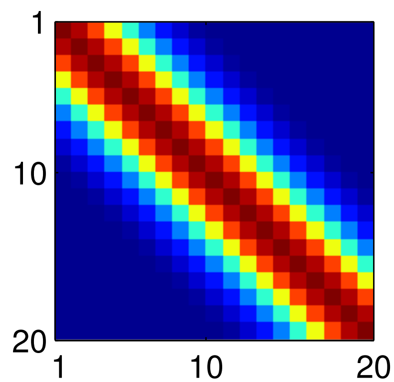

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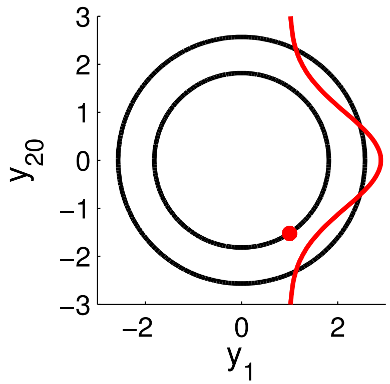

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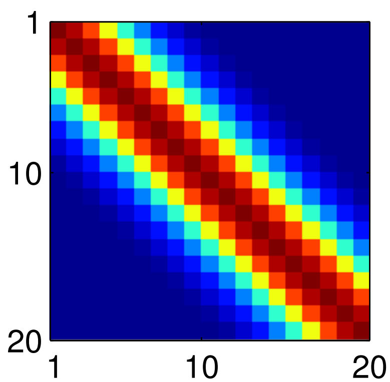

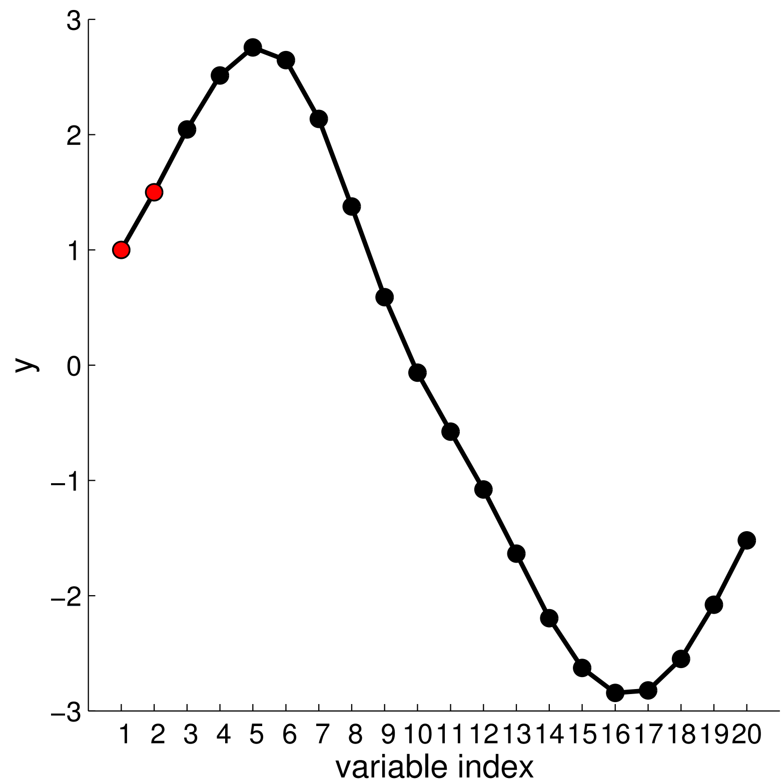

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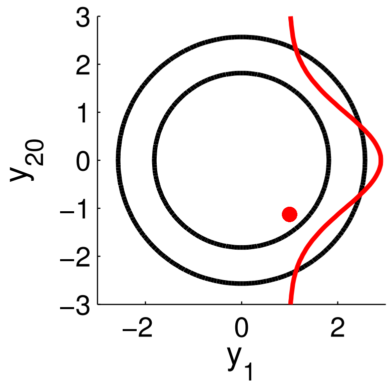

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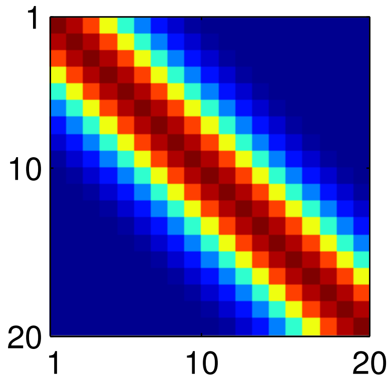

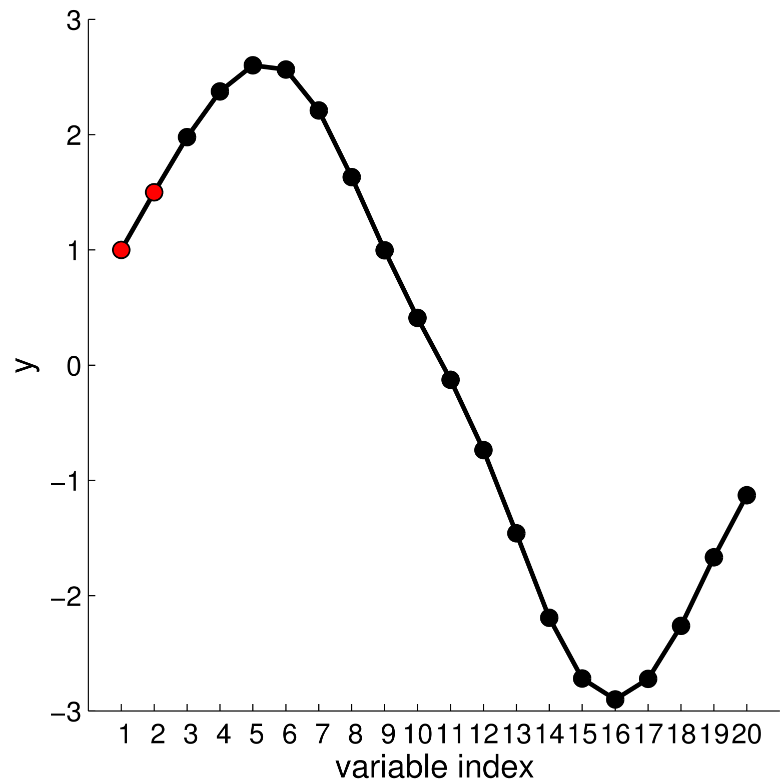

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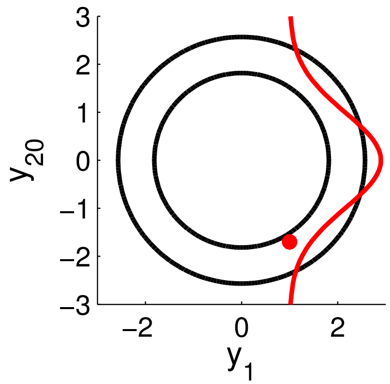

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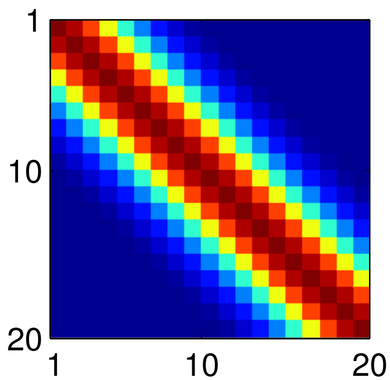

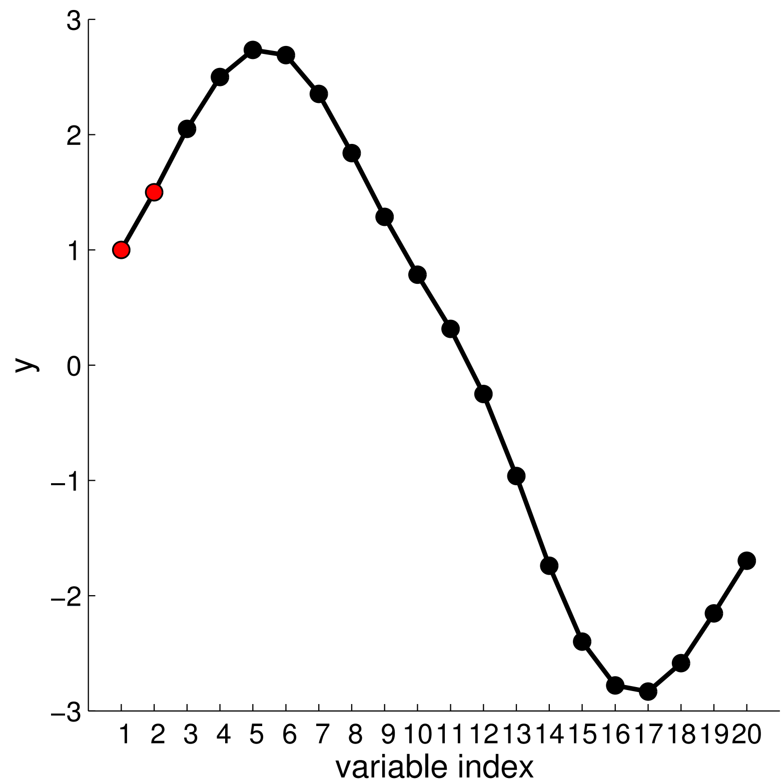

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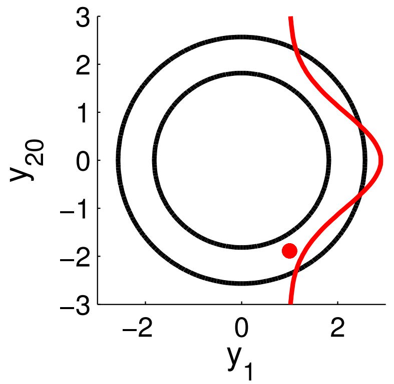

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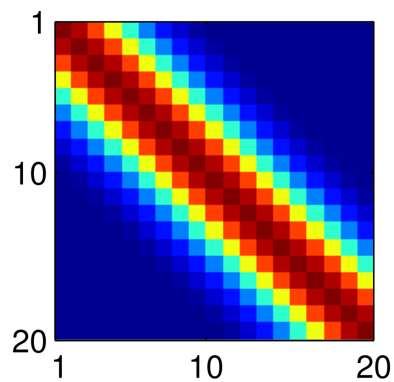
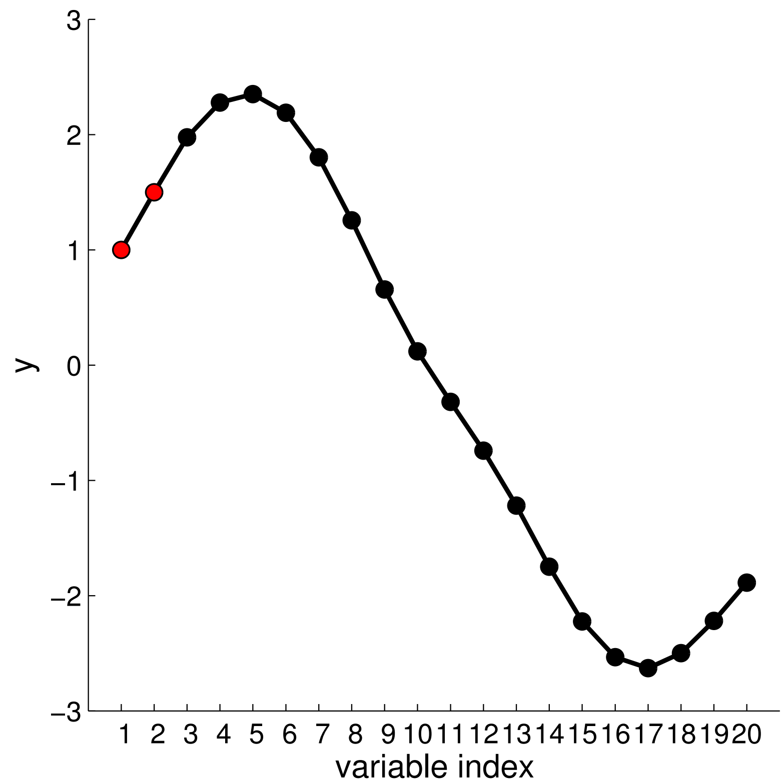
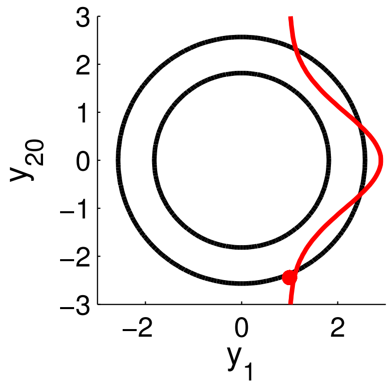
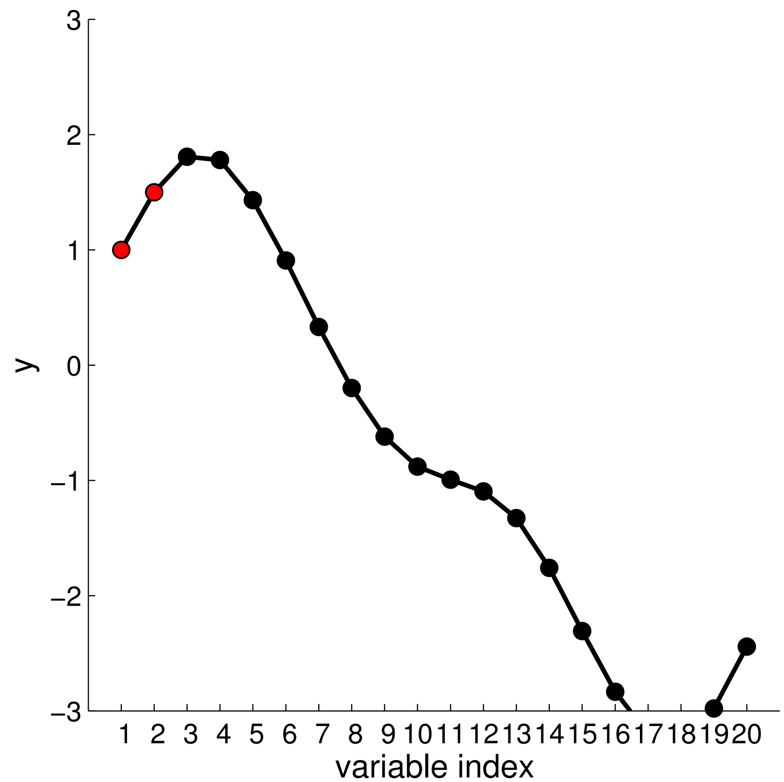




New visualisation





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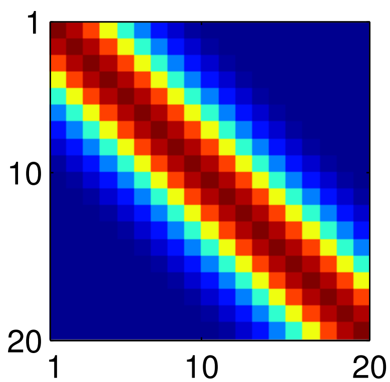

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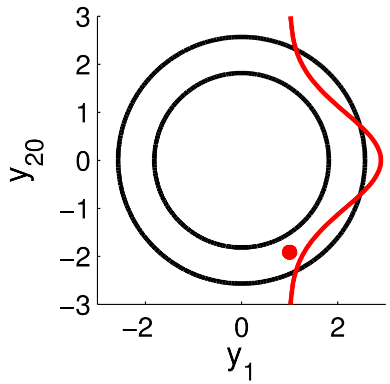
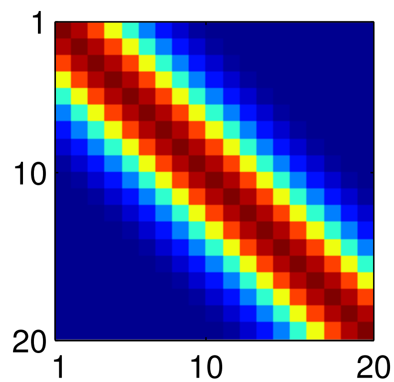
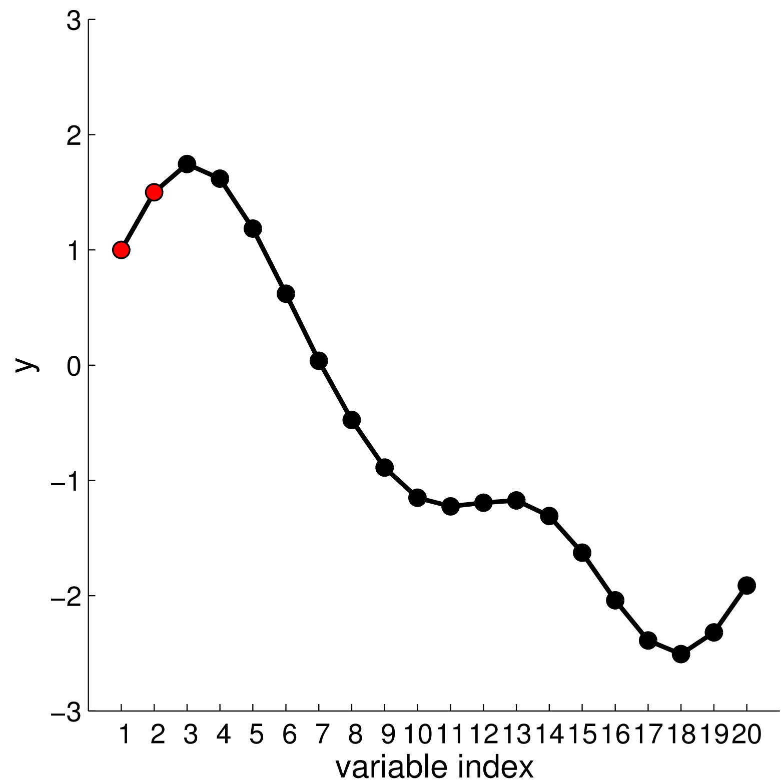


$\Sigma =$ 



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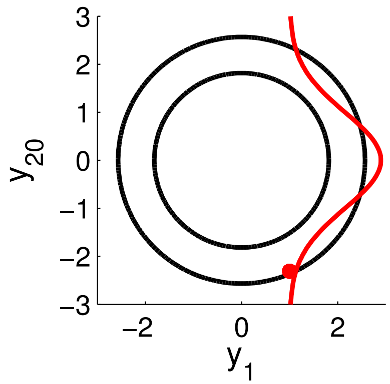

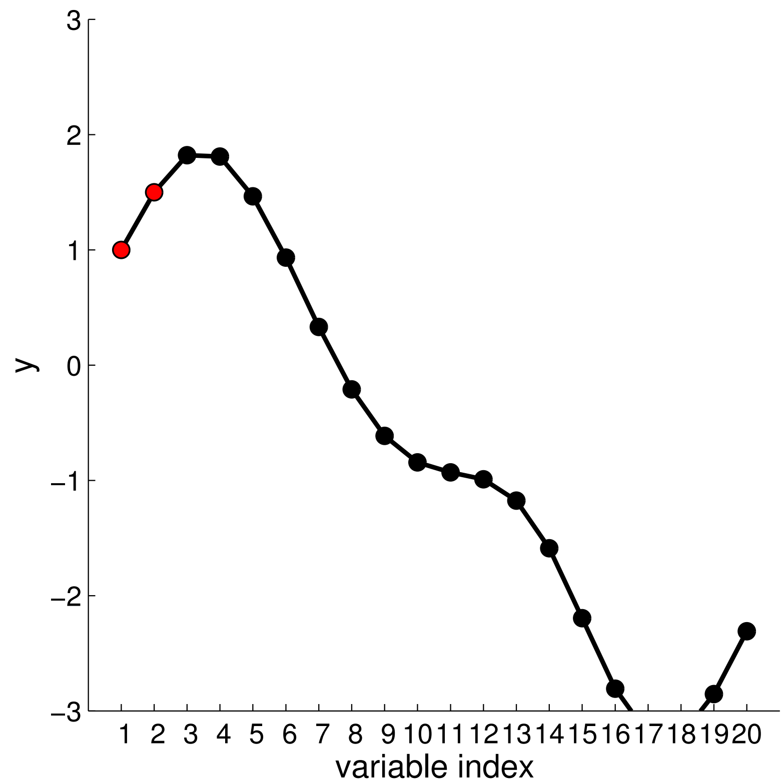

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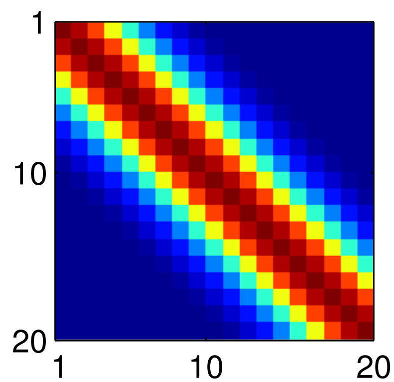

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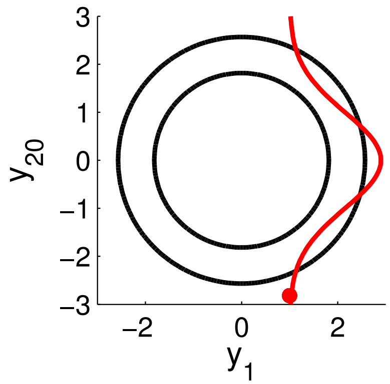

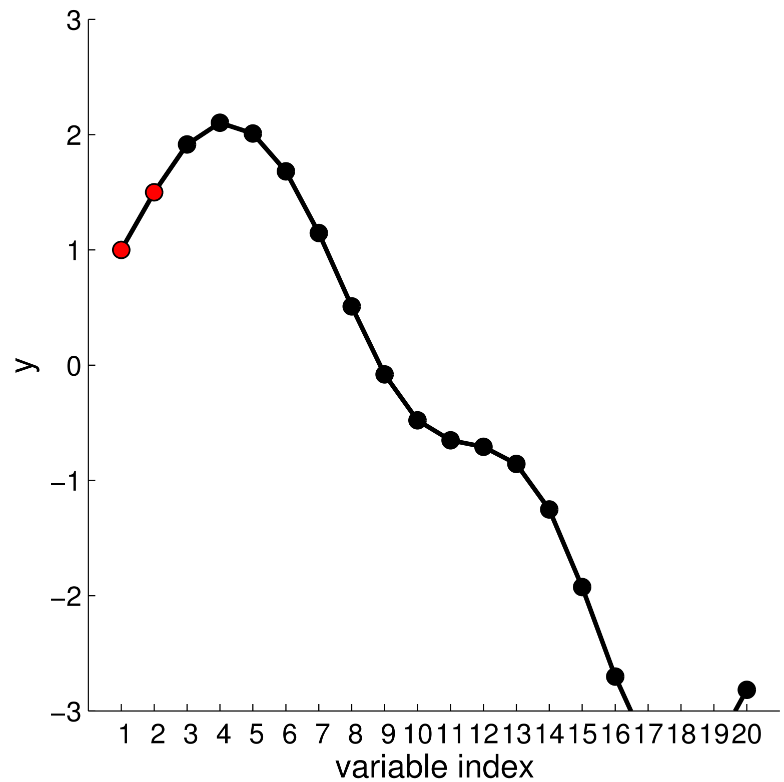

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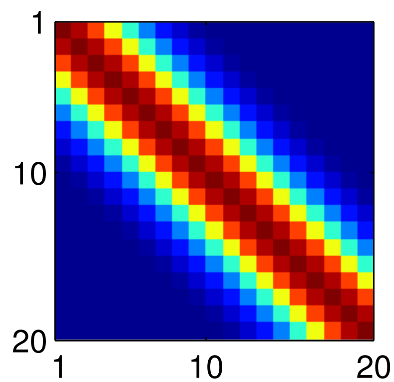

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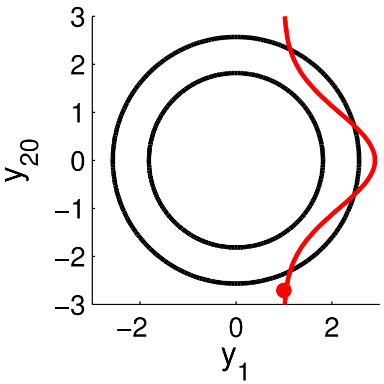
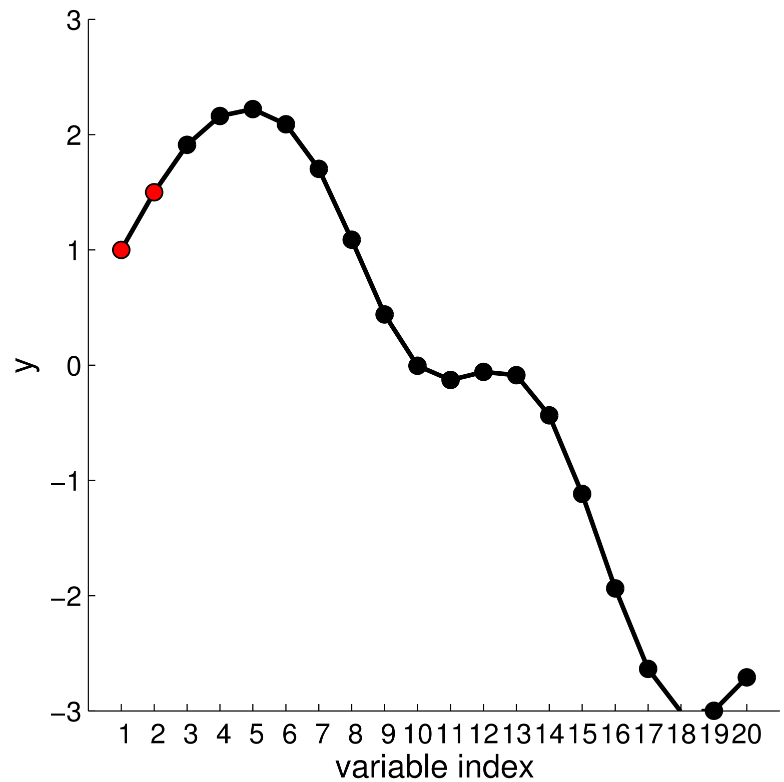
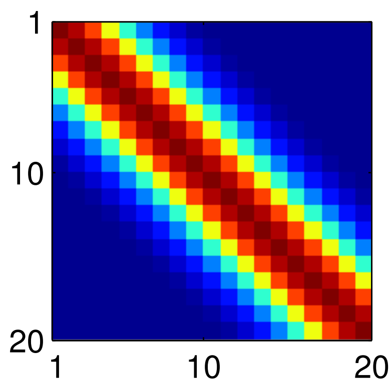




$$\Sigma =$$



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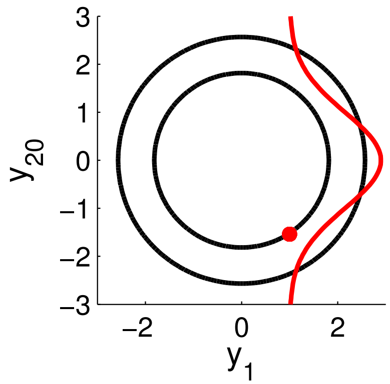

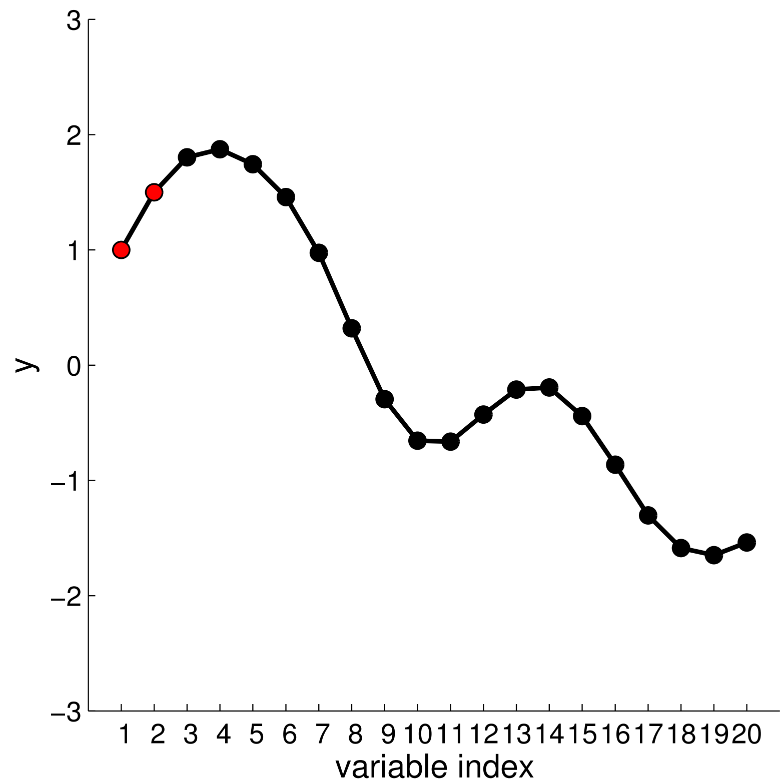

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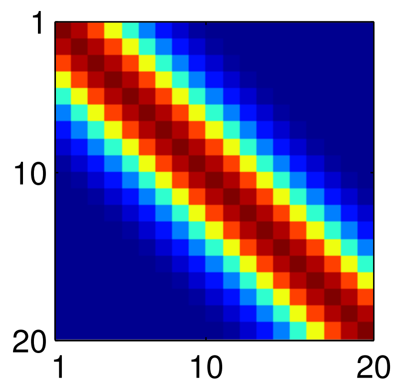

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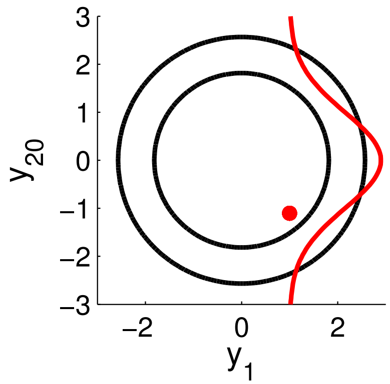

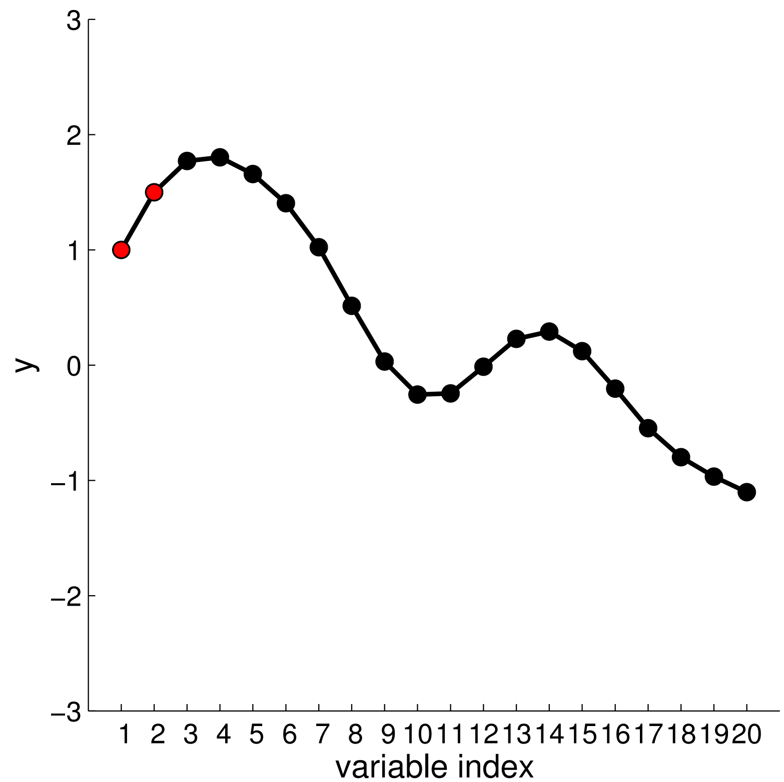

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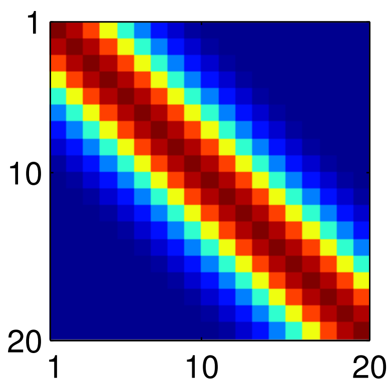

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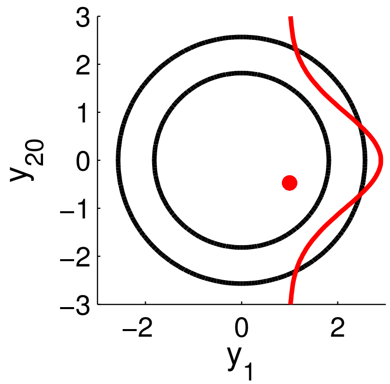

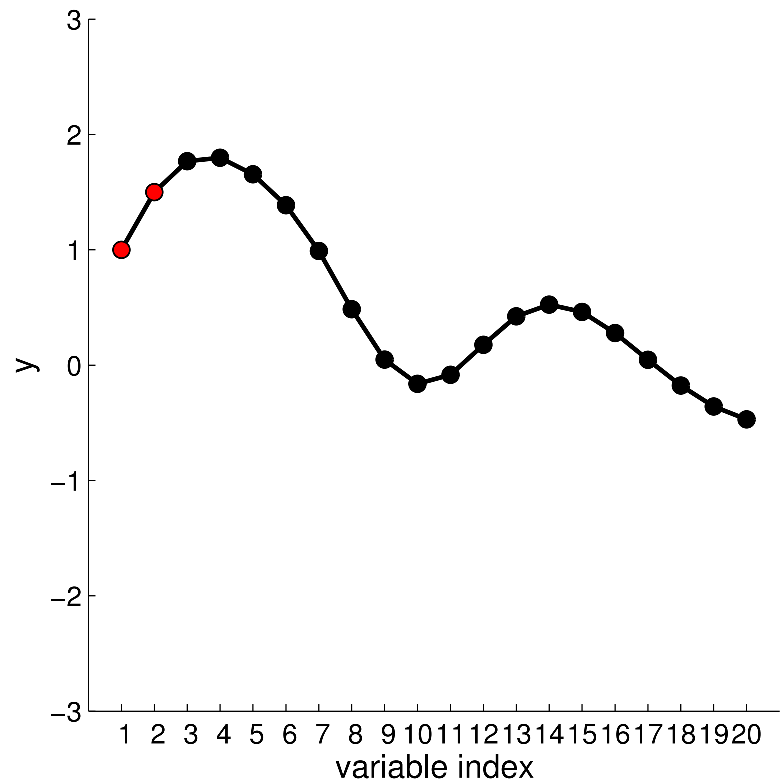

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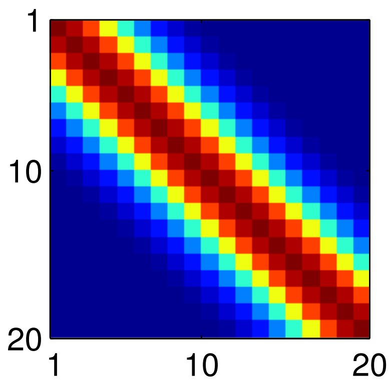

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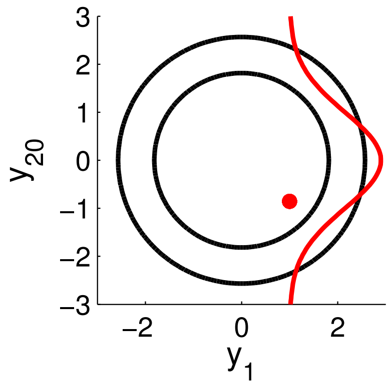

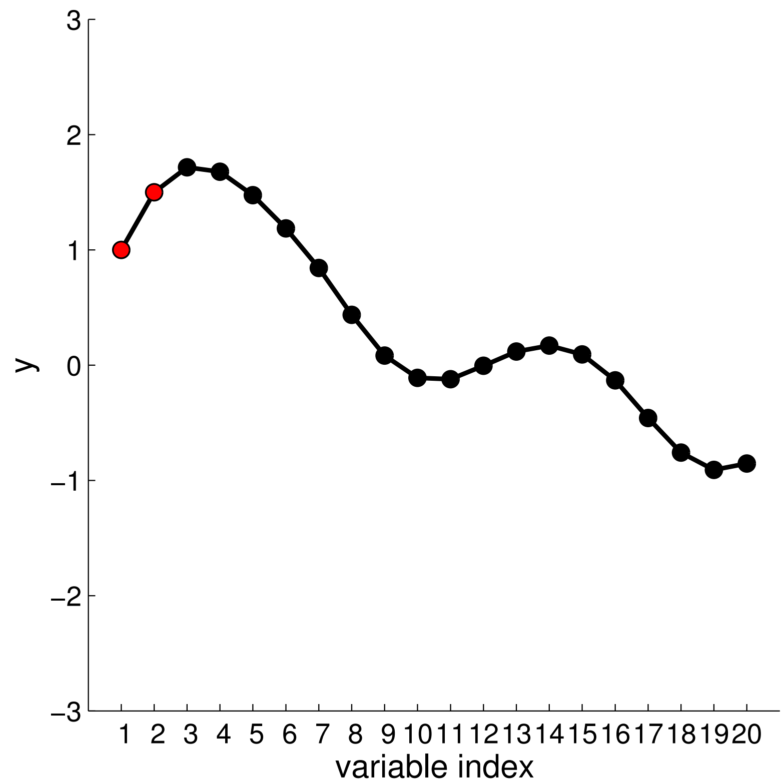

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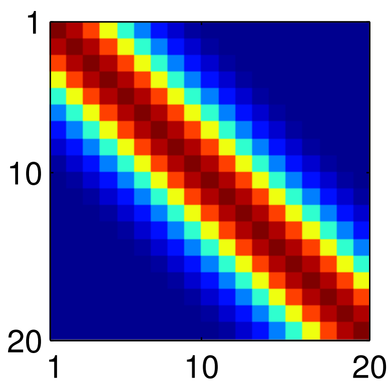

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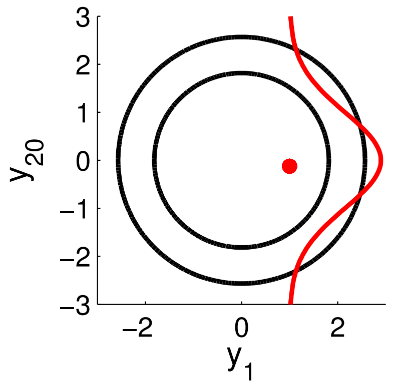

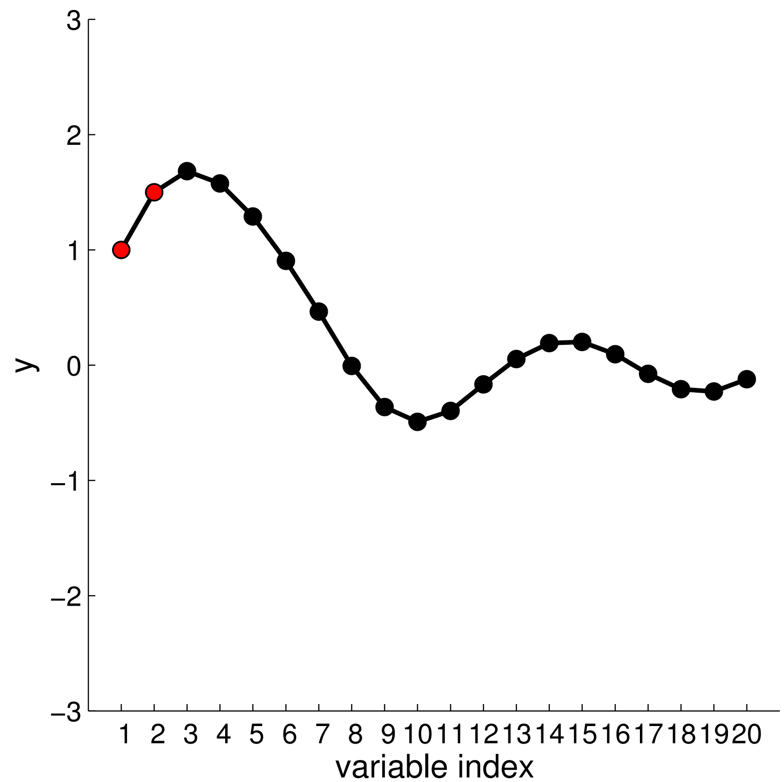

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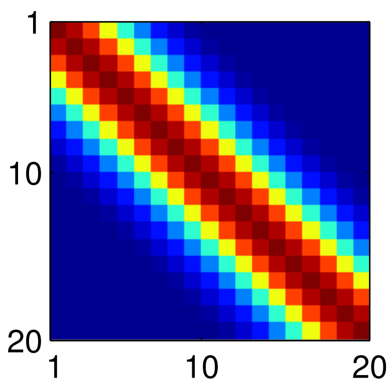

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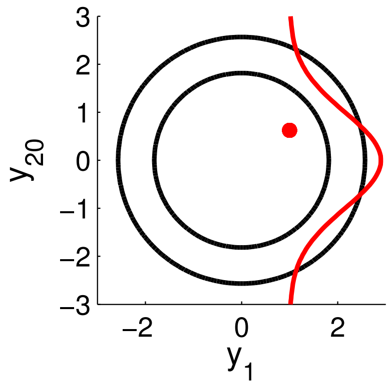

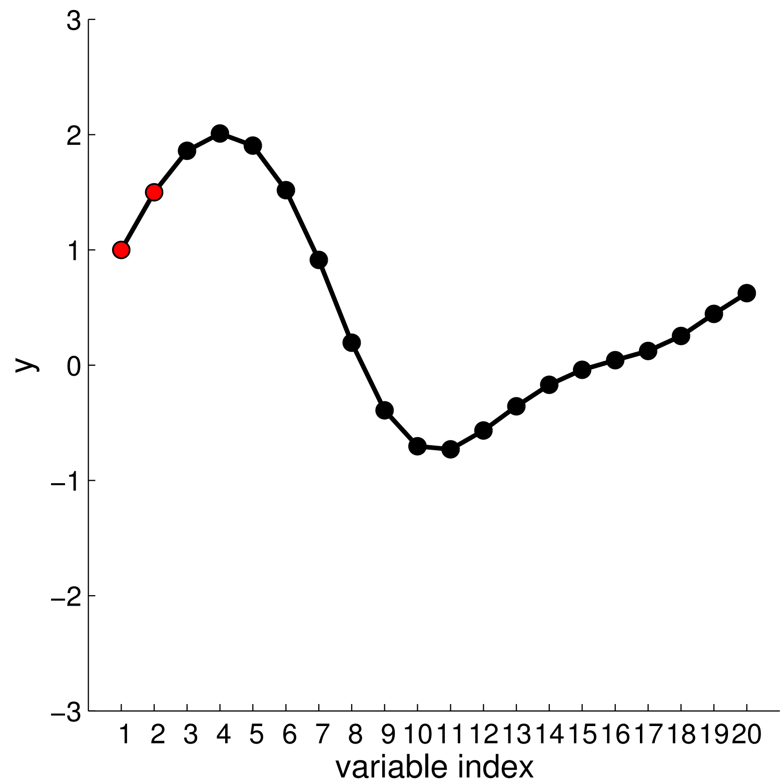

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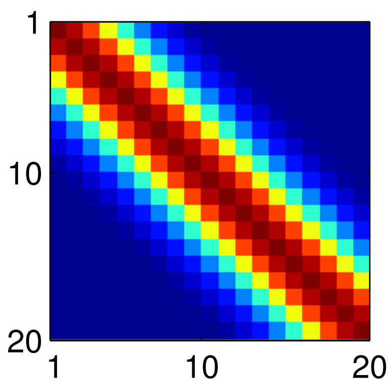

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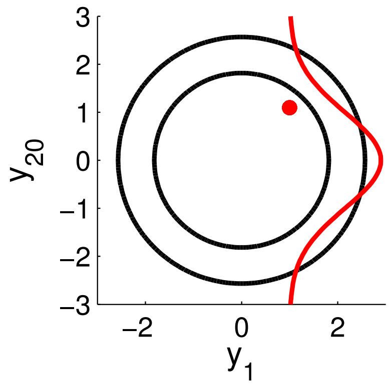

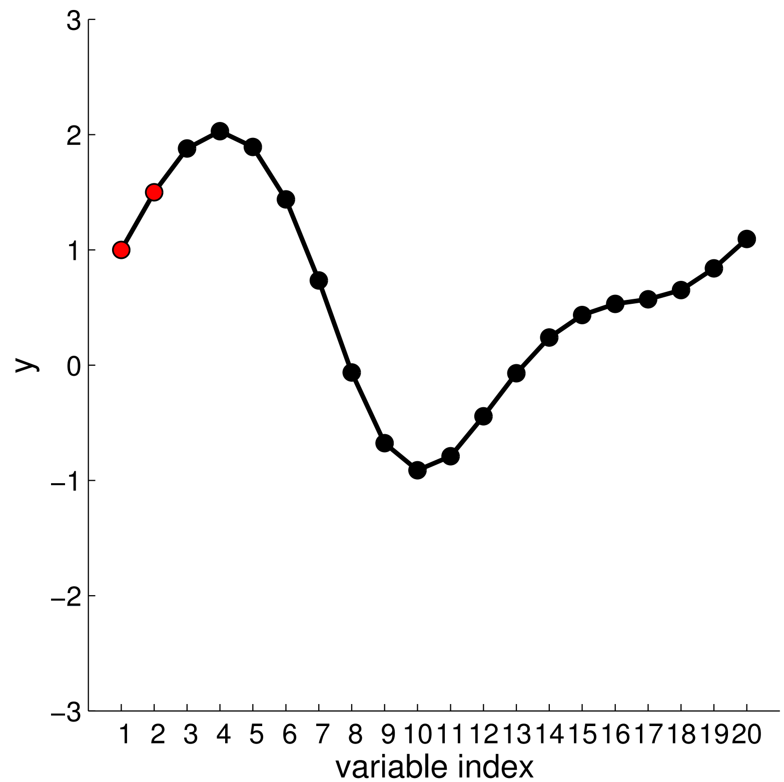

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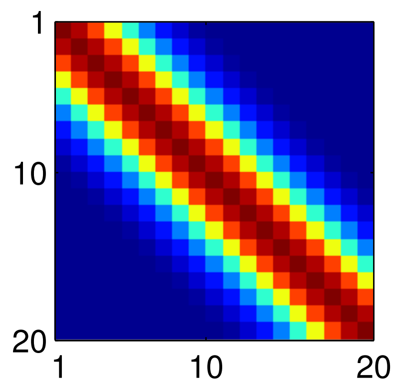

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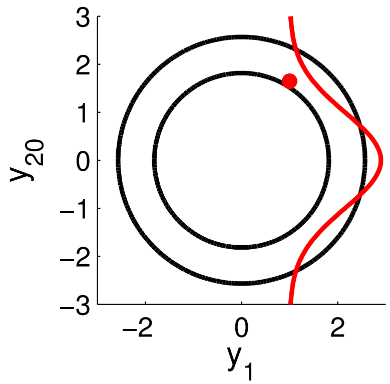

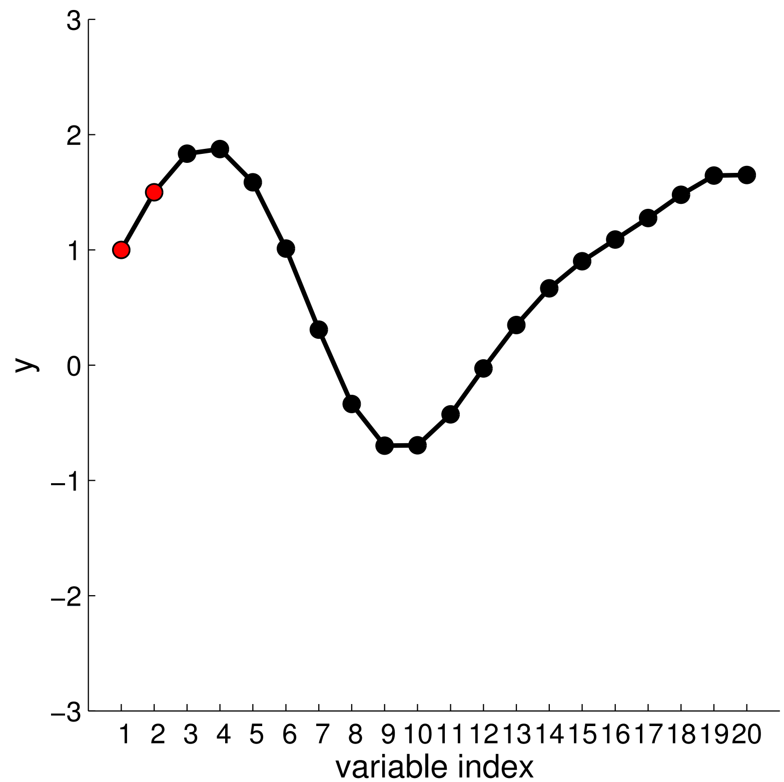

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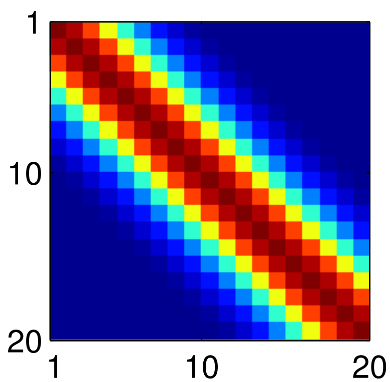

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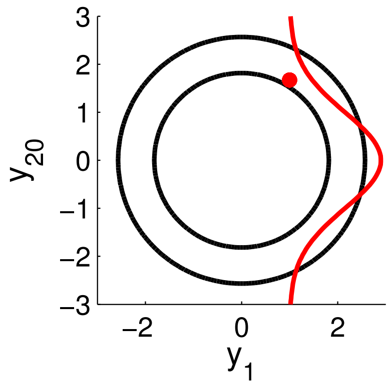

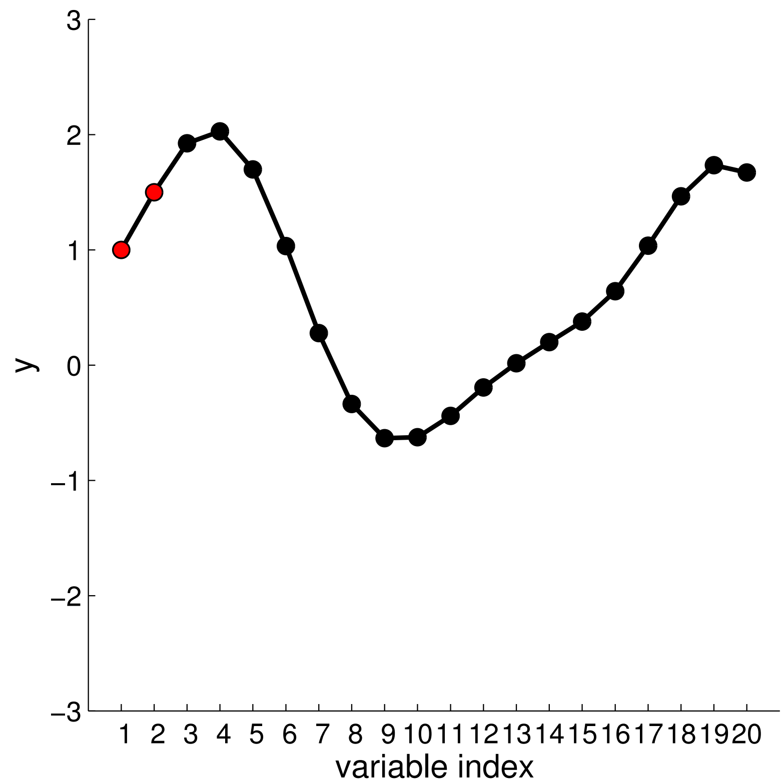

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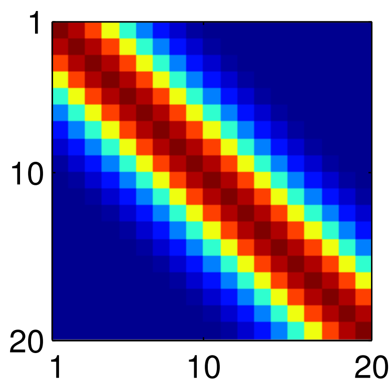

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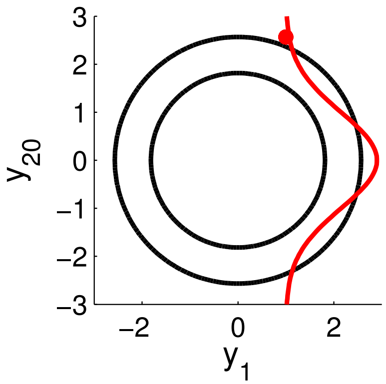

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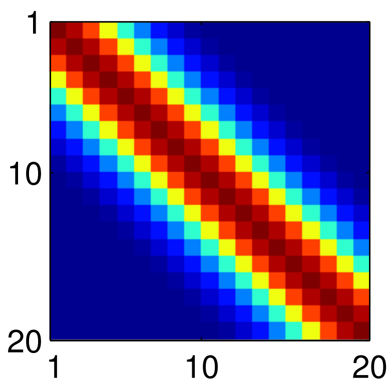

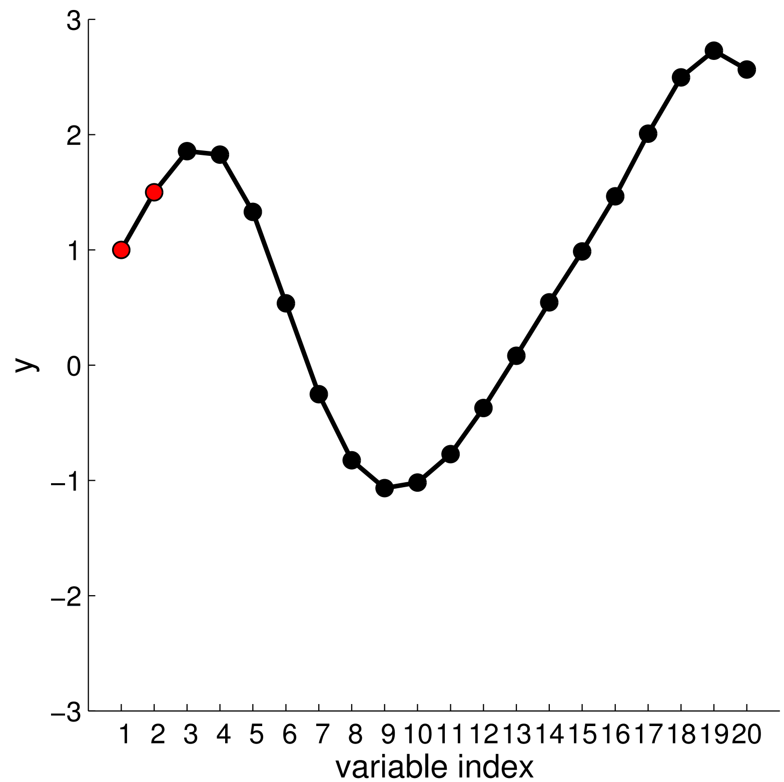

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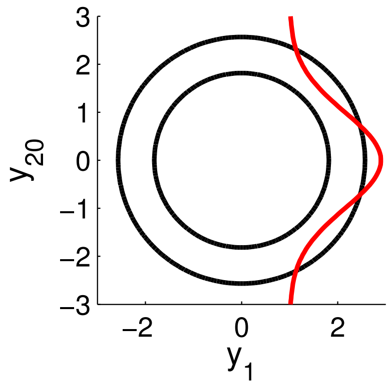

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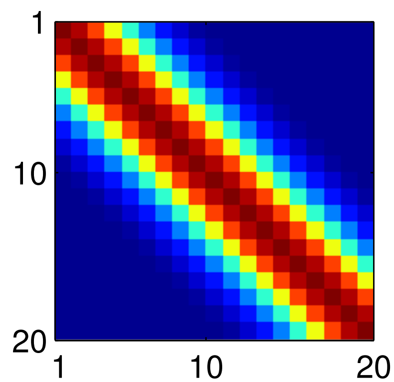
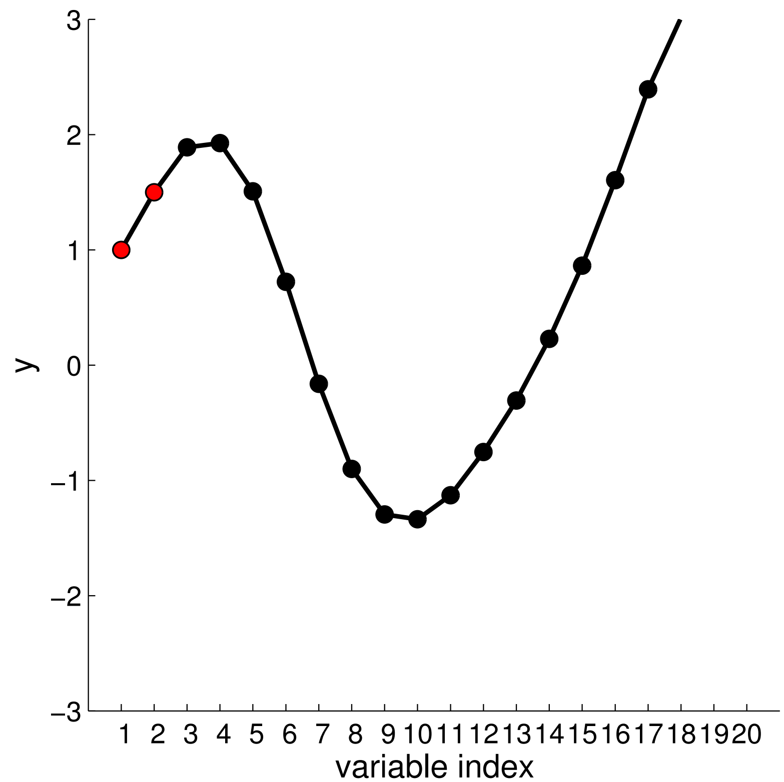
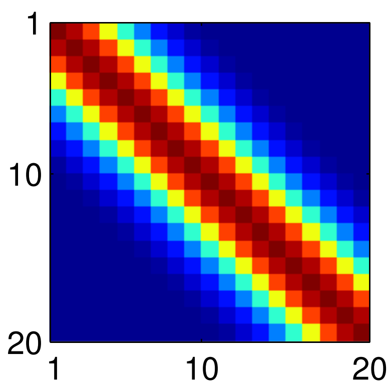
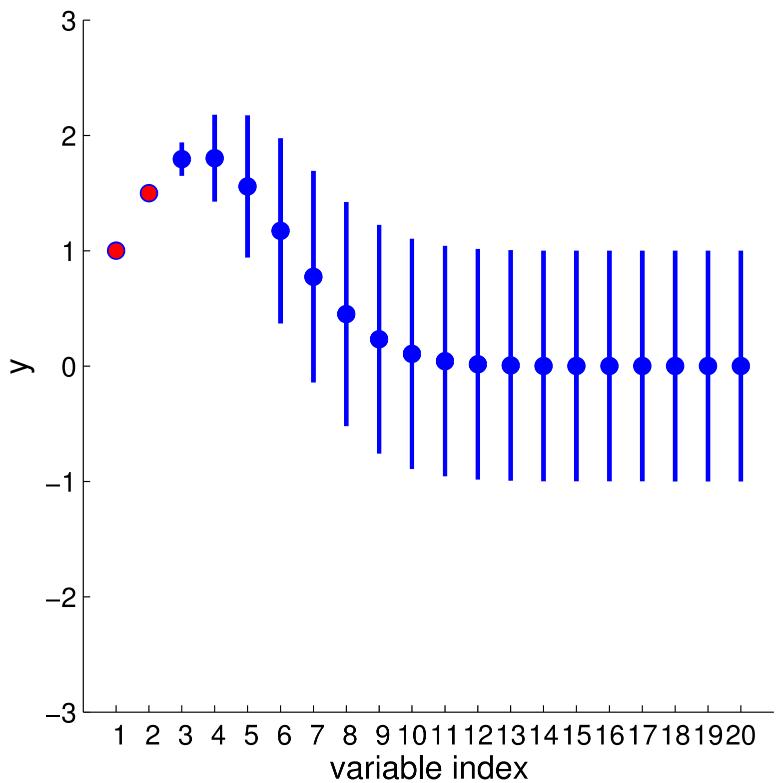




Regression using Gaussians

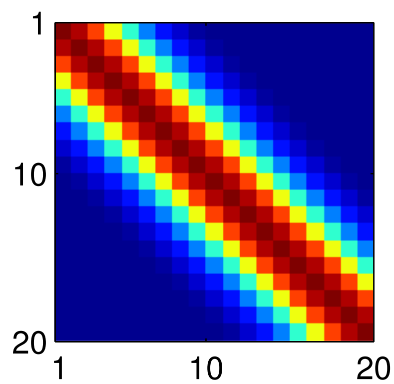
$\Sigma =$

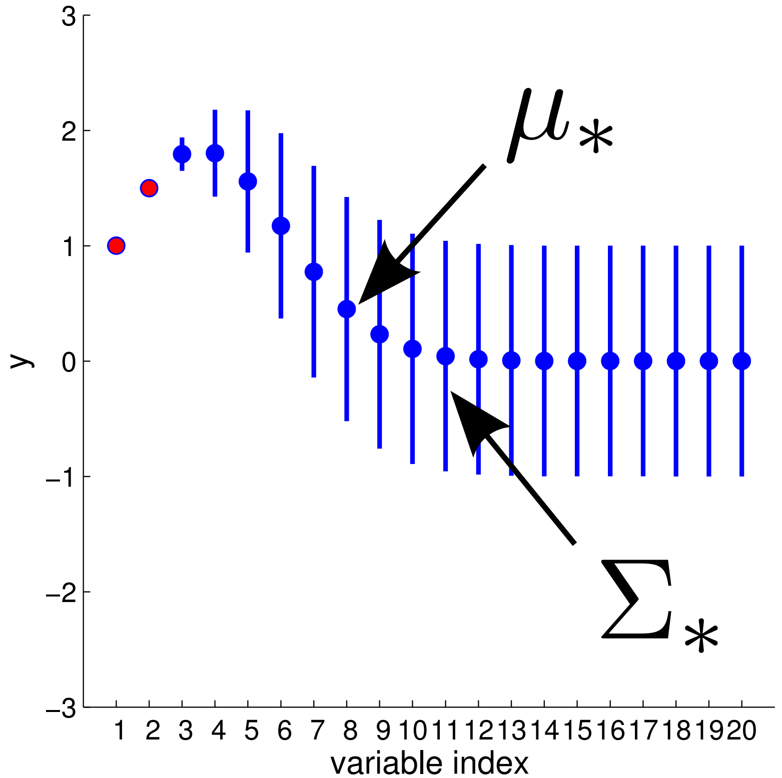




Regression using Gaussians

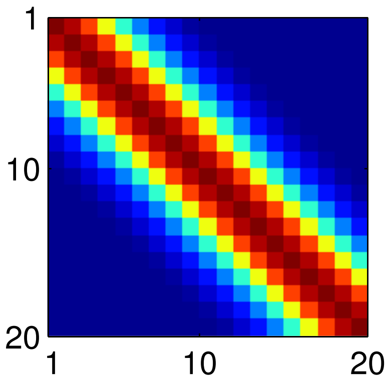
$\Sigma =$

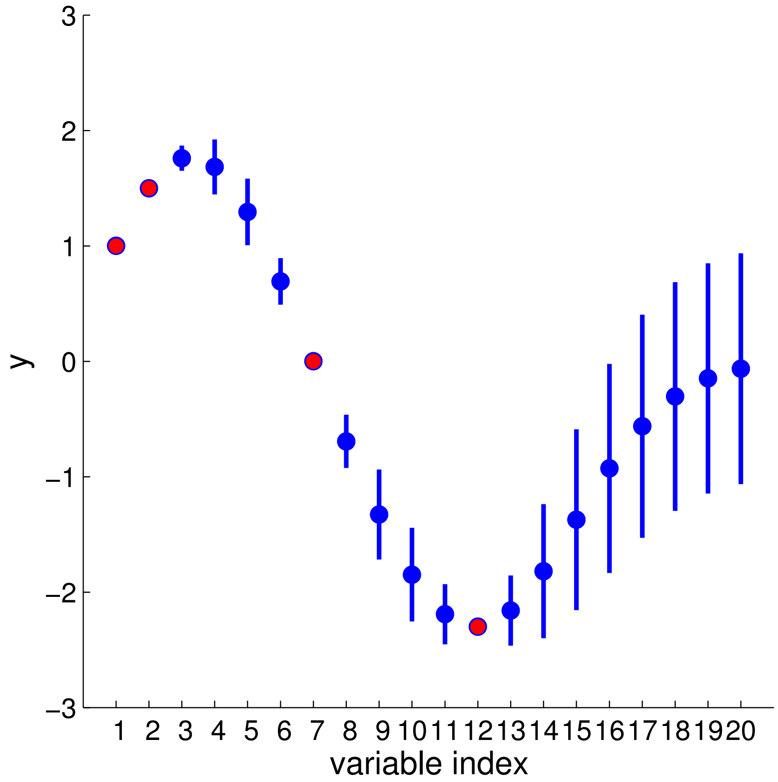




Regression using Gaussians

$\Sigma =$



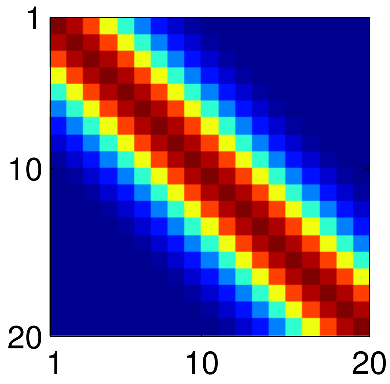


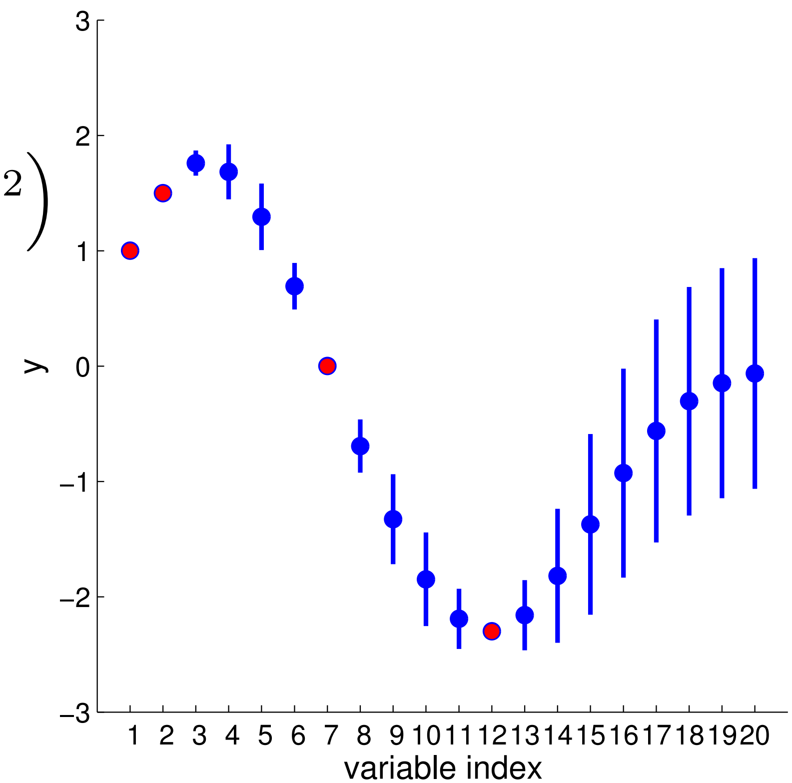
Regression using Gaussians

$$\Sigma(\mathsf{x}_1, \mathsf{x}_2) = \mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) + \mathsf{I}\sigma_{\mathsf{y}}^2$$

$$\mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) = \sigma^2 \exp\left(-\frac{1}{2\mathsf{l}^2}(\mathsf{x}_1 - \mathsf{x}_2)^2\right)$$

$\Sigma =$

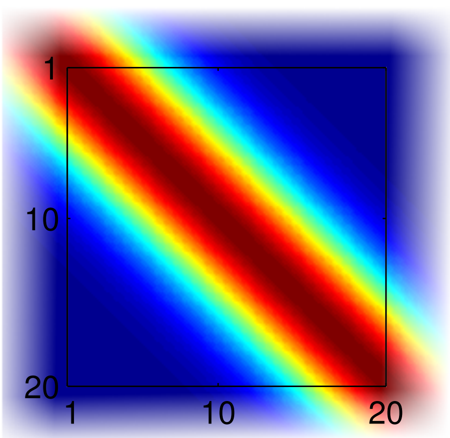


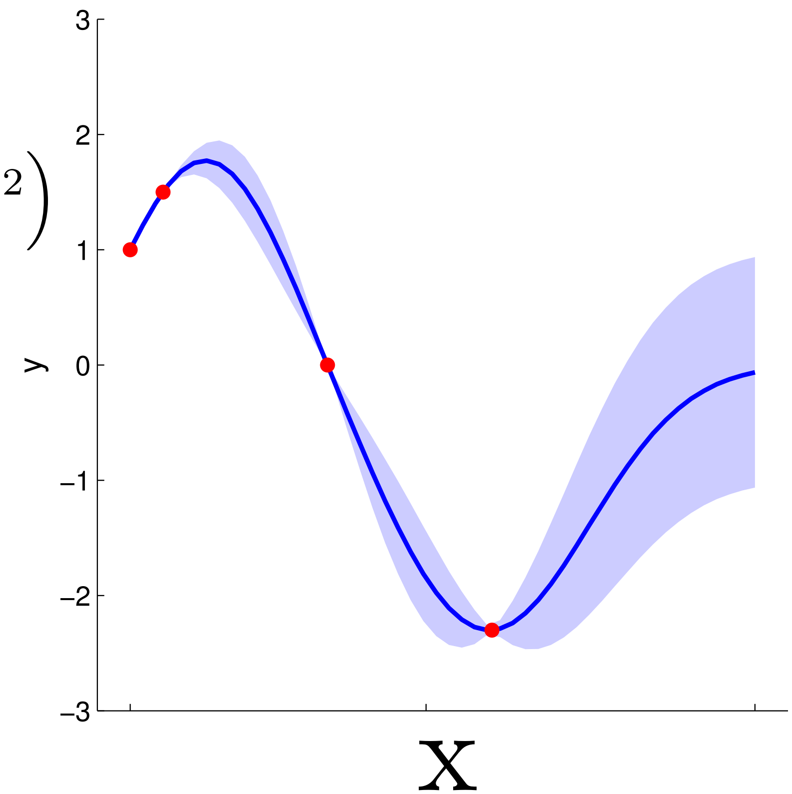


Regression: probabilistic inference in function space

$$\Sigma(x_1, x_2) = K(x_1, x_2) + I\sigma_y^2$$

$$K(x_1, x_2) = \sigma^2 \exp\left(-\frac{1}{2l^2}(x_1 - x_2)^2\right)$$

$\Sigma =$ 



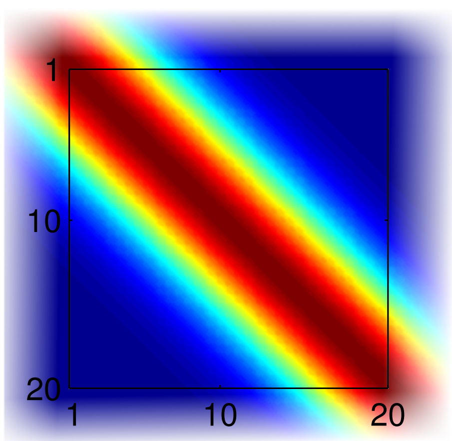
Regression: probabilistic inference in function space

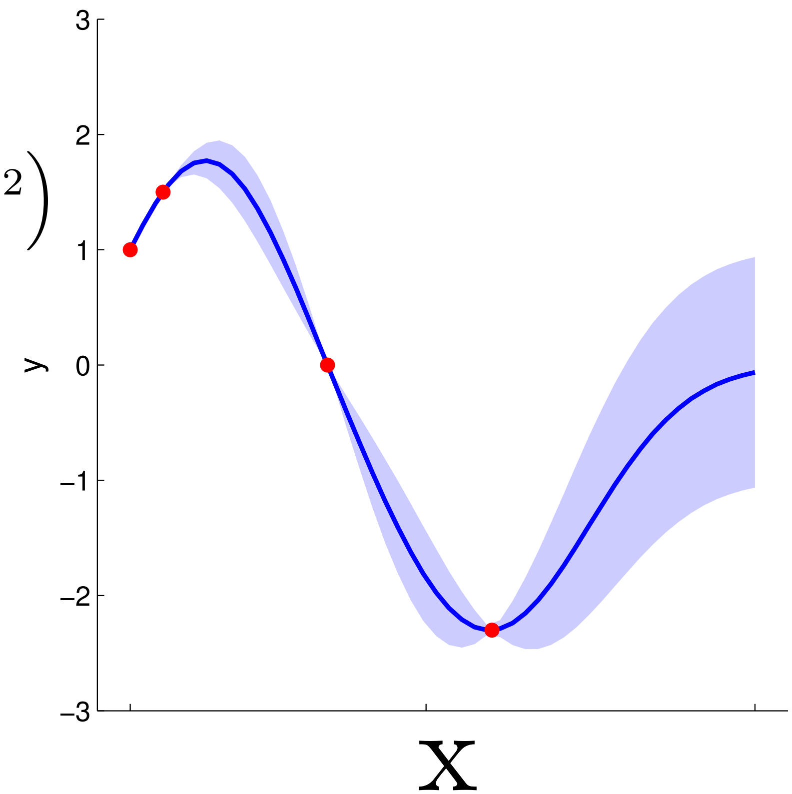
Non-parametric (∞-parametric)

$$p(\mathsf{y}|\theta) = \mathcal{N}(0, \Sigma)$$

$$\Sigma(\mathsf{x}_1, \mathsf{x}_2) = \mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) + \mathsf{I}\sigma_{\mathsf{y}}^2$$

$$\mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) = \sigma^2 \exp\left(-\frac{1}{2\mathsf{l}^2}(\mathsf{x}_1 - \mathsf{x}_2)^2\right)$$

$\Sigma =$ 



Parametric model

$$\mathsf{y}(\mathsf{x}) = f(\mathsf{x}; \theta) + \sigma_{\mathsf{y}}\epsilon$$

$$\epsilon \sim \mathcal{N}(0, 1)$$

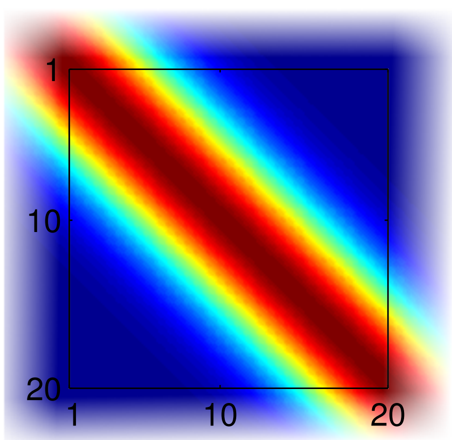
Regression: probabilistic inference in function space

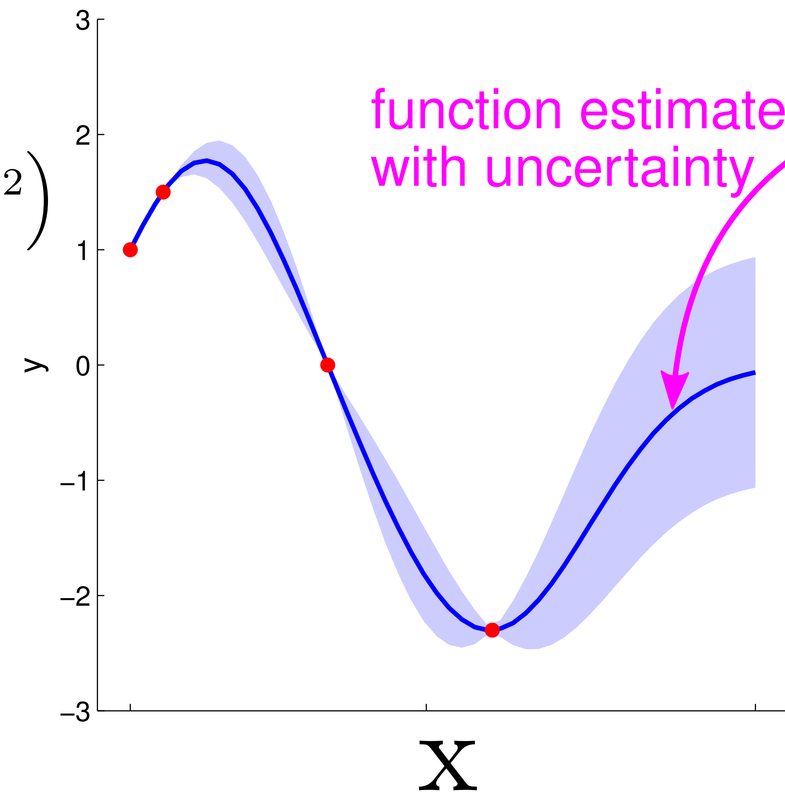
Non-parametric (∞-parametric)

$$p(\mathsf{y}|\theta) = \mathcal{N}(0, \Sigma)$$

$$\Sigma(\mathsf{x}_1, \mathsf{x}_2) = \mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) + \mathsf{I}\sigma_\mathsf{y}^2$$

$$\mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) = \sigma^2 \exp\left(-\frac{1}{2\mathsf{l}^2}(\mathsf{x}_1 - \mathsf{x}_2)^2\right)$$

$\Sigma =$ 



Parametric model

$$\mathsf{y}(\mathsf{x}) = f(\mathsf{x}; \theta) + \sigma_\mathsf{y}\epsilon$$

$$\epsilon \sim \mathcal{N}(0, 1)$$

Regression: probabilistic inference in function space

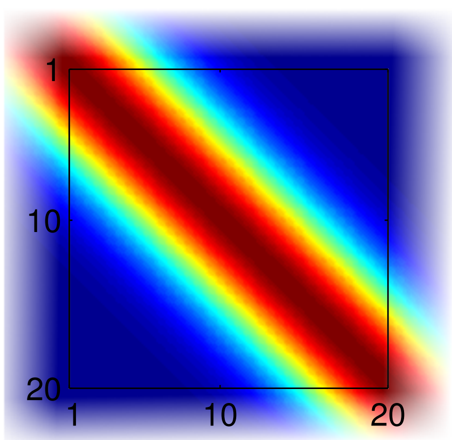
Non-parametric (∞-parametric)

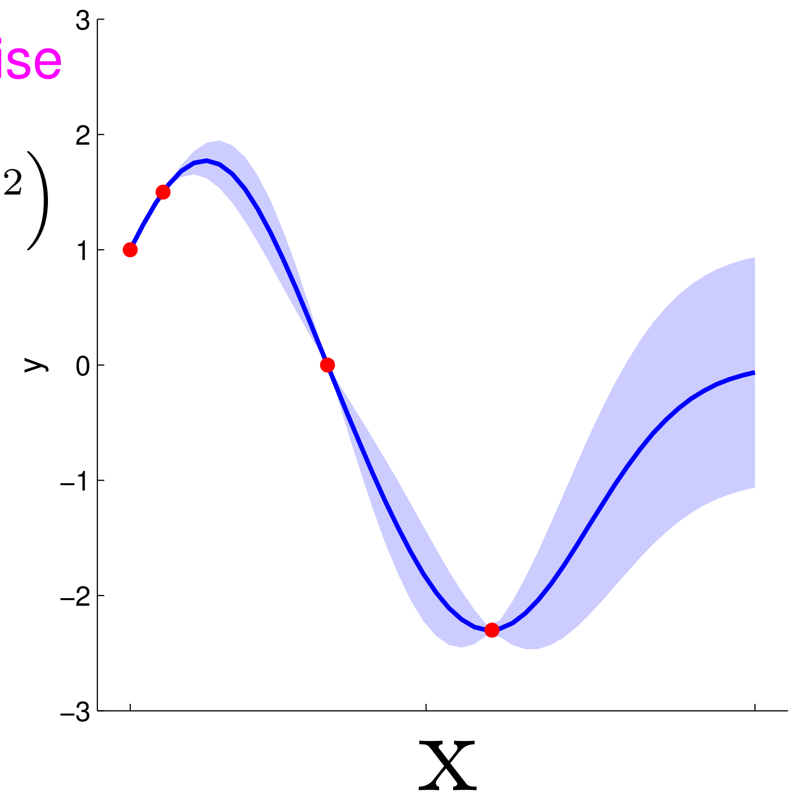
$$p(\mathsf{y}|\theta) = \mathcal{N}(0, \Sigma)$$

$$\Sigma(\mathsf{x}_1, \mathsf{x}_2) = \mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) + \mathsf{I}\sigma_{\mathsf{y}}^2 \leftarrow \text{noise}$$

$$\mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) = \sigma^2 \exp\left(-\frac{1}{2\mathsf{l}^2}(\mathsf{x}_1 - \mathsf{x}_2)^2\right)$$

$\Sigma =$





Parametric model

$$\mathsf{y}(\mathsf{x}) = f(\mathsf{x}; \theta) + \sigma_{\mathsf{y}}\epsilon$$

$$\epsilon \sim \mathcal{N}(0, 1)$$

Regression: probabilistic inference in function space

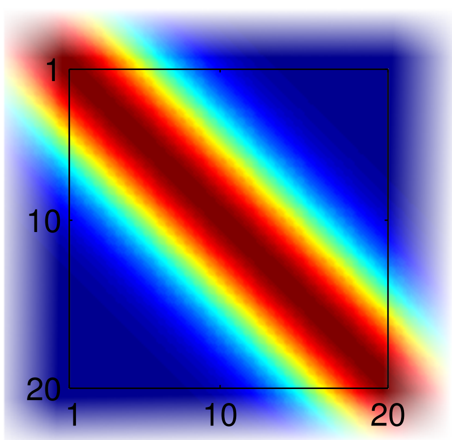
Non-parametric (∞-parametric)

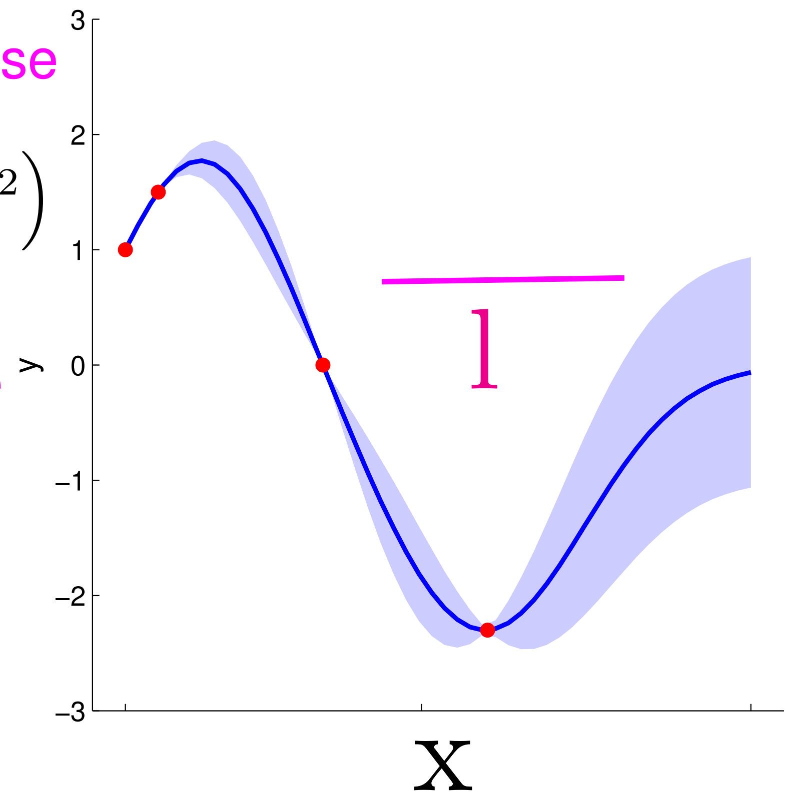
$$p(\mathsf{y}|\theta) = \mathcal{N}(0, \Sigma)$$

$$\Sigma(\mathsf{x}_1, \mathsf{x}_2) = \mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) + \mathsf{I}\sigma_\mathsf{y}^2$$ ← noise

$$\mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) = \sigma^2 \exp\left(-\frac{1}{2\mathsf{l}^2}(\mathsf{x}_1 - \mathsf{x}_2)^2\right)$$

↑ horizontal-scale

$\Sigma =$ 



Parametric model

$$\mathsf{y}(\mathsf{x}) = f(\mathsf{x}; \theta) + \sigma_\mathsf{y}\epsilon$$

$$\epsilon \sim \mathcal{N}(0, 1)$$

Regression: probabilistic inference in function space

Non-parametric (∞-parametric)

$$p(\mathsf{y}|\theta) = \mathcal{N}(0, \Sigma)$$

$$\Sigma(\mathsf{x}_1, \mathsf{x}_2) = \mathsf{K}(\mathsf{x}_1, \mathsf{x}_2) + \mathsf{I}\sigma_{\mathsf{y}}^2$$ ← noise

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↑ vertical-scale ↑ horizontal-scale

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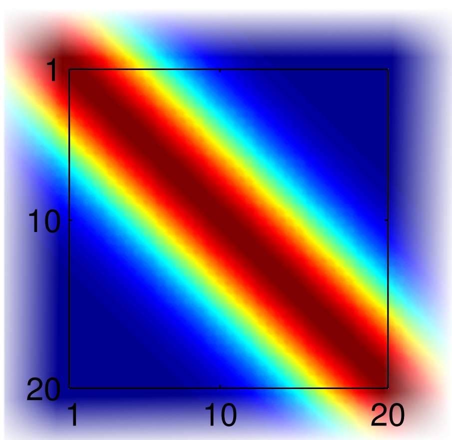

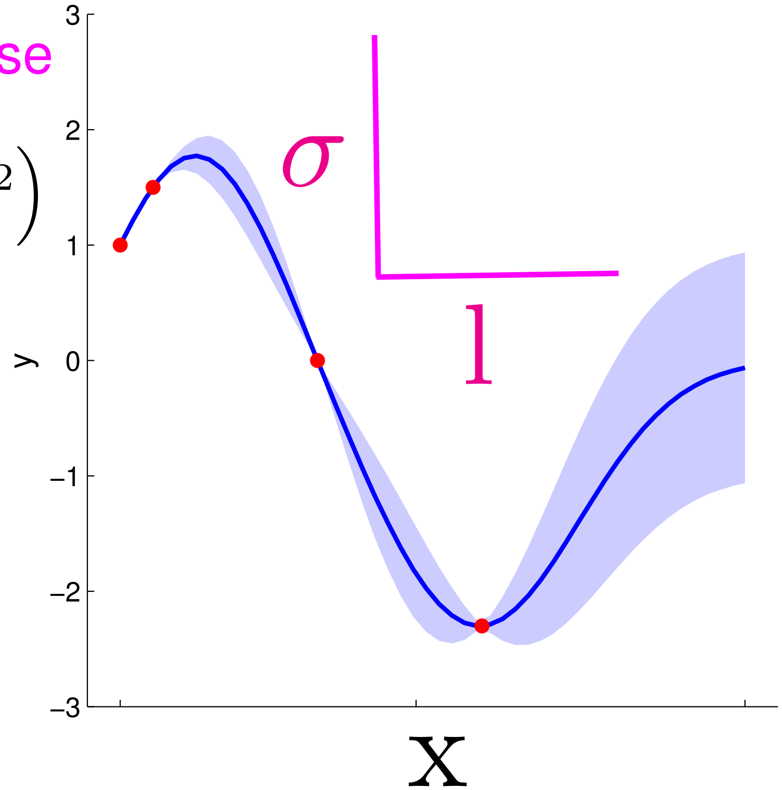

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Mathematical Foundations: Definition

Gaussian process = generalization of multivariate Gaussian distribution to infinitely many variables.

> **Definition**: a Gaussian process is a collection of random variables, any finite number of which have (consistent) Gaussian distributions.

A Gaussian distribution is fully specified by a mean vector, $\boldsymbol{\mu}$, and covariance matrix Σ:

$$\mathbf{f} = (\mathsf{f}_1, \ldots, \mathsf{f}_n) \sim \mathcal{N}(\mu, \Sigma), \quad \text{indices} \quad i = 1, \ldots, n$$

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

$$f(\mathbf{x}) \sim \mathcal{GP}\left(m(\mathbf{x}), \mathsf{K}(\mathbf{x}, \mathbf{x}')\right), \quad \text{indices} \quad \mathbf{x}$$

Mathematical Foundations: Marginalisation

Q1. A GP is "like" a Gaussian distribution with an infinitely long mean vector and an "infinite by infinite" covariance matrix, so how do we represent it on a computer?

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$\implies$ Entries in a precision matrix depend on what other data we are considering

Precisions tell us about the conditional independence relationships between pairs of variables (are $\mathbf{y}_1$ and $\mathbf{y}_2$ independent given all other variables).

Mathematical Foundations: Regression

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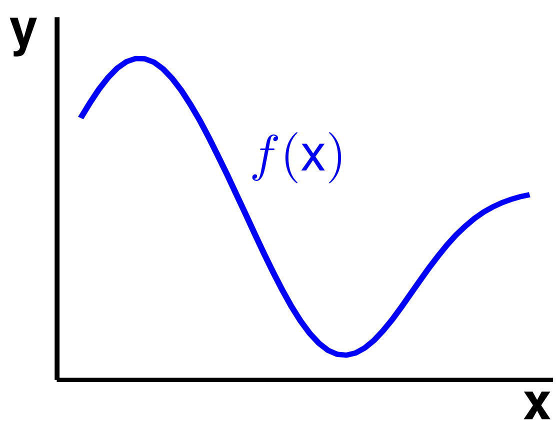
Generative model (like non-linear regression)

$$y(x) = f(x) + \epsilon\sigma_y$$



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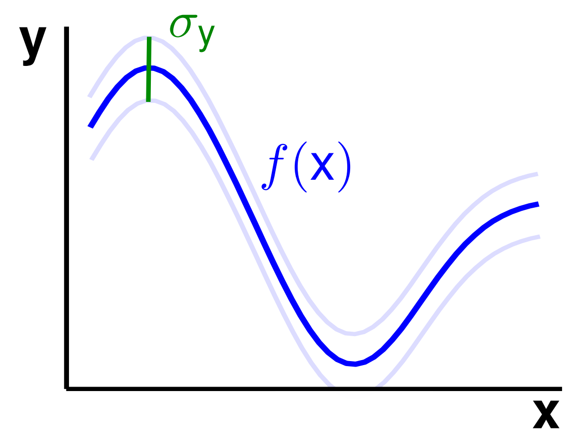

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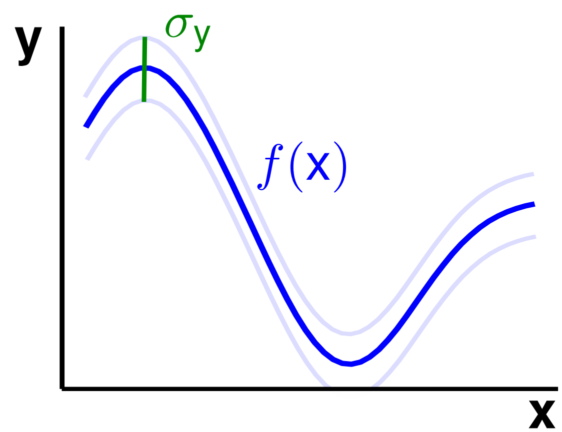

place GP prior over the non-linear function

$$p(f(\mathsf{x})|\theta) = \mathcal{GP}(0, \mathsf{K}(\mathsf{x}, \mathsf{x}'))$$

$$\mathsf{K}(\mathsf{x}, \mathsf{x}') = \sigma^2 \exp\left(-\frac{1}{2l^2}(\mathsf{x} - \mathsf{x}')^2\right)$$

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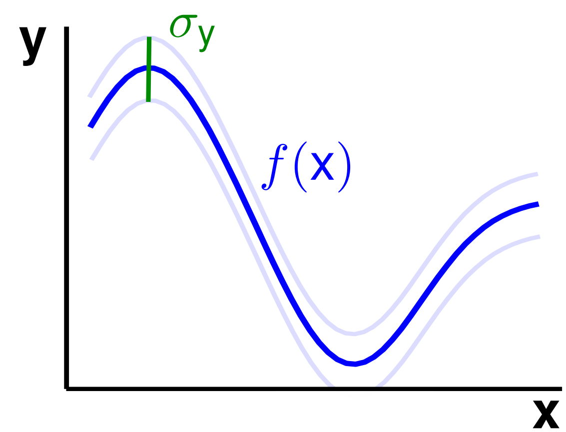

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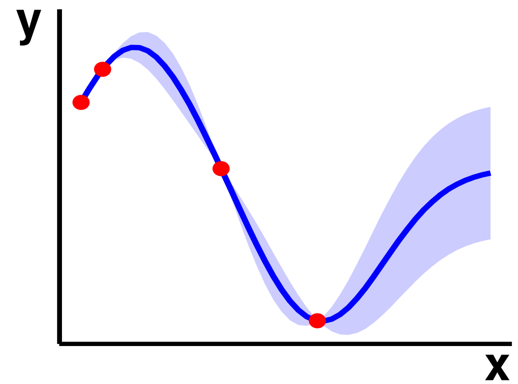
since the sum of two Gaussians is a Gaussian, the model induces a GP over $y(x)$

$$p(y(x)|\theta) = \mathcal{GP}(0, K(x, x') + I\sigma_y^2)$$

Mathematical foundations: Prediction

Q4. How do we make predictions?



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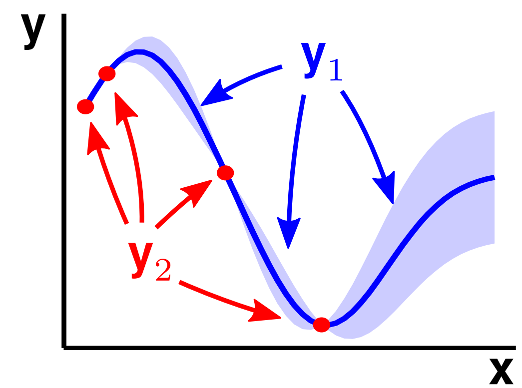

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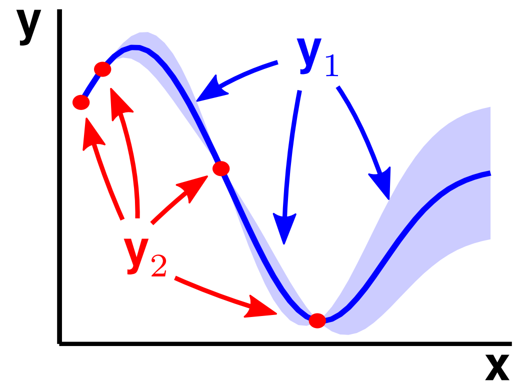

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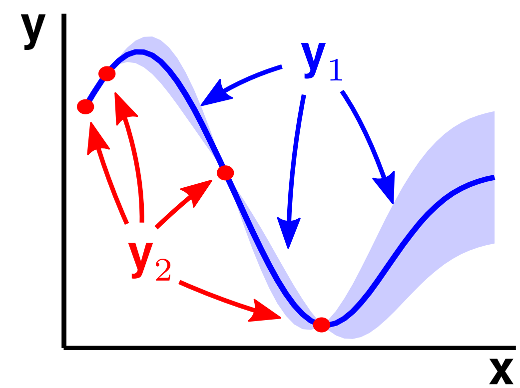

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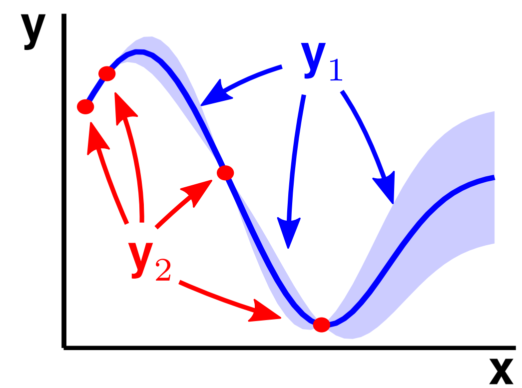

$$\Longrightarrow \quad p(\mathbf{y}_1 | \mathbf{y}_2) = \mathcal{N}(\mathbf{a} + \mathsf{B}\mathsf{C}^{-1}(\mathbf{y}_2 - \mathbf{b}), \mathsf{A} - \mathsf{B}\mathsf{C}^{-1}\mathsf{B}^\mathsf{T})$$

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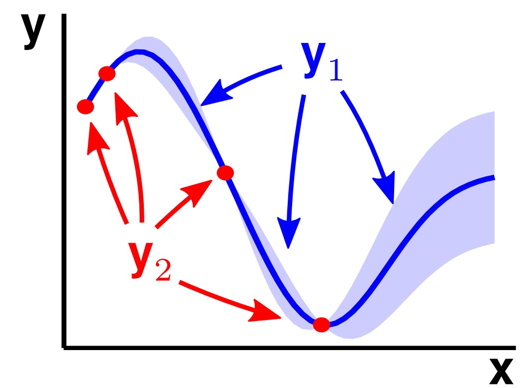

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predictive mean

$$\mu_{\mathbf{y}_1|\mathbf{y}_2} = \mathbf{a} + \mathsf{B}\mathsf{C}^{-1}(\mathbf{y}_2 - \mathbf{b})$$

$$= \mathsf{B}\mathsf{C}^{-1}\mathbf{y}_2$$

$$= \mathsf{W}\mathbf{y}_2$$

linear in the data

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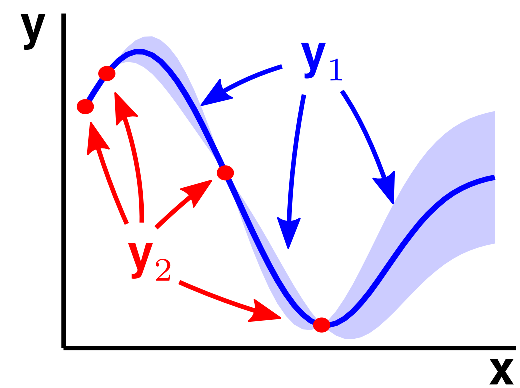

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$$= \mathsf{B}\mathsf{C}^{-1}\mathbf{y}_2$$
$$= \mathsf{W}\mathbf{y}_2$$

linear in the data

predictive covariance

$$\Sigma_{\mathbf{y}_1|\mathbf{y}_2} = \mathsf{A} - \mathsf{B}\mathsf{C}^{-1}\mathsf{B}^\top$$

predictive uncertainty = prior uncertainty − reduction in uncertainty

predictions more confident than prior

What effect do the hyper-parameters have?

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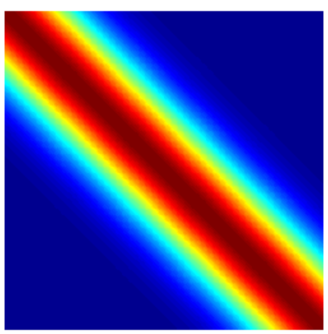
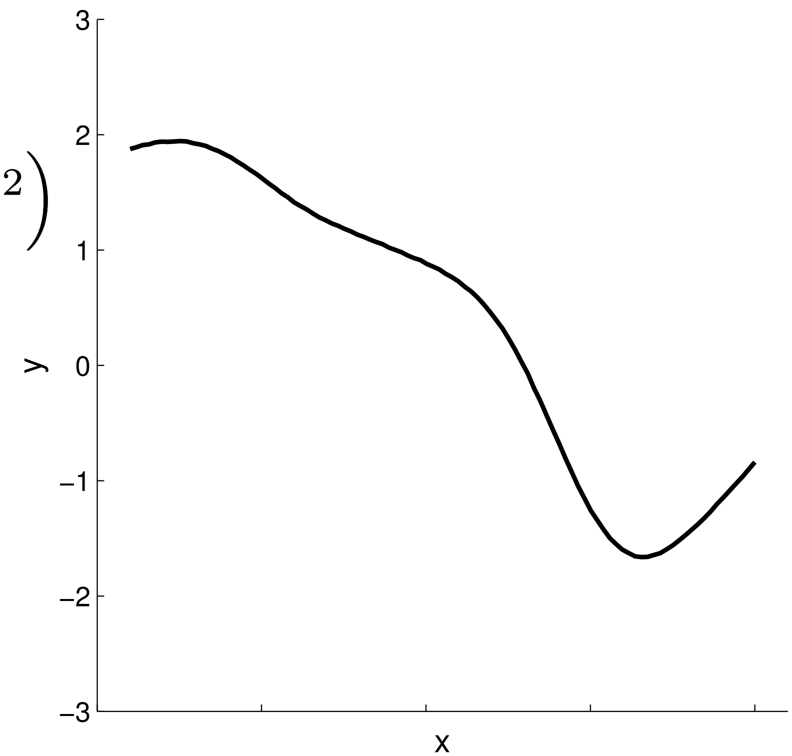
$\Sigma =$ 



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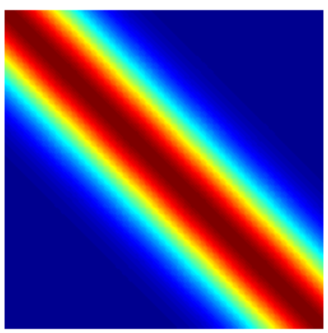
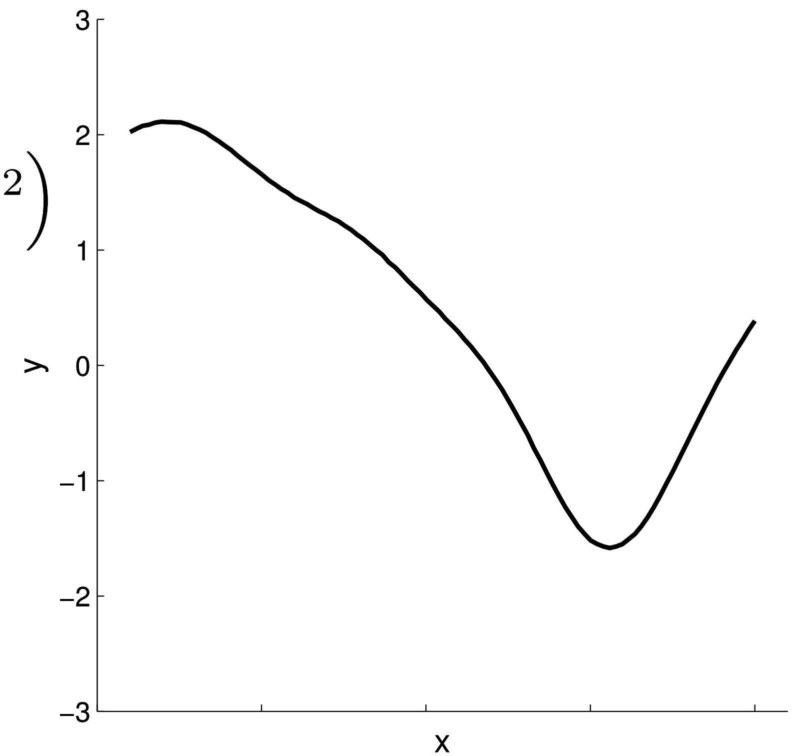
$\Sigma =$ 



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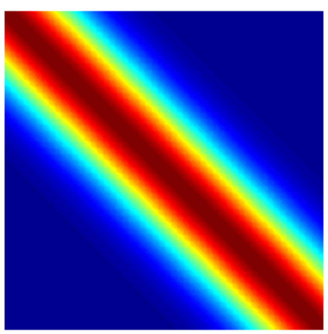
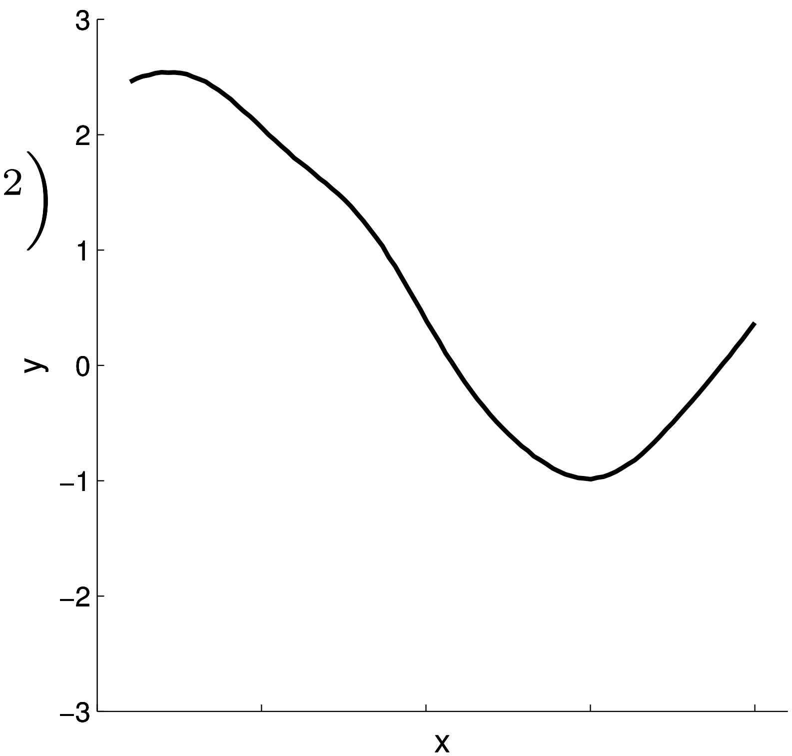
$\Sigma =$ 



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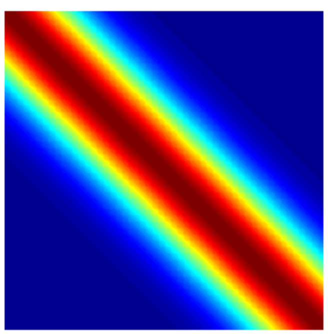
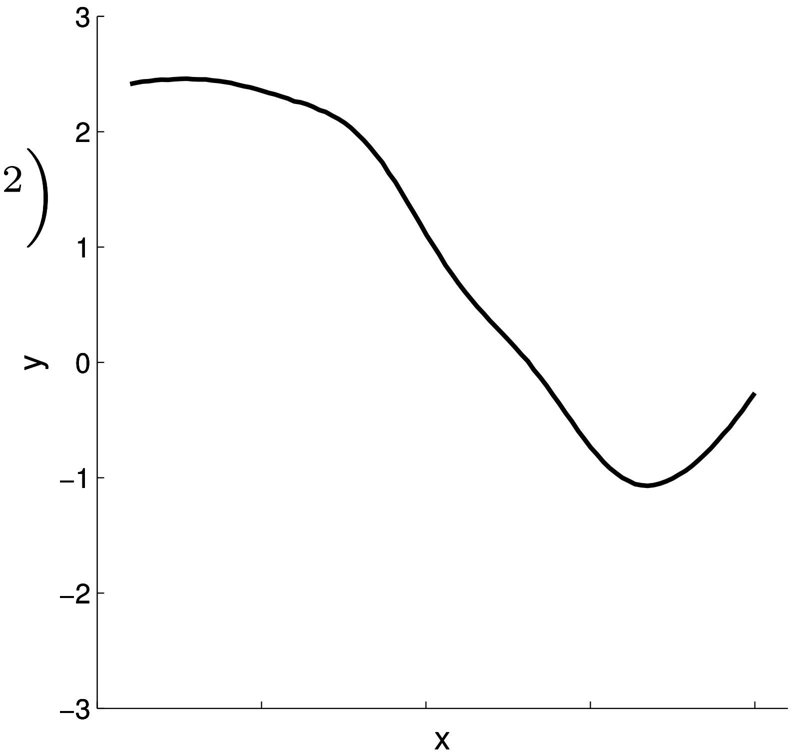
$\Sigma =$ 



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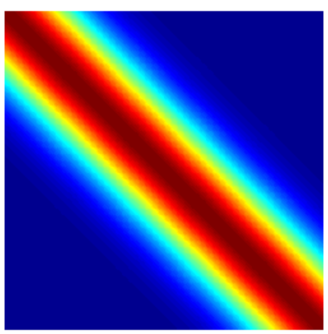
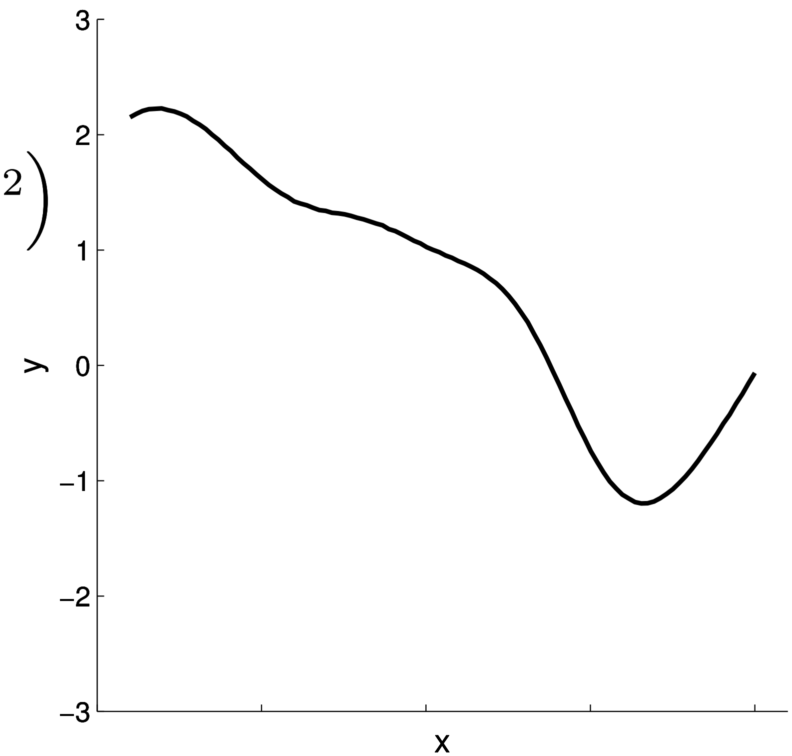
$\Sigma =$ 



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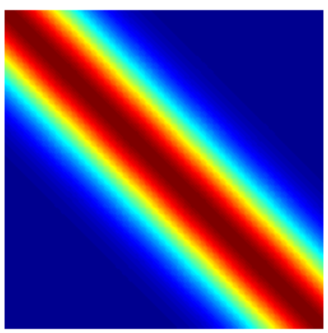
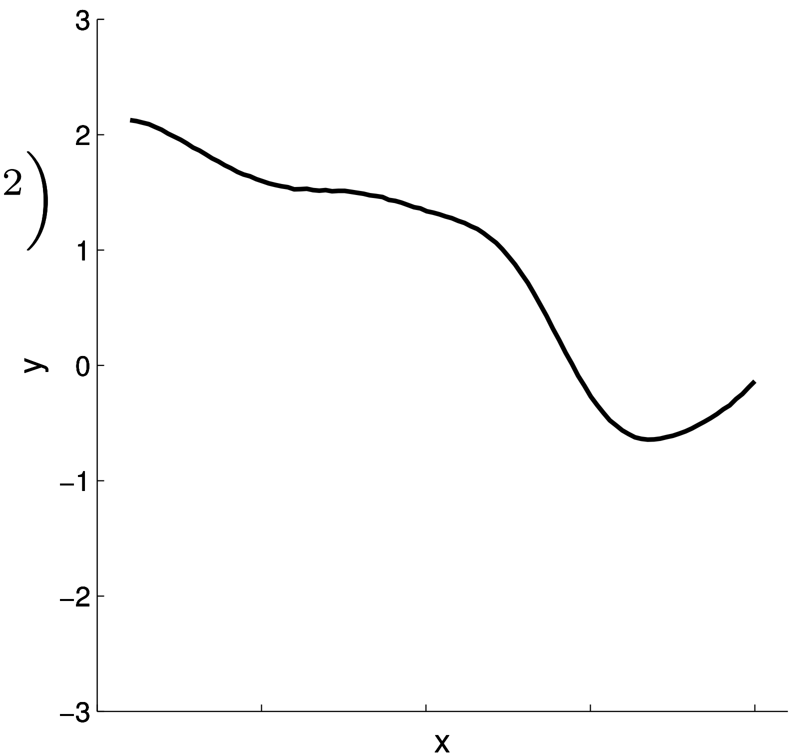
$\Sigma =$ 



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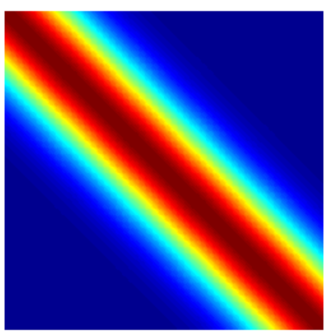
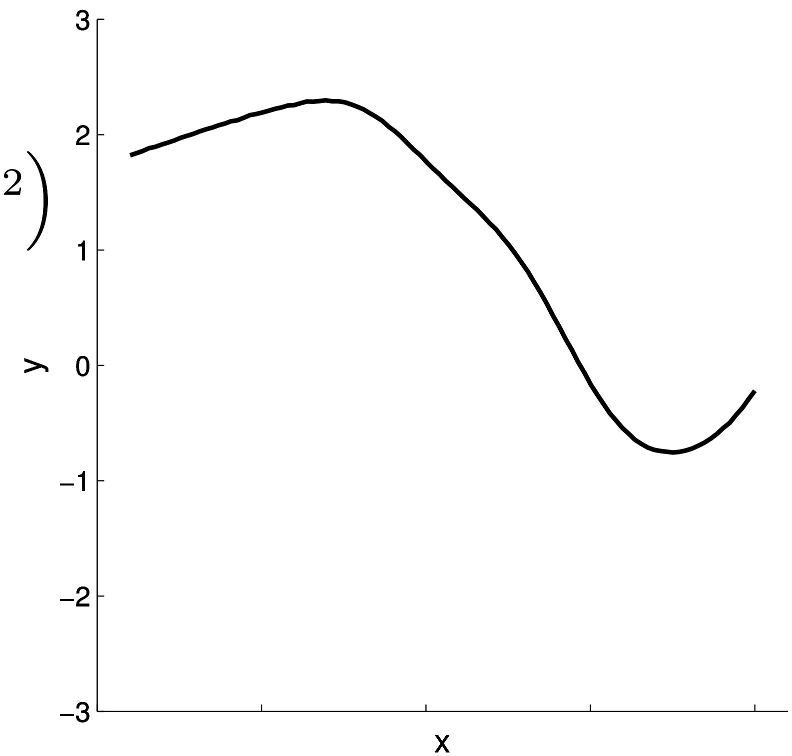
$\Sigma =$ 



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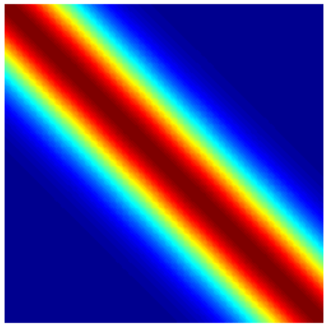
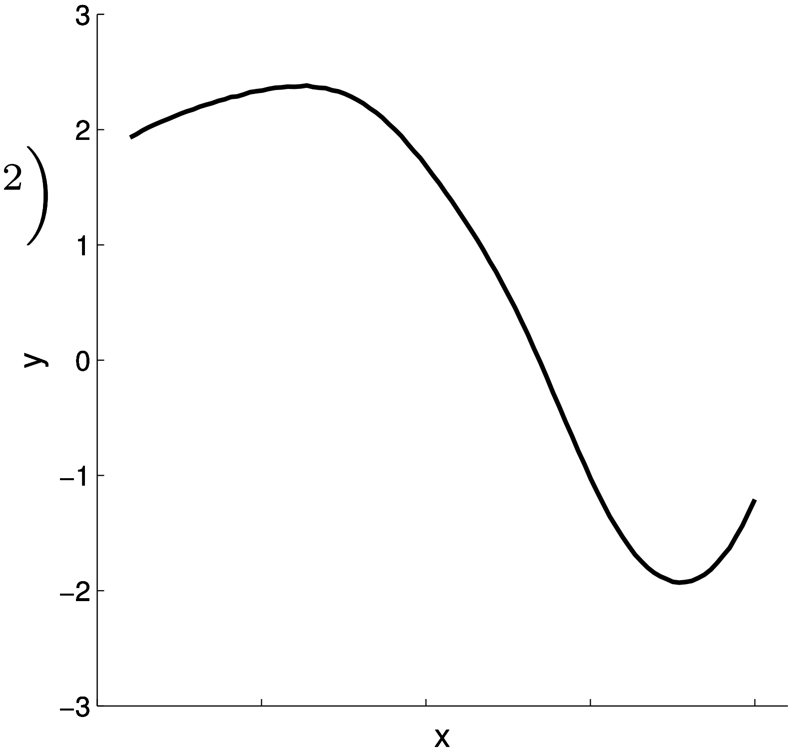
$\Sigma =$ 



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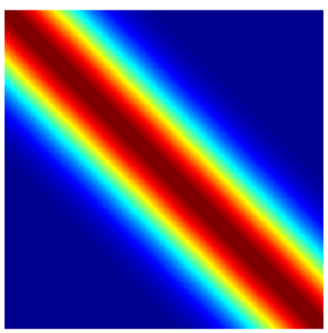
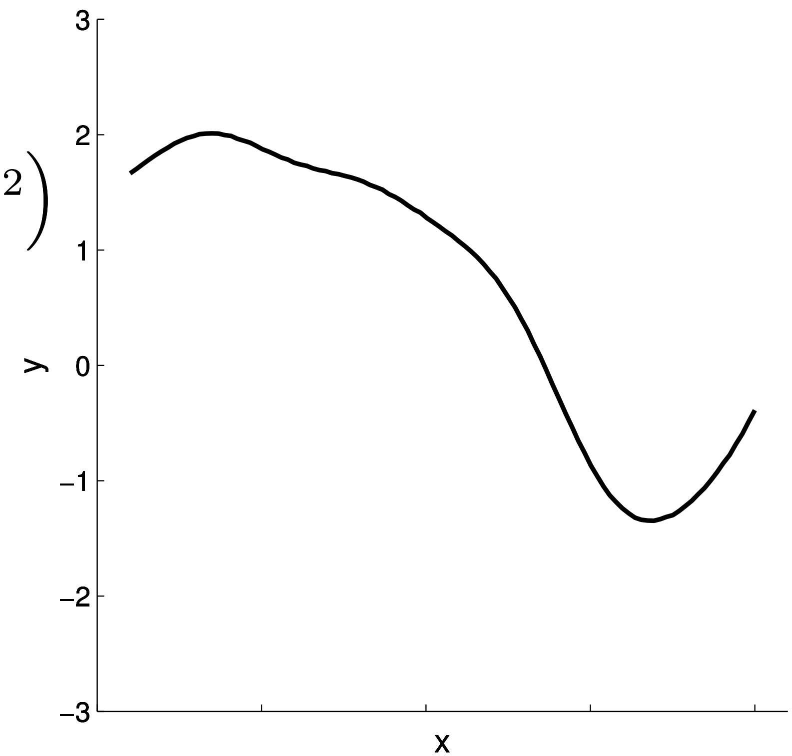
$\Sigma =$ 



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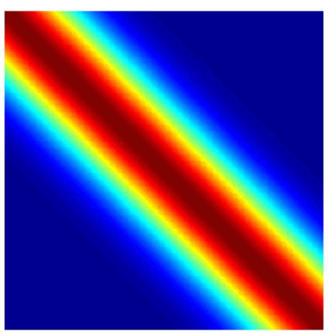
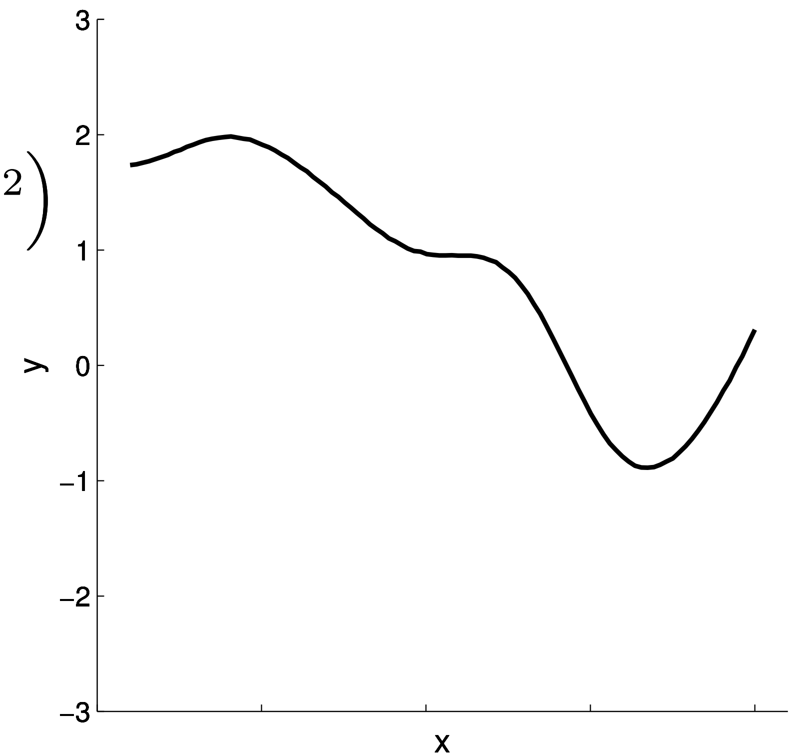
$\Sigma =$ 



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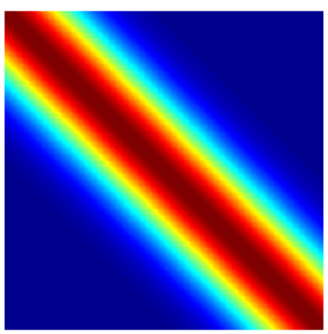
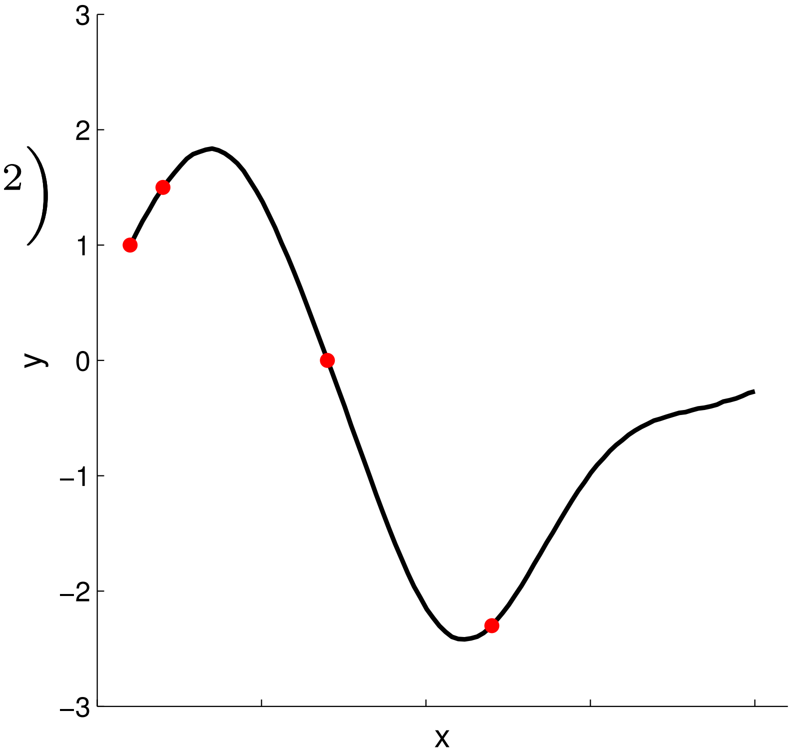
$\Sigma =$ 



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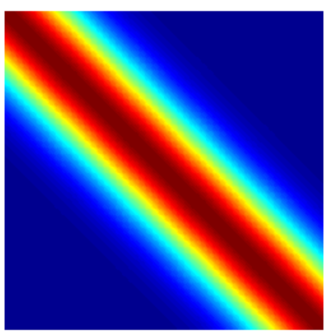

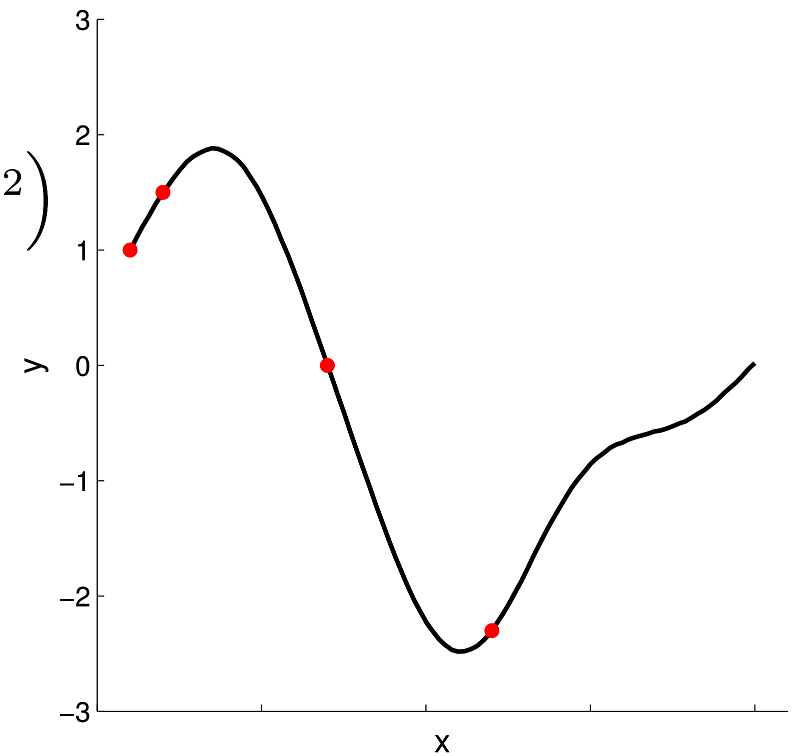

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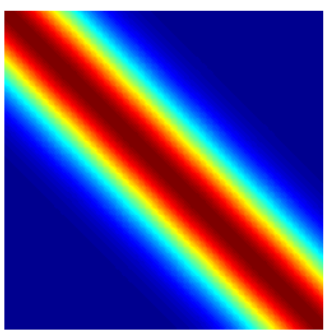
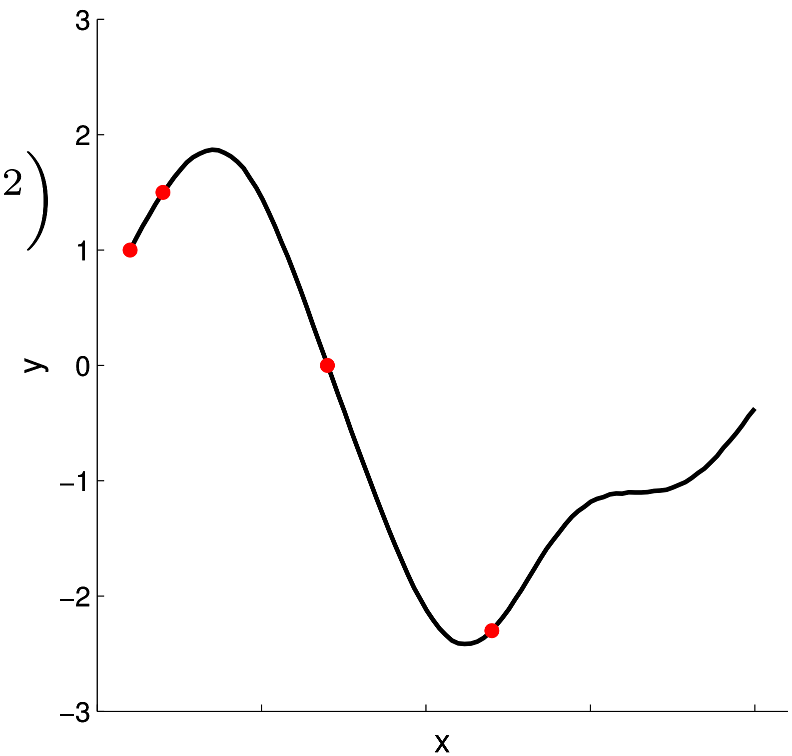
$\Sigma =$ 



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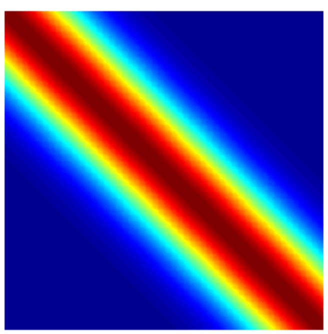
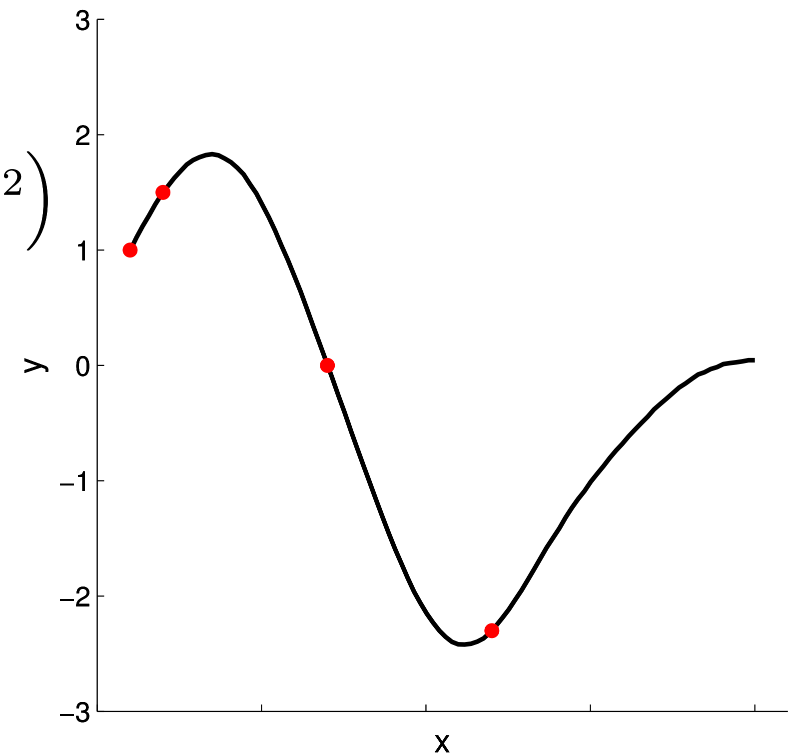
$\Sigma =$ 



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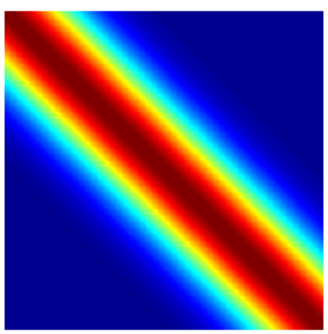

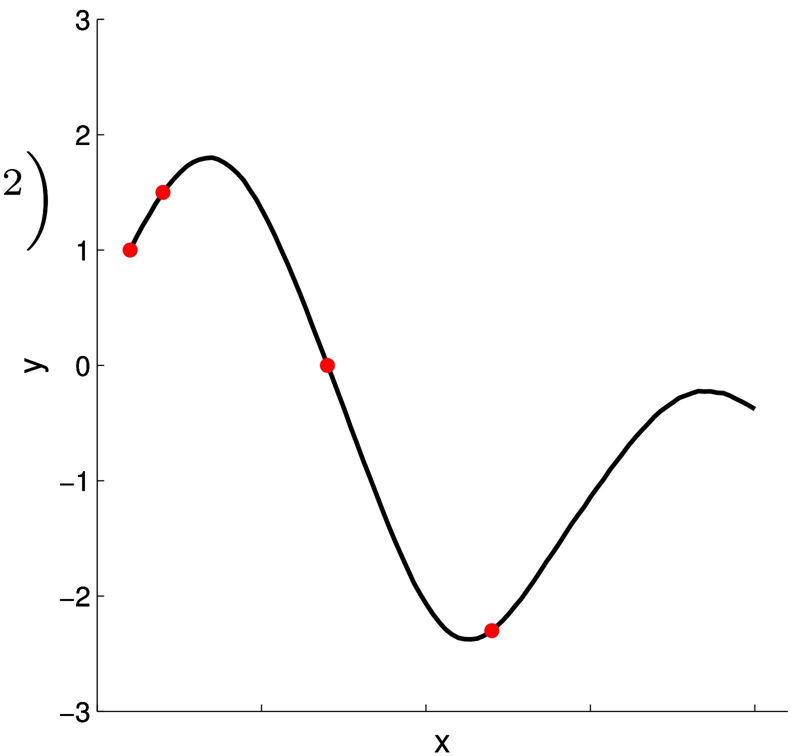

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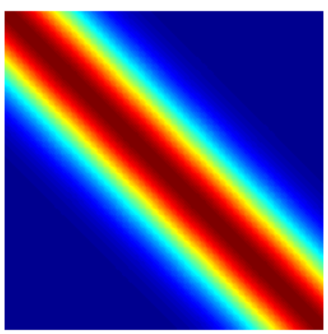

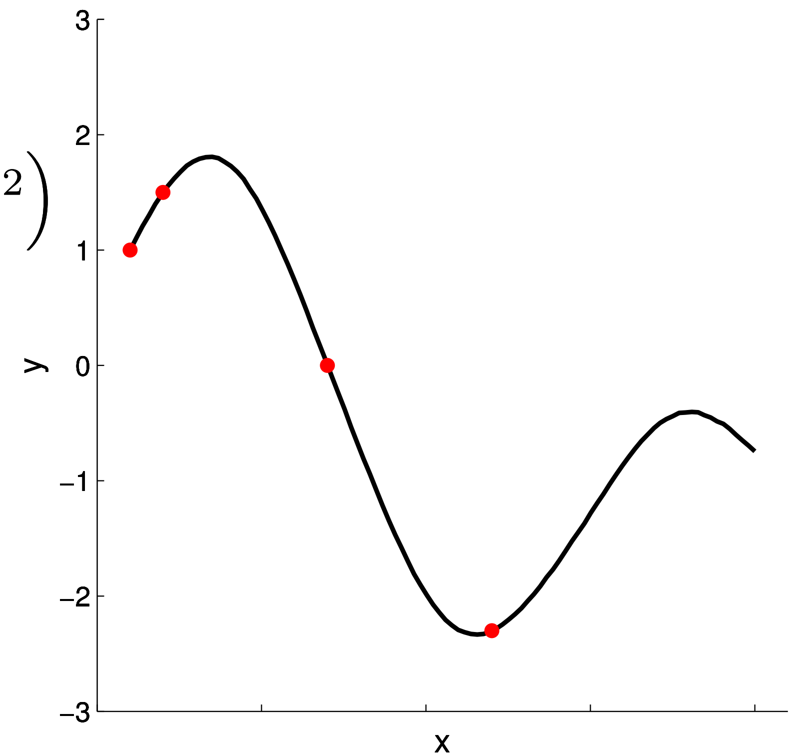

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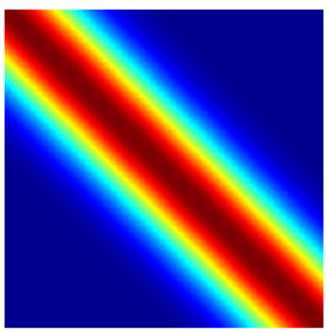

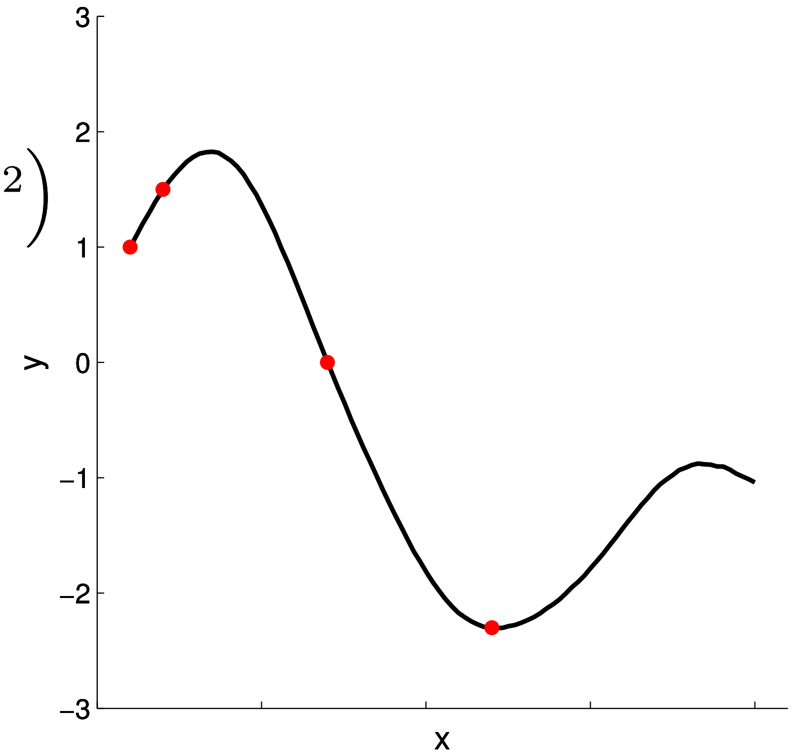

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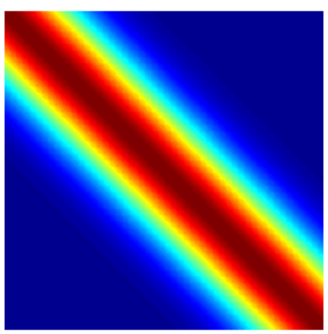
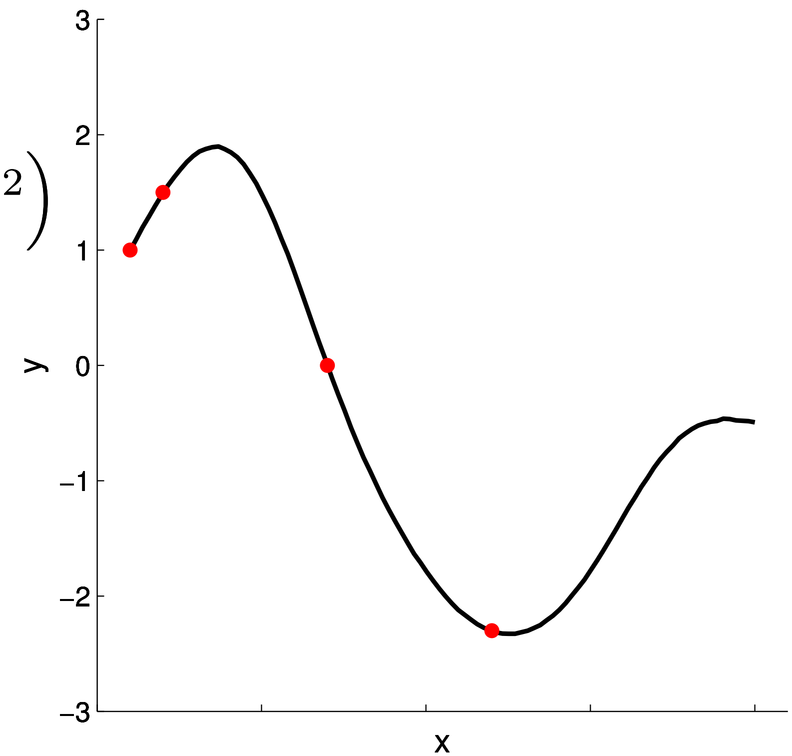
$\Sigma =$ 



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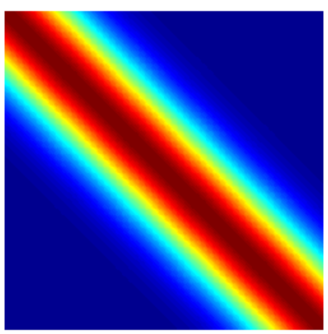
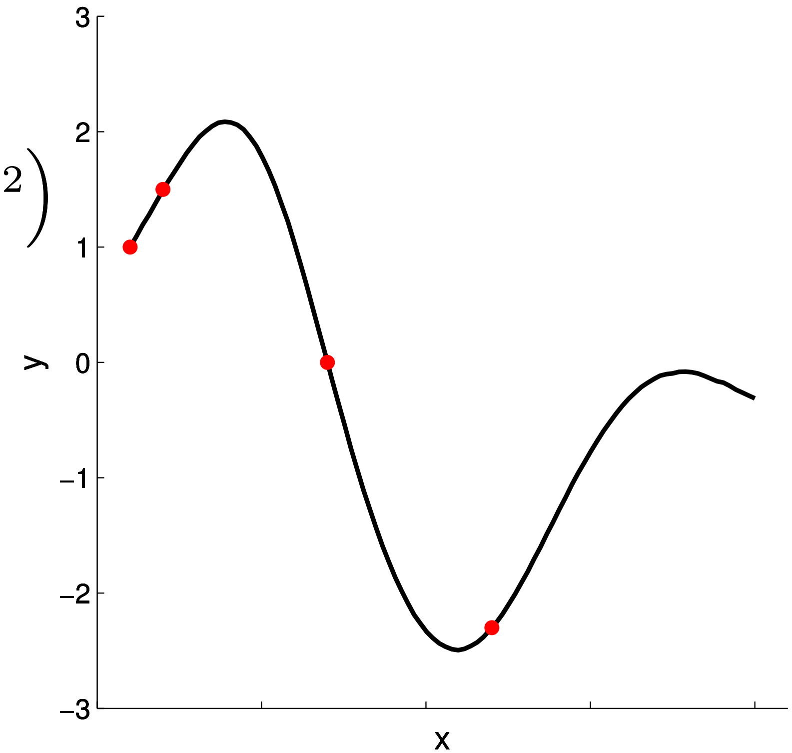
$\Sigma =$ 



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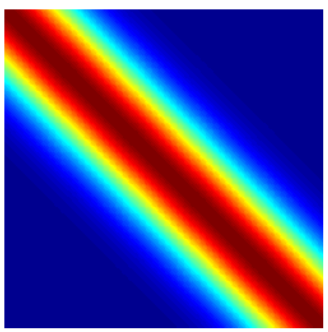
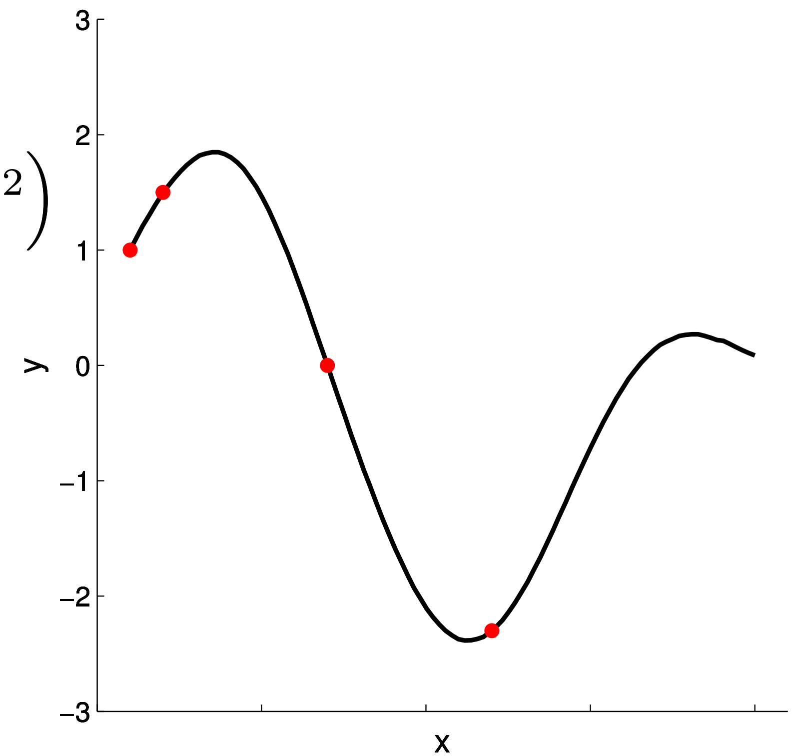
$\Sigma =$ 



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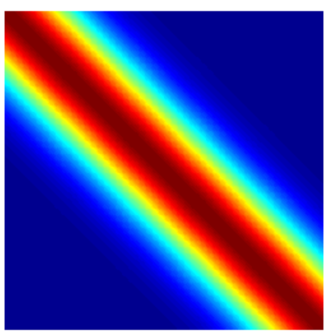

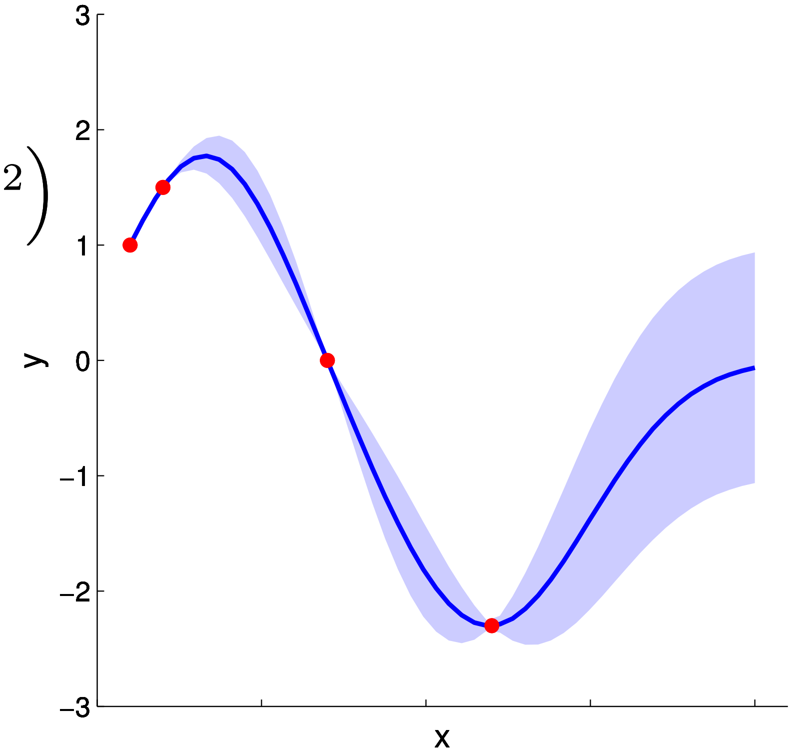

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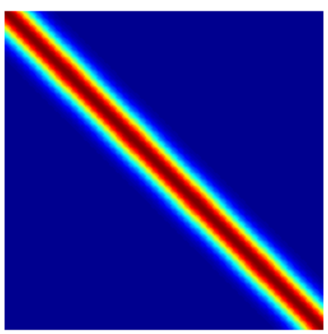
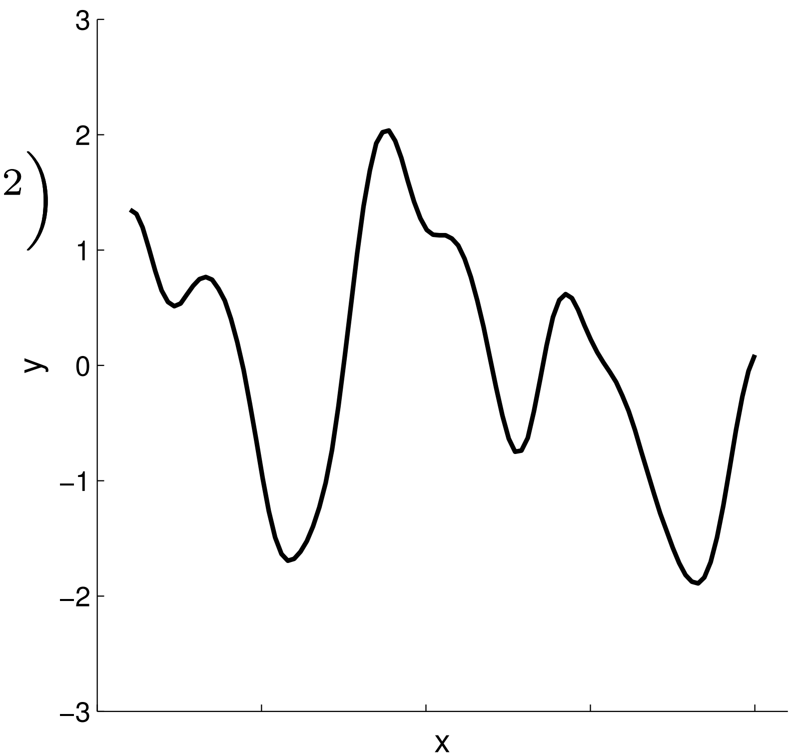
$\Sigma =$ 



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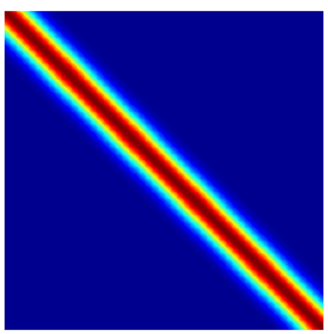
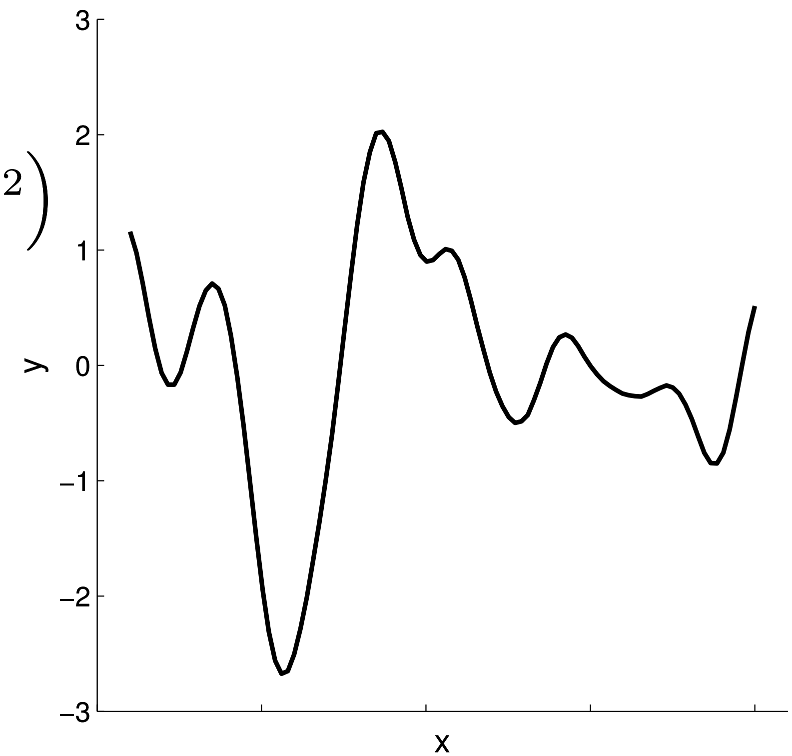
$\Sigma =$ 



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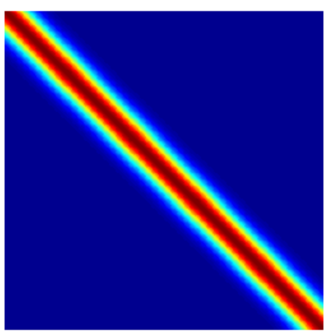

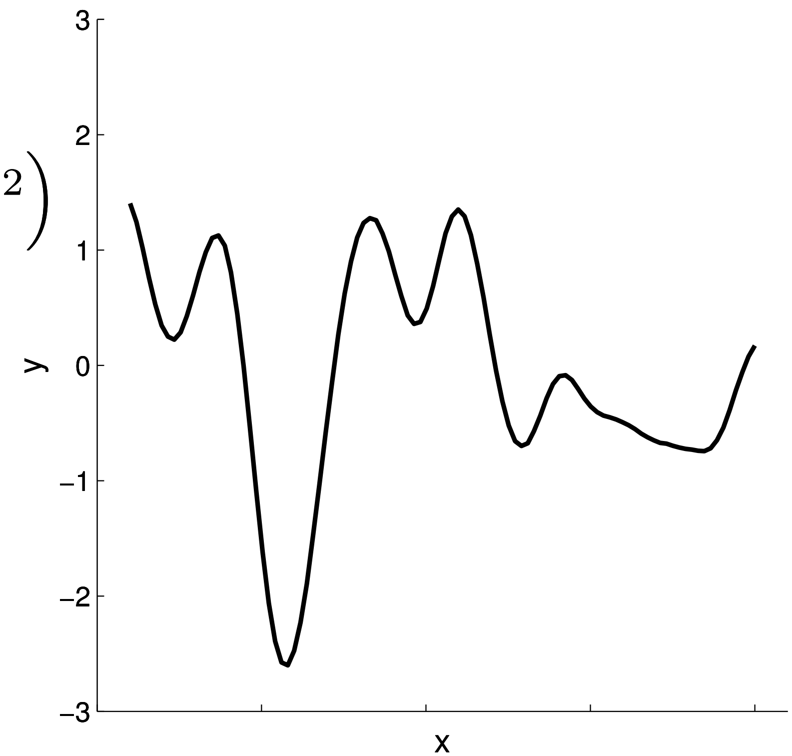

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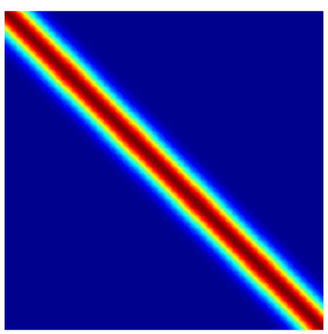
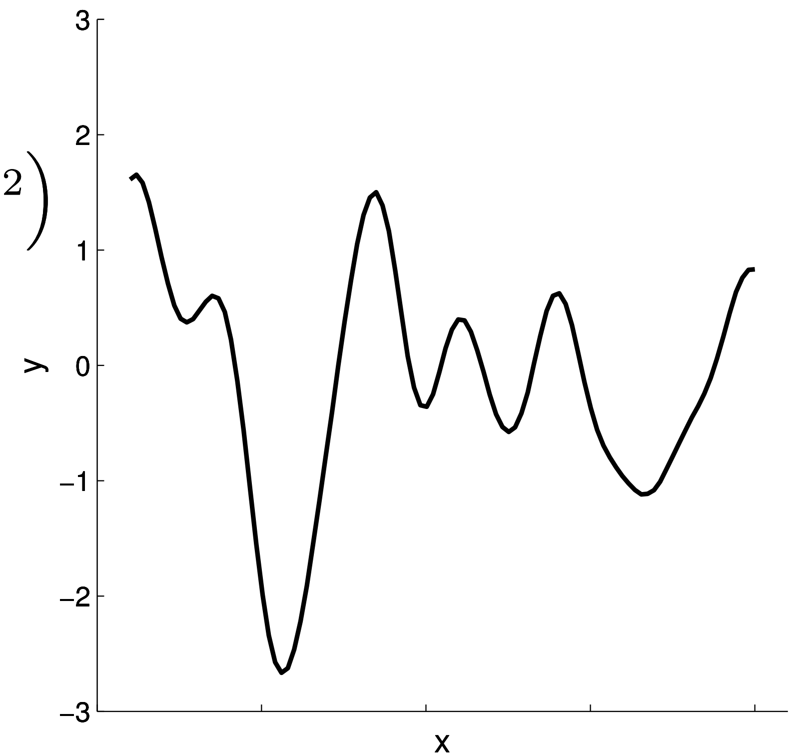
$\Sigma =$ 



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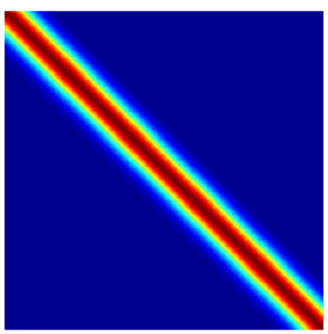
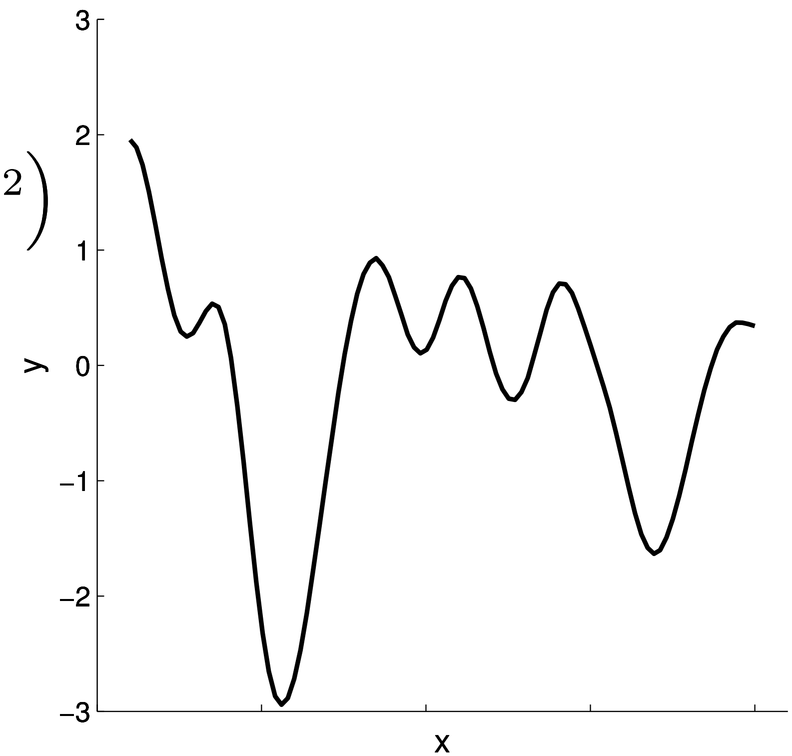
$\Sigma =$ 



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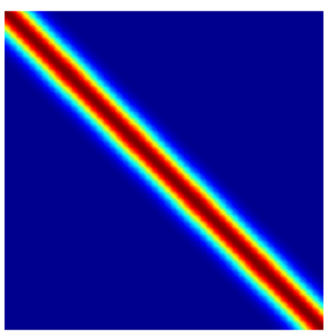
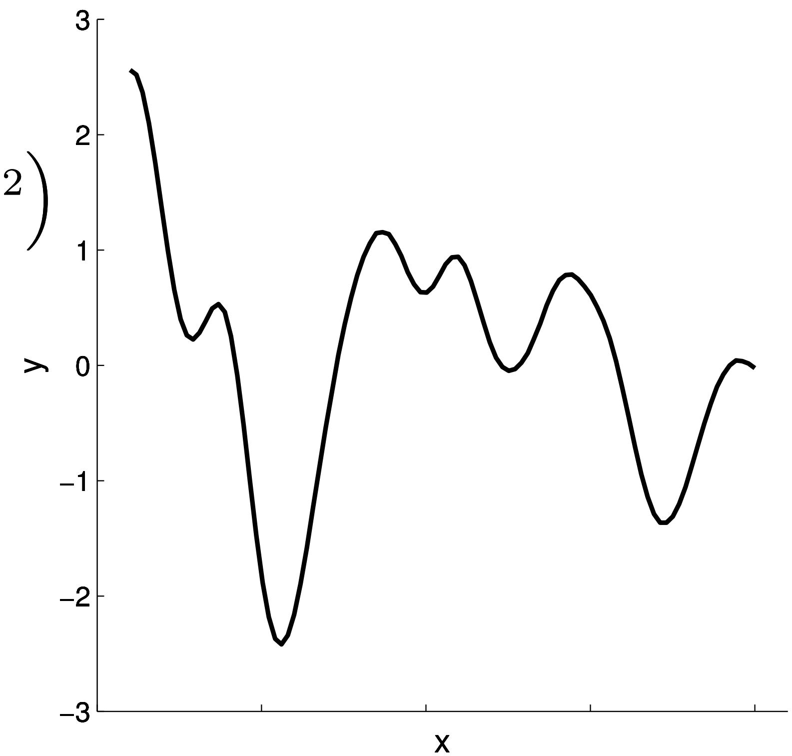
$\Sigma =$ 



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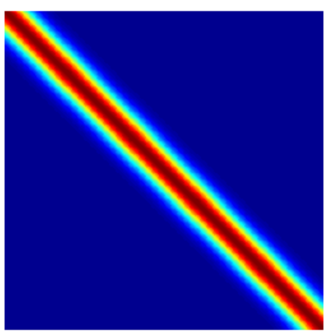

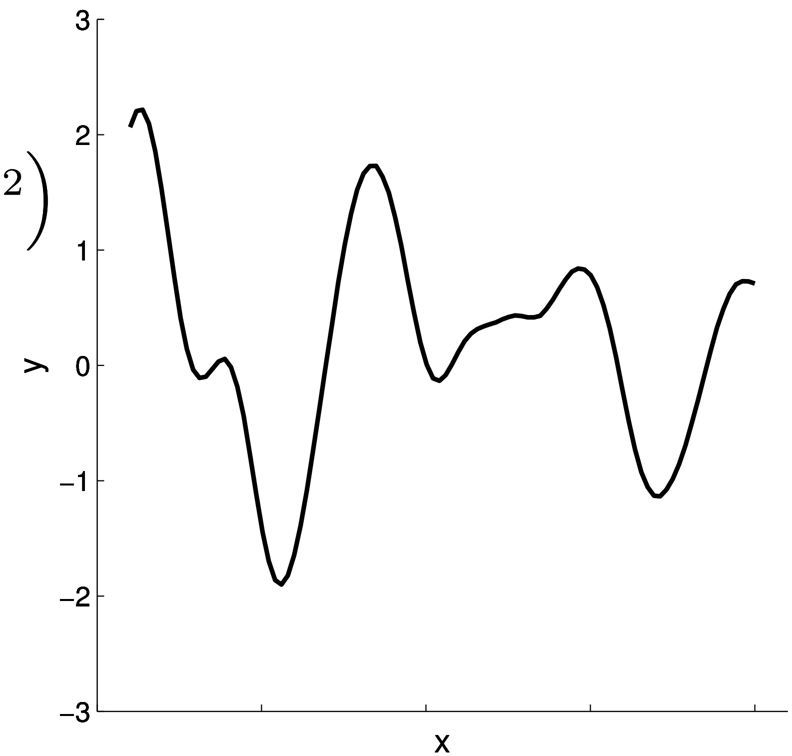

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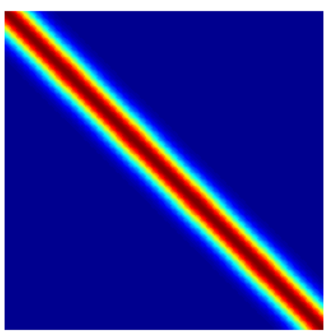
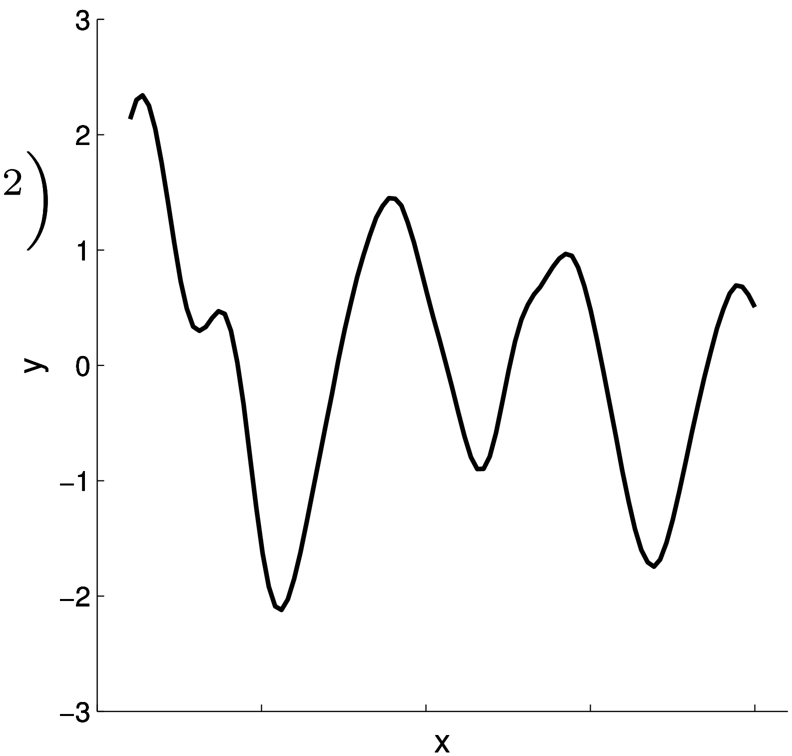
$\Sigma =$ 



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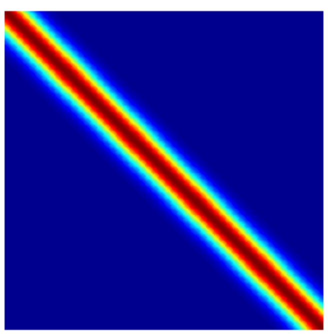
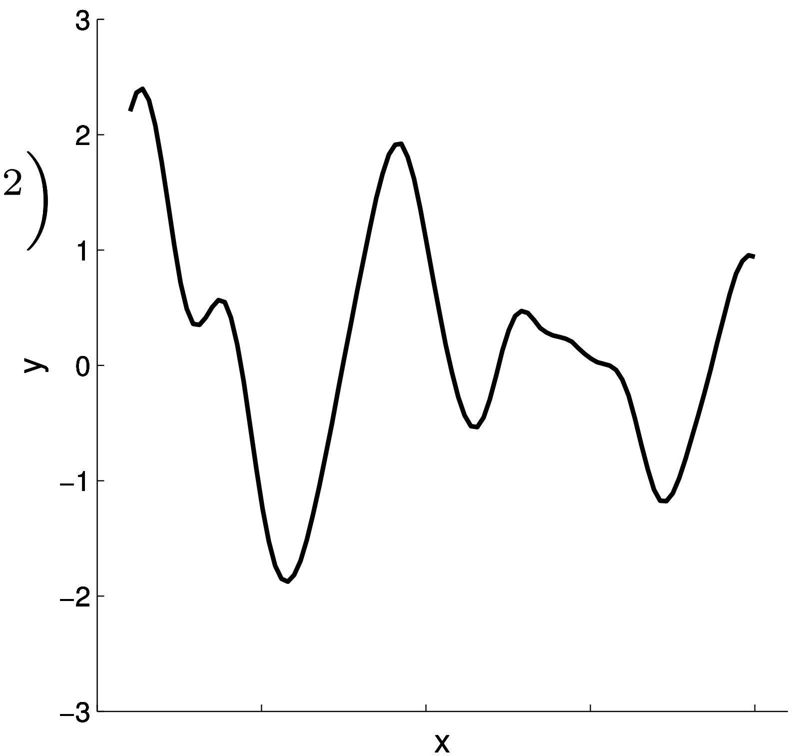
$\Sigma =$ 



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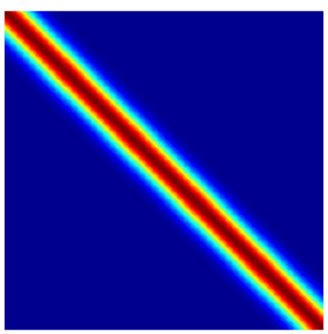
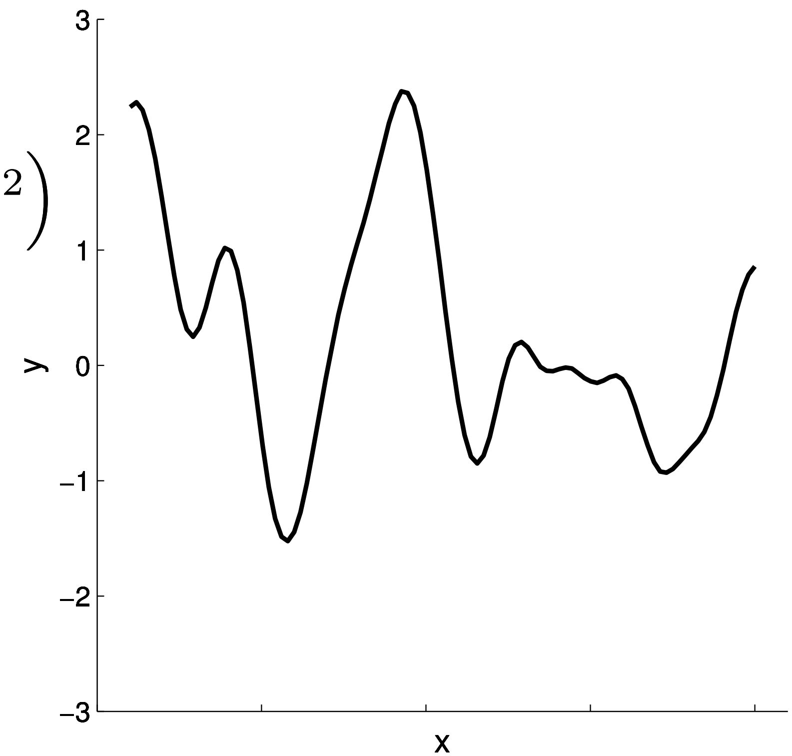
$\Sigma =$ 



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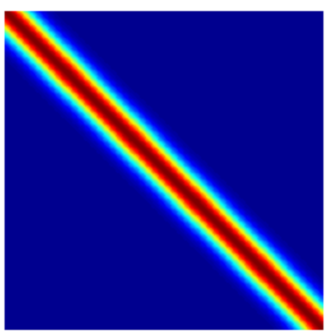

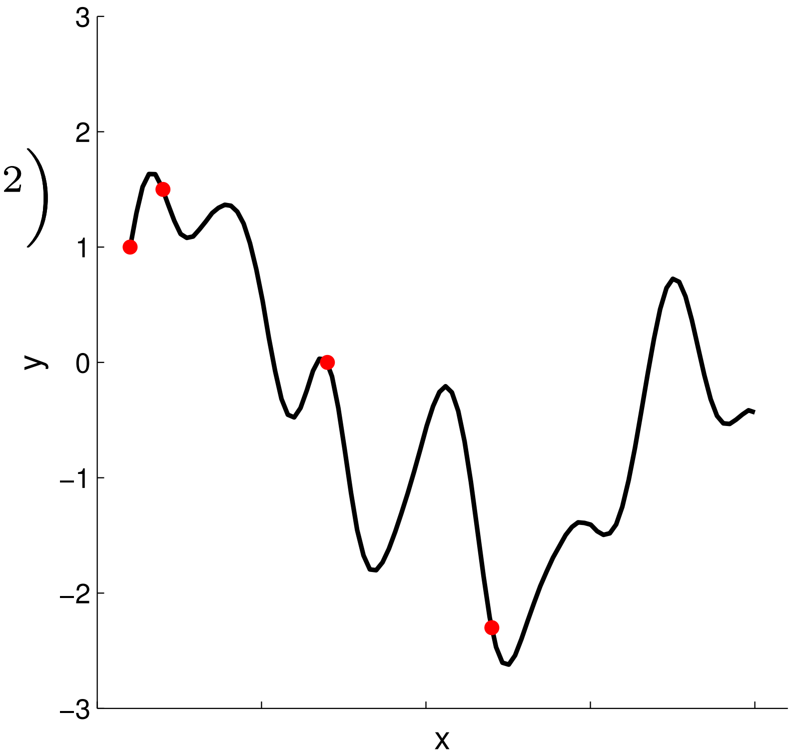

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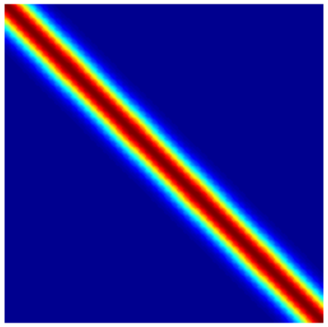
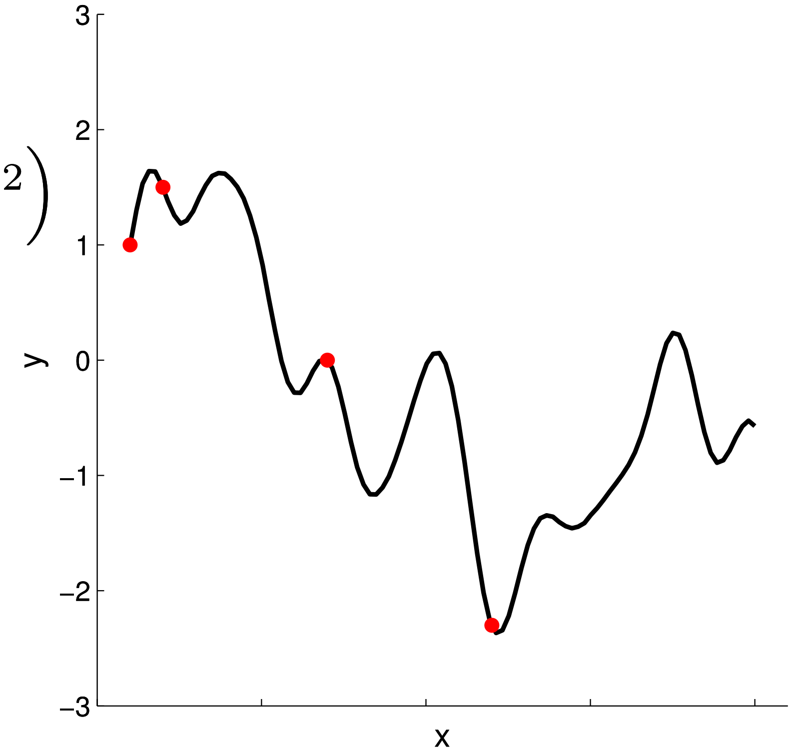
$\Sigma =$ 



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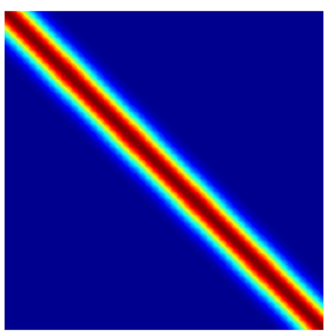
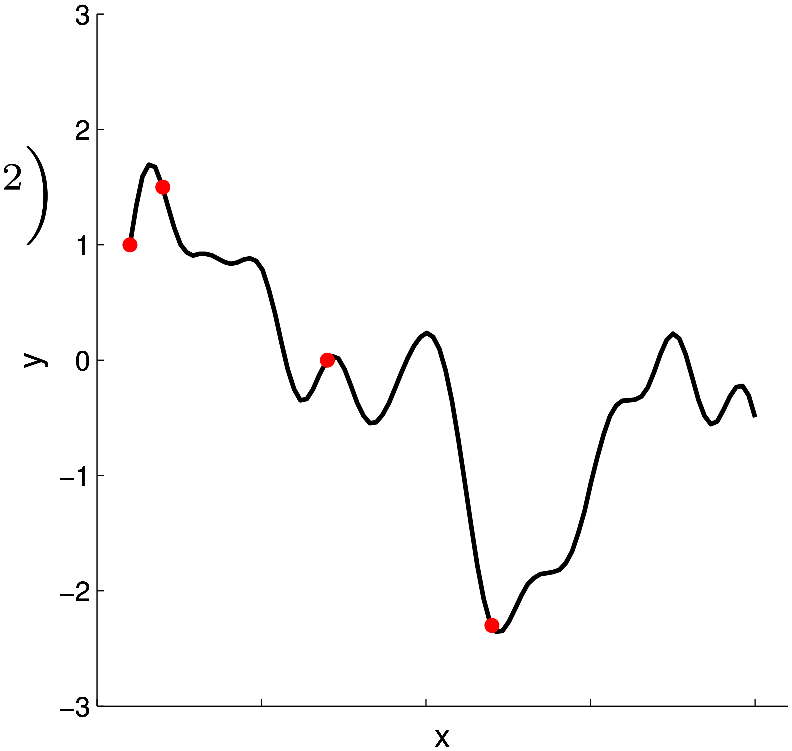
$\Sigma =$ 



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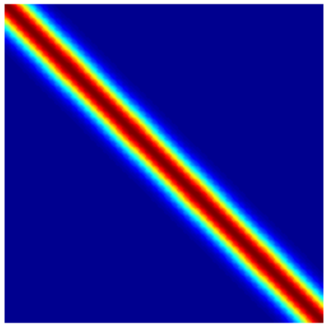

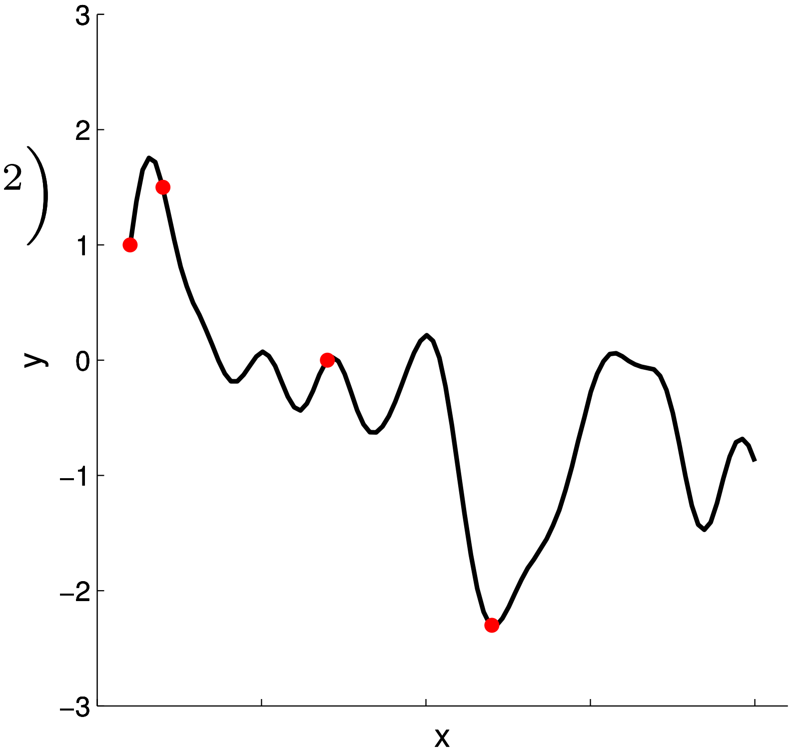

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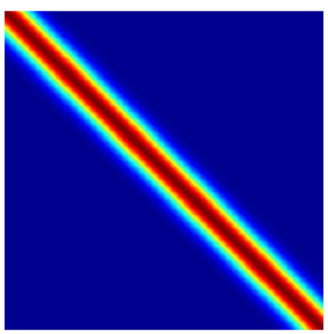
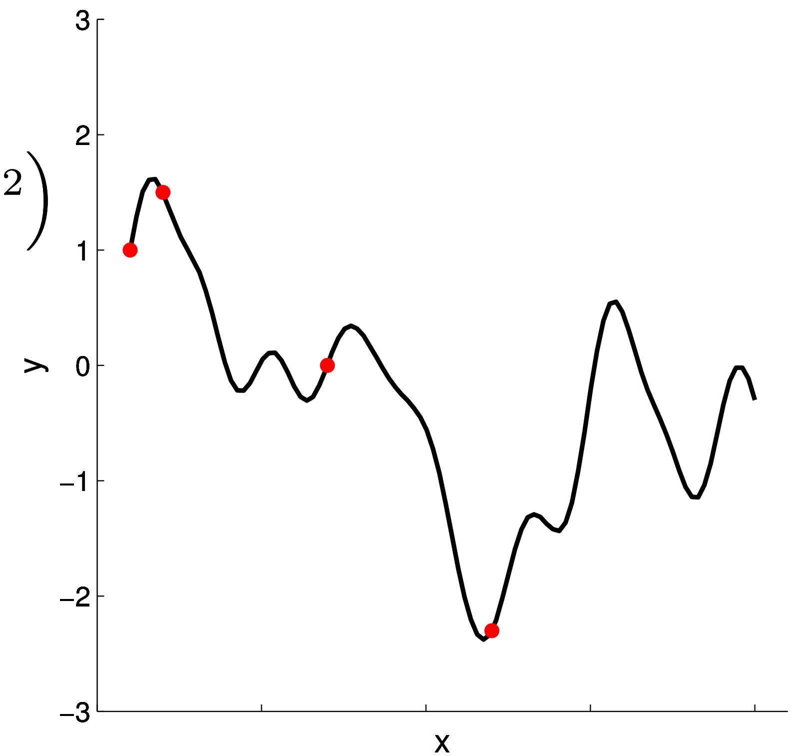
$\Sigma =$ 



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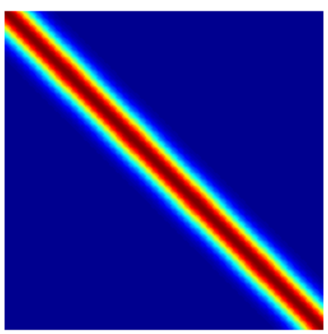
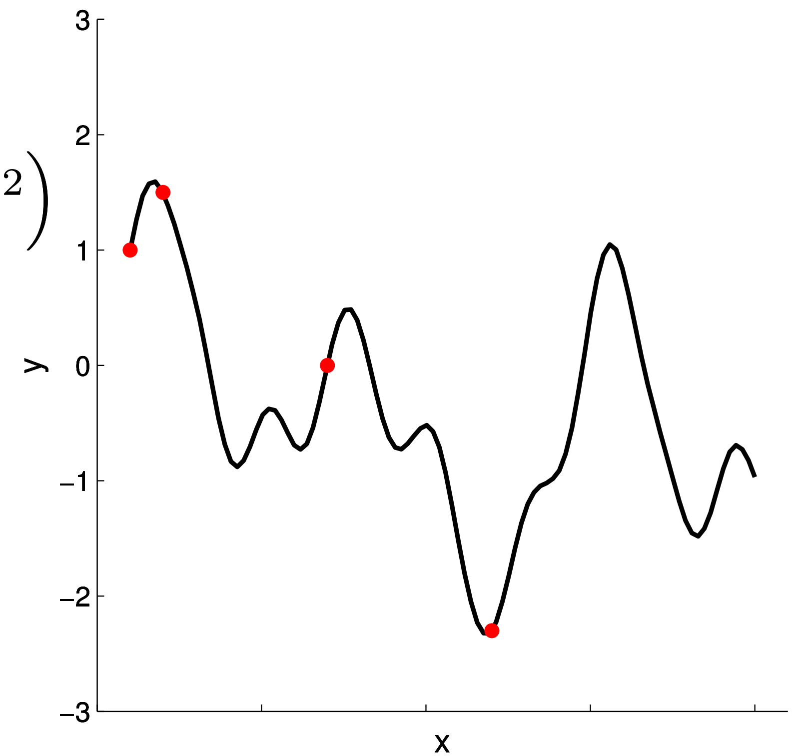
$\Sigma =$ 



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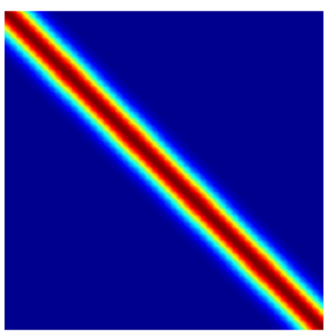
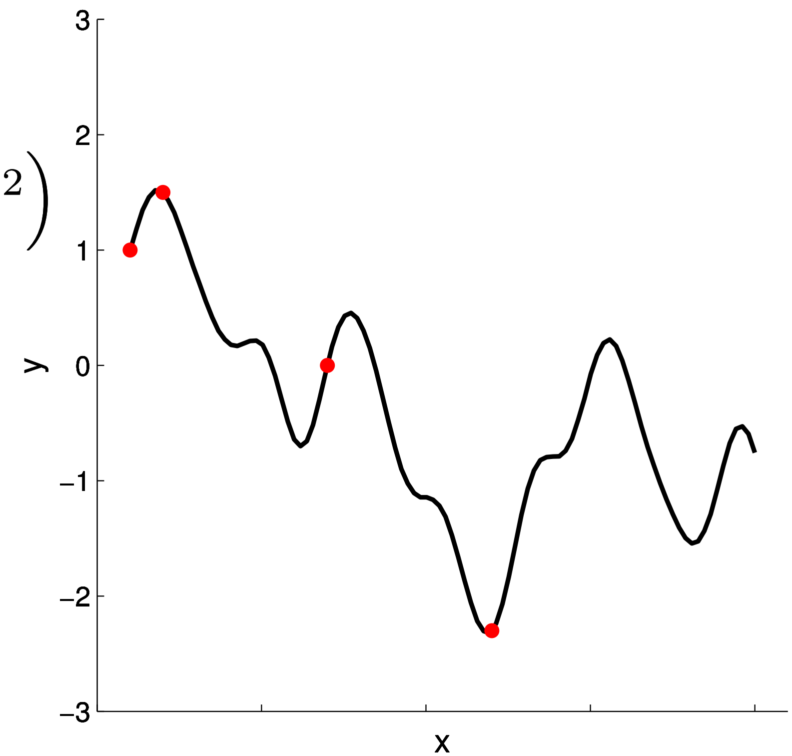
$\Sigma =$ 



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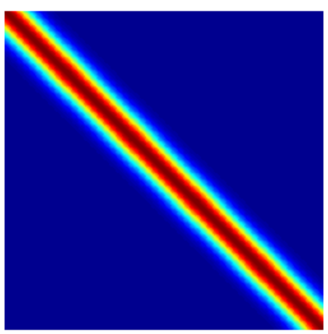
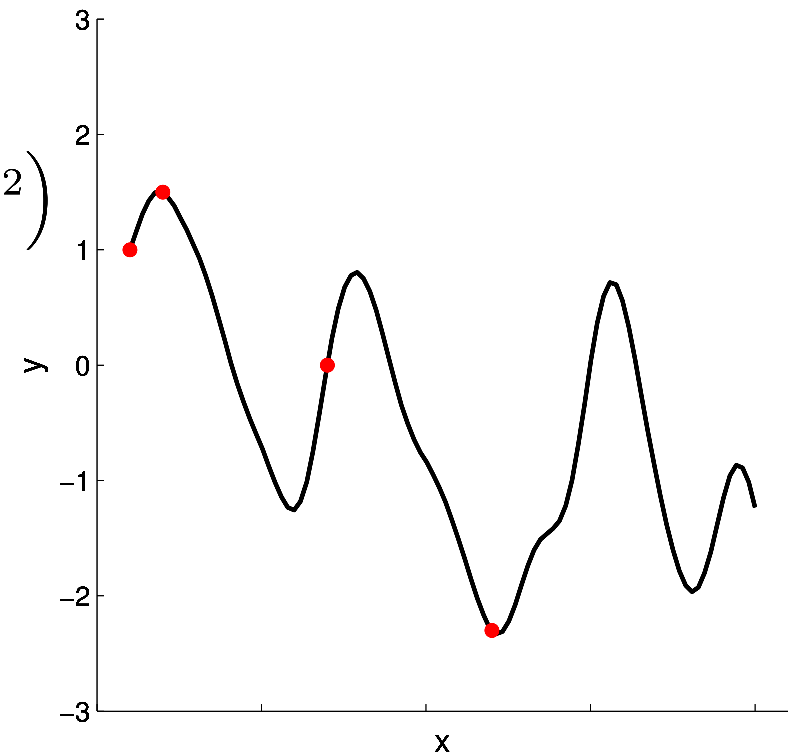
$\Sigma =$ 



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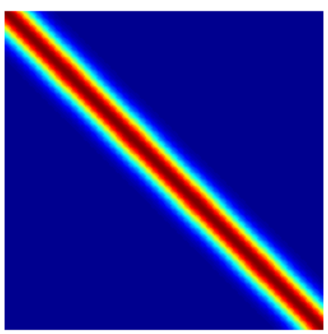
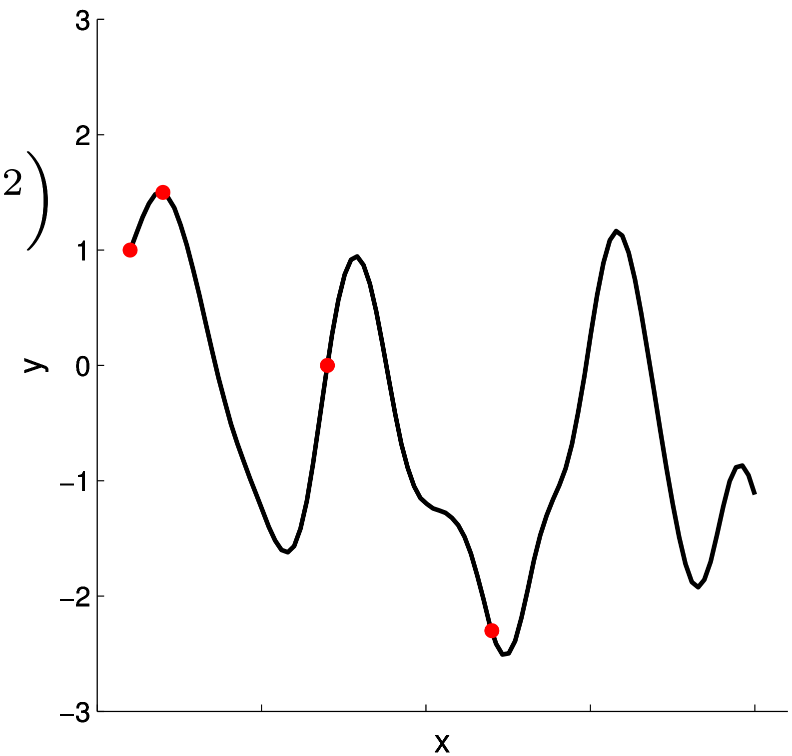
$\Sigma =$ 



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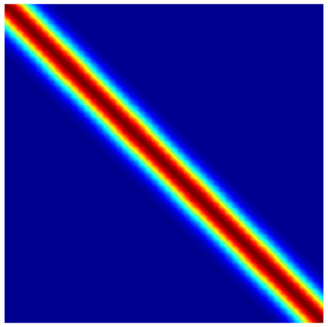
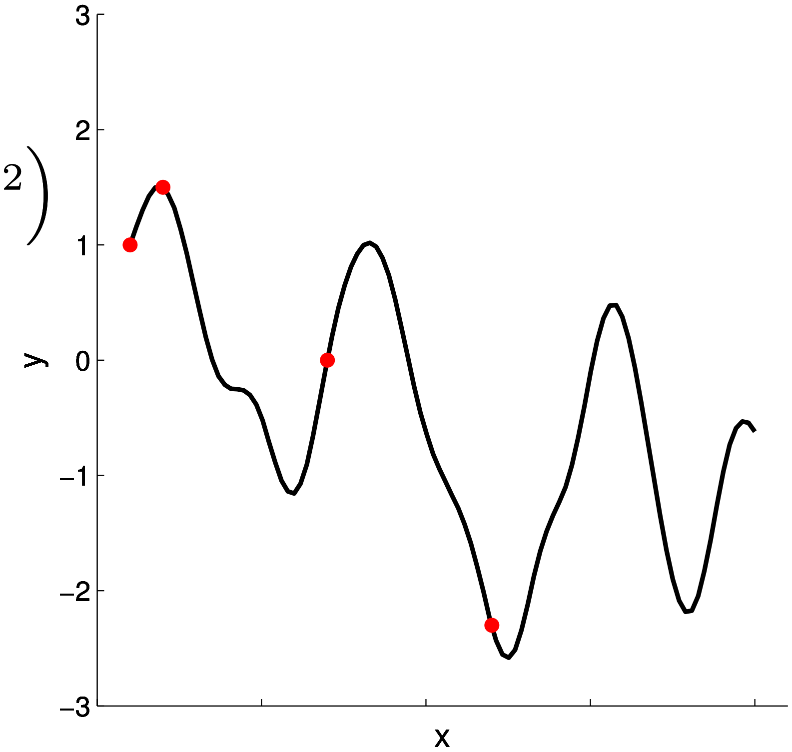
$\Sigma =$ 



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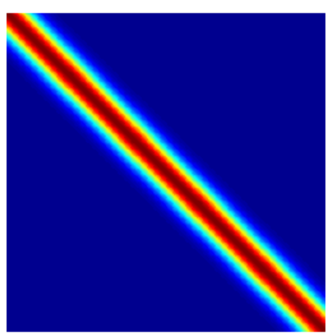
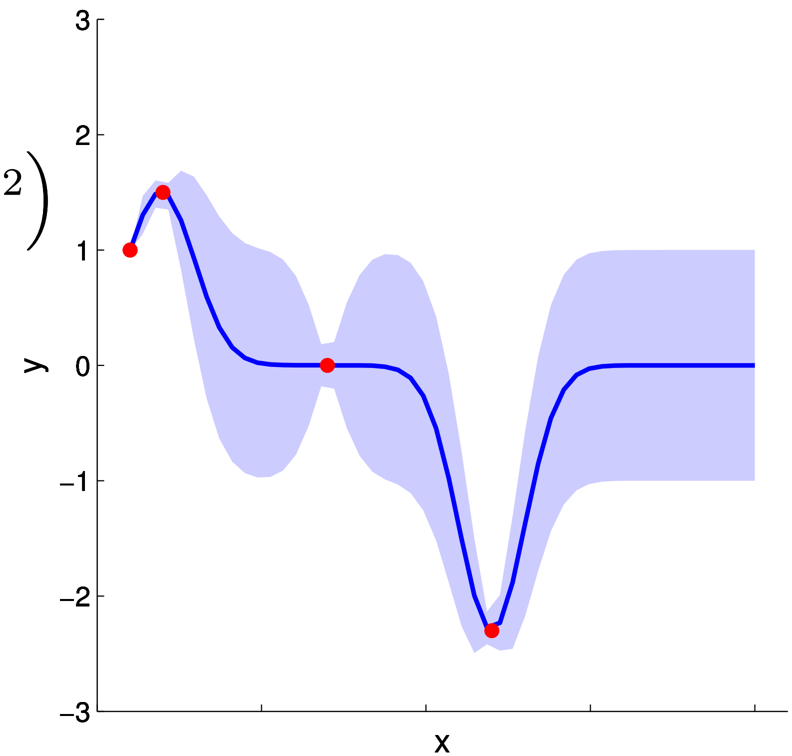
$\Sigma =$ 



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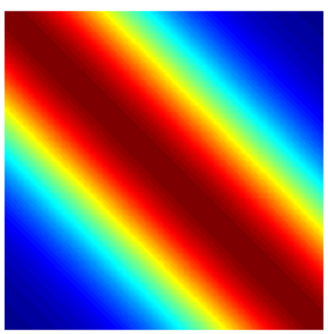
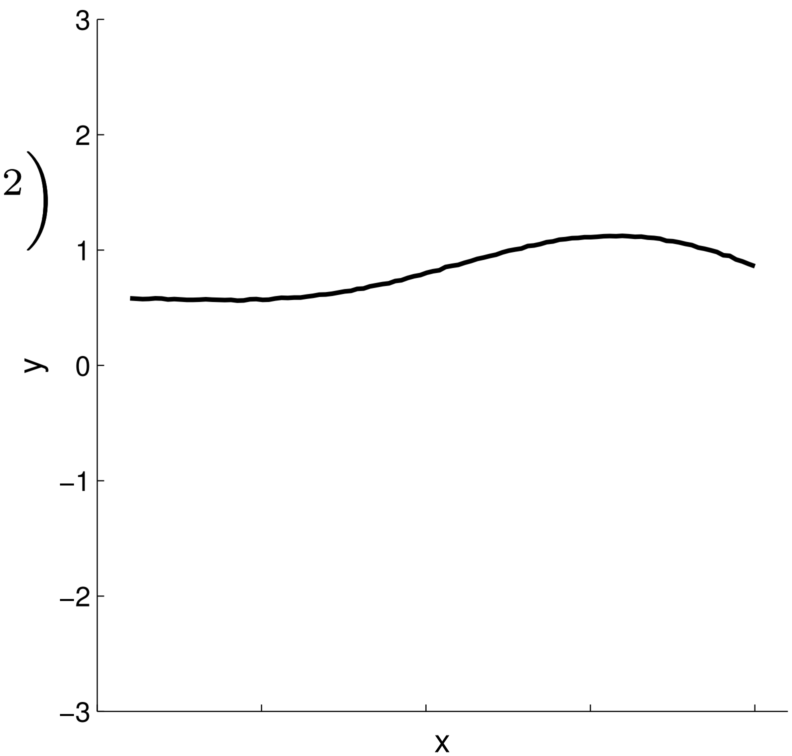
$\Sigma =$ 



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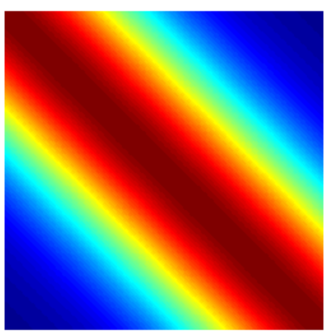
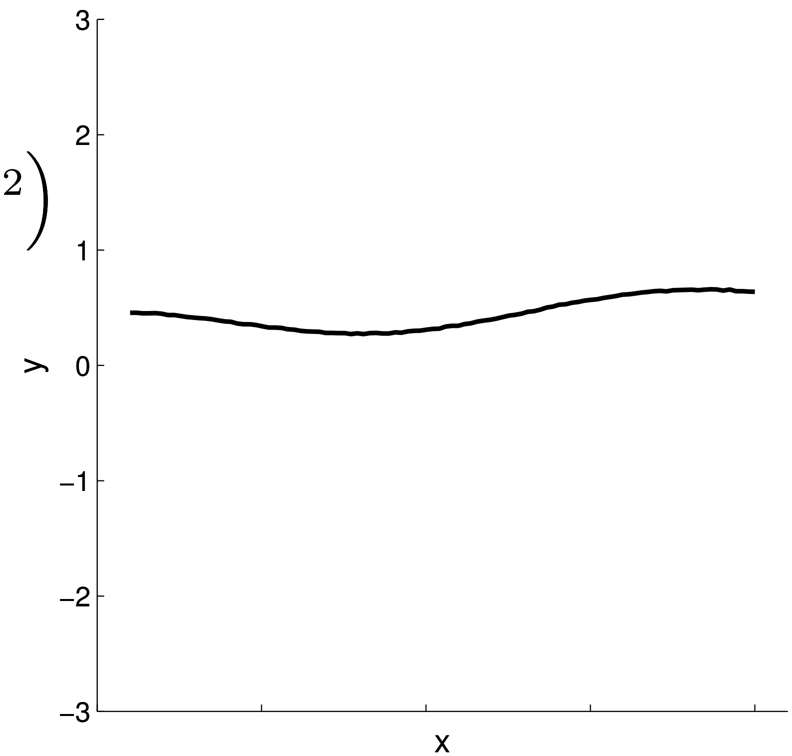
$\Sigma =$ 



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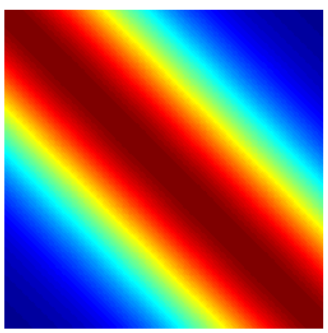

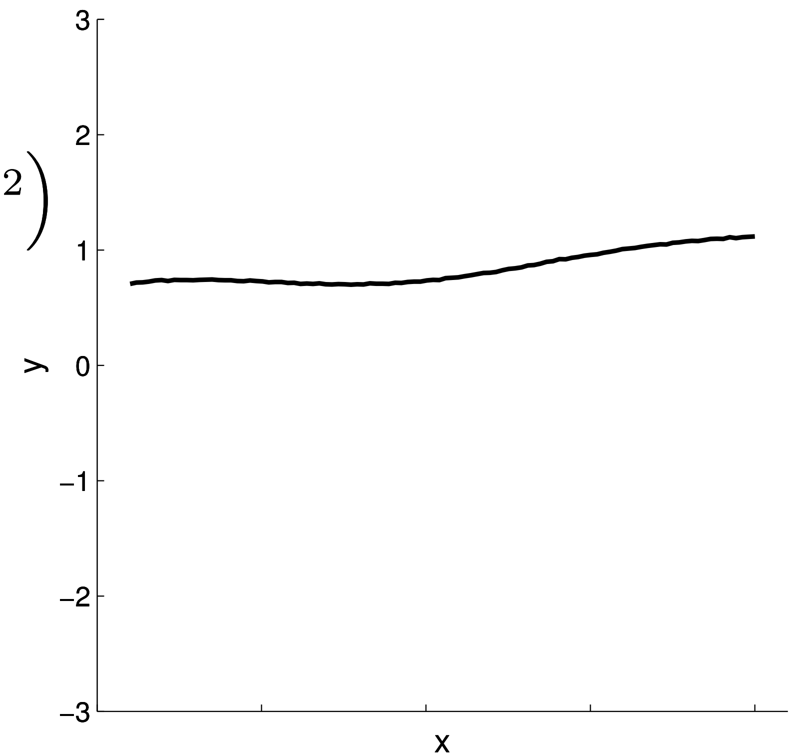

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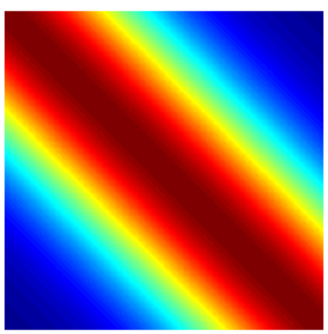
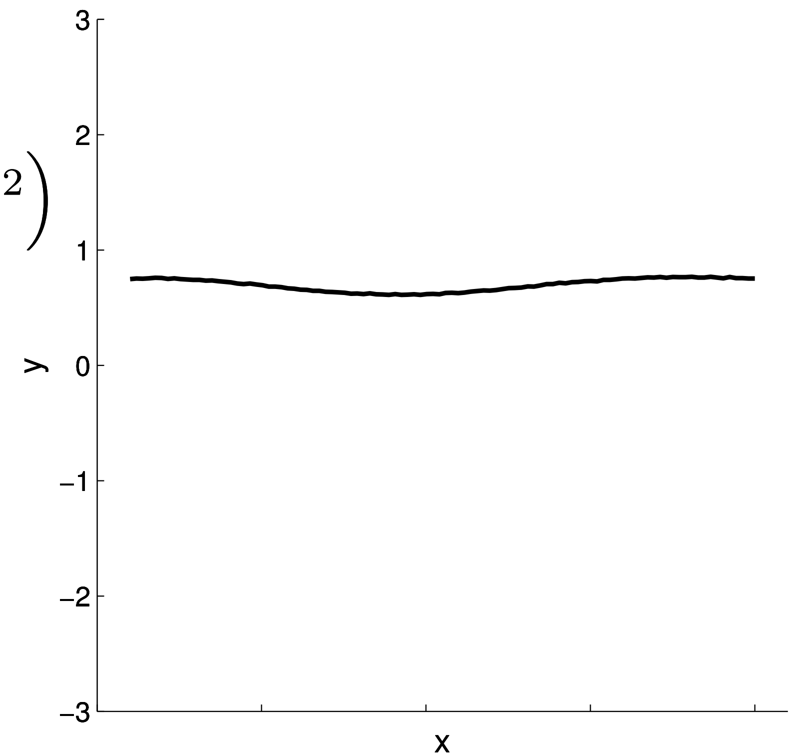
$\Sigma =$ 



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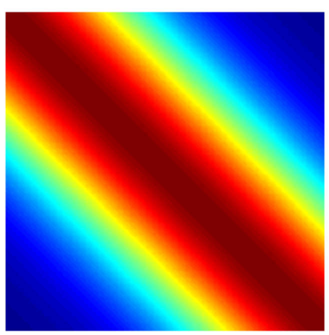
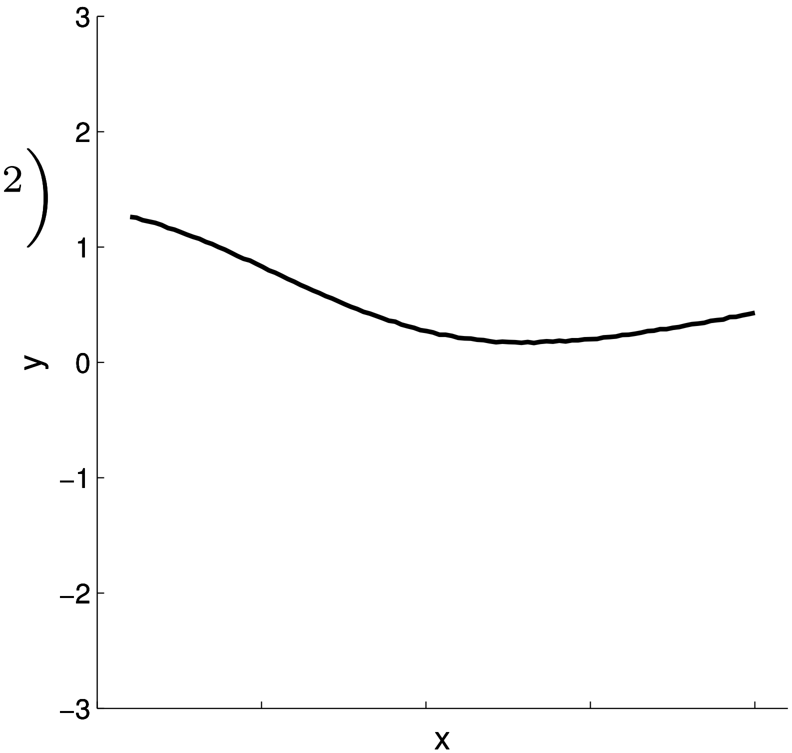
$\Sigma =$ 



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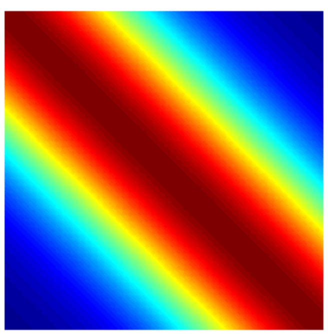

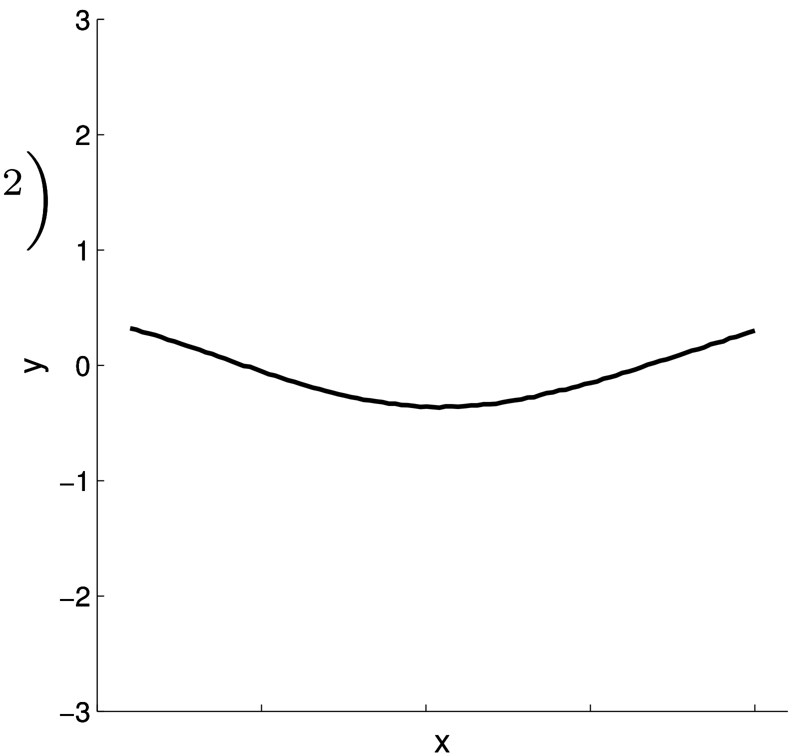

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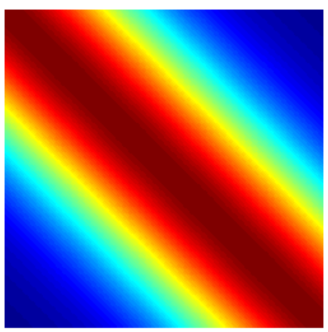
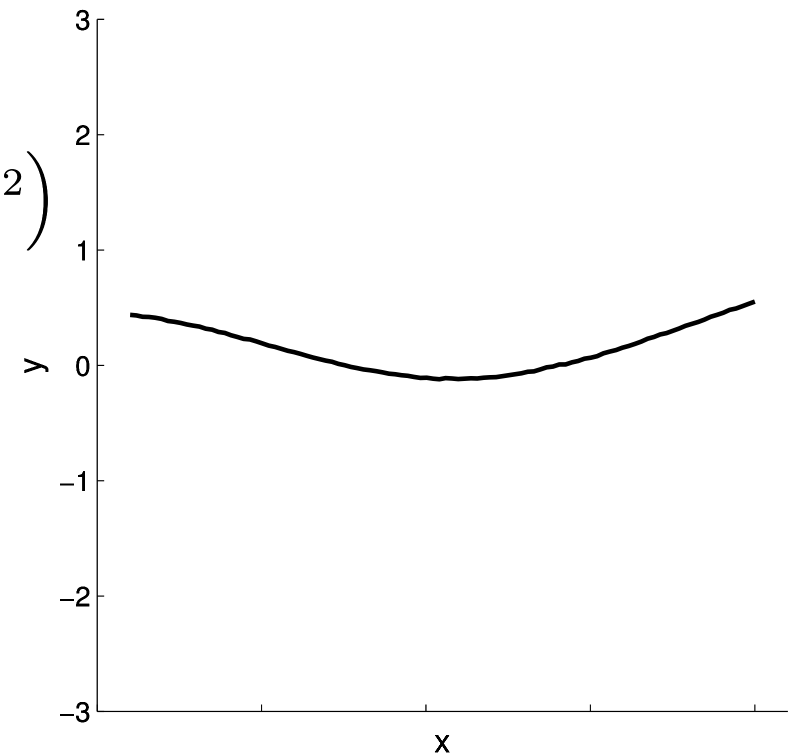
$\Sigma =$ 



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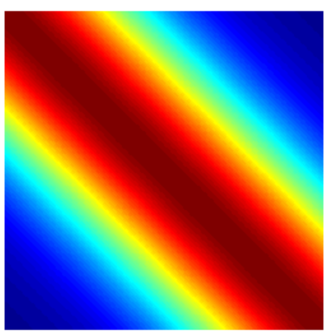

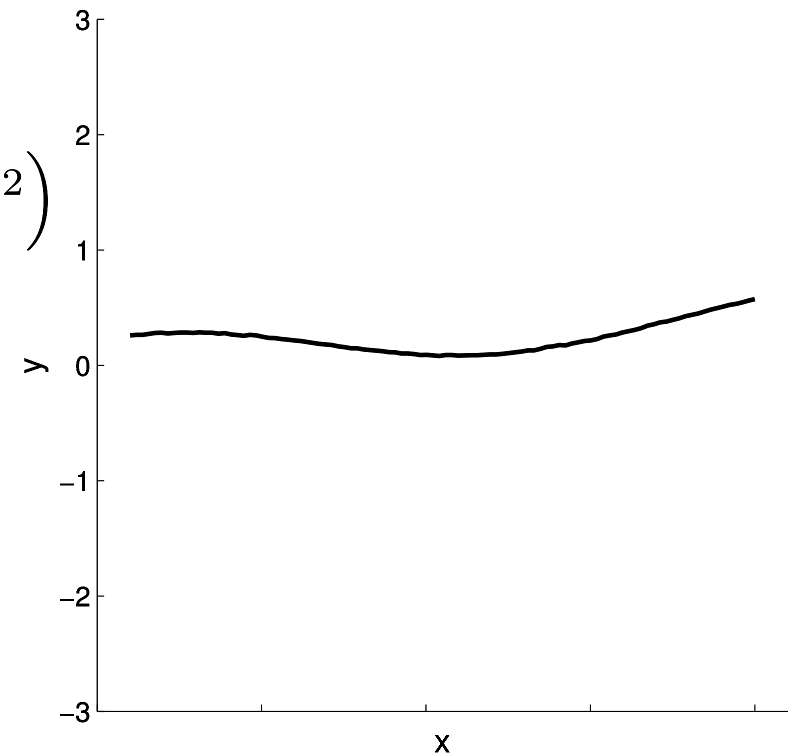

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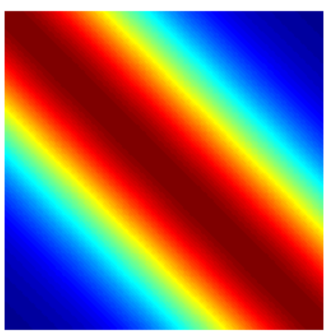
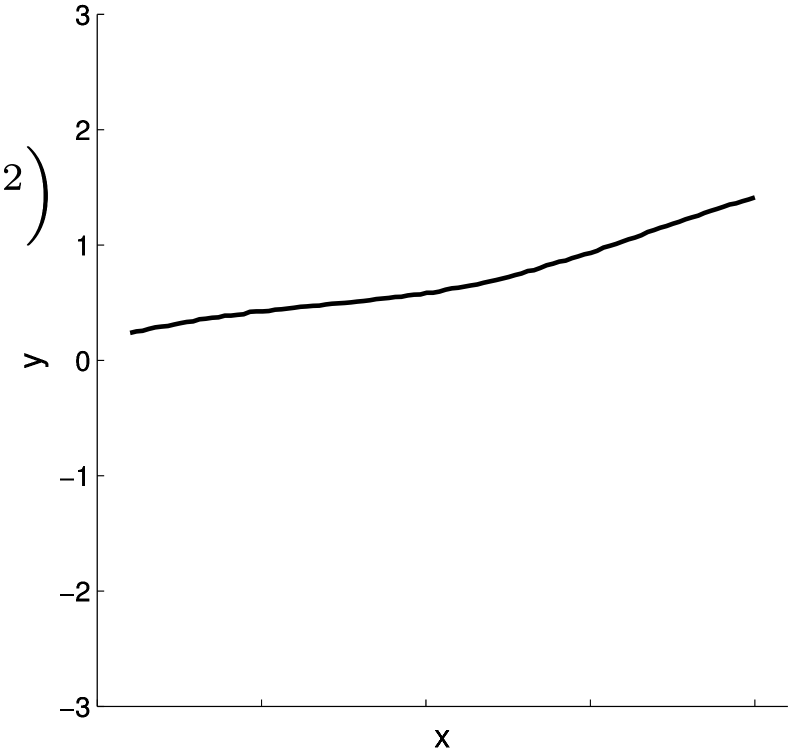
$\Sigma =$ 



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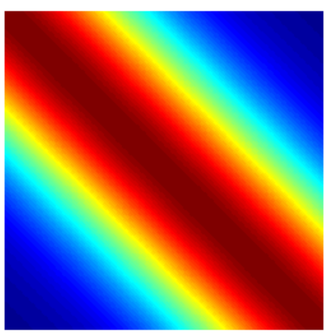
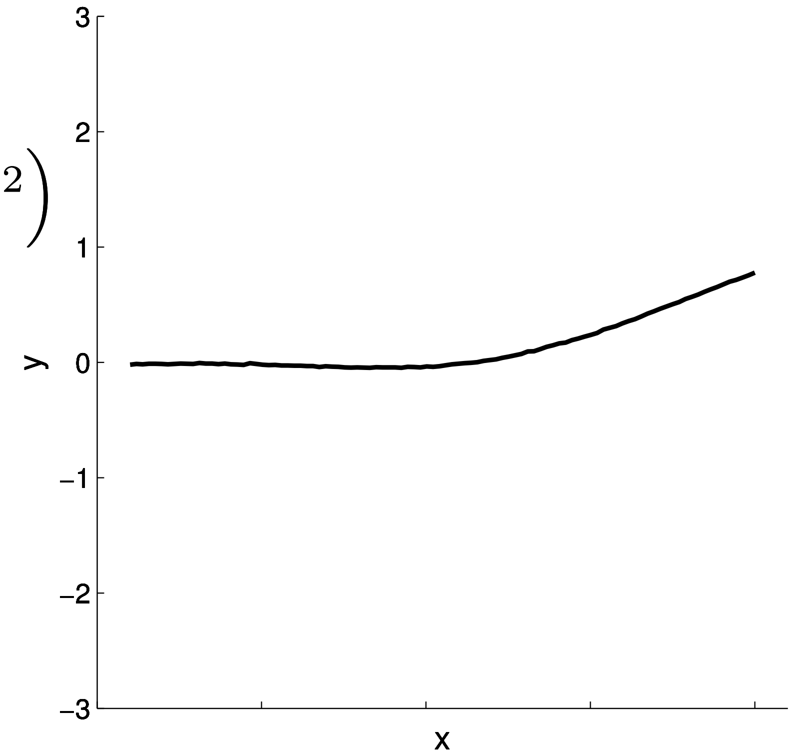
$\Sigma =$ 



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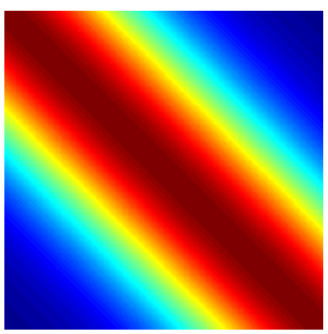
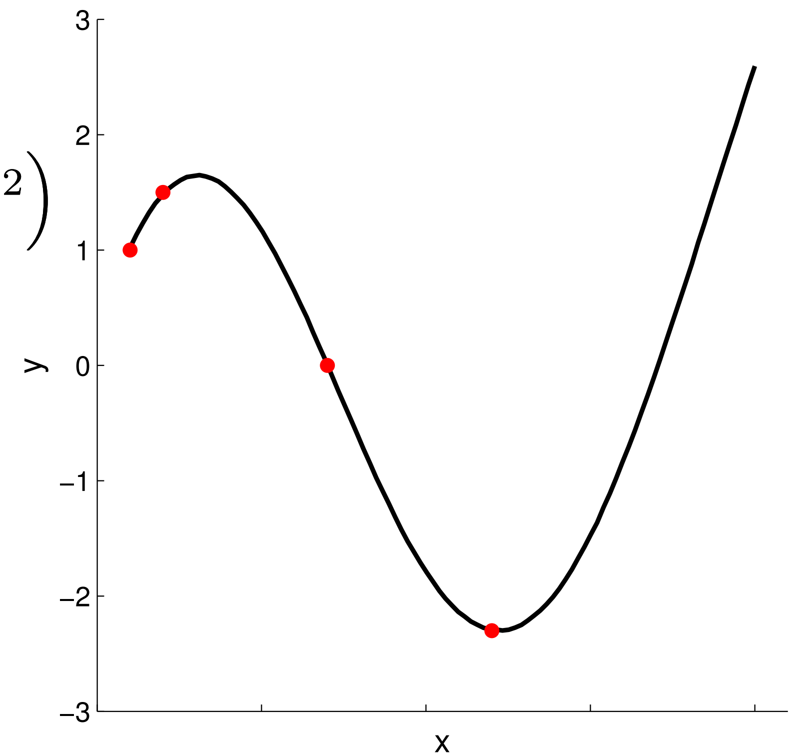
$\Sigma =$ 



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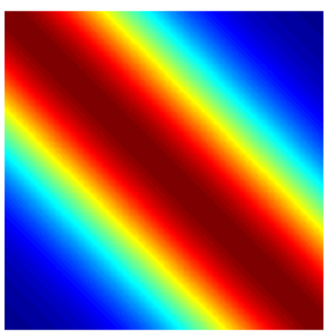

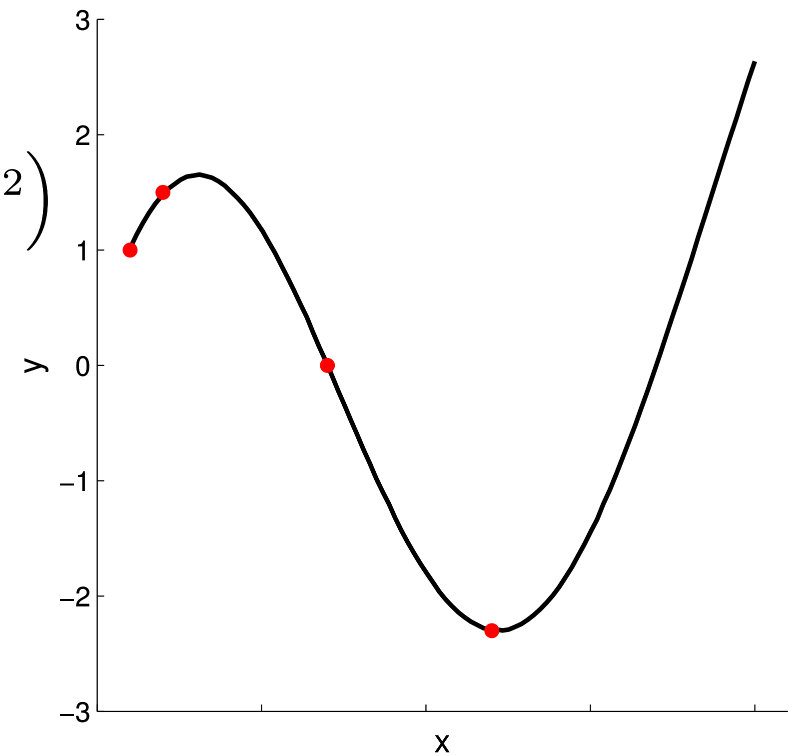

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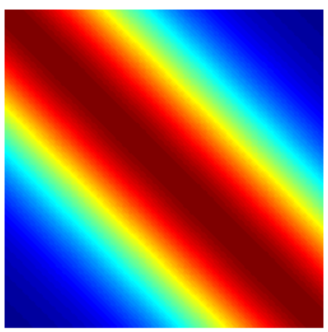

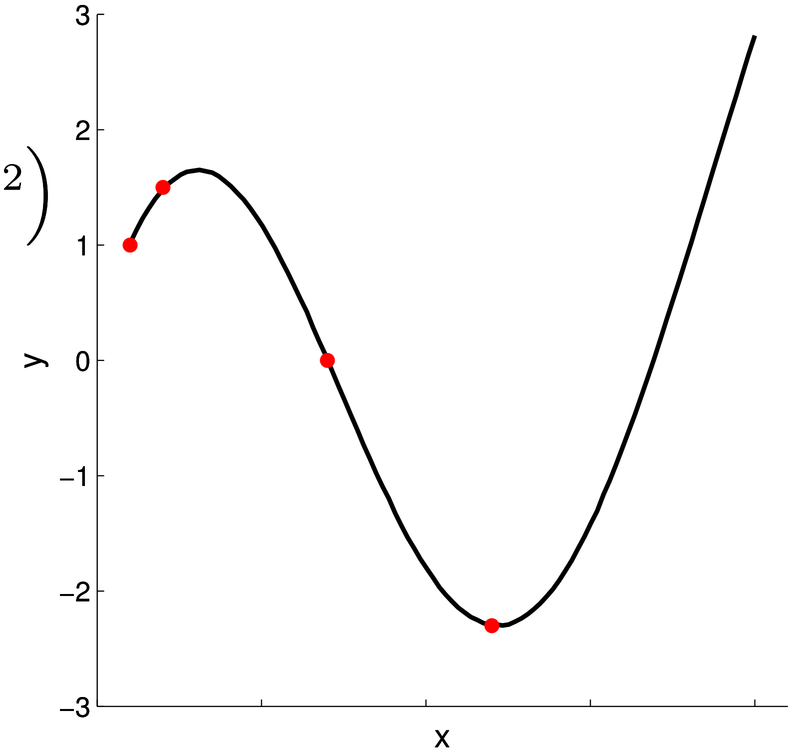

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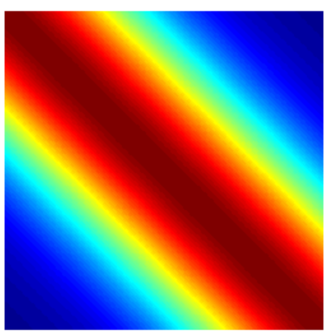
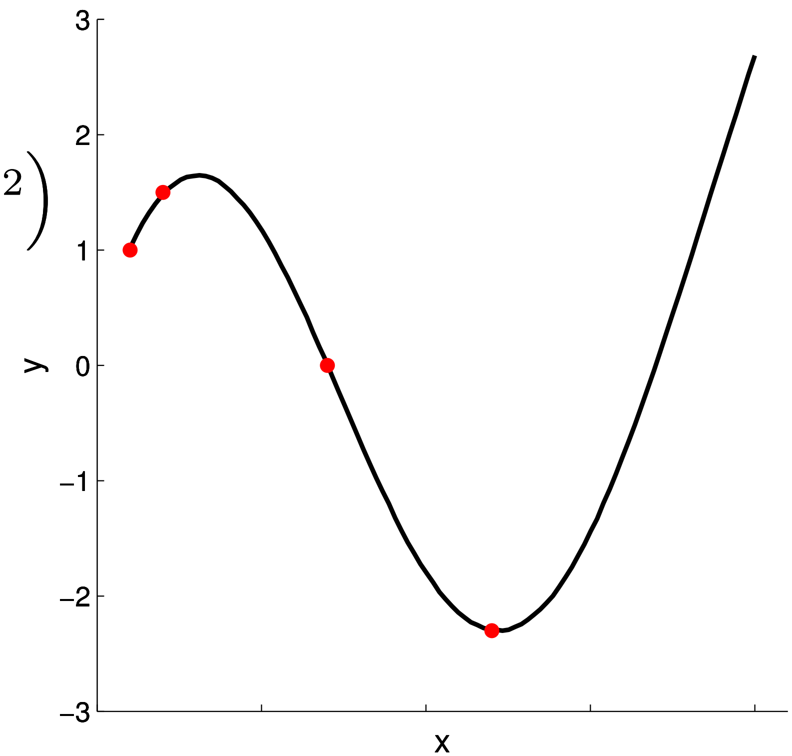
$\Sigma =$ 



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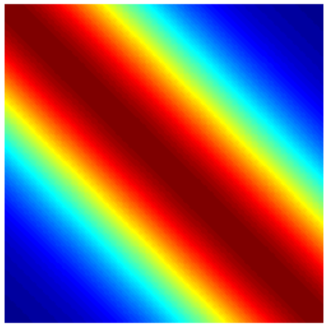

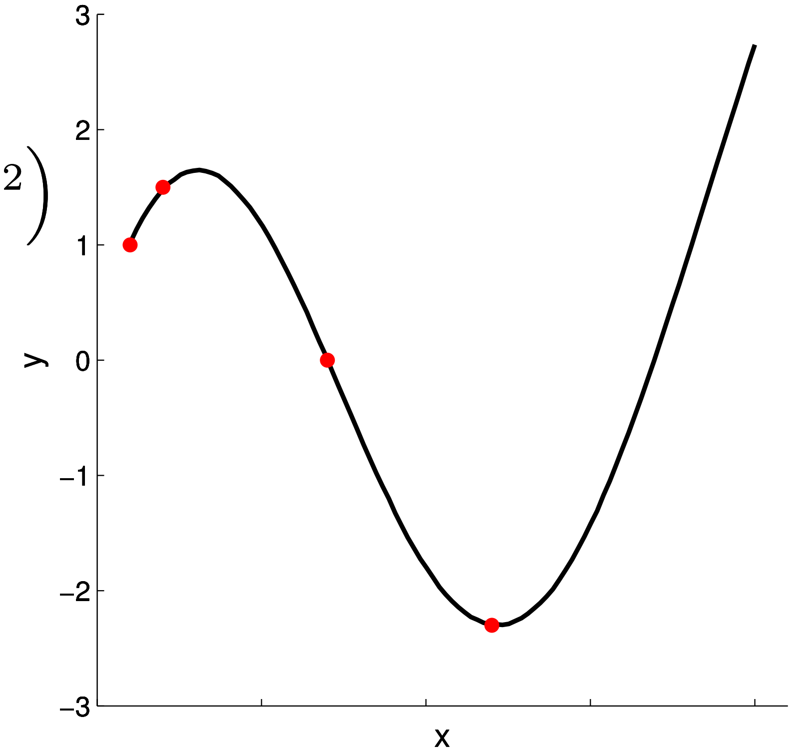

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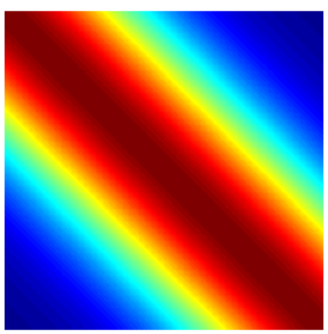

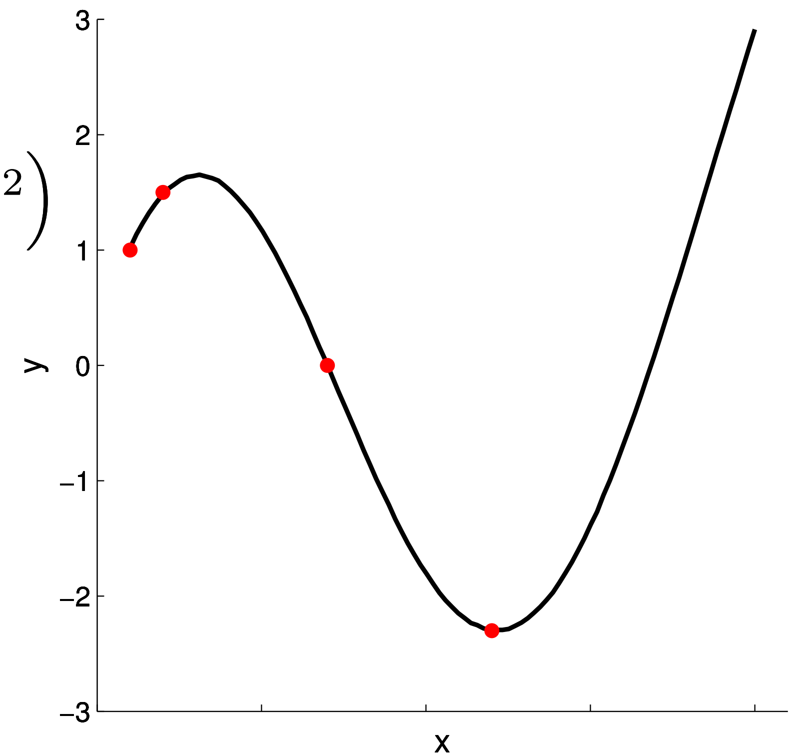

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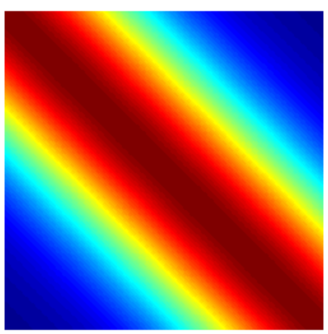
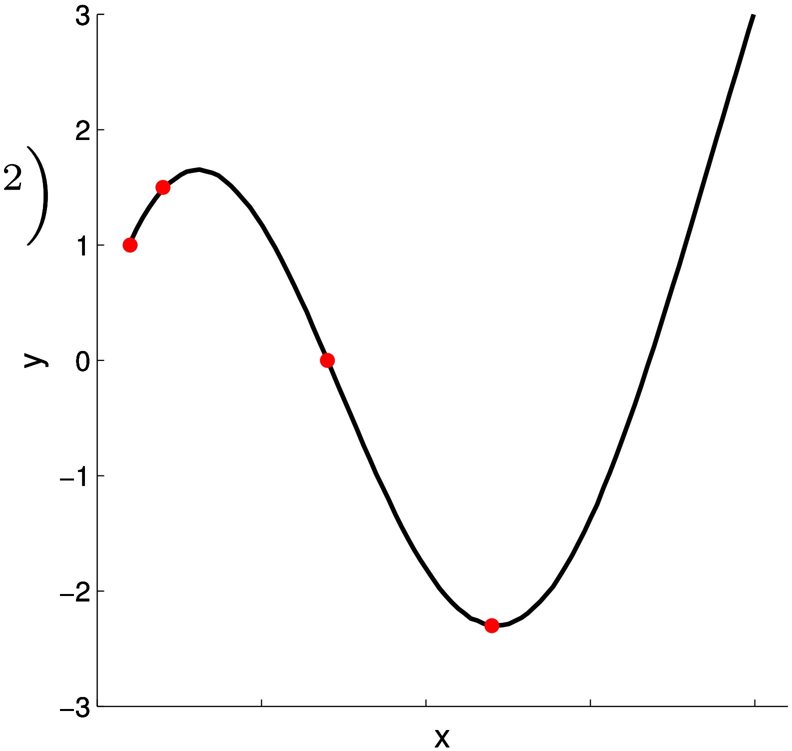
$\Sigma =$ 



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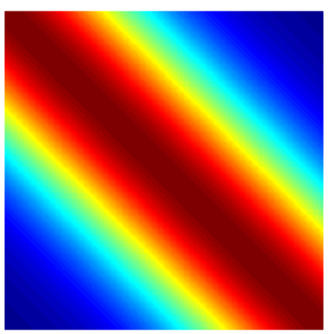
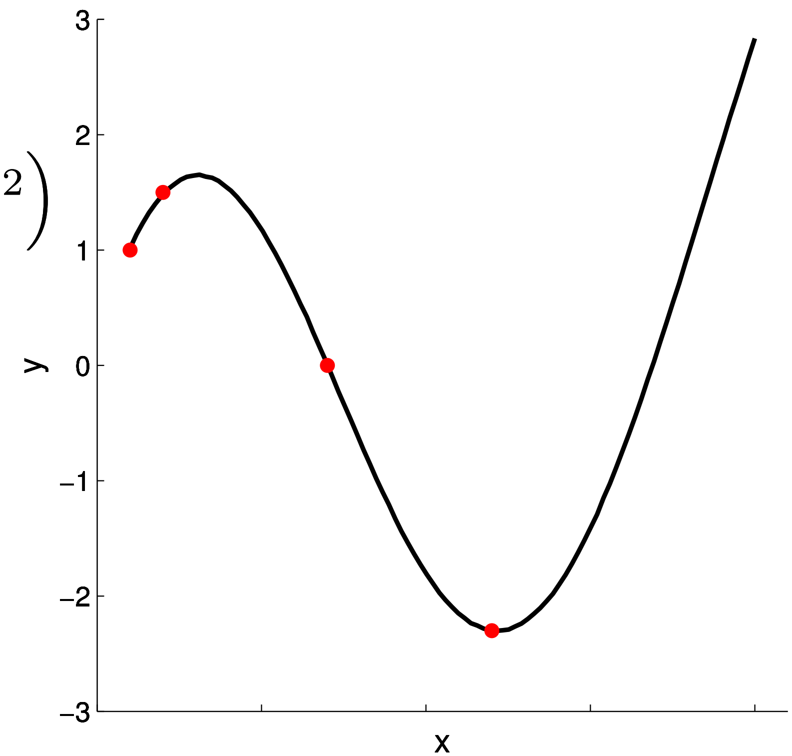
$\Sigma =$ 



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What effect do the hyper-parameters have?

long horizontal length-scale

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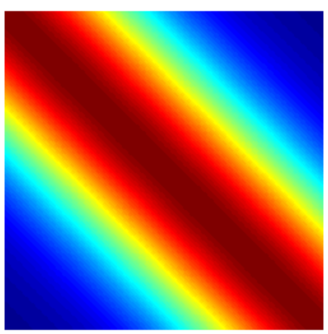

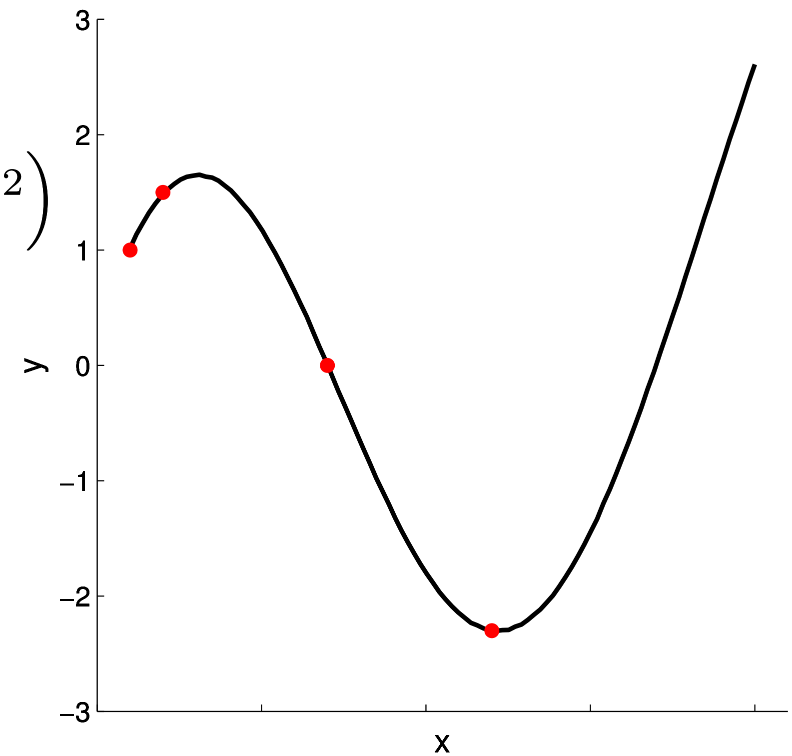

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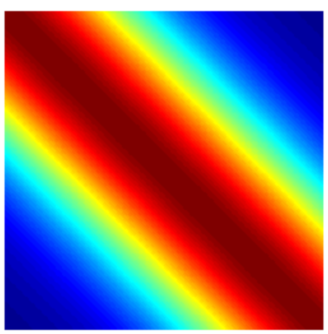

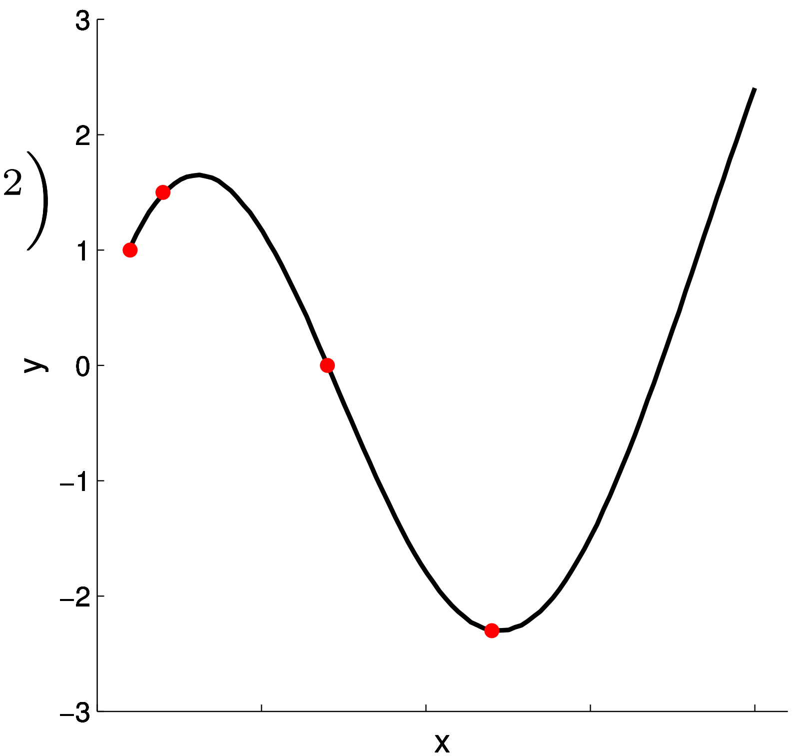

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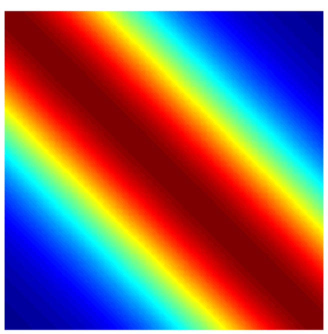
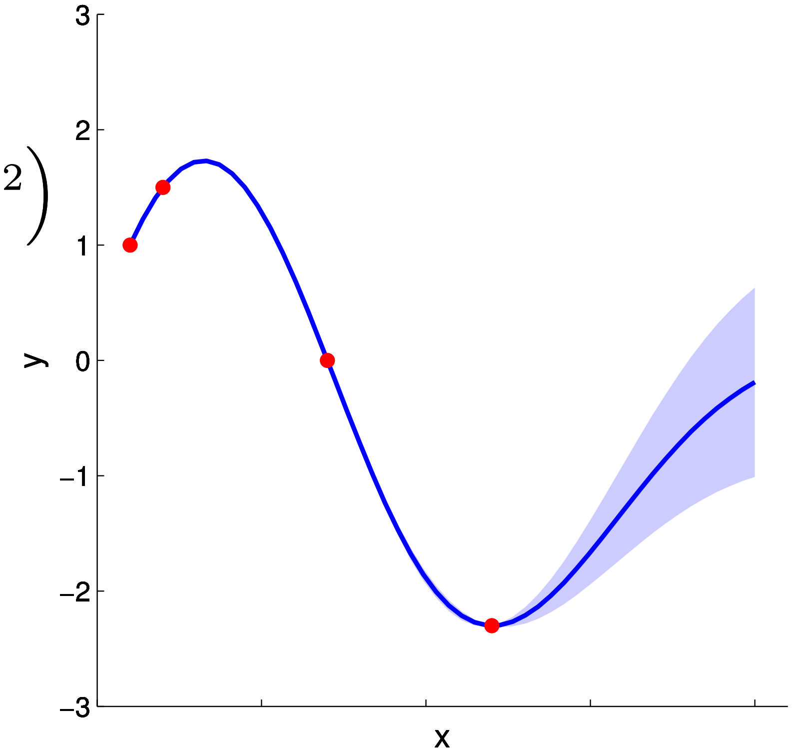
$\Sigma =$ 



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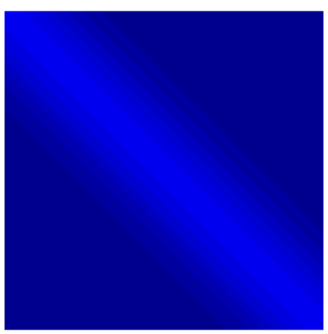
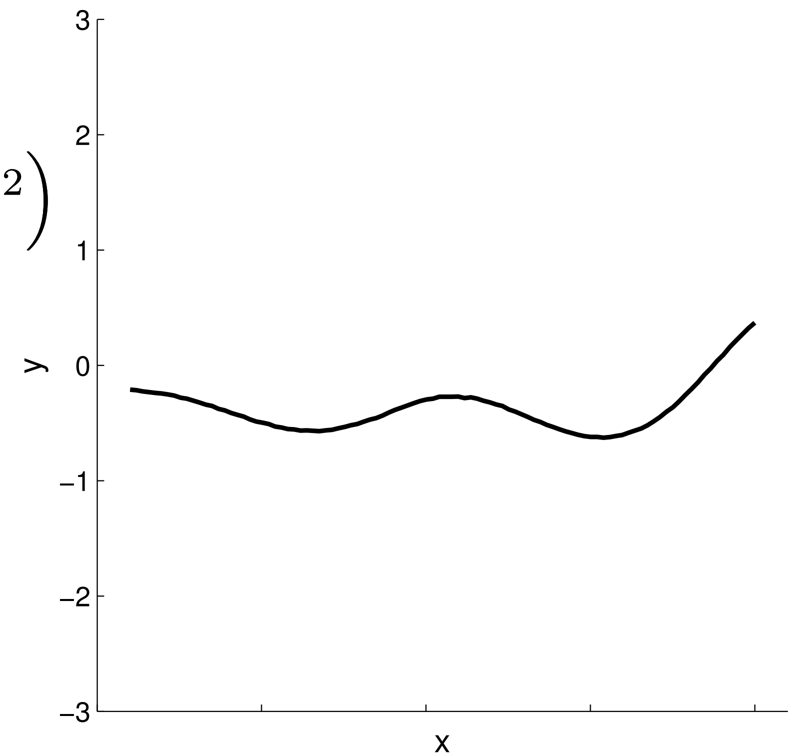
$\Sigma =$ 



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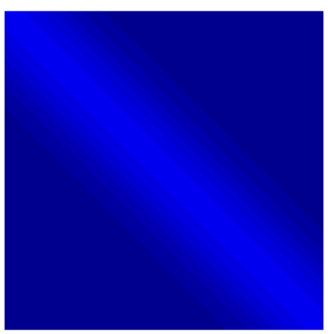

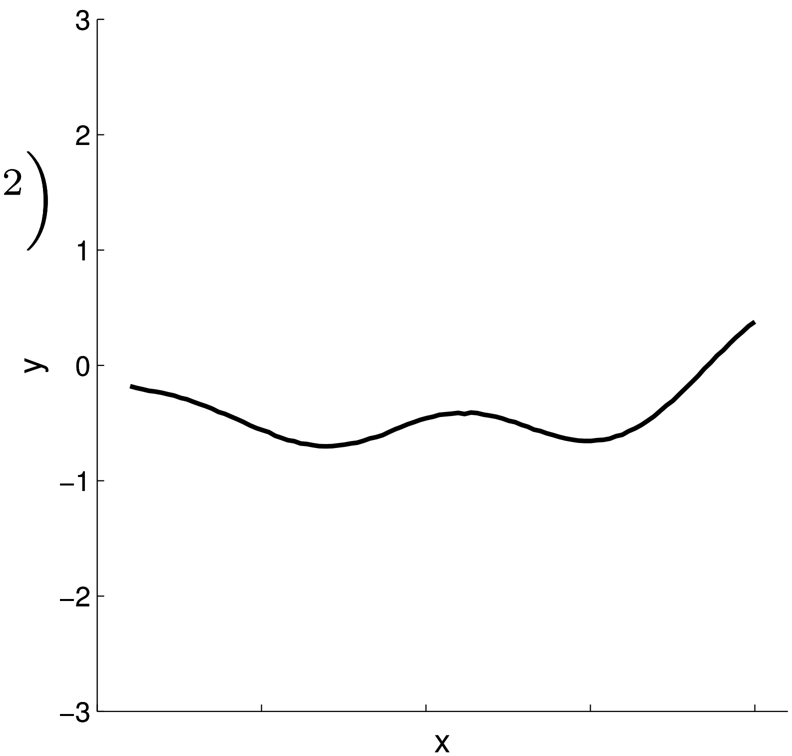

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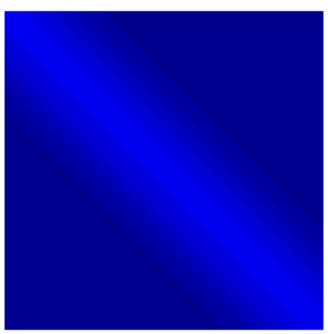
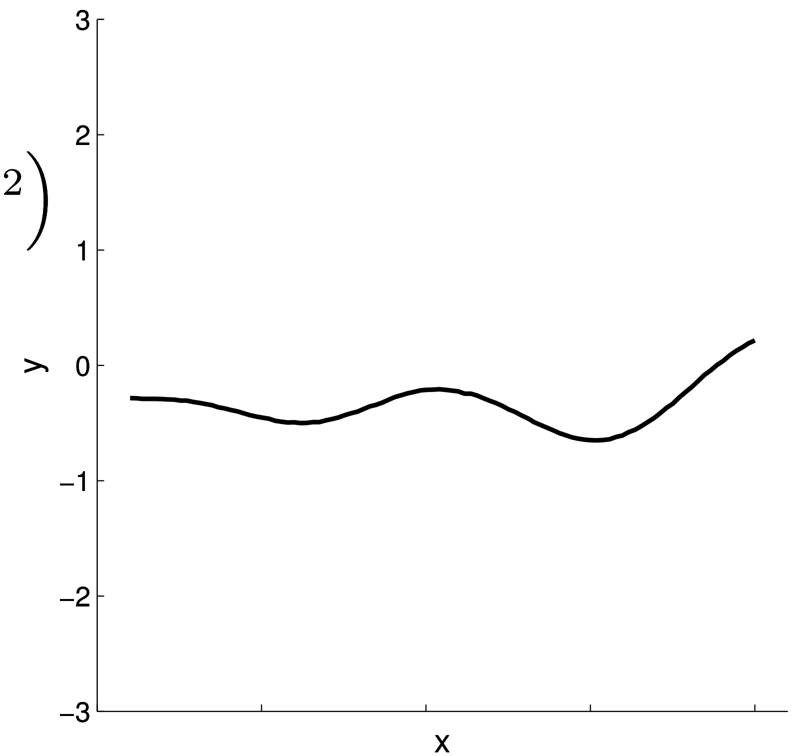
$\Sigma =$ 



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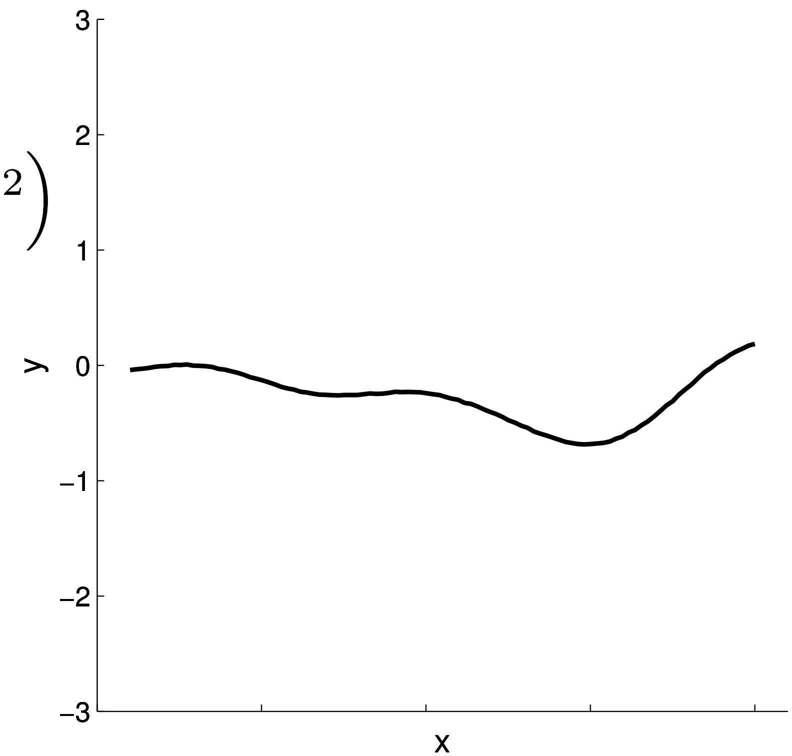

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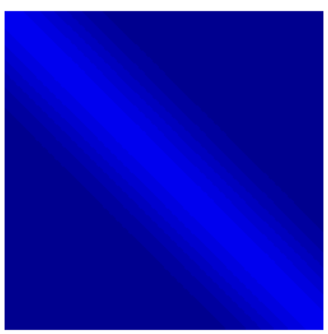
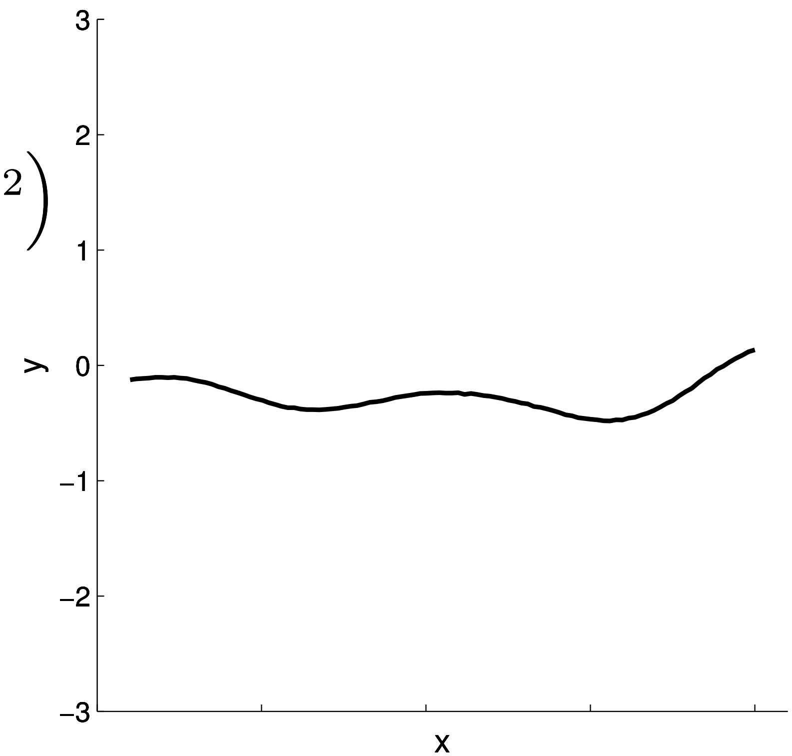
$\Sigma =$ 



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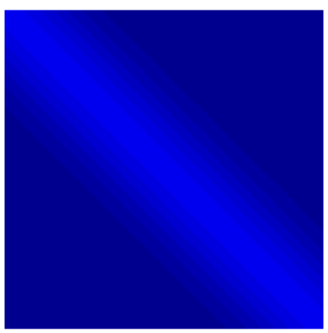
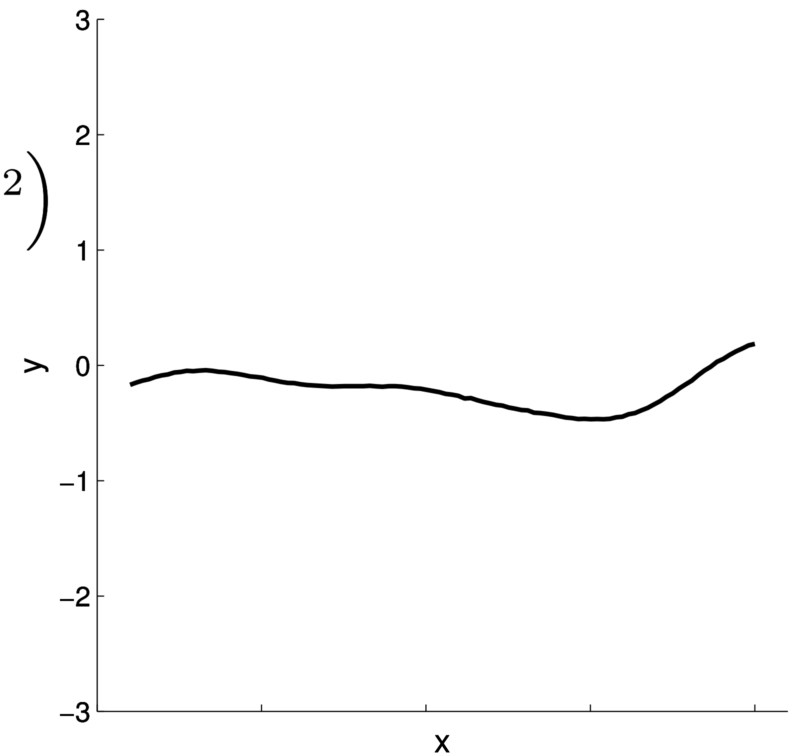
$\Sigma =$ 



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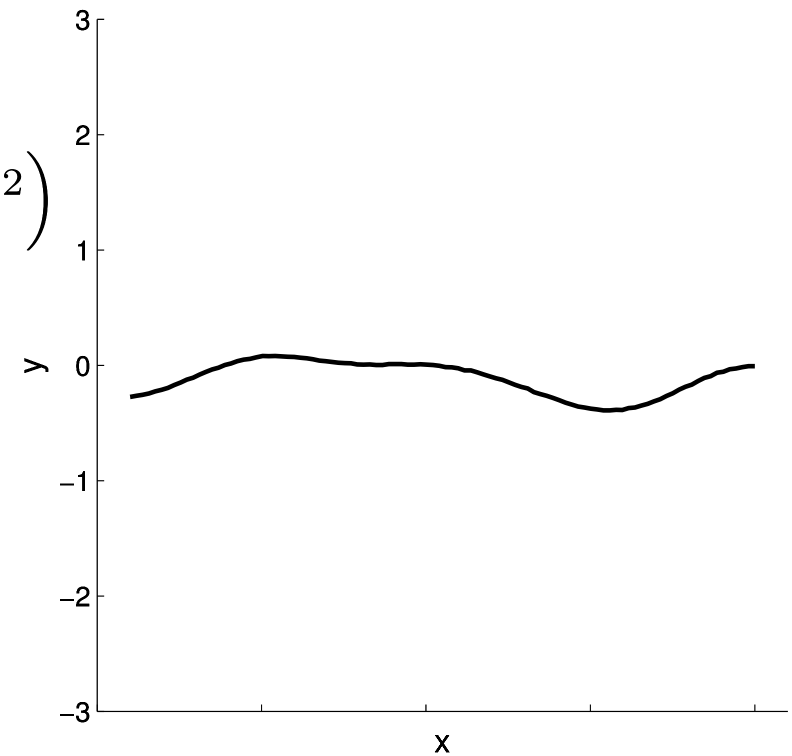

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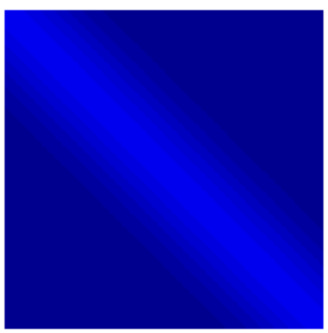
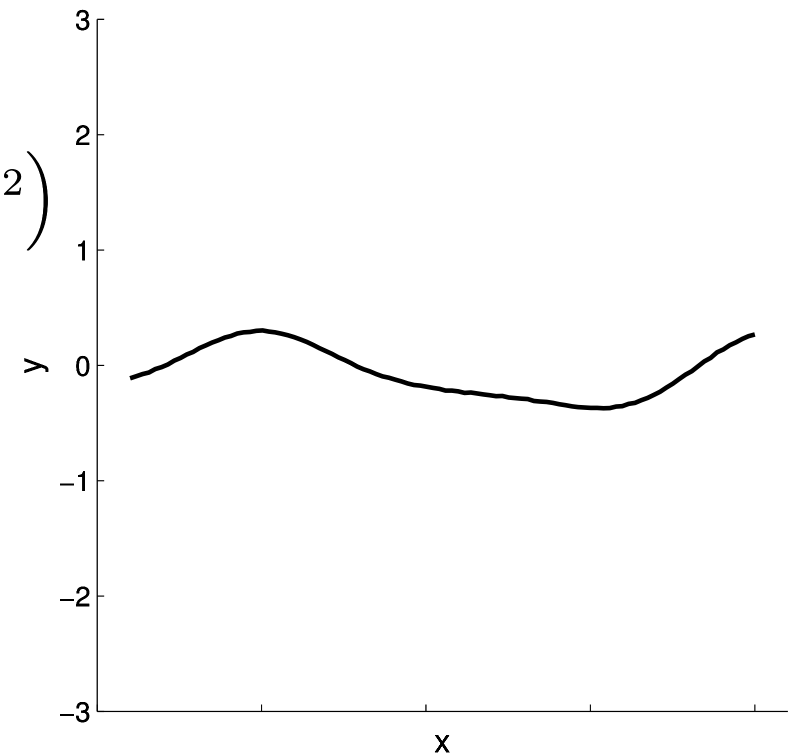
$\Sigma =$ 



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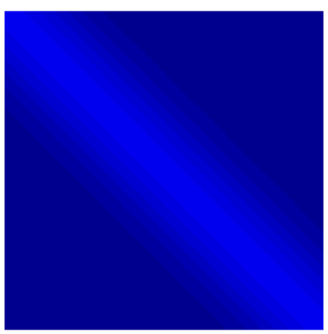
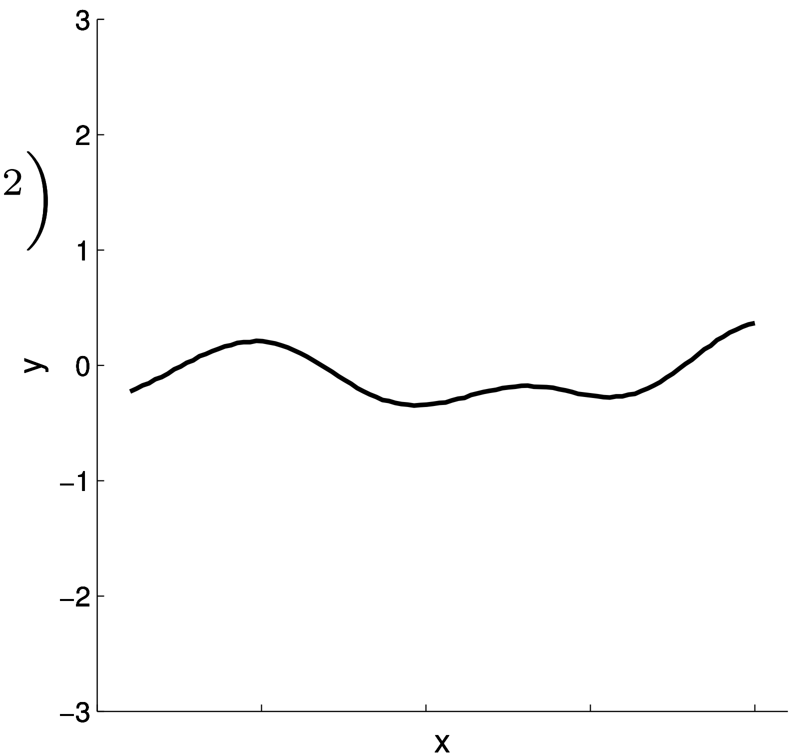
$\Sigma =$ 



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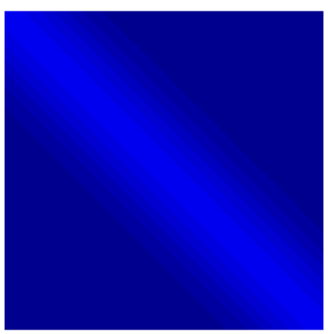
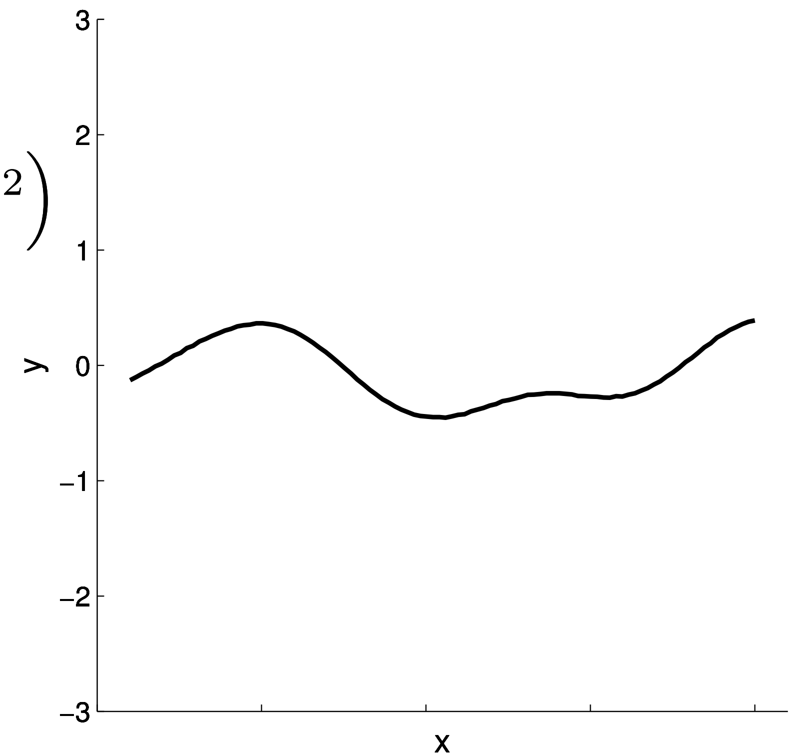
$\Sigma =$ 



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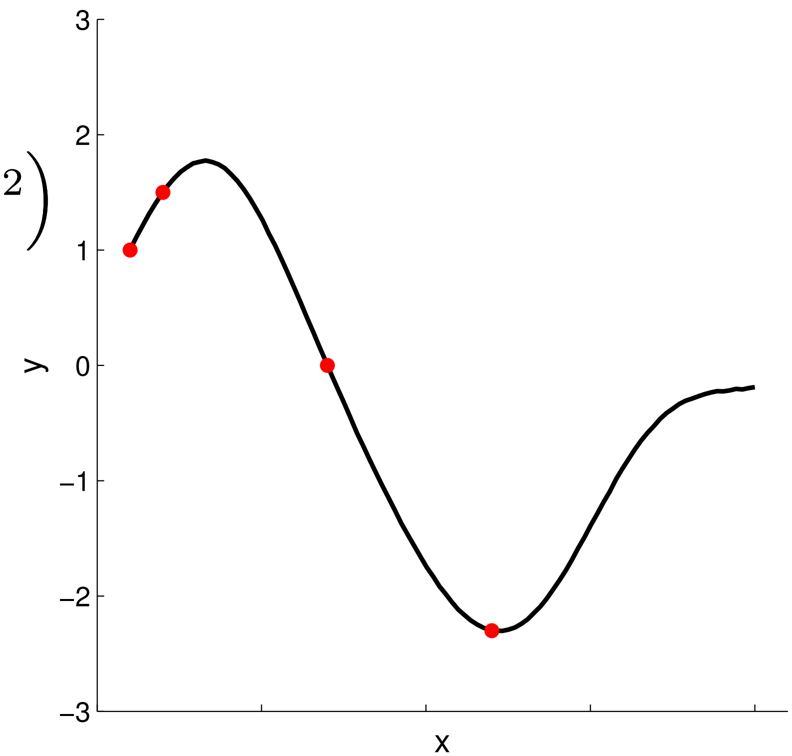

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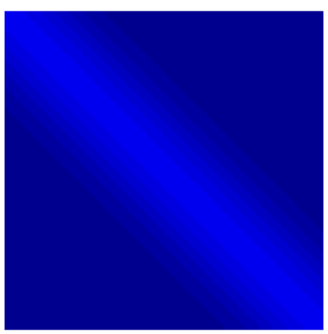

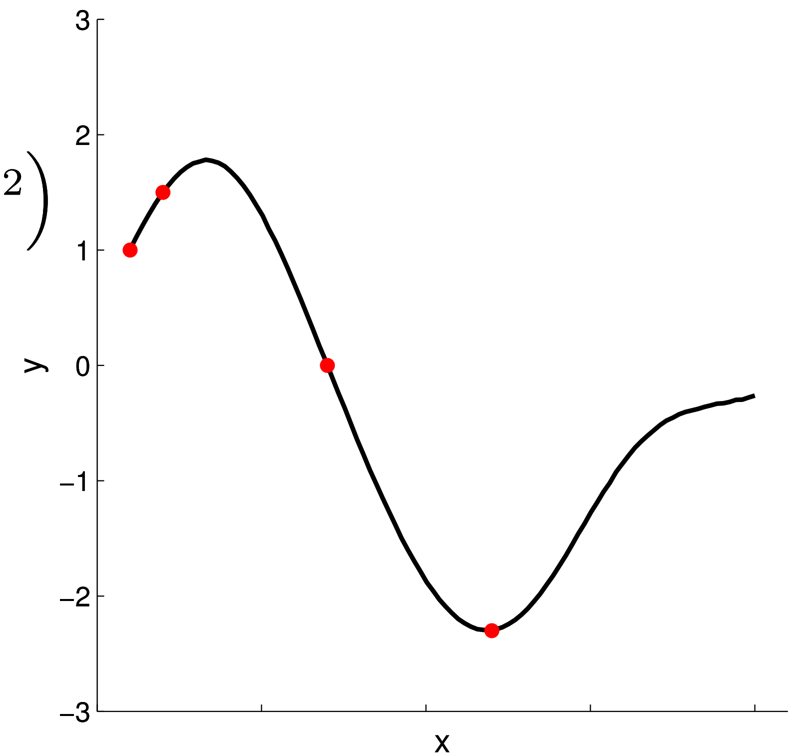

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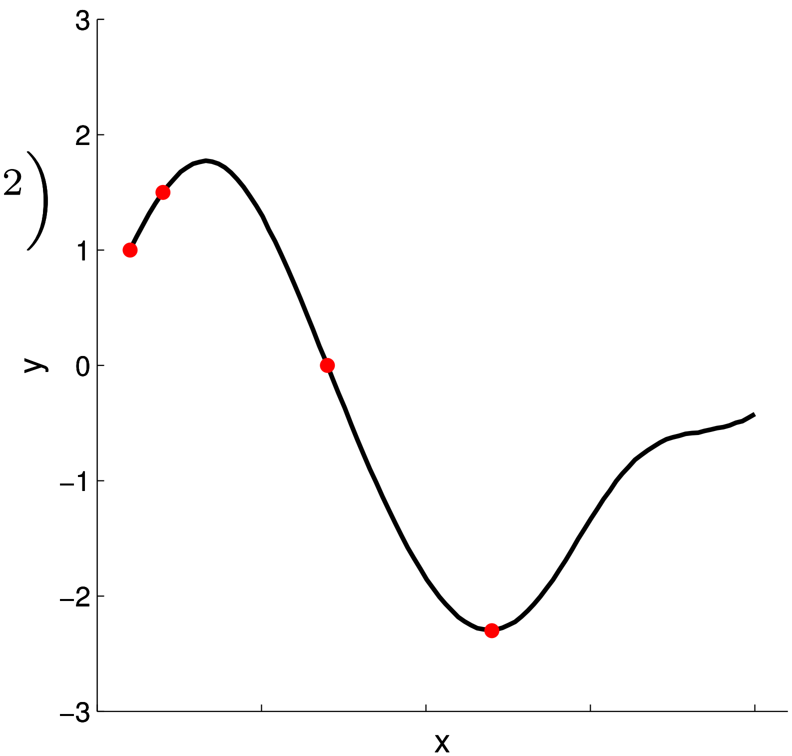

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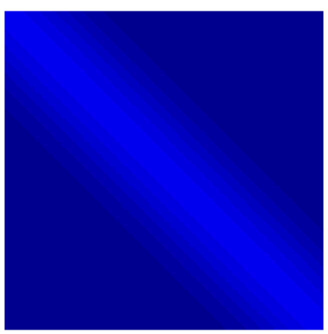

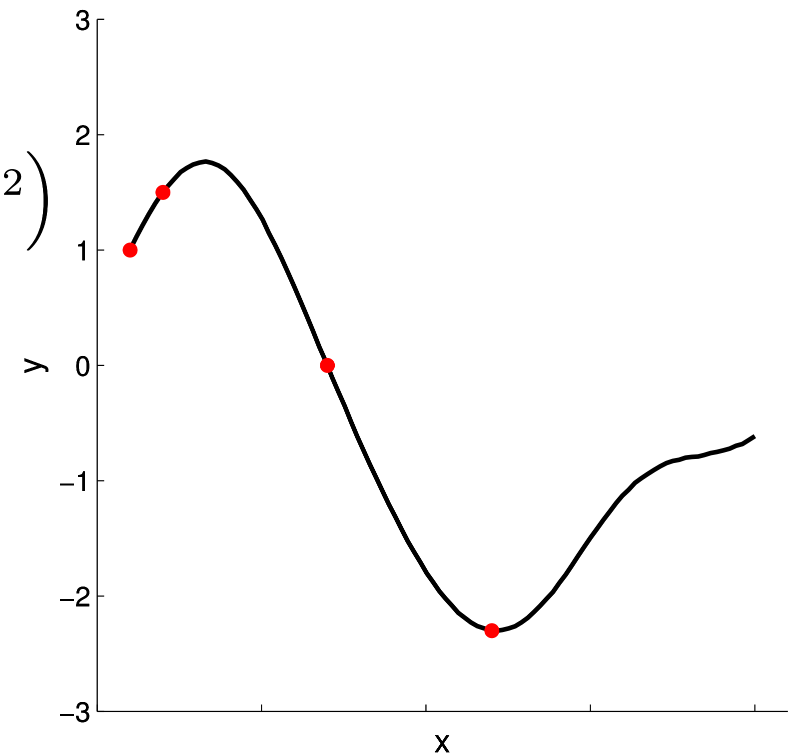

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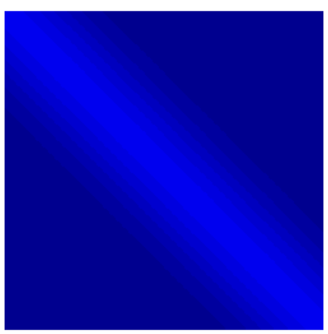
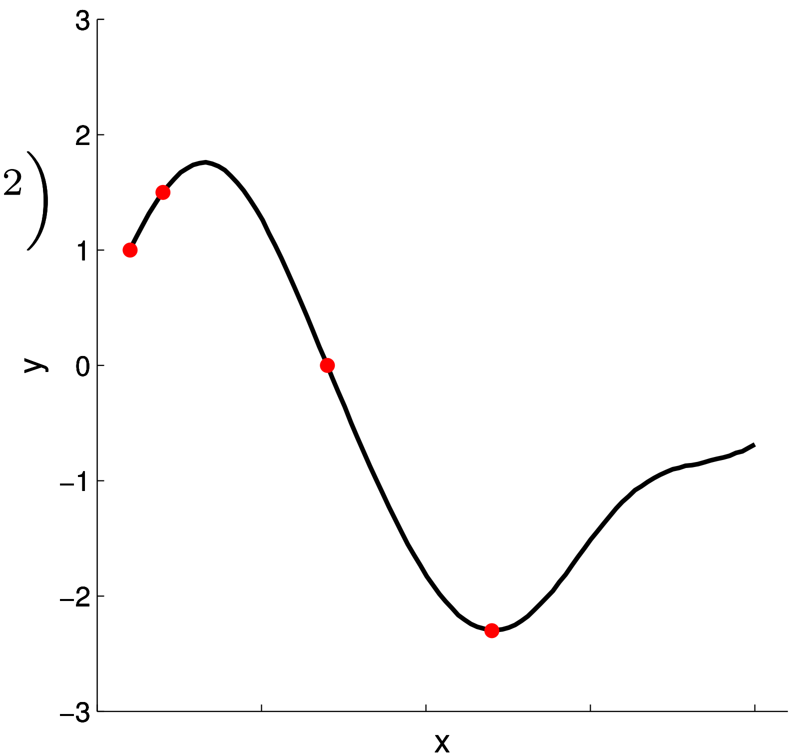
$\Sigma =$ 



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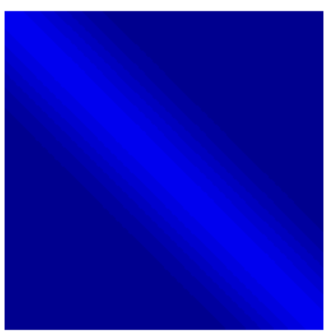
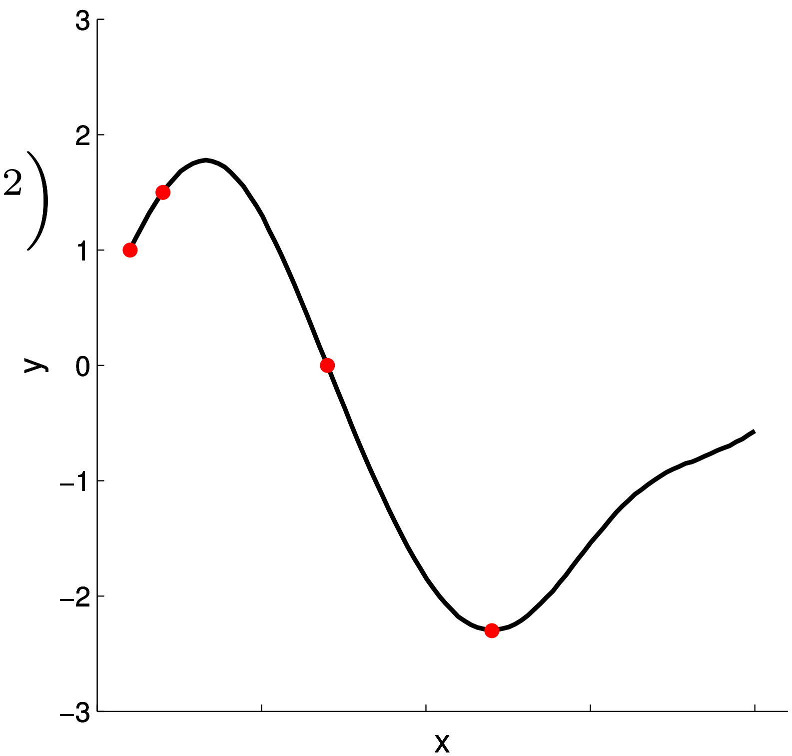
$\Sigma =$ 



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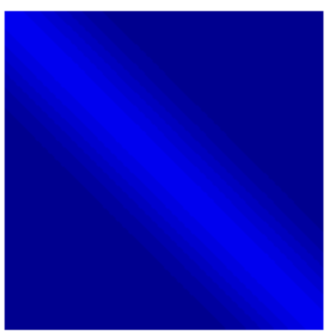

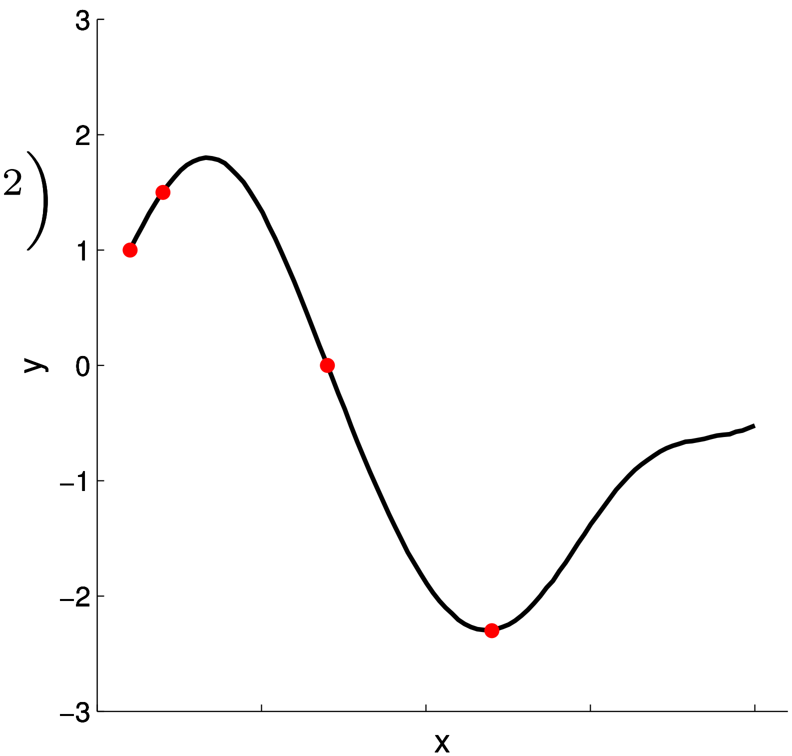

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$\epsilon \sim \mathcal{N}(0, 1)$

What effect do the hyper-parameters have?

small vertical scale

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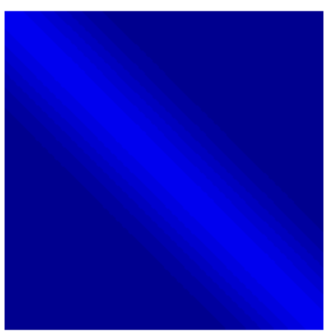

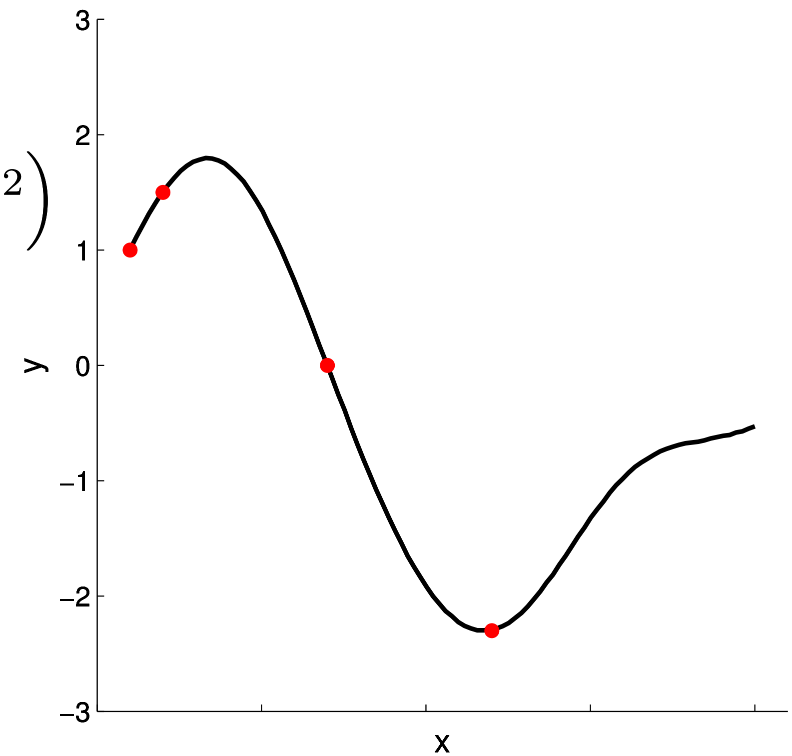

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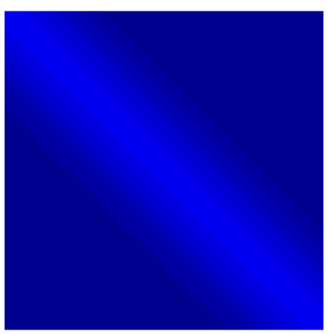
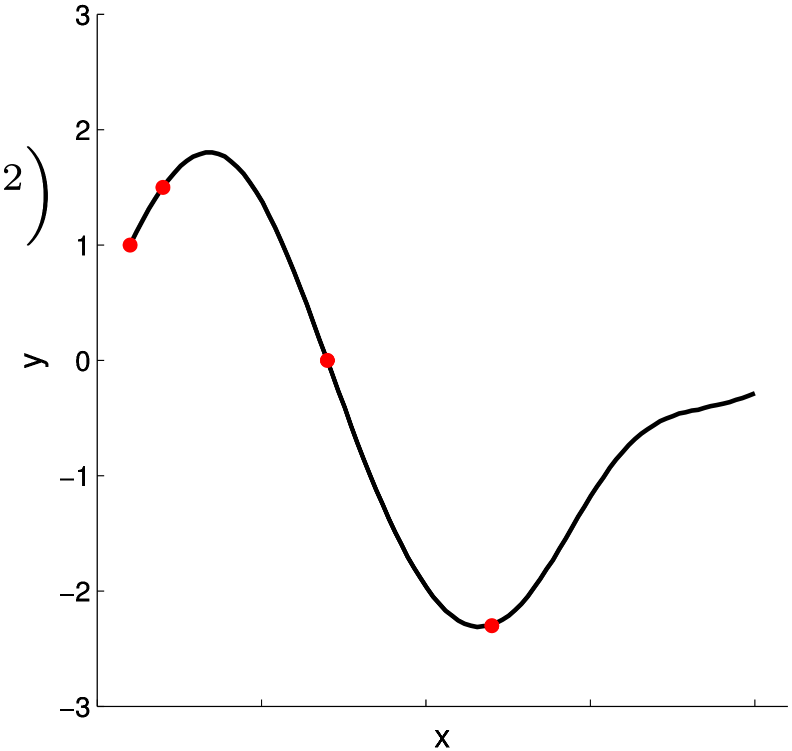
$\Sigma =$ 



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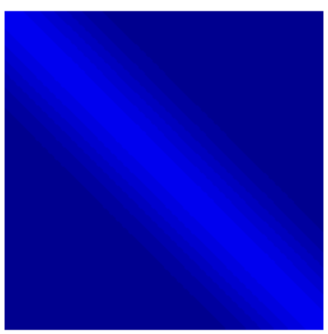
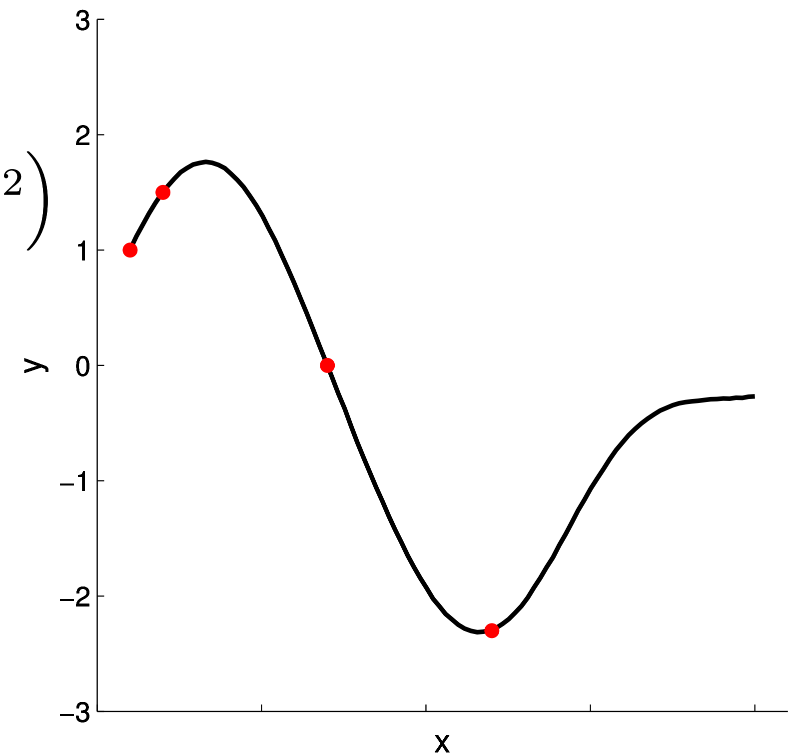
$\Sigma =$ 



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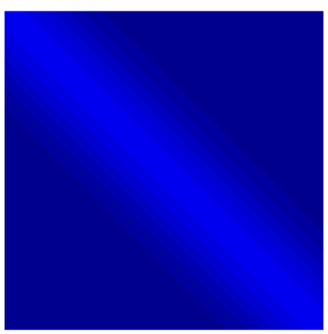
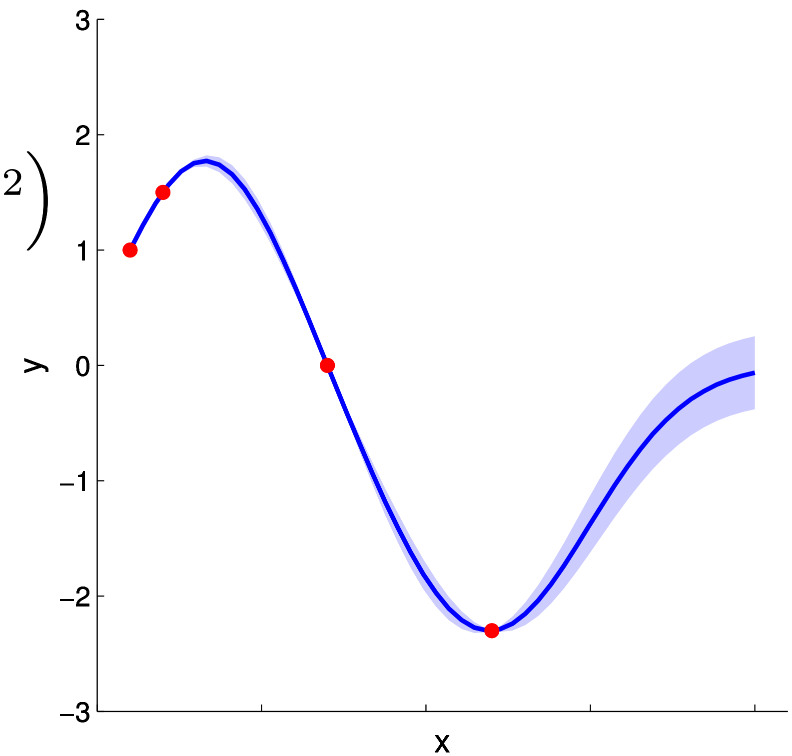
$\Sigma =$ 



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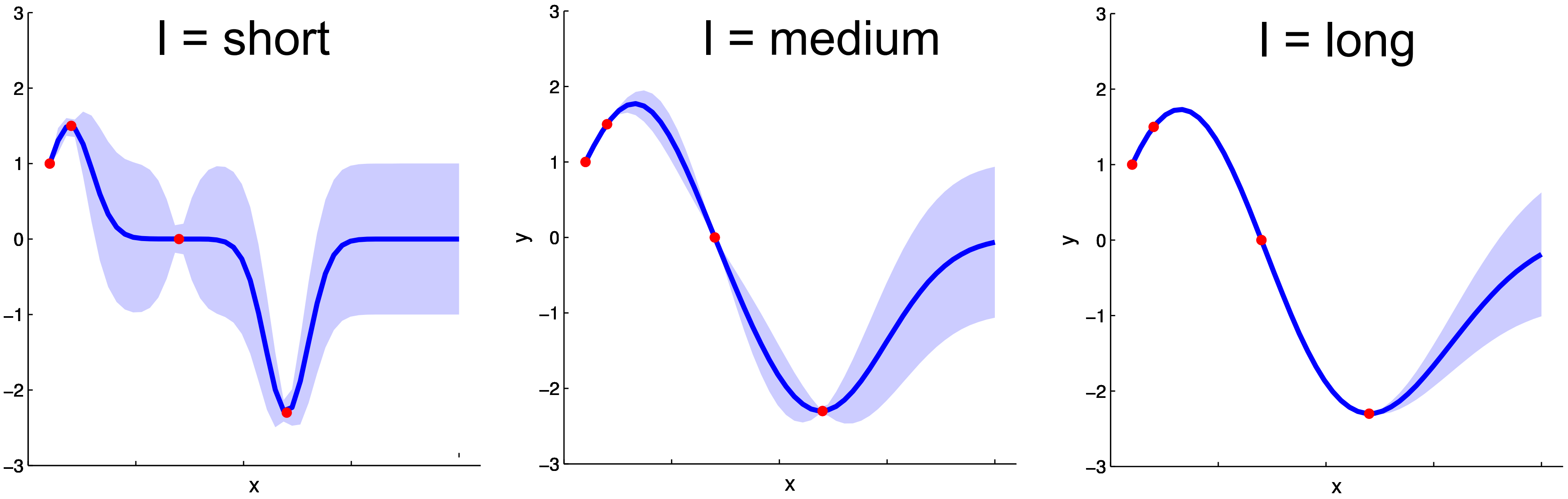
What effect do the hyper-parameters have?

$$K(x_1, x_2) = \sigma^2 \exp\left(-\frac{1}{2l^2}(x_1 - x_2)^2\right)$$

- Hyper-parameters have a strong effect
  - l controls the horizontal length-scale
  - σ^2 controls the vertical scale of the data
- $\Longrightarrow$ we need automatic ways of learning the hyper-parameters from data



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$p(\mathbf{y}_{1:N}|\theta)$ = likelihood of the parameters

= how well did θ predict the data we observed

$$p(\mathbf{y}_{1:N}|\theta) = \frac{1}{\det(2\pi\Sigma(\theta))^{-1/2}} \exp\left(-\frac{1}{2}\mathbf{y}_{1:N}^{\intercal}\Sigma^{-1}(\theta)\mathbf{y}_{1:N}\right)$$

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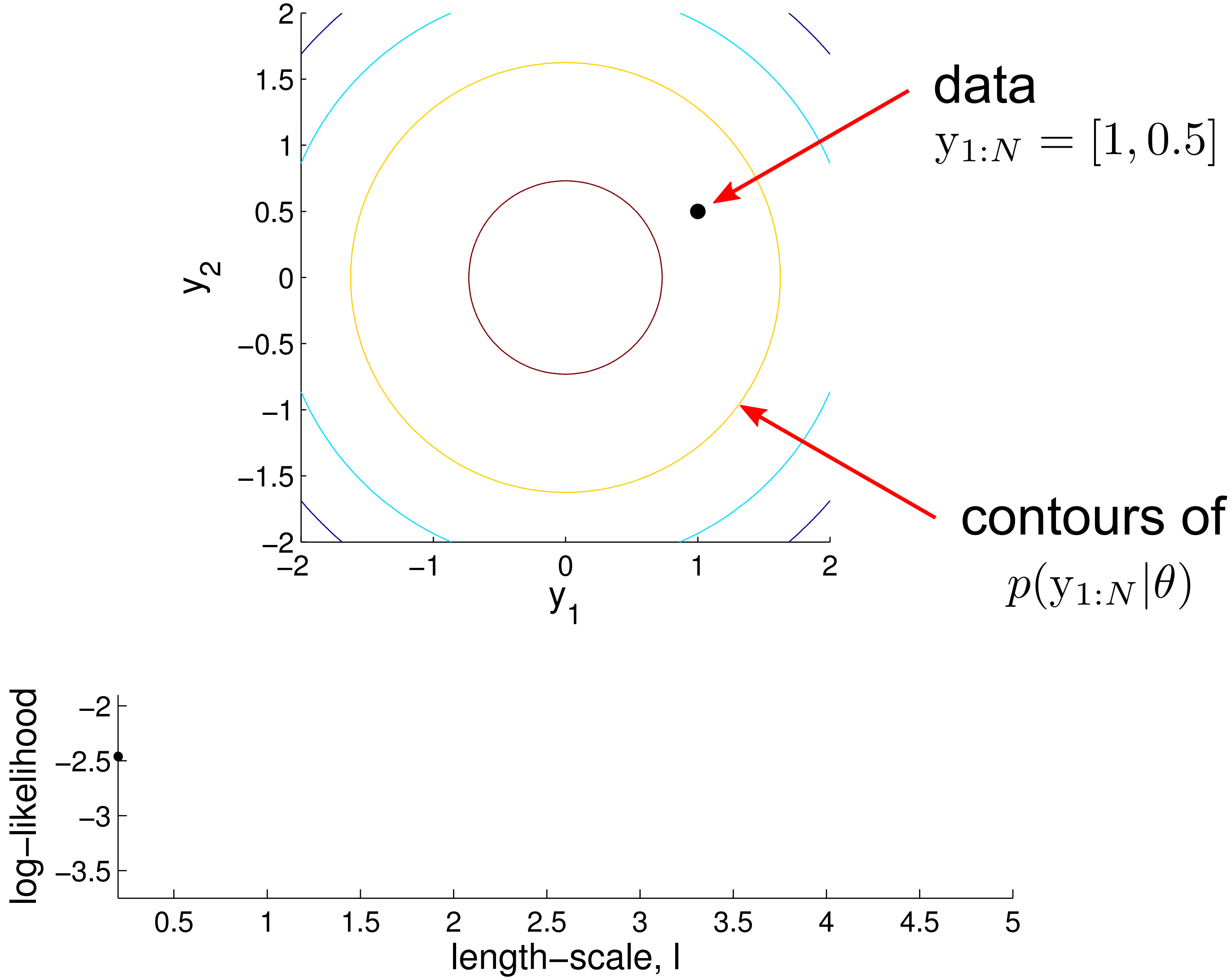

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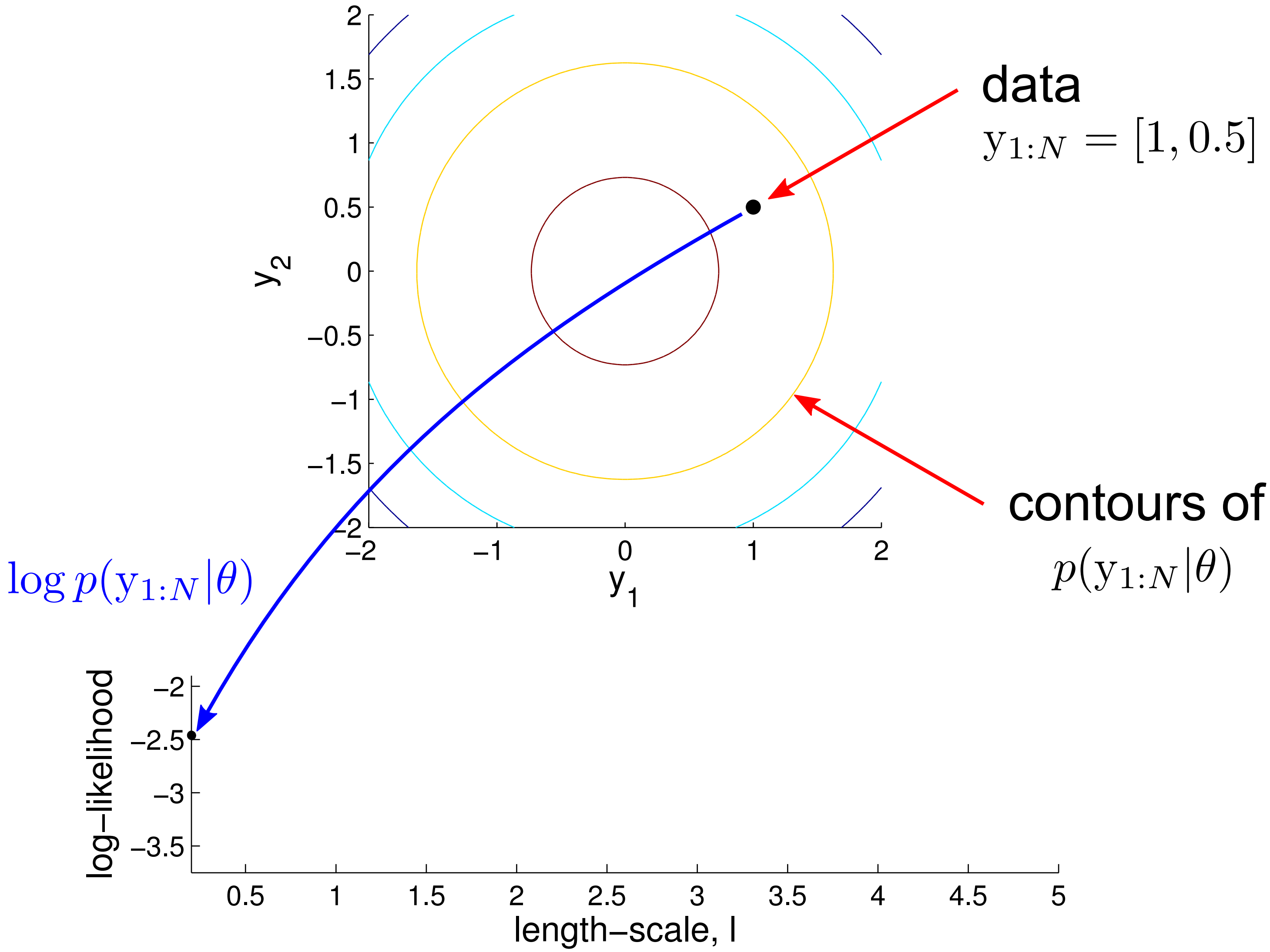

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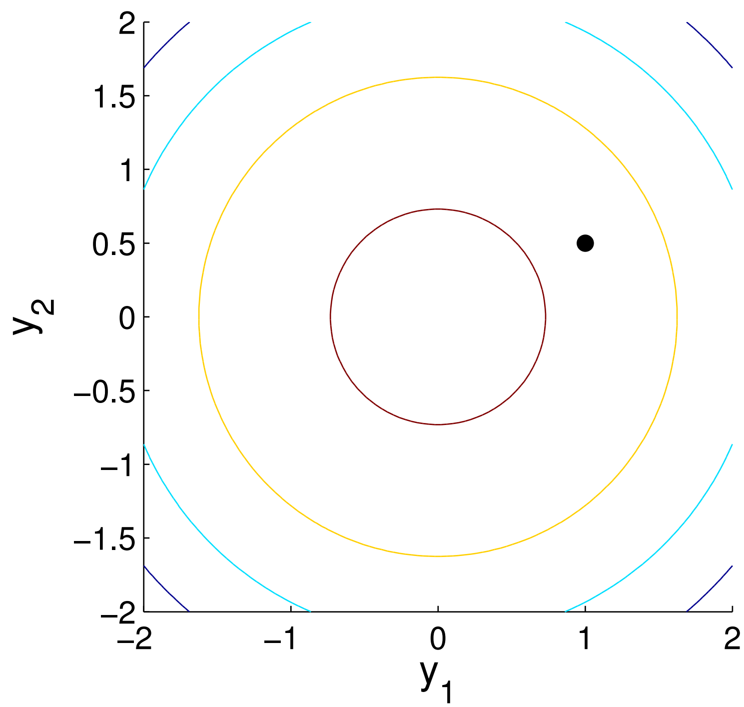

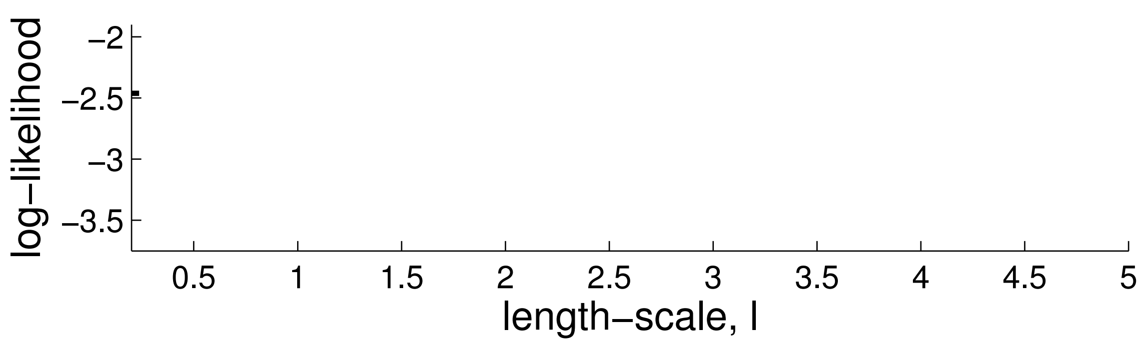

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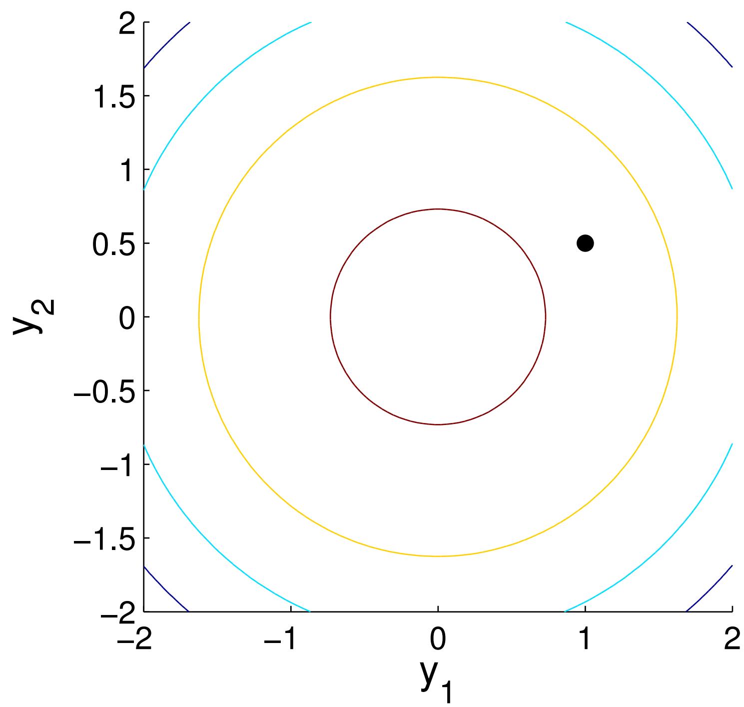

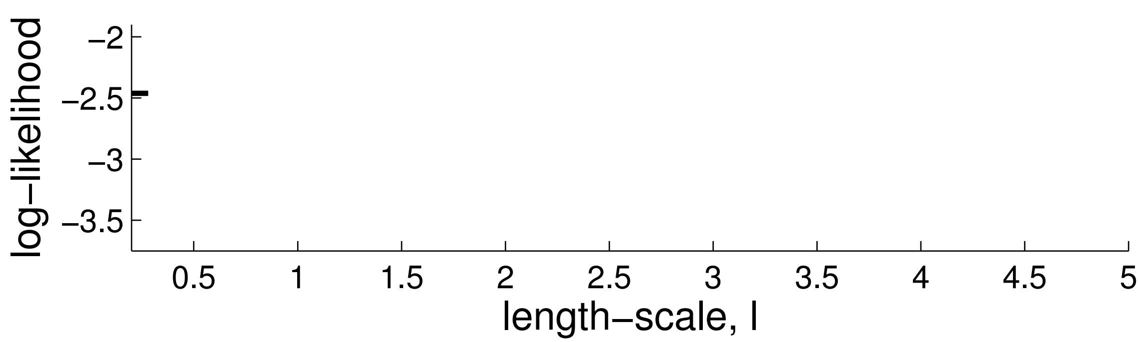

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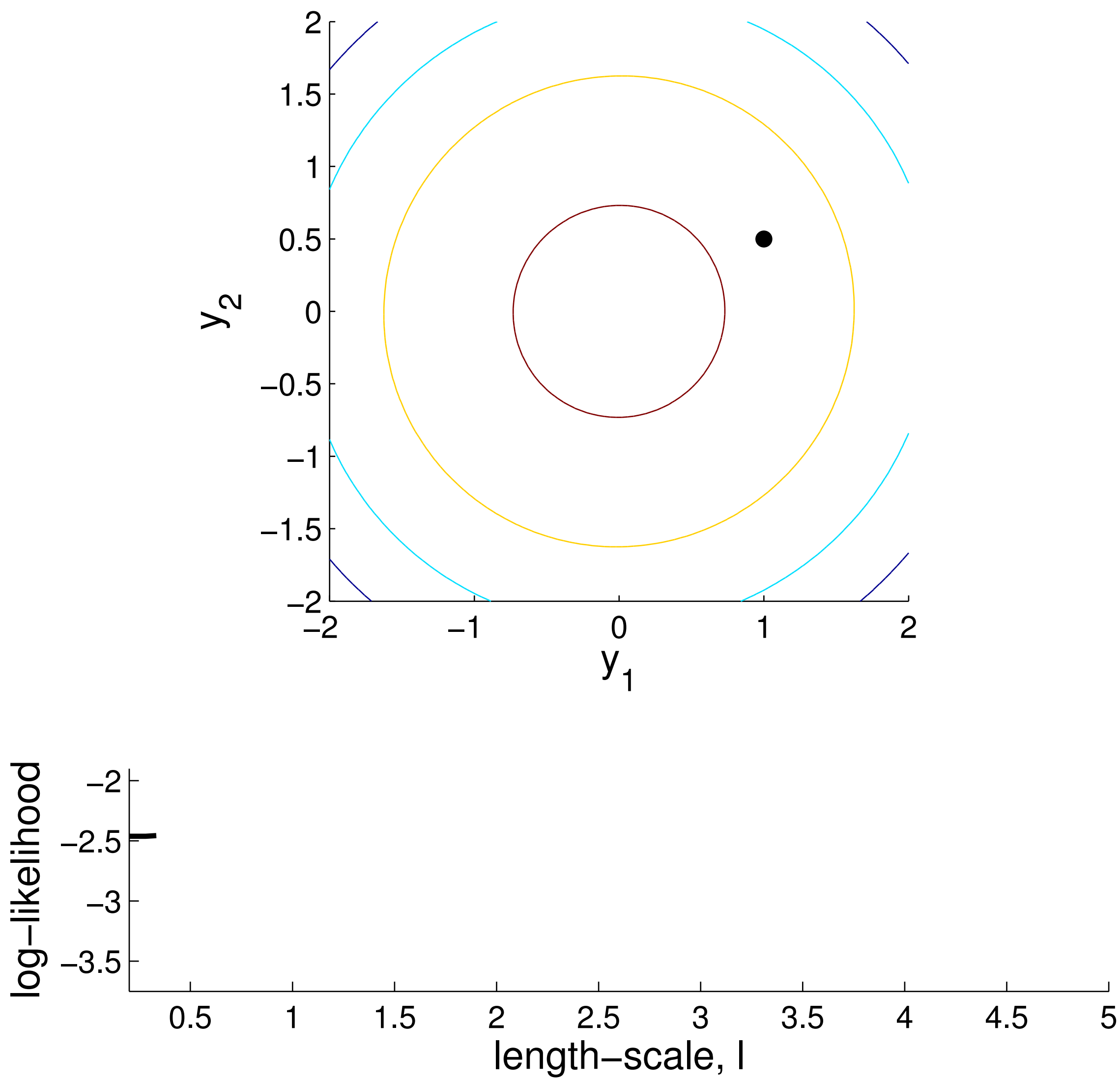

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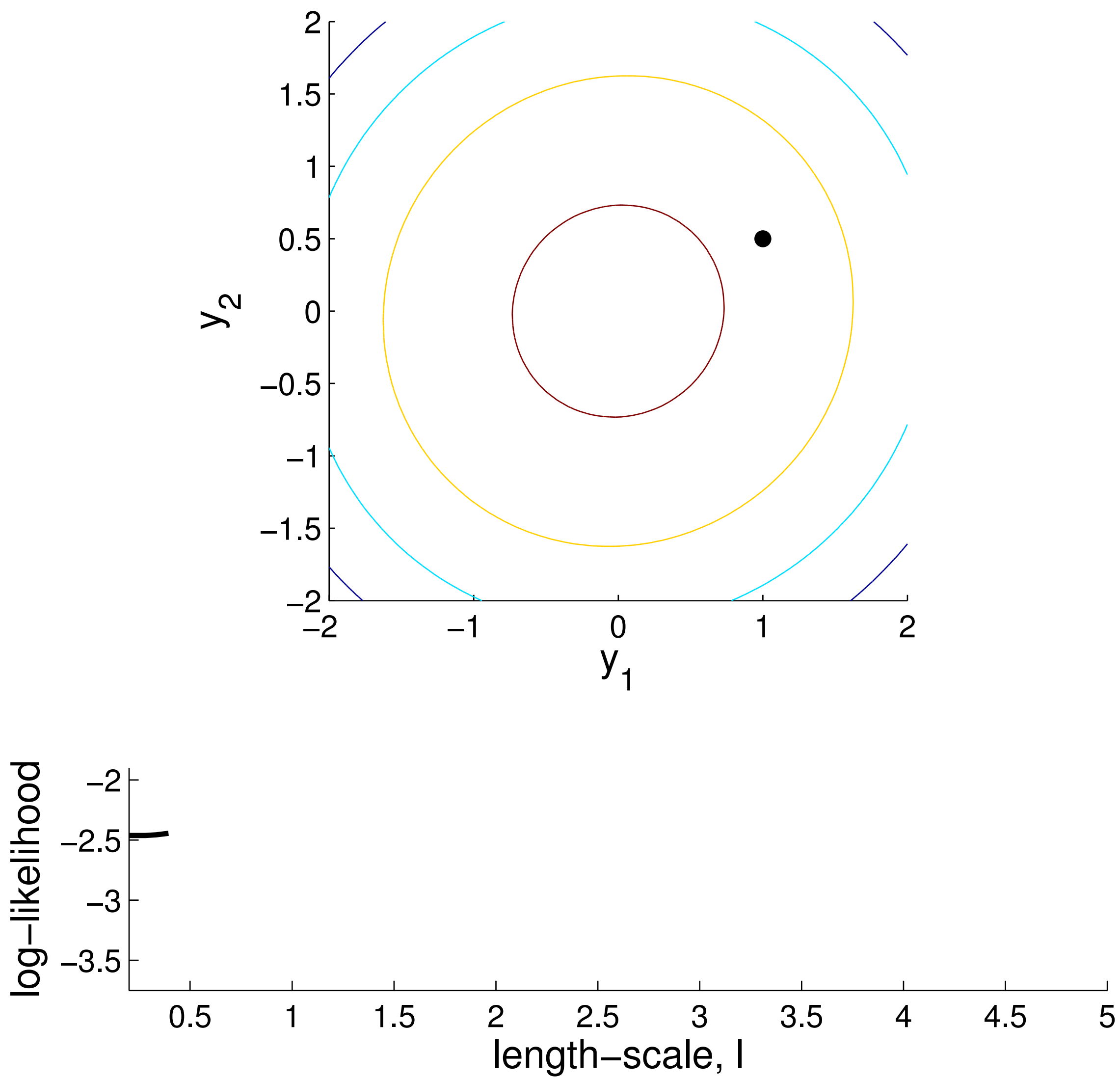

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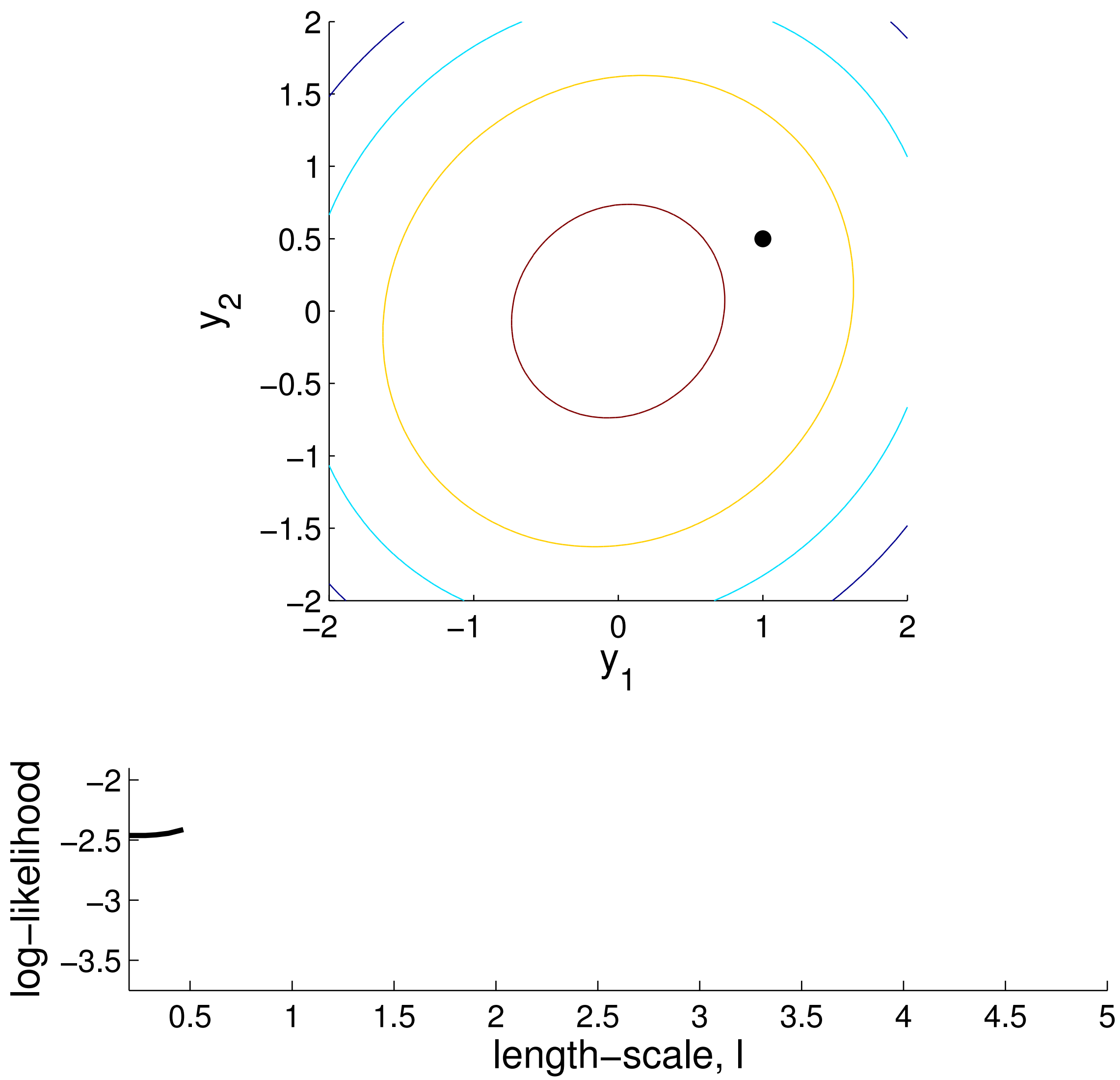

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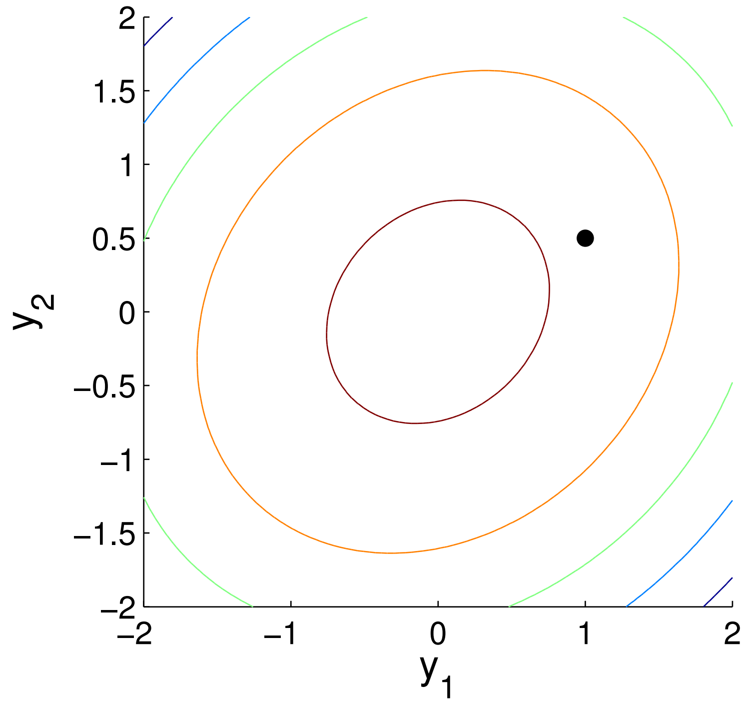

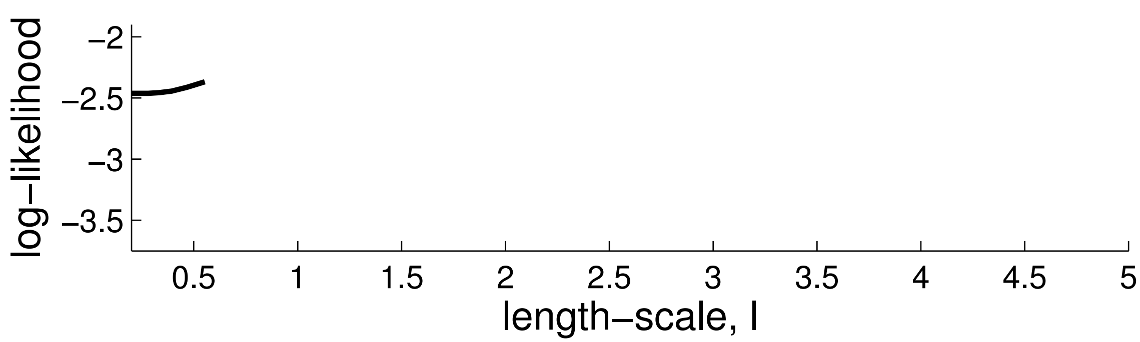

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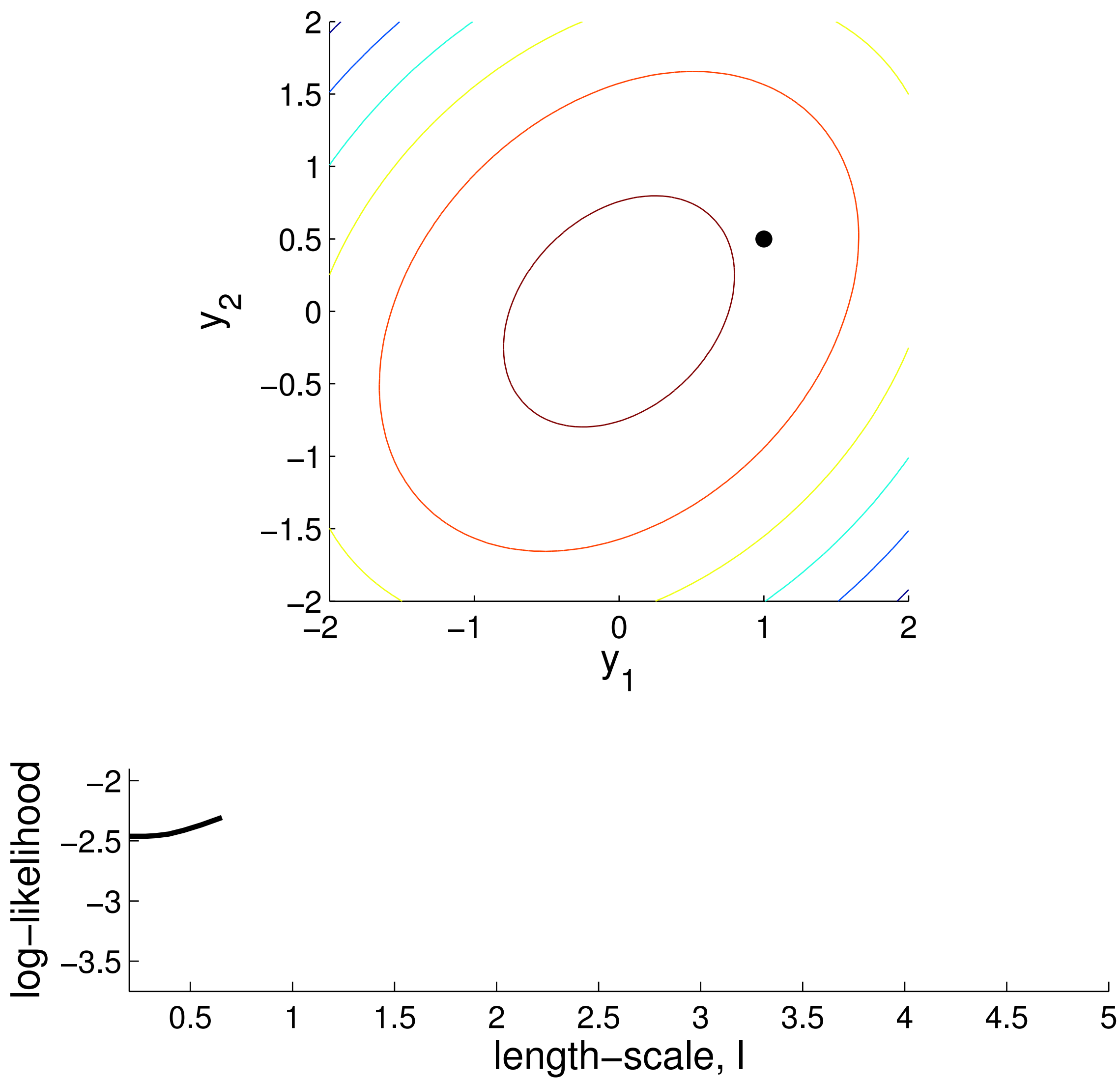

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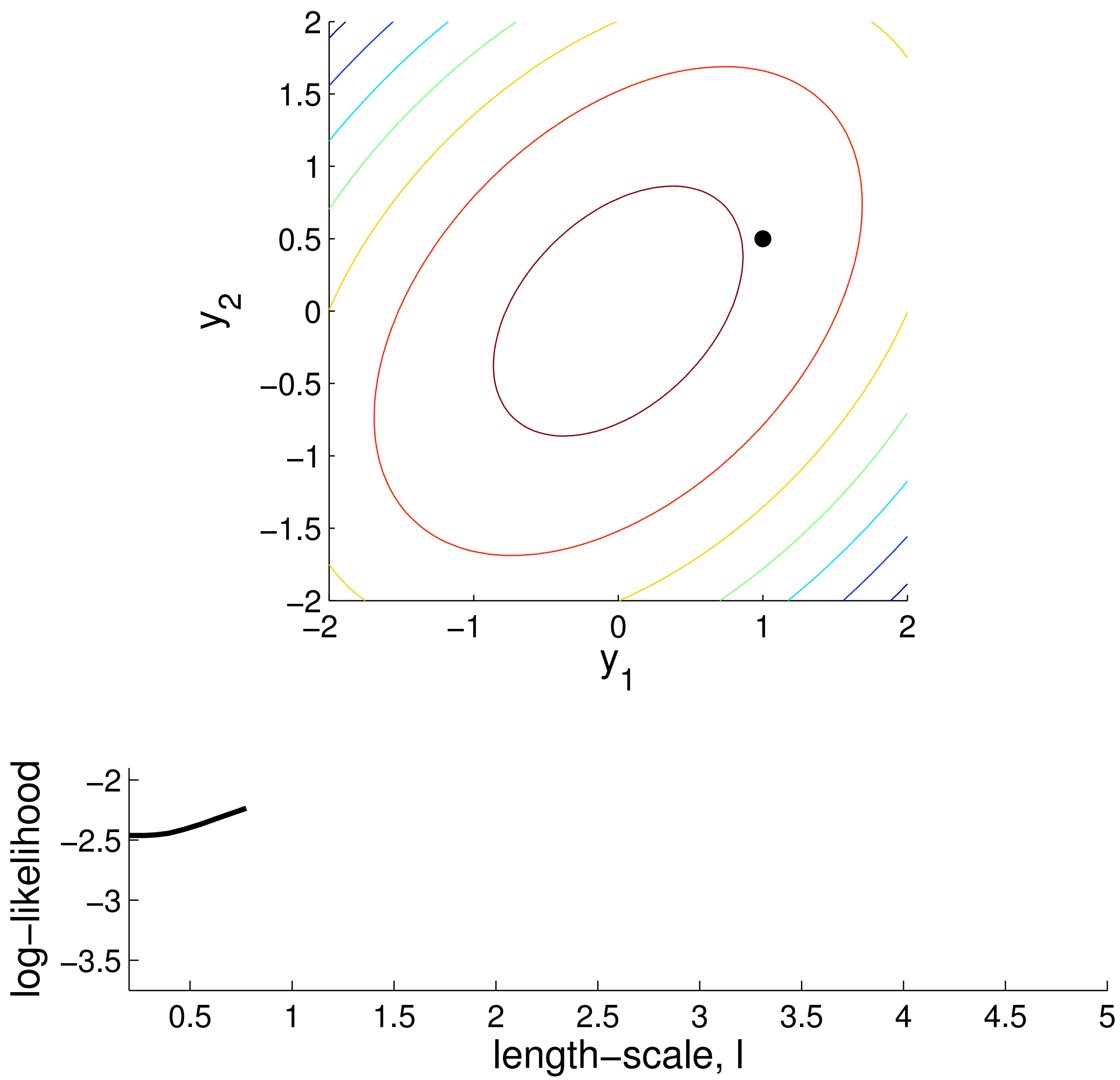

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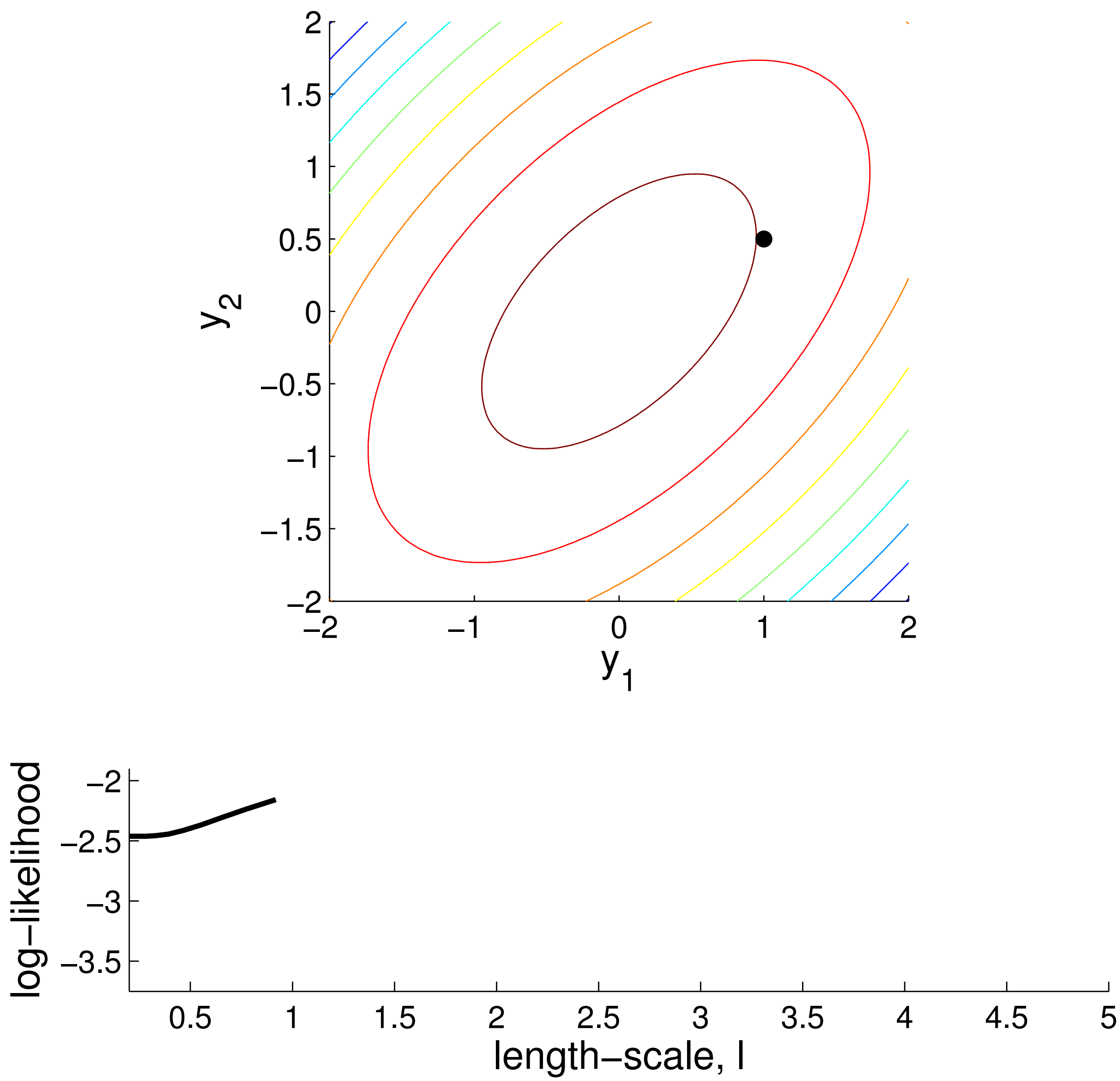

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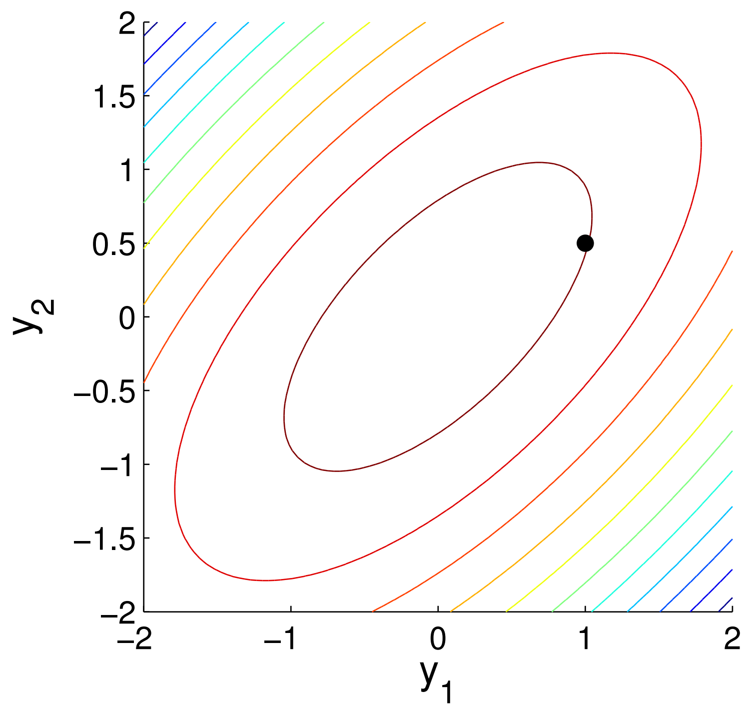

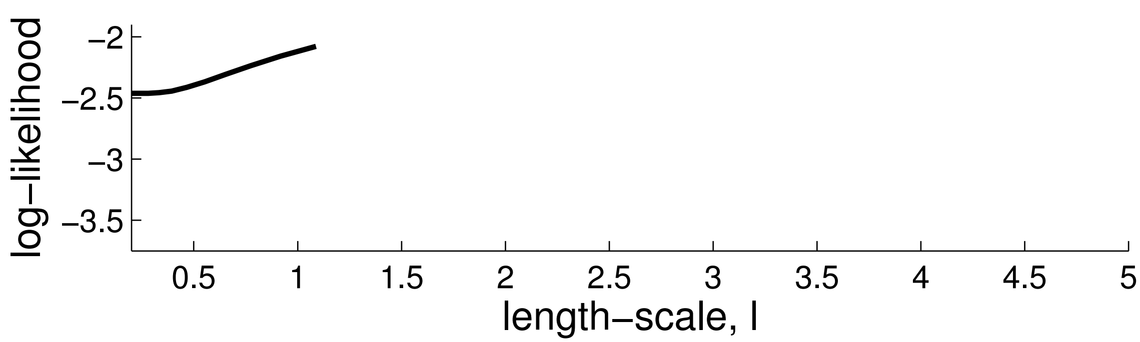

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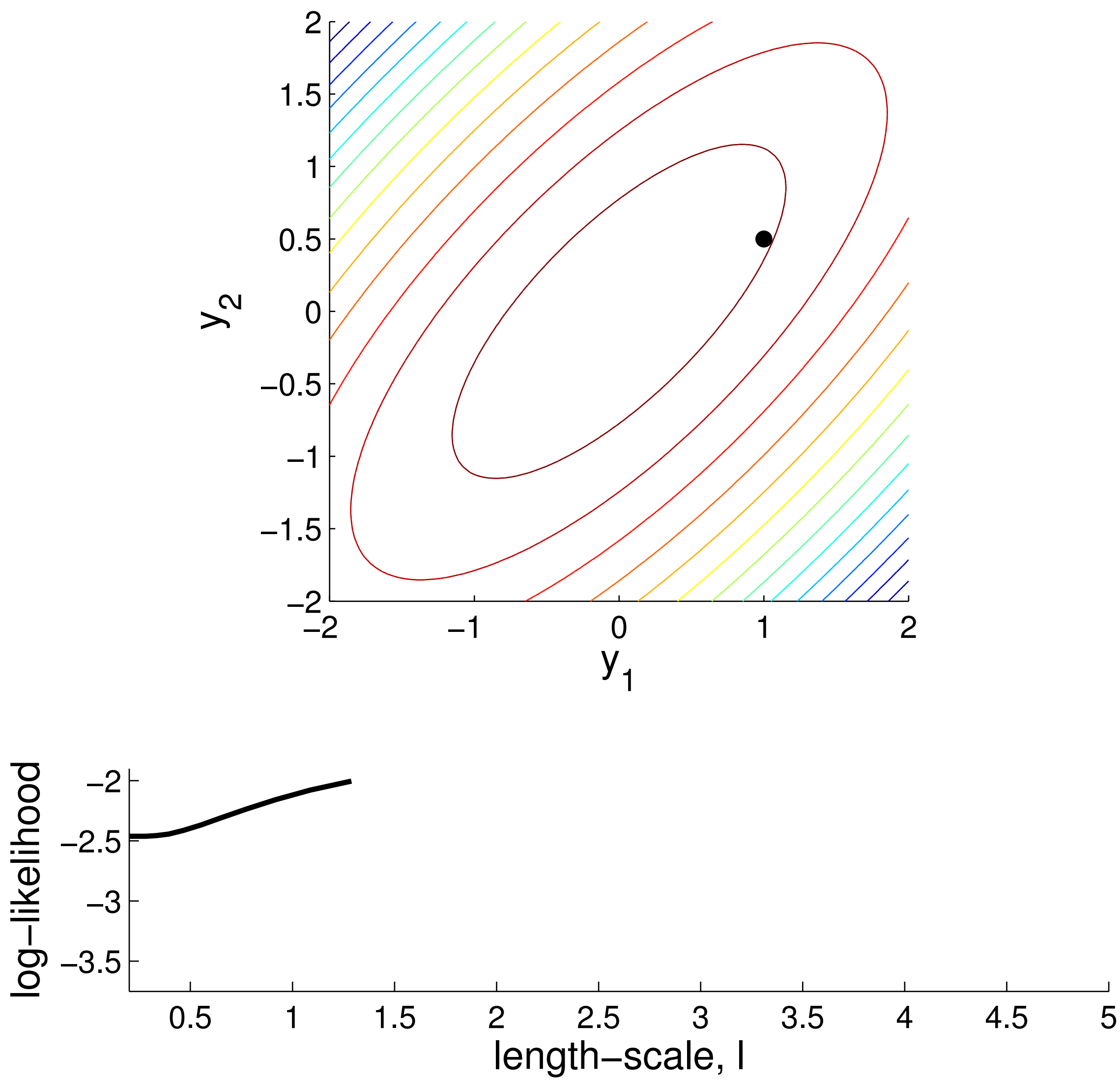

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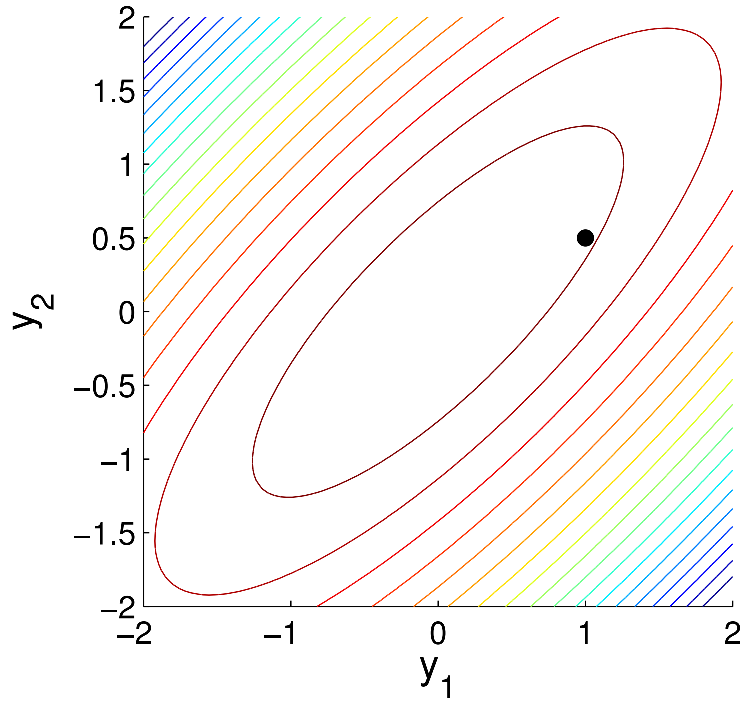

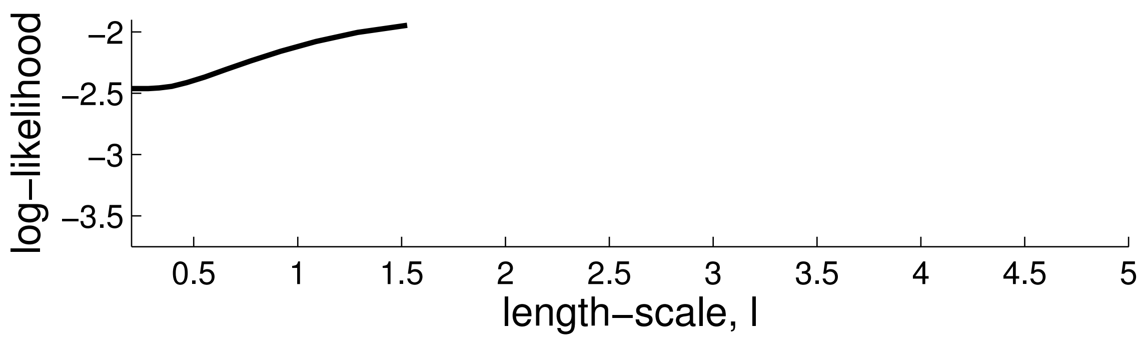

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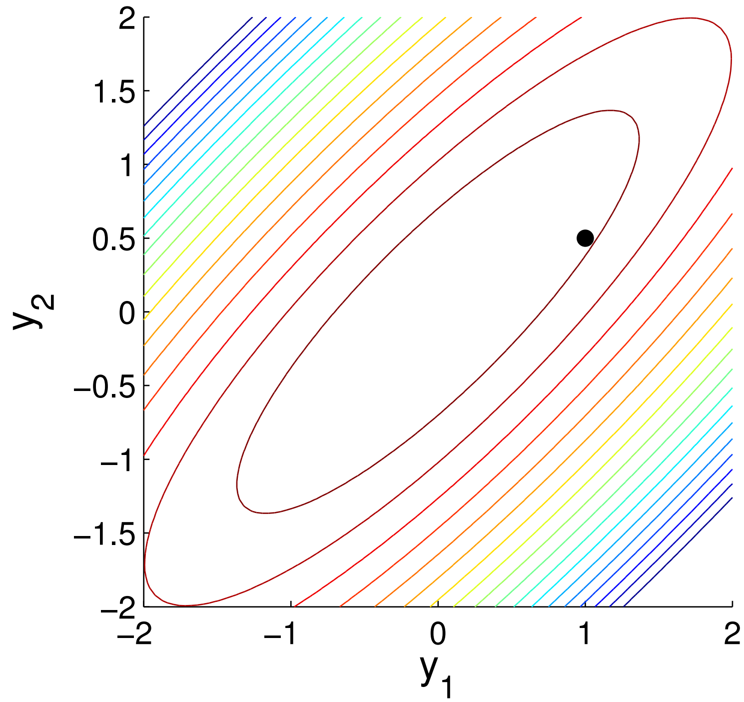

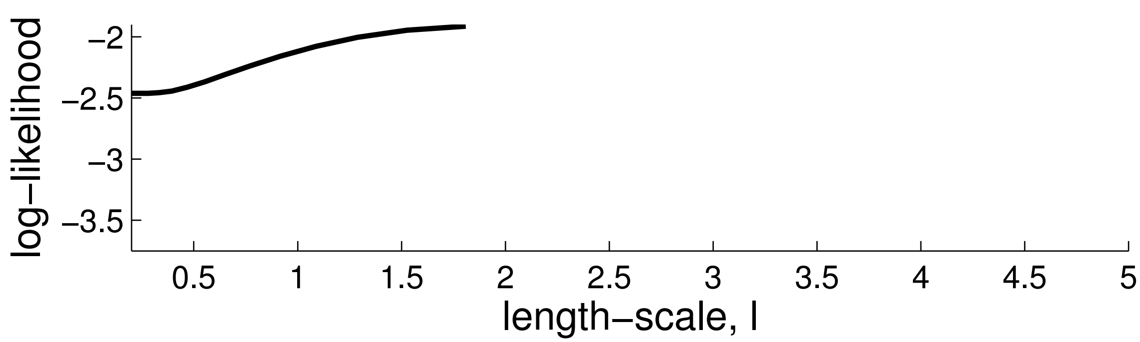

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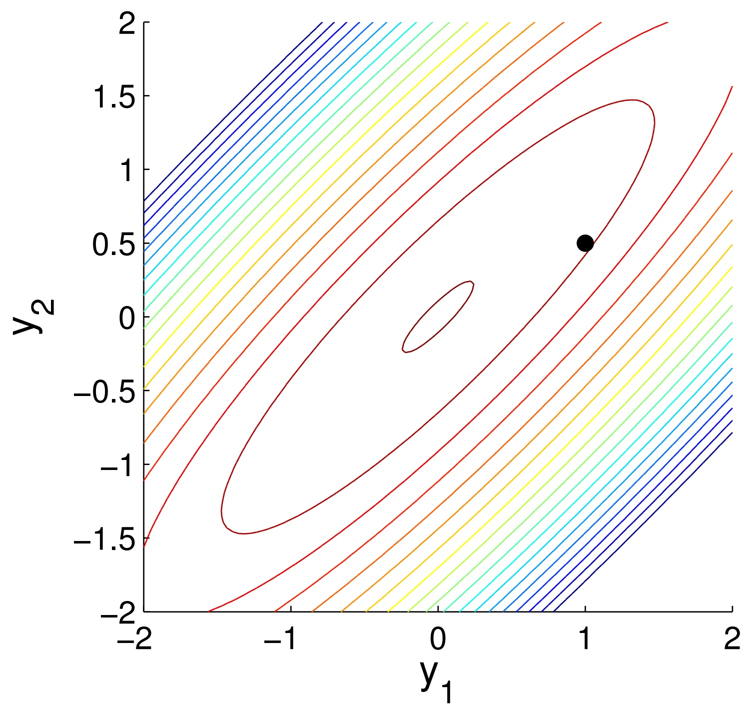

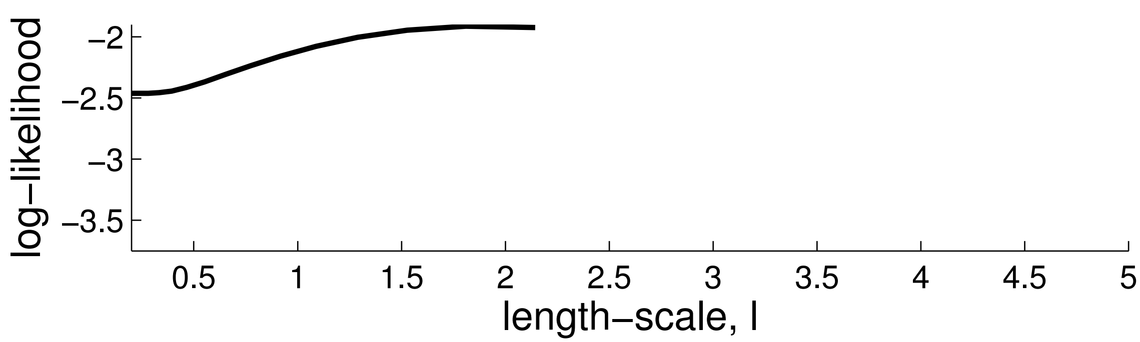

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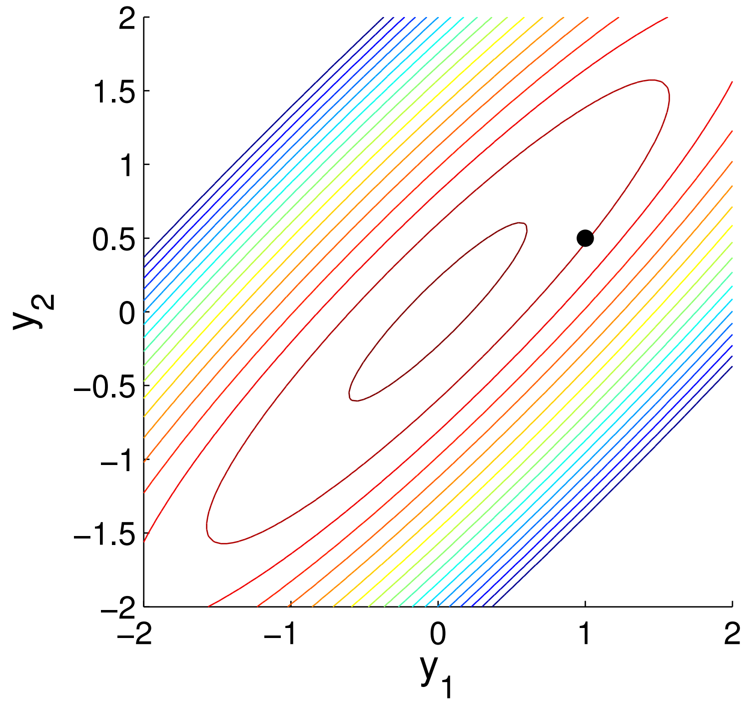

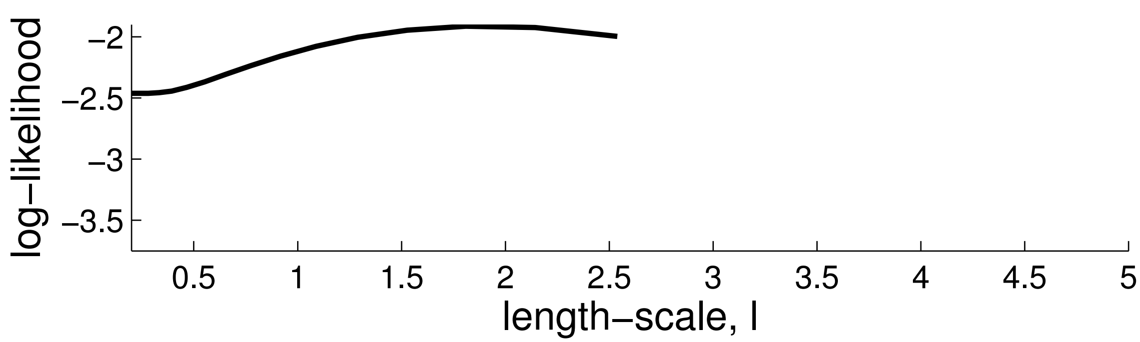

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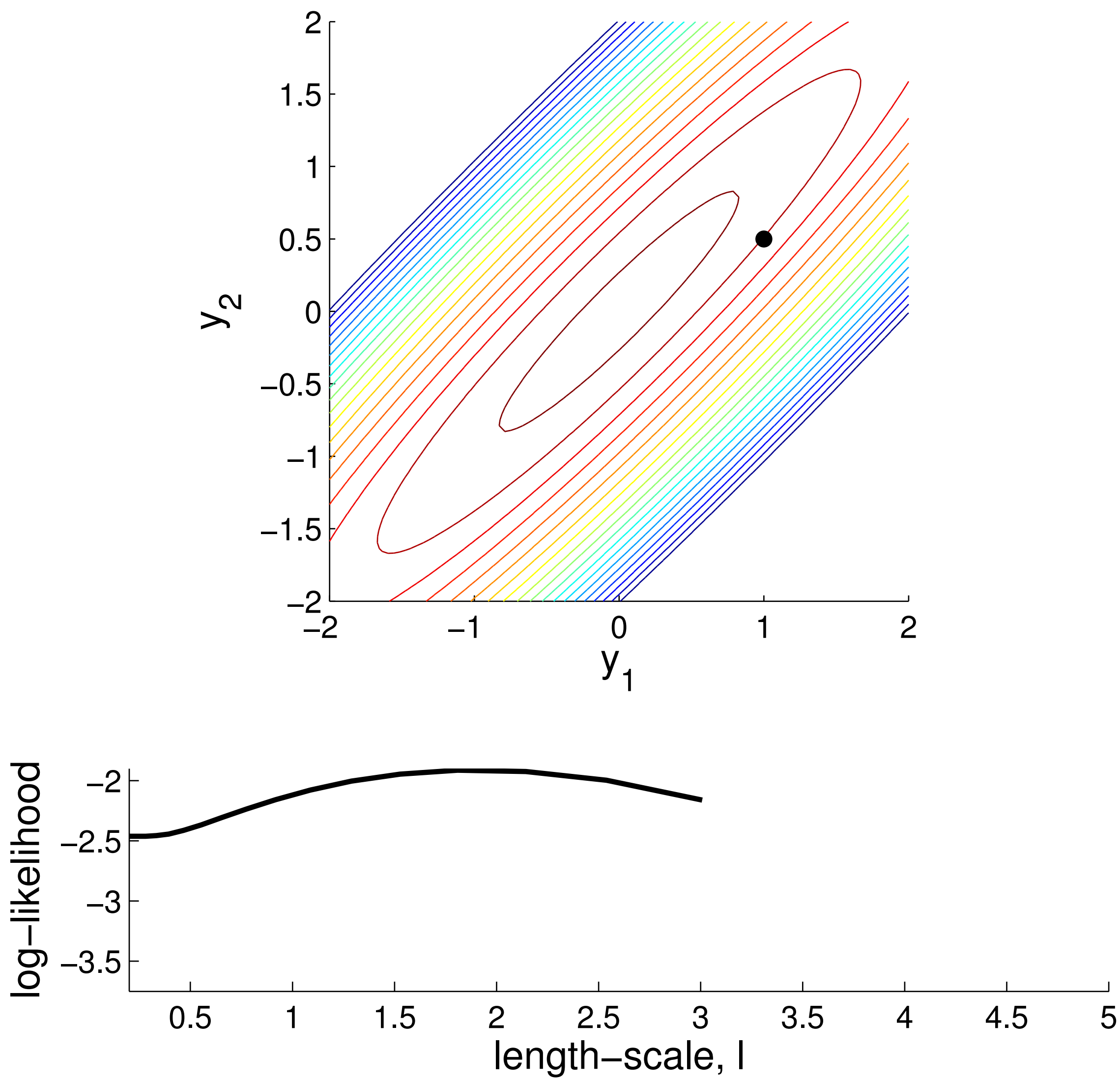

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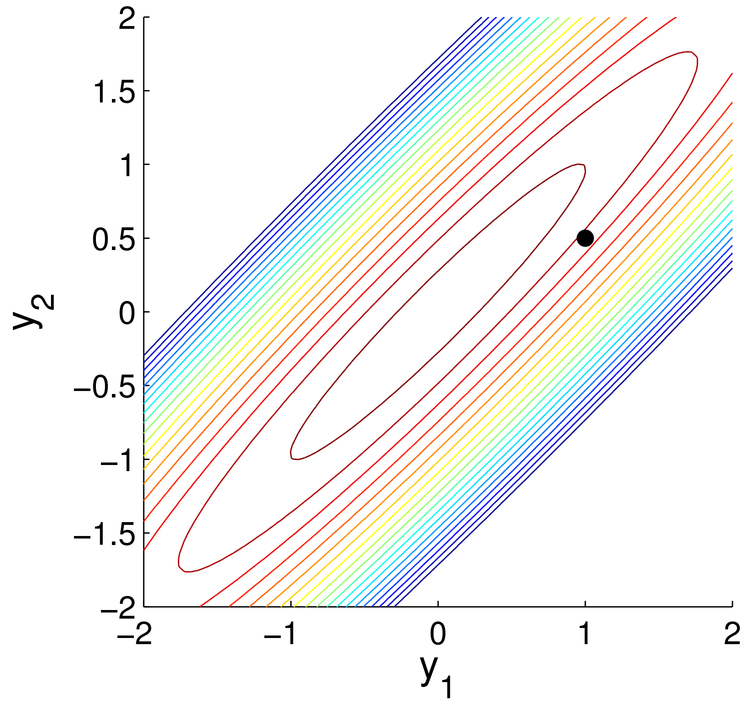

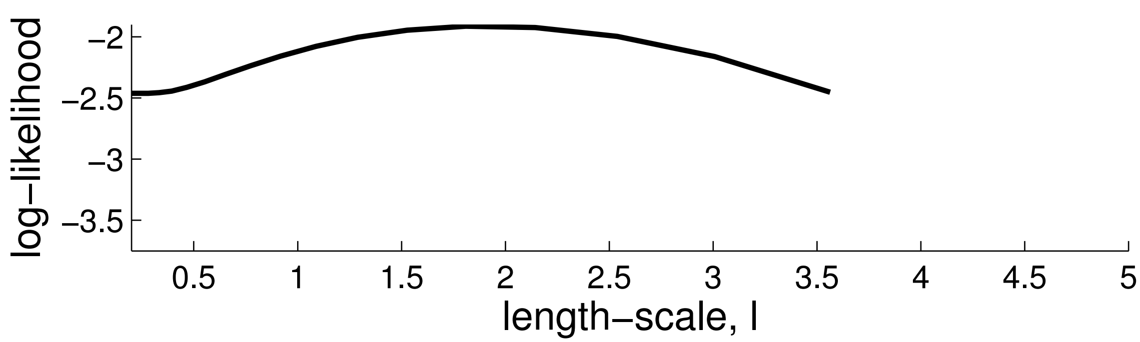

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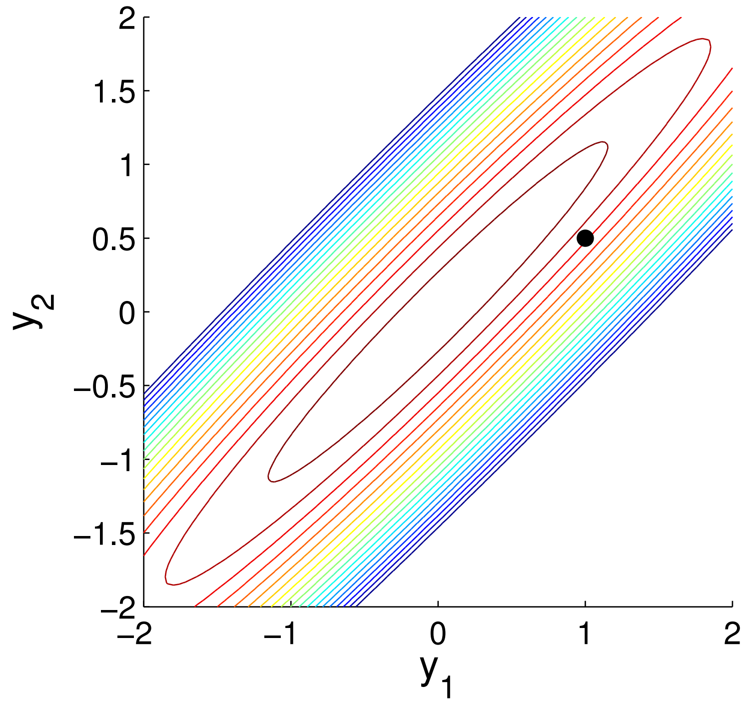

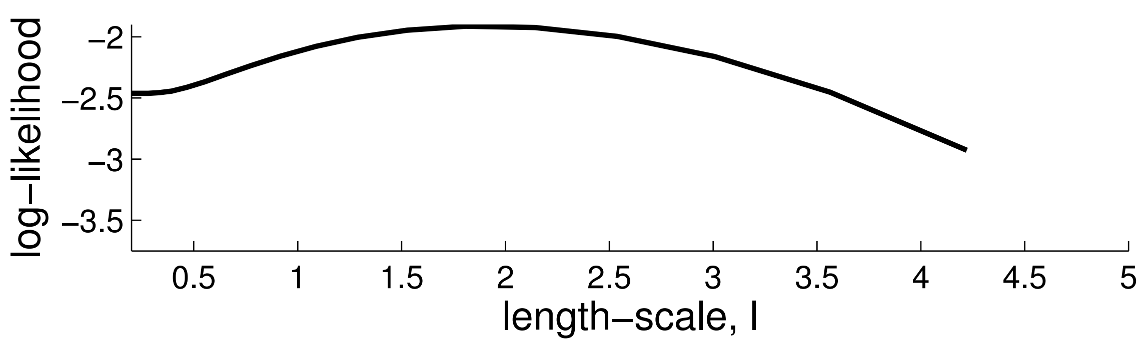

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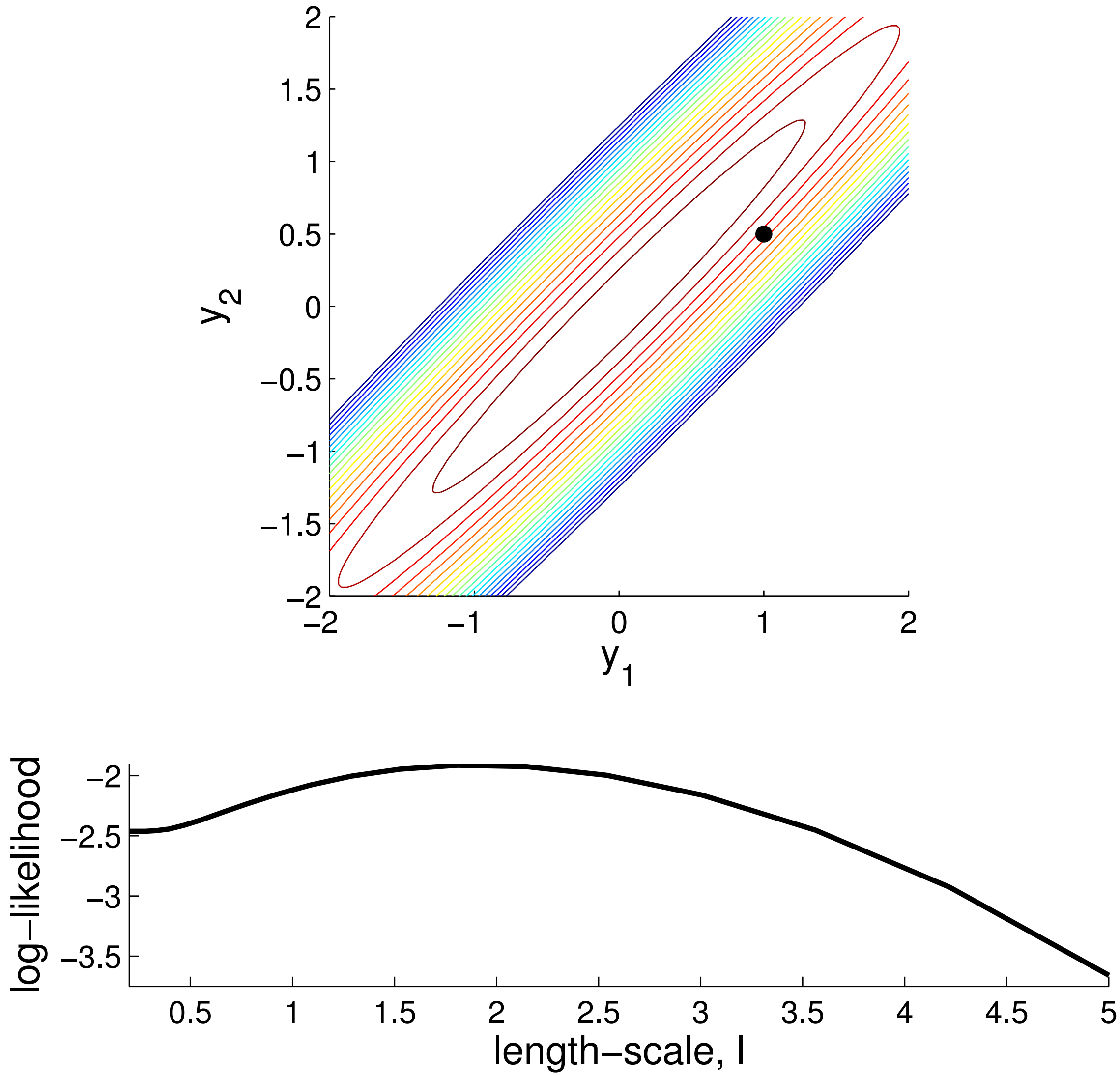

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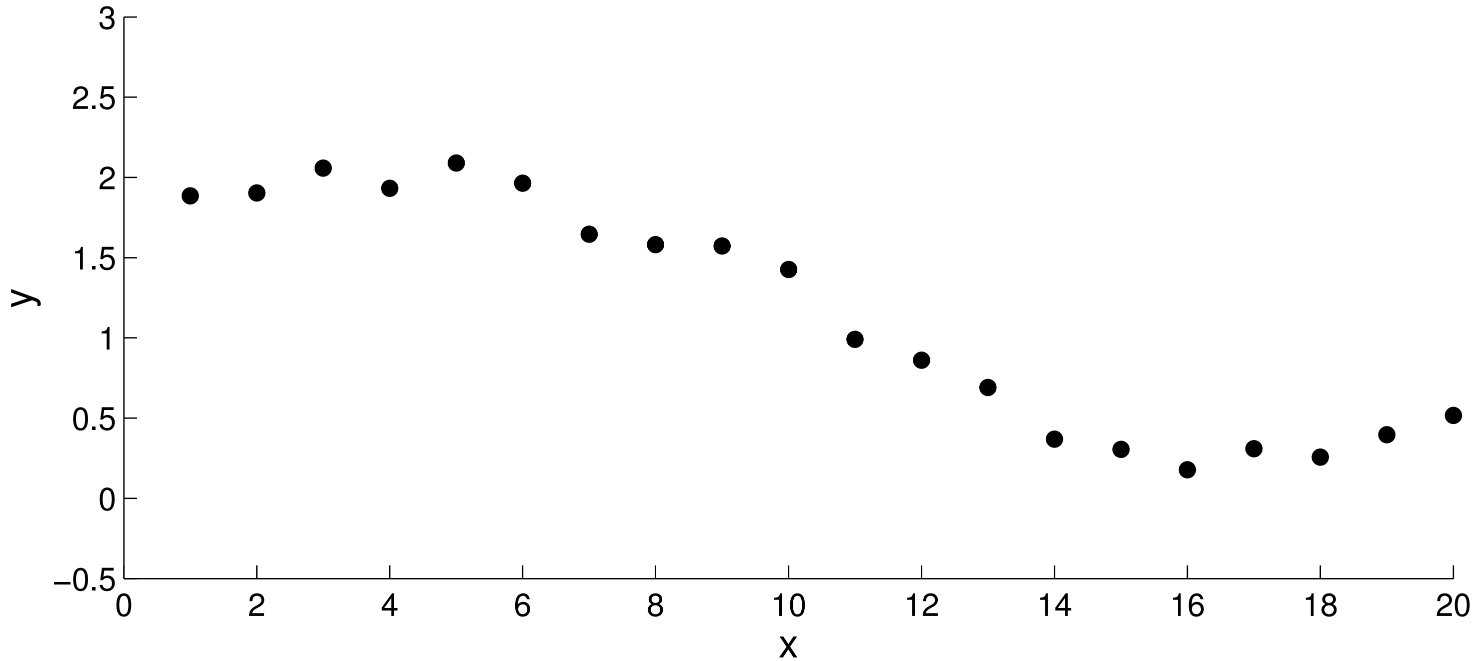

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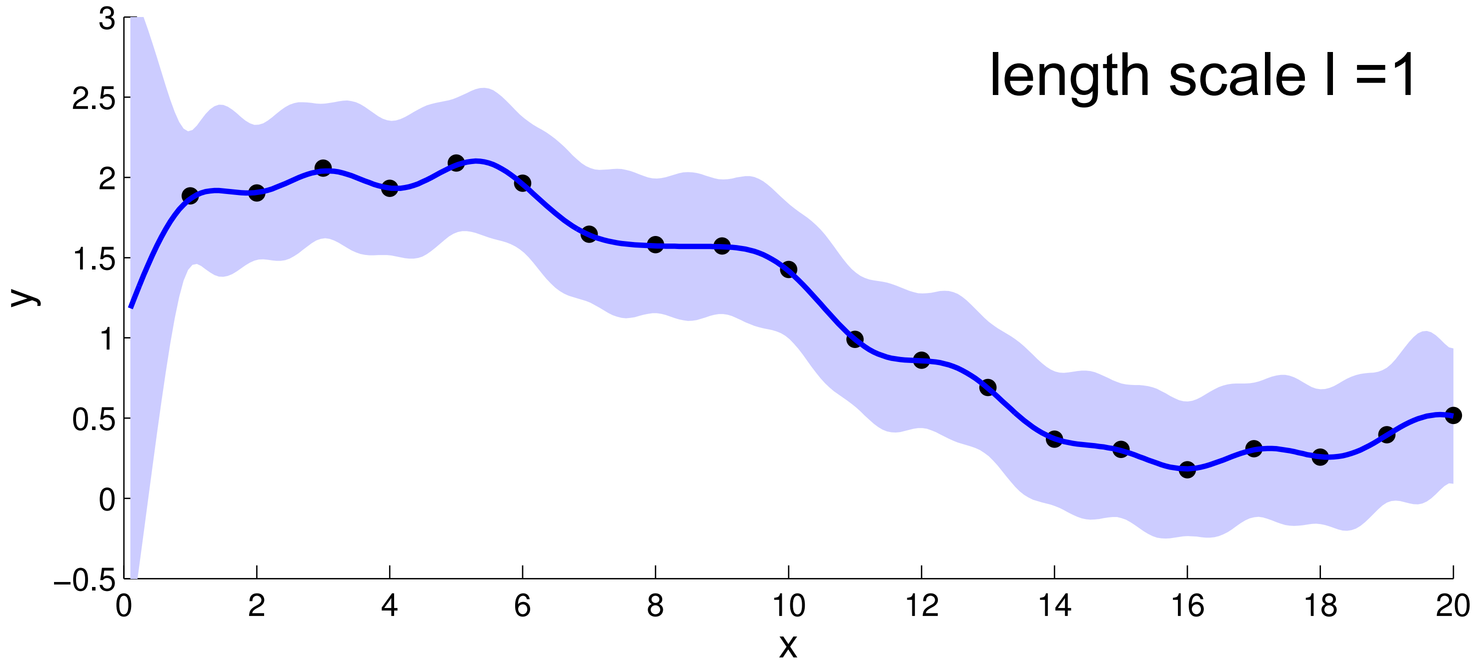

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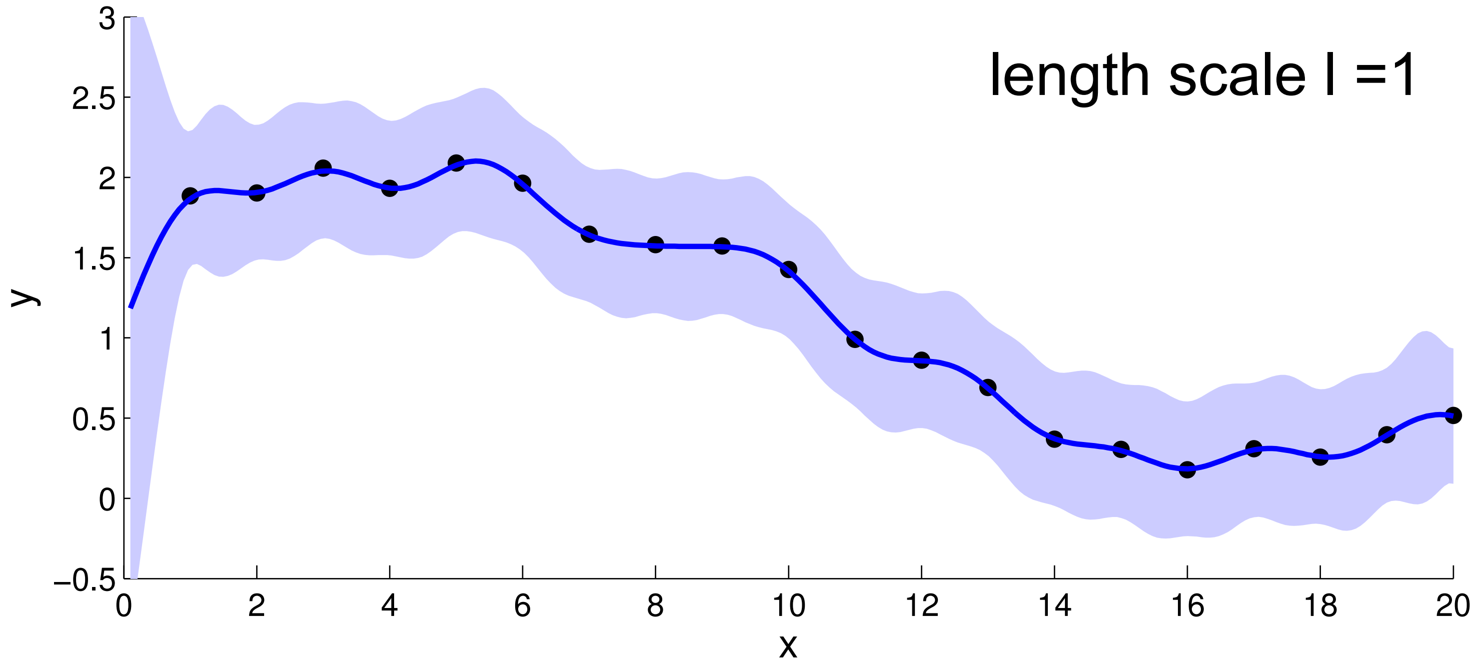

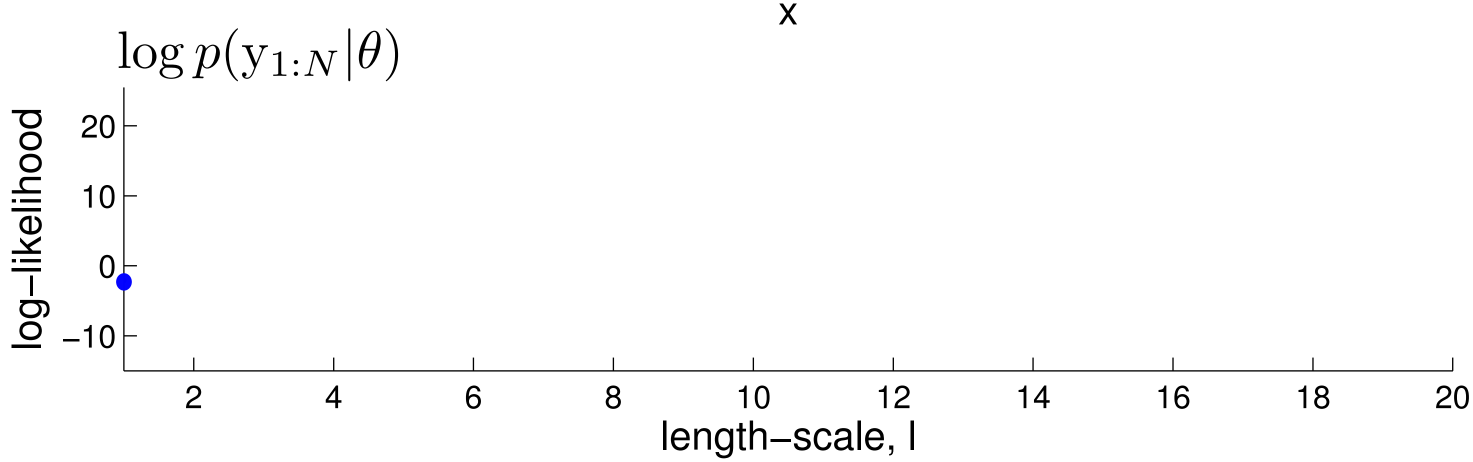

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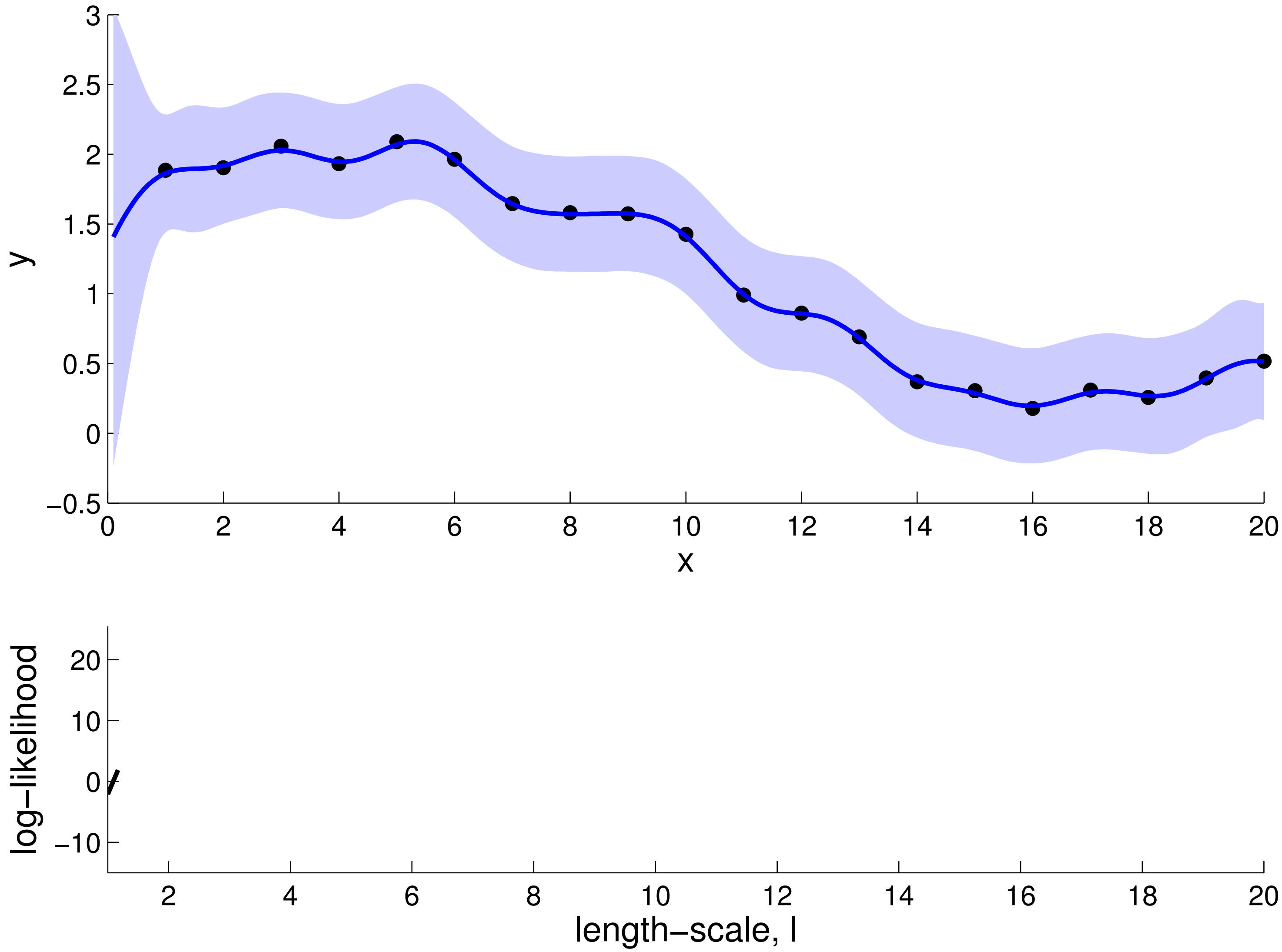

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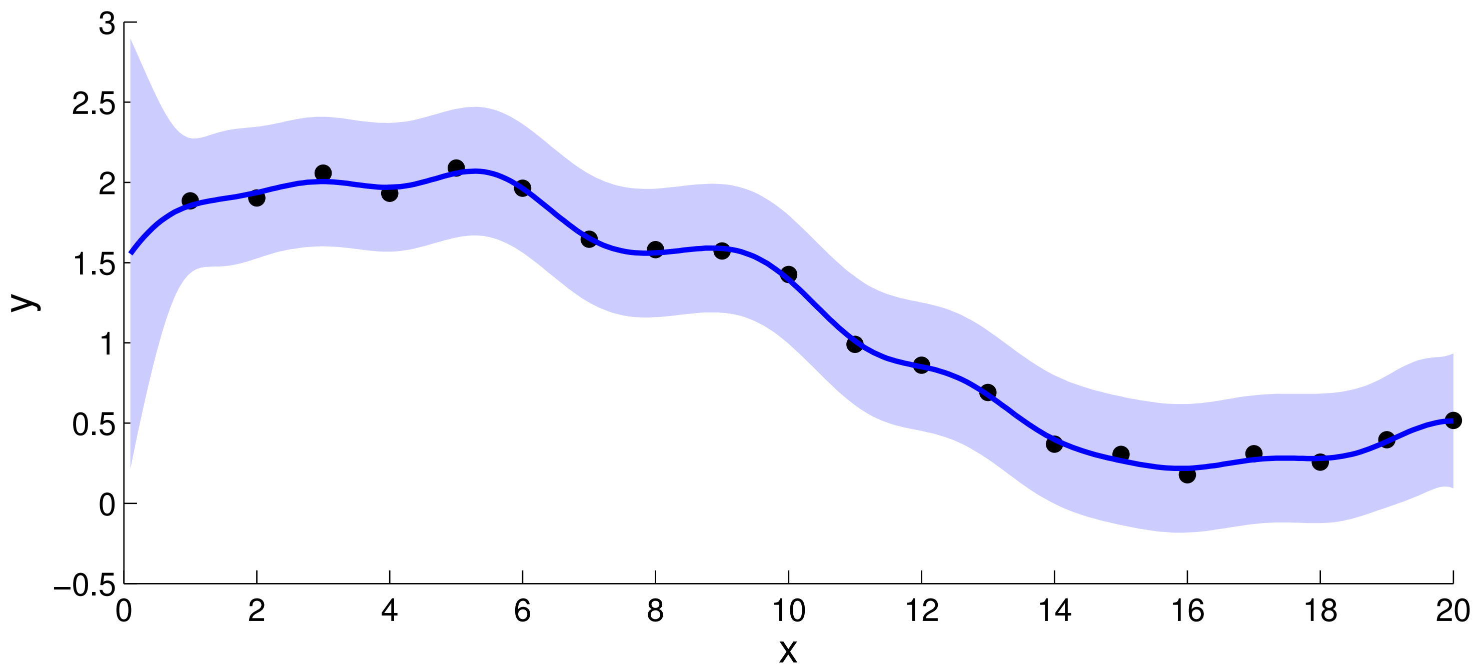

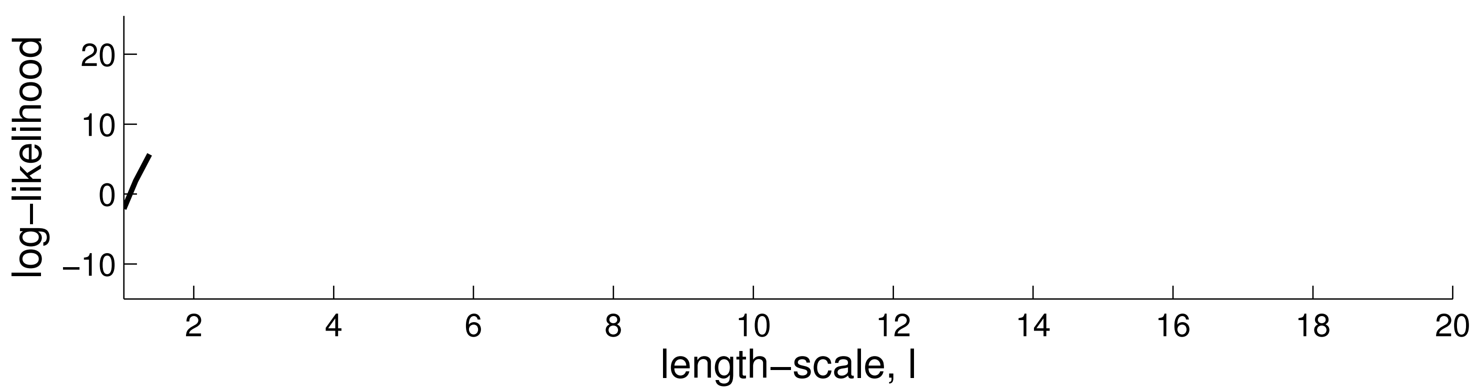

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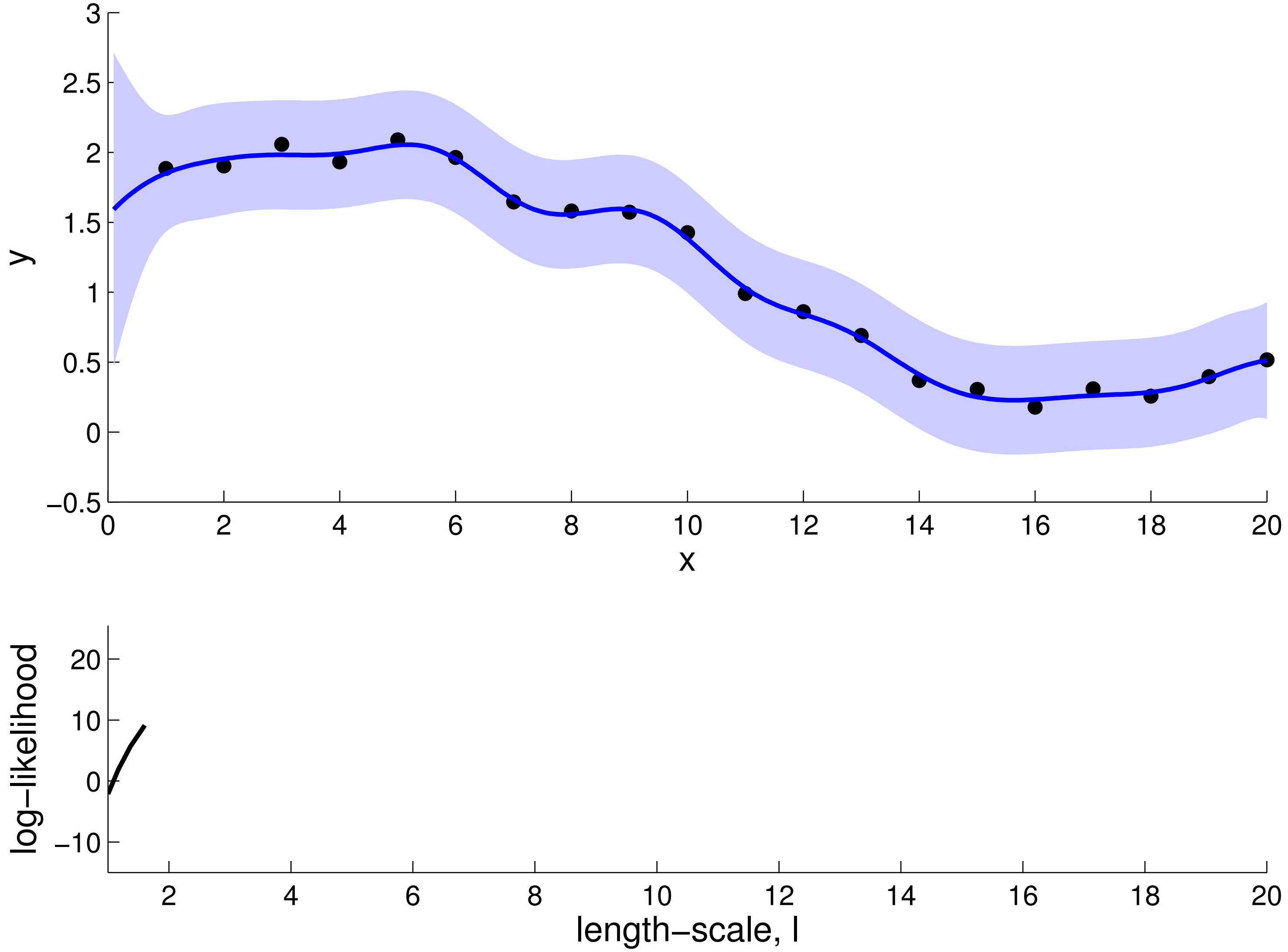

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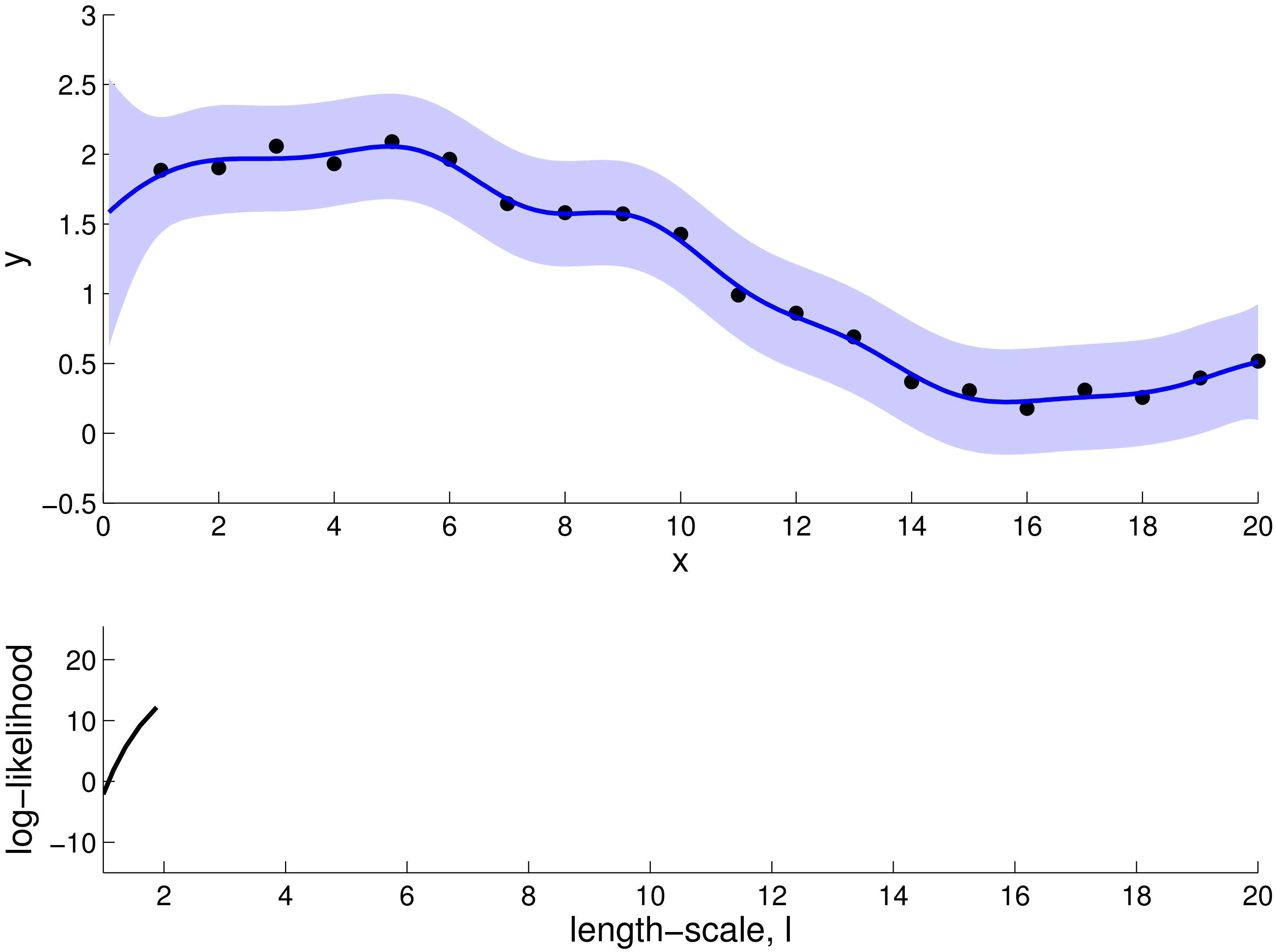

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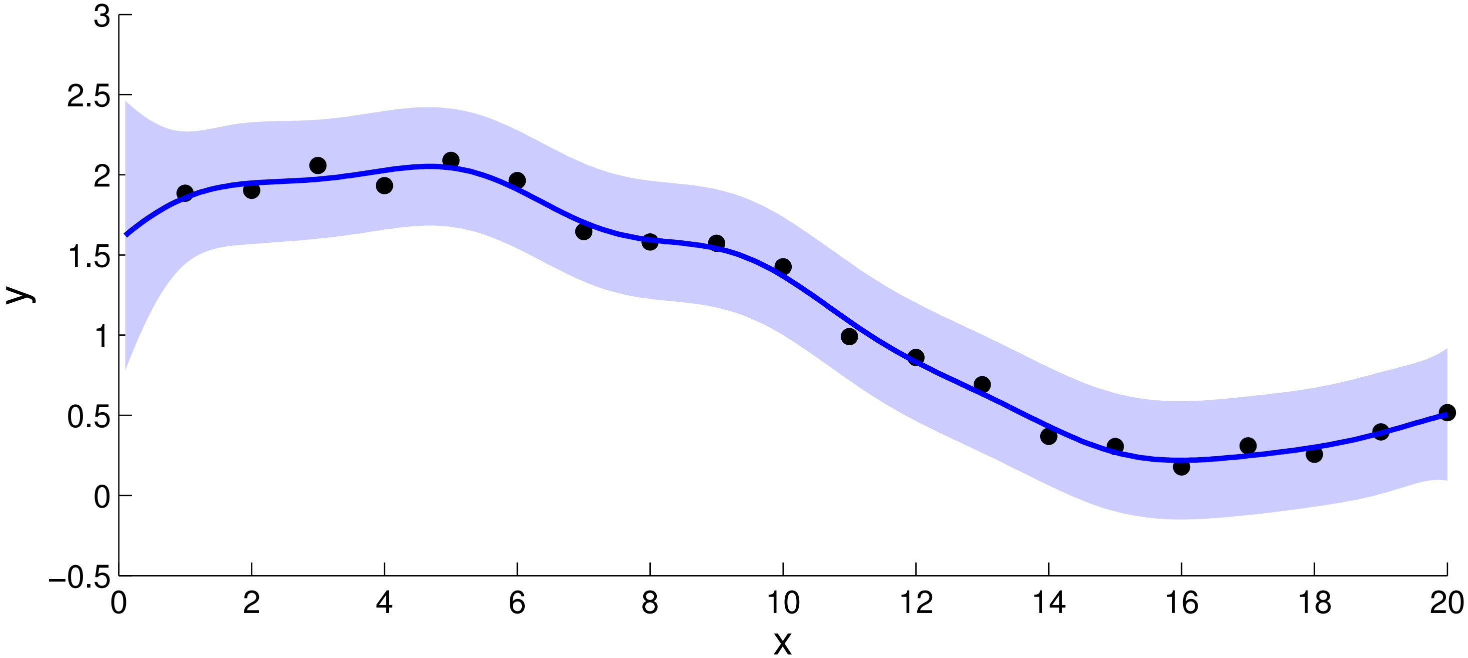

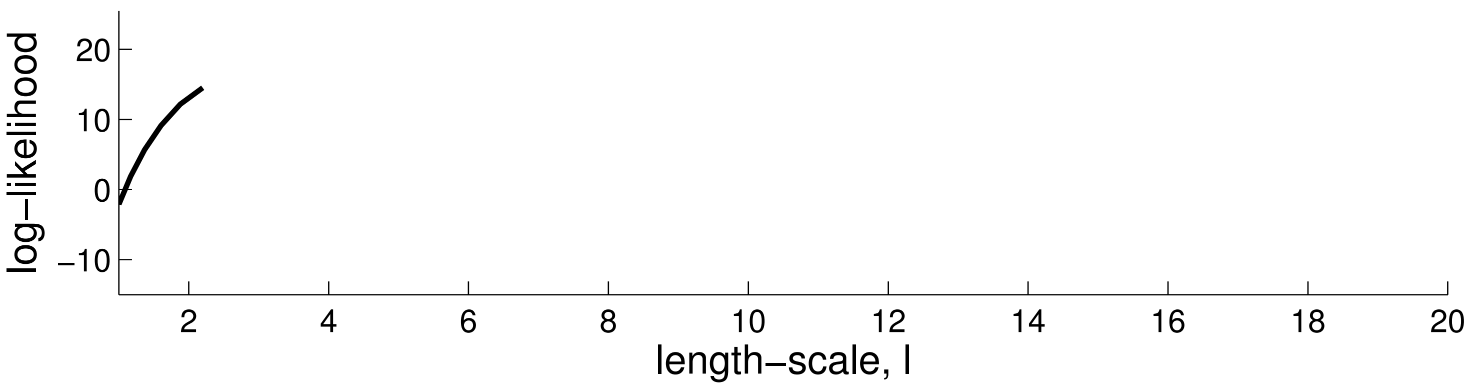

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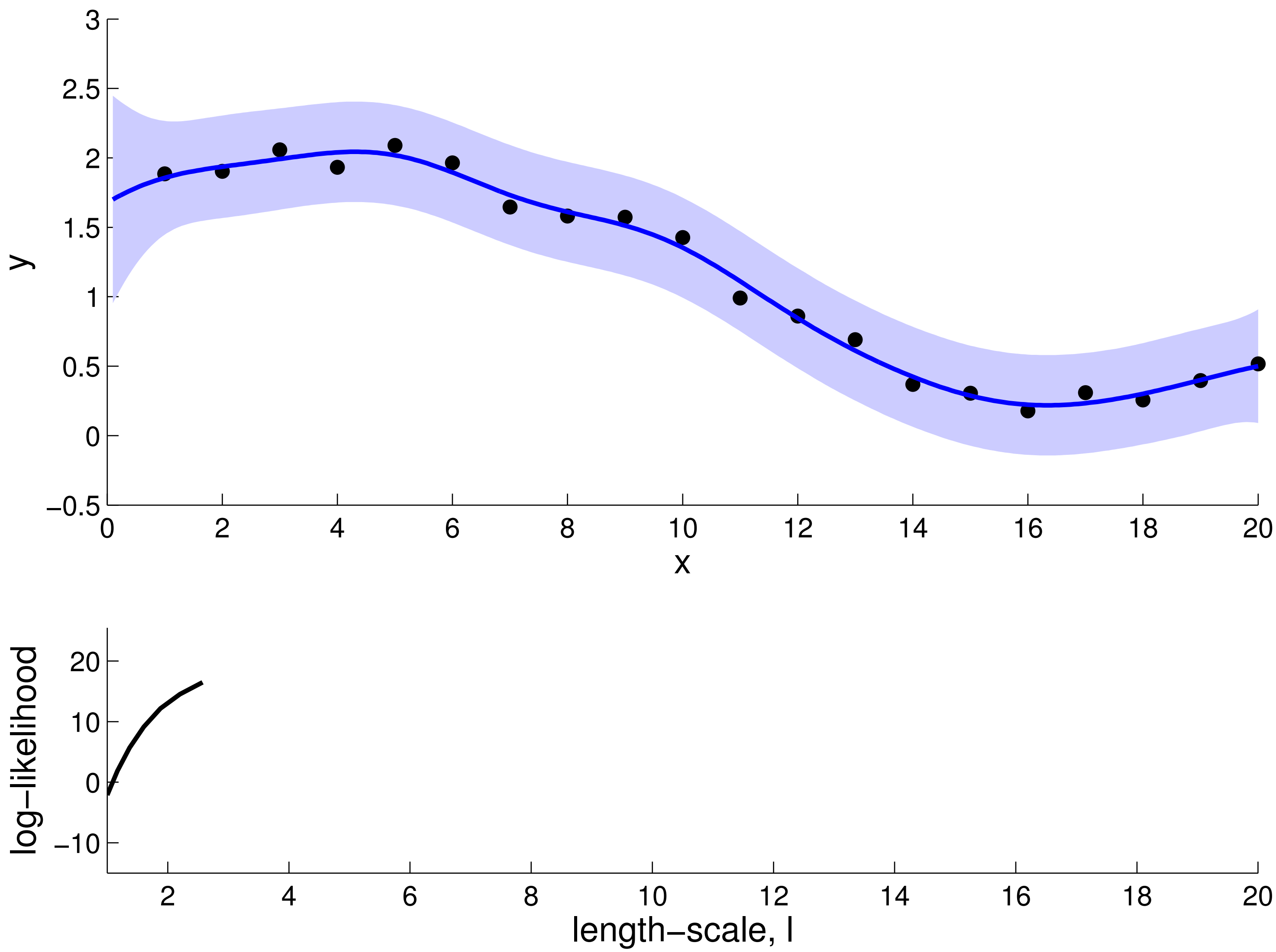

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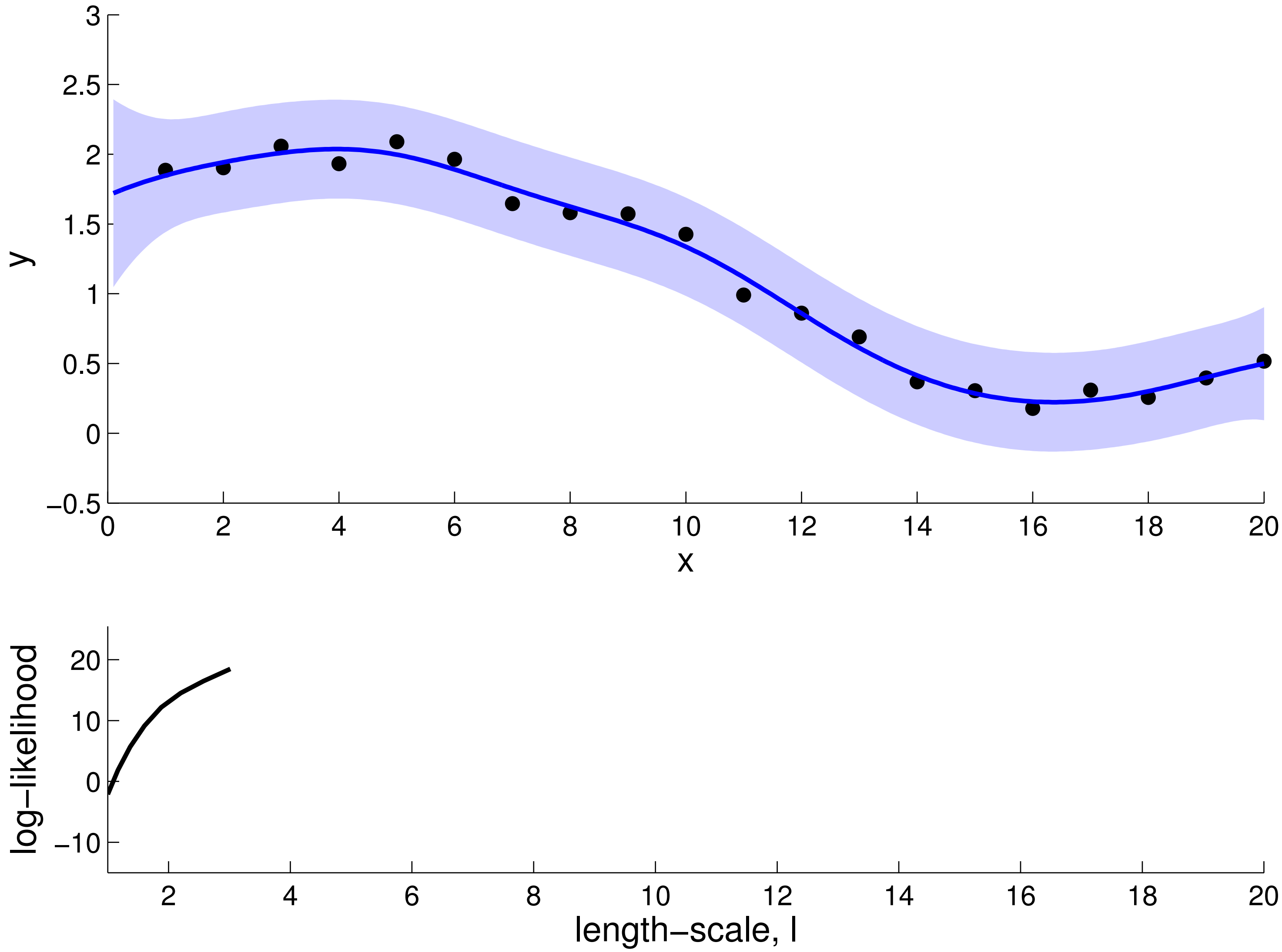

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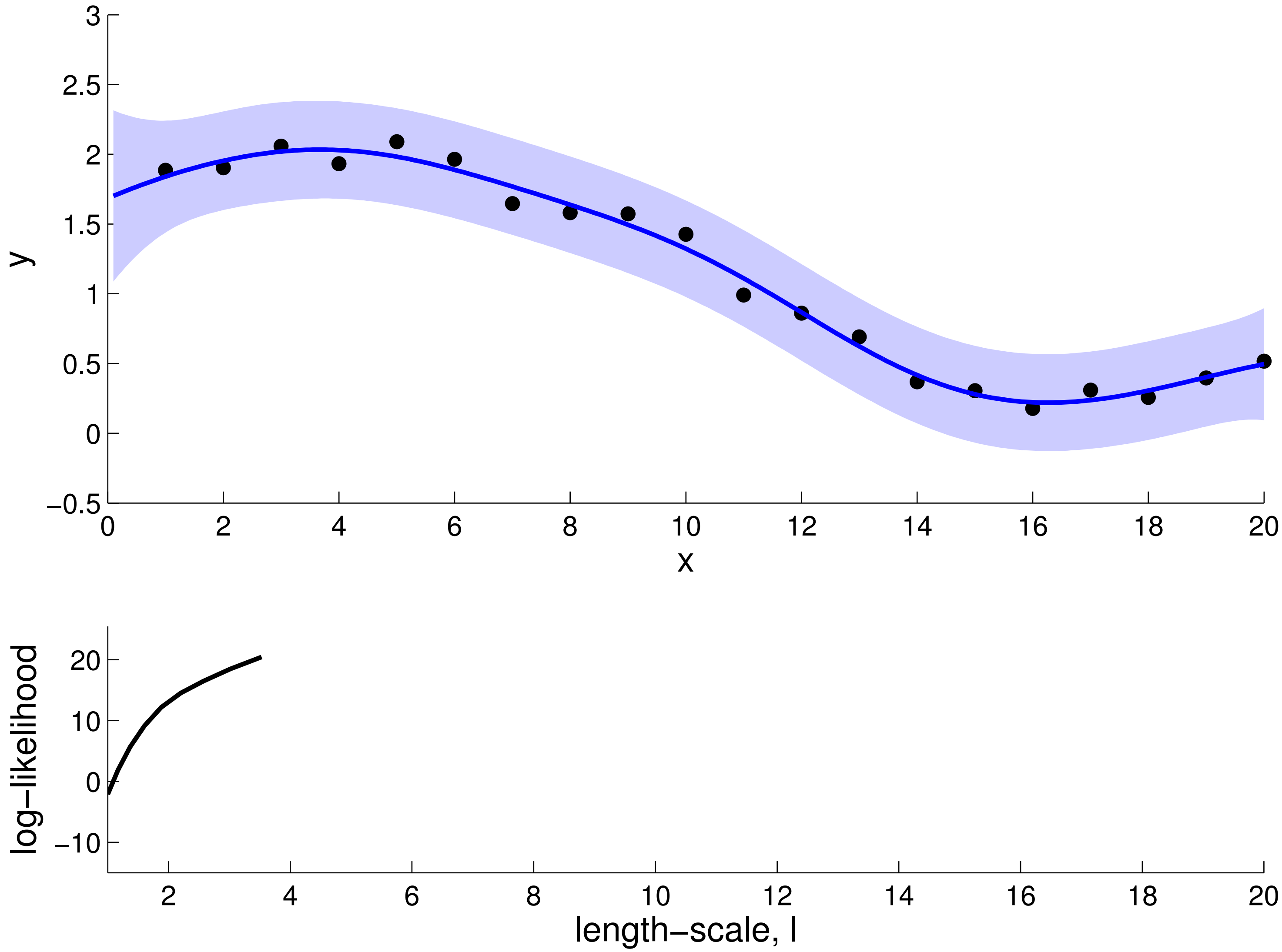

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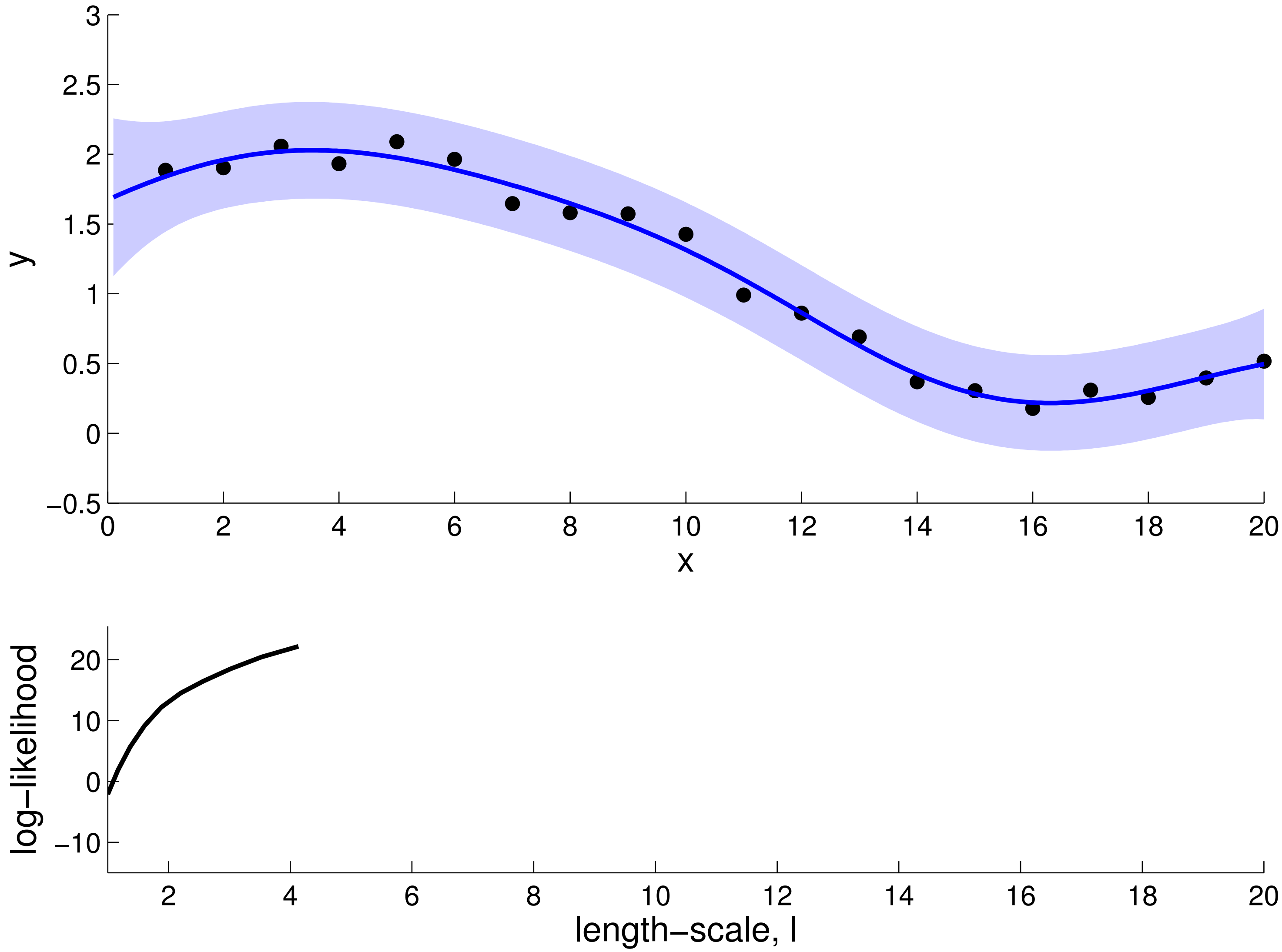

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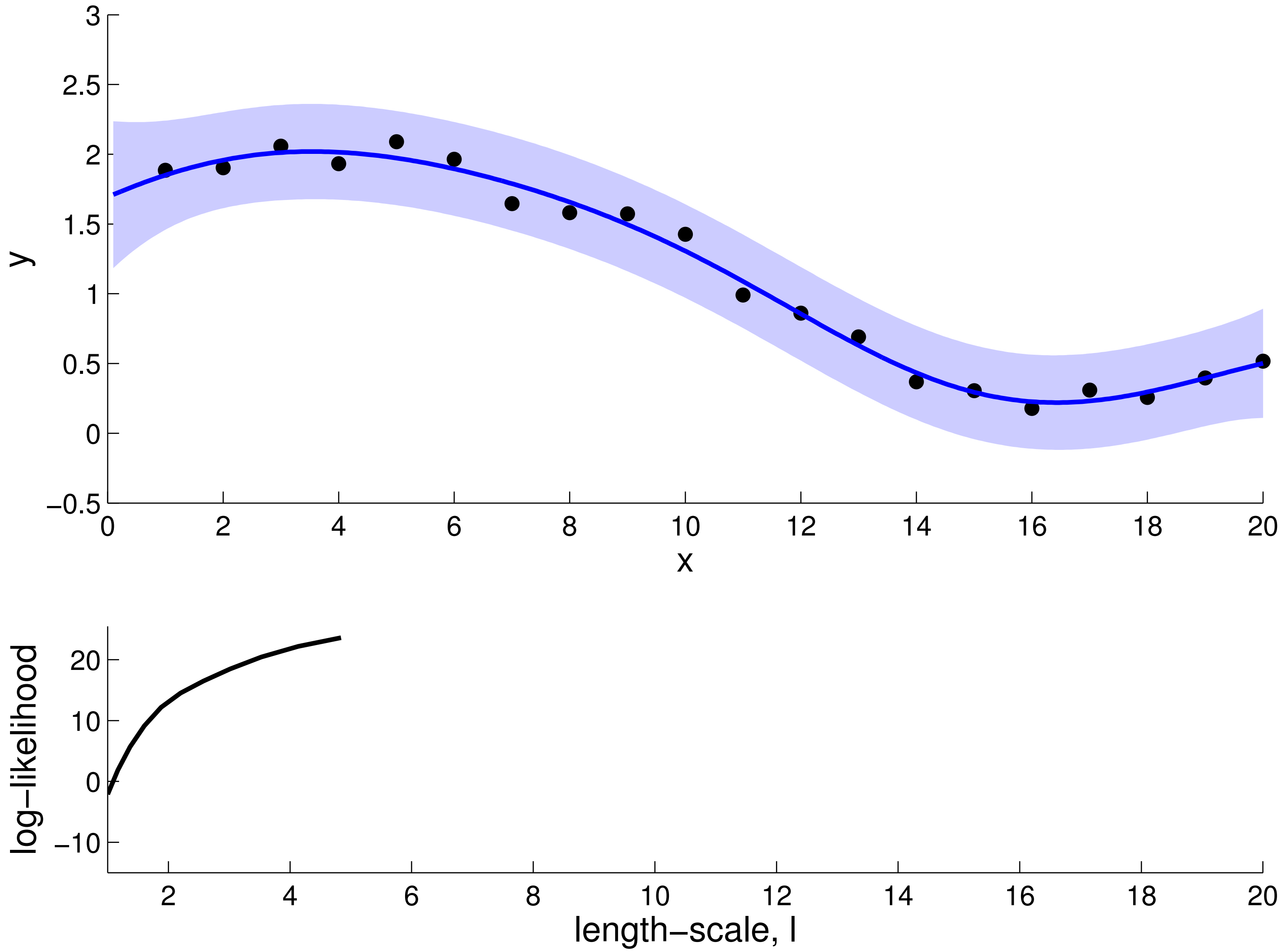

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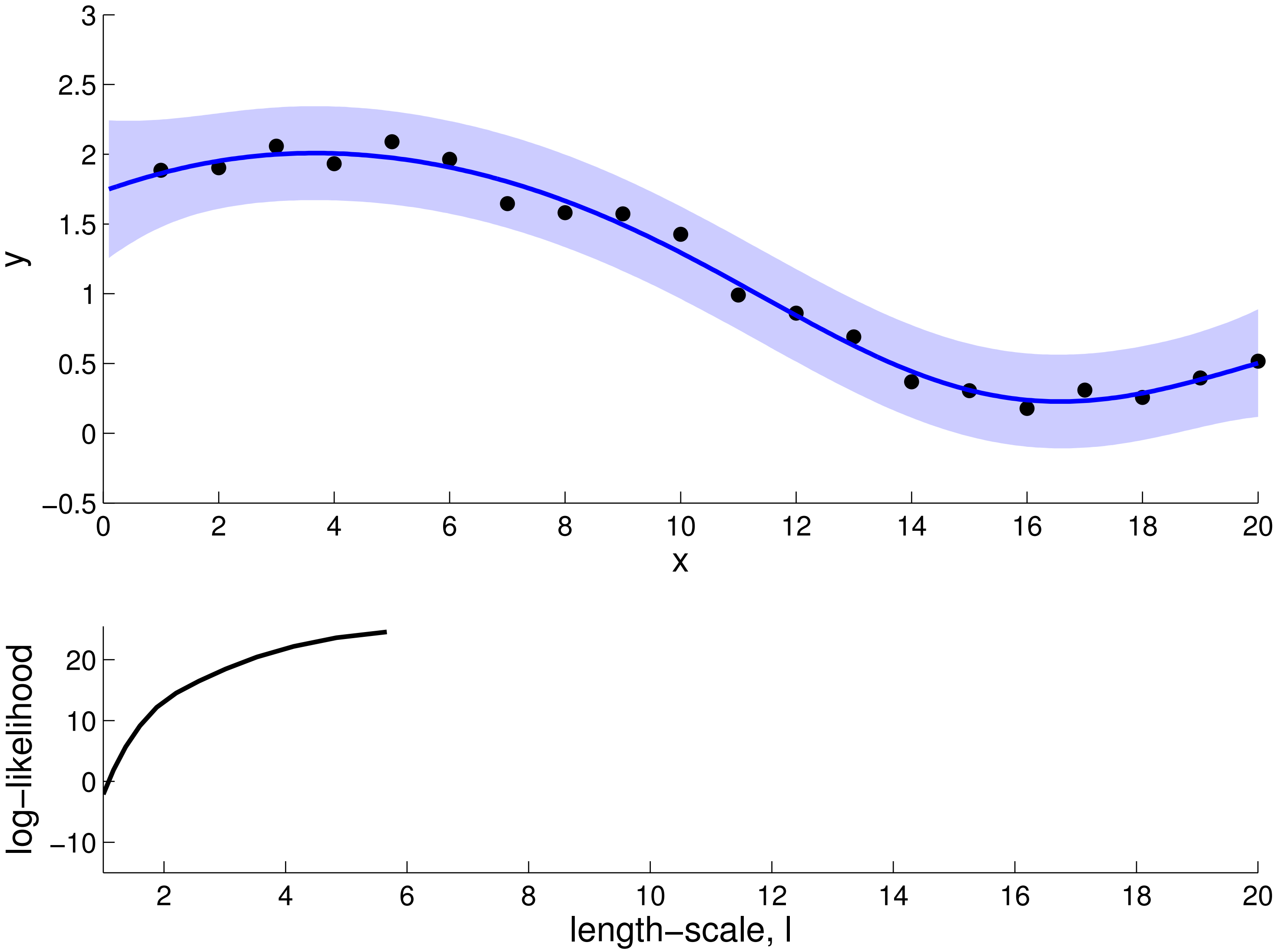

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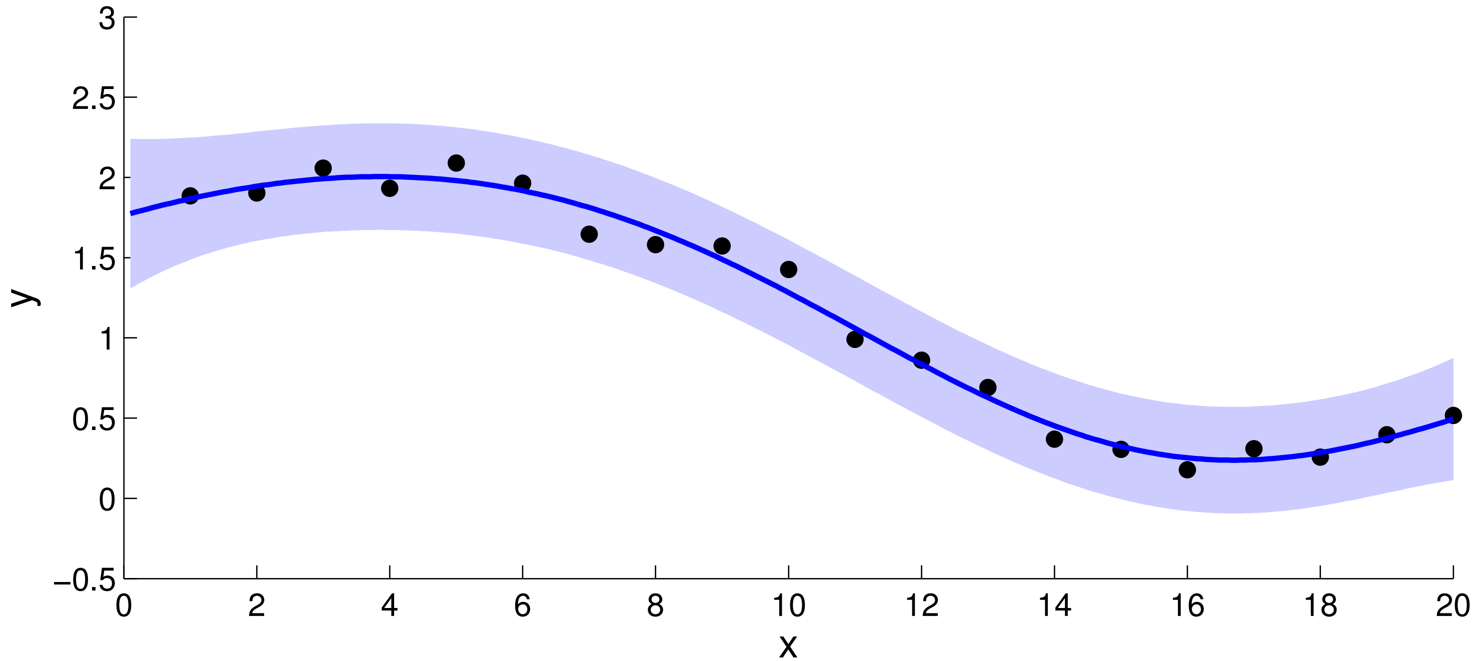

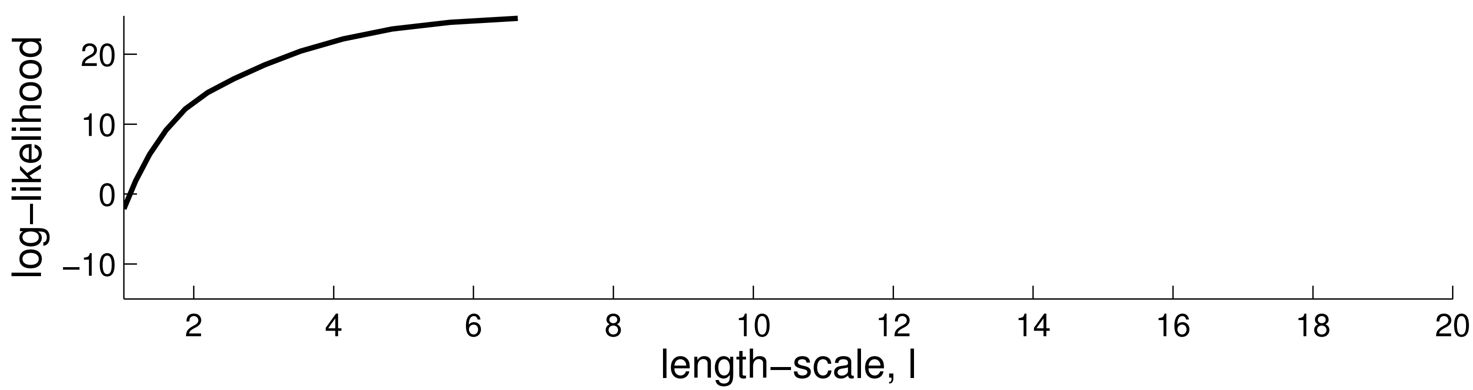

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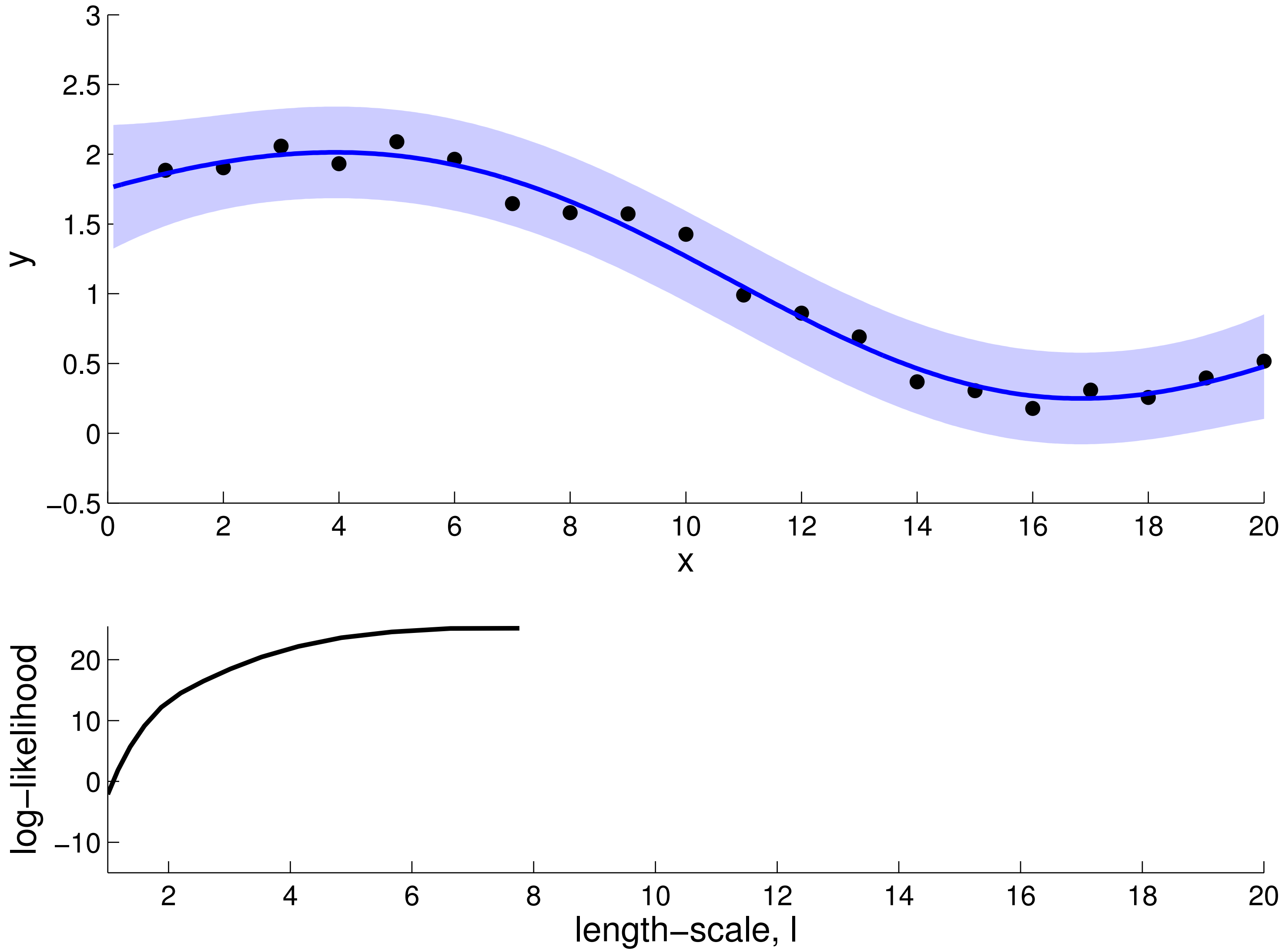

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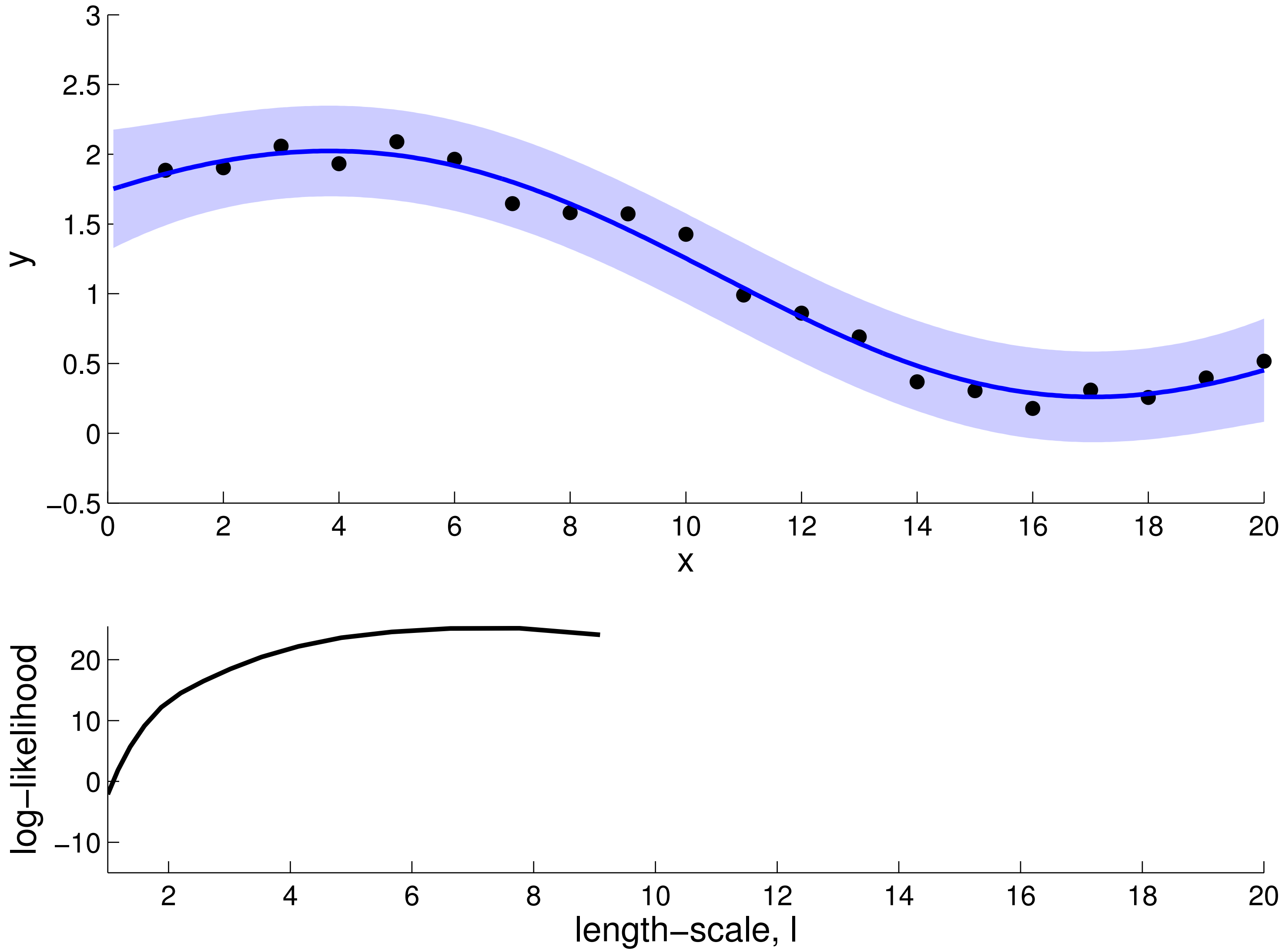

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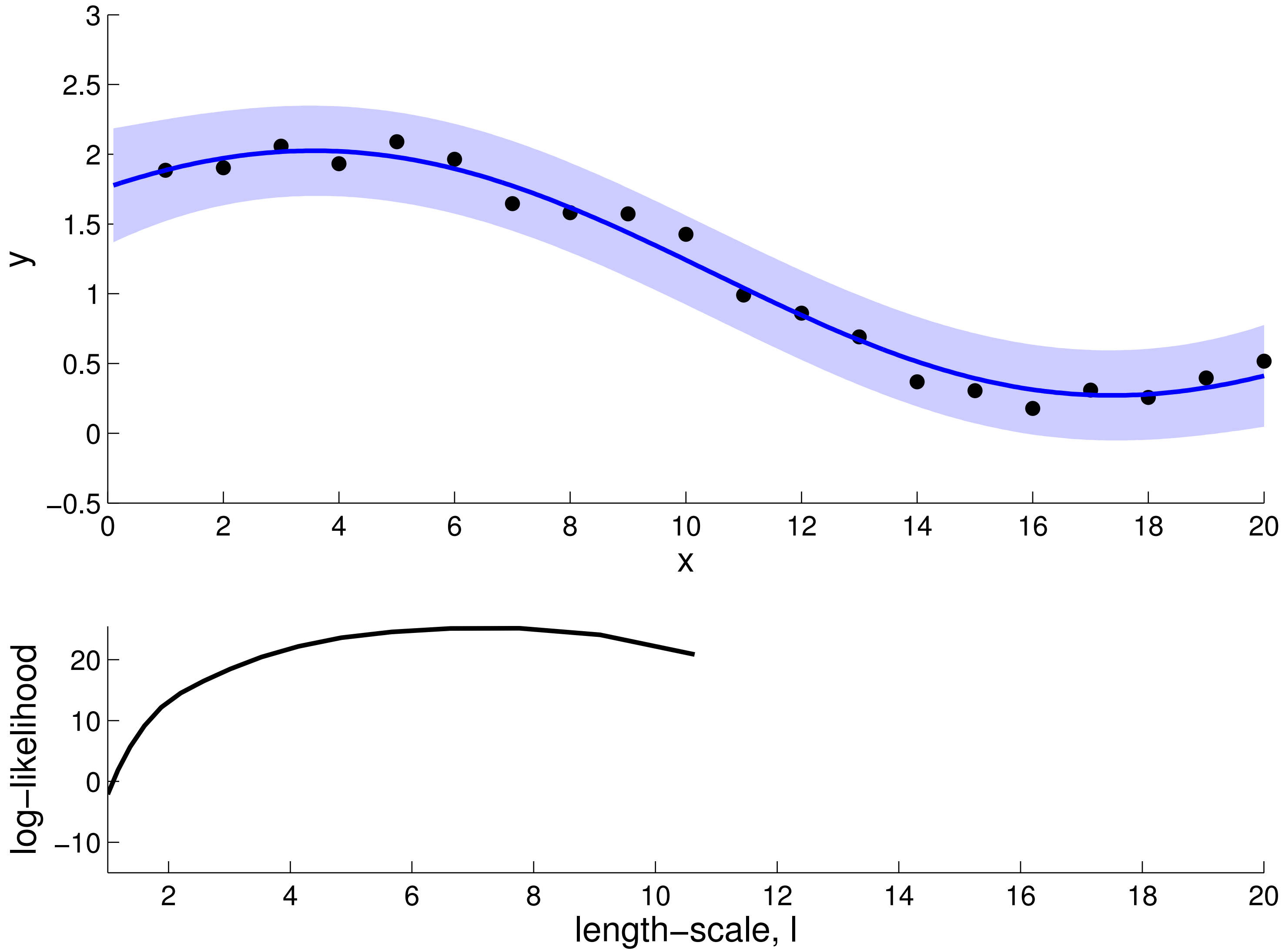

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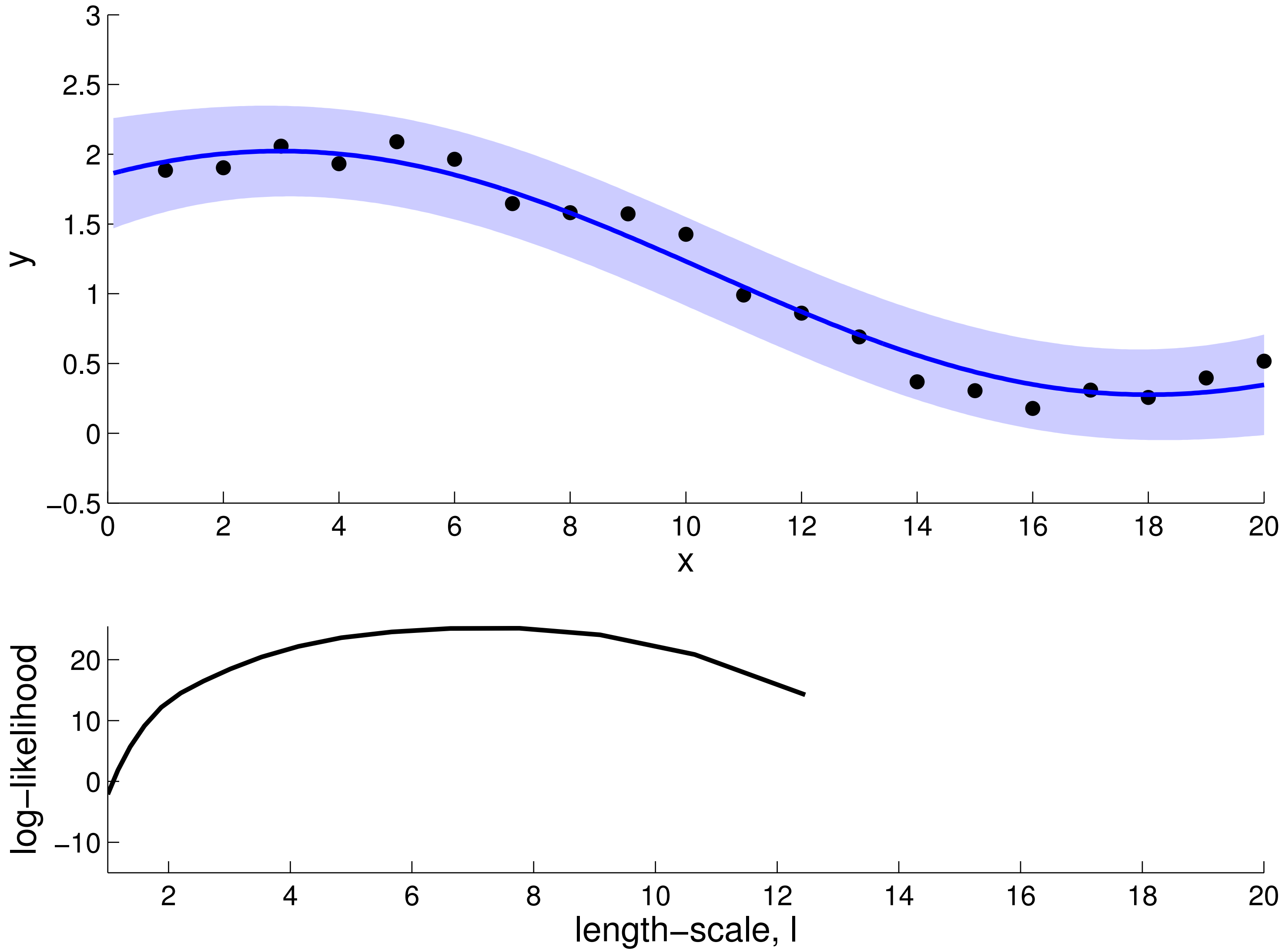

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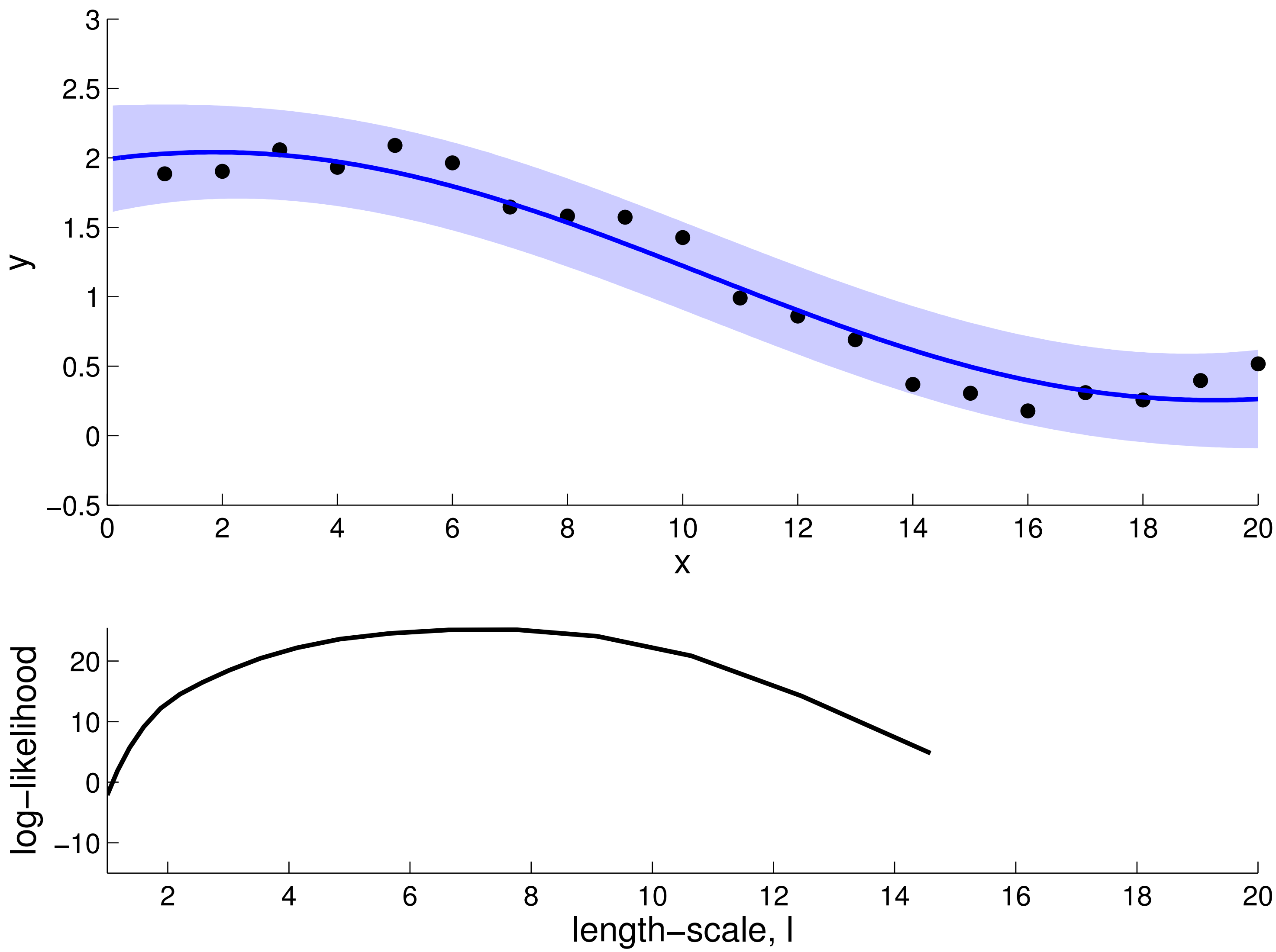

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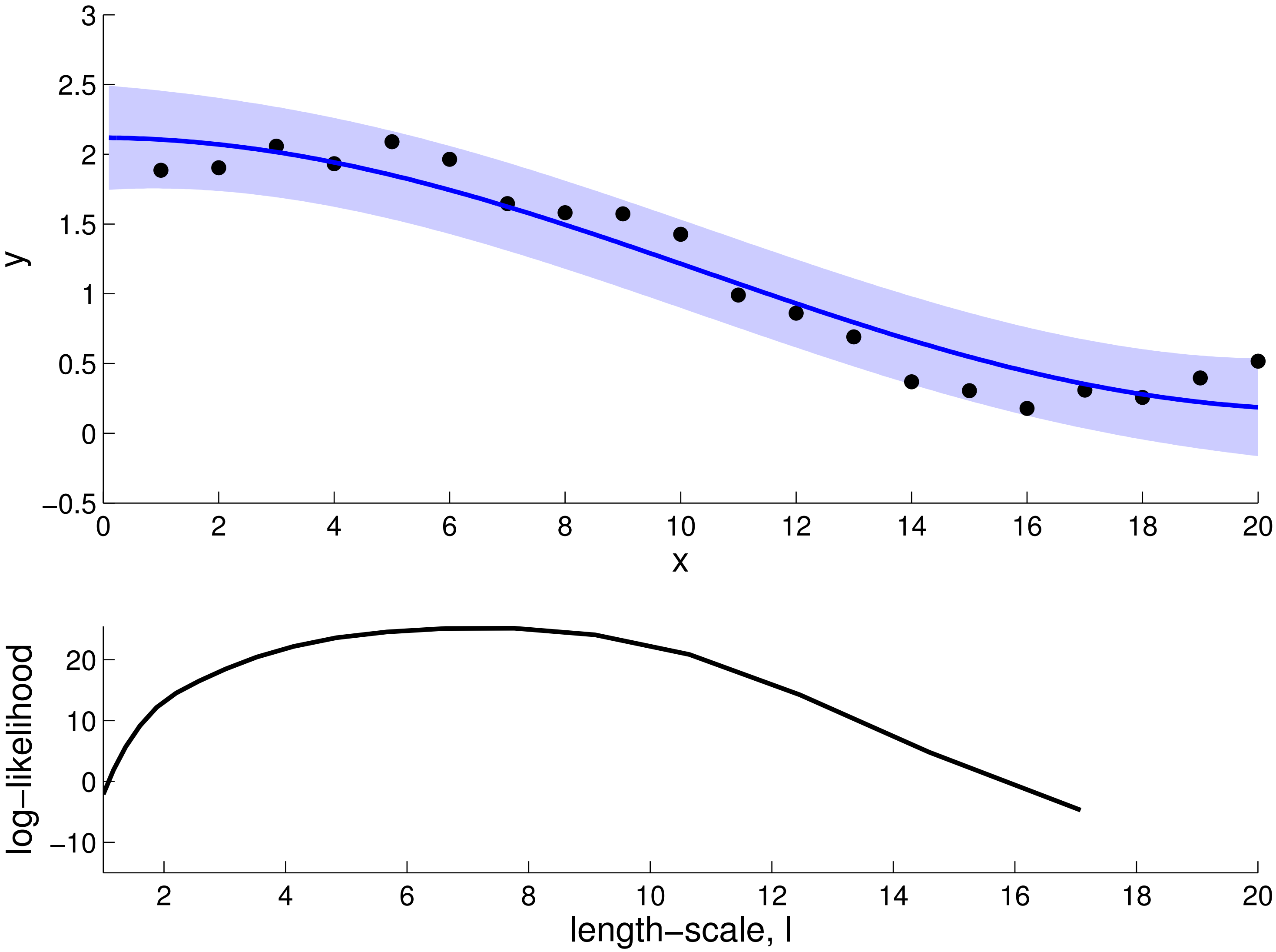

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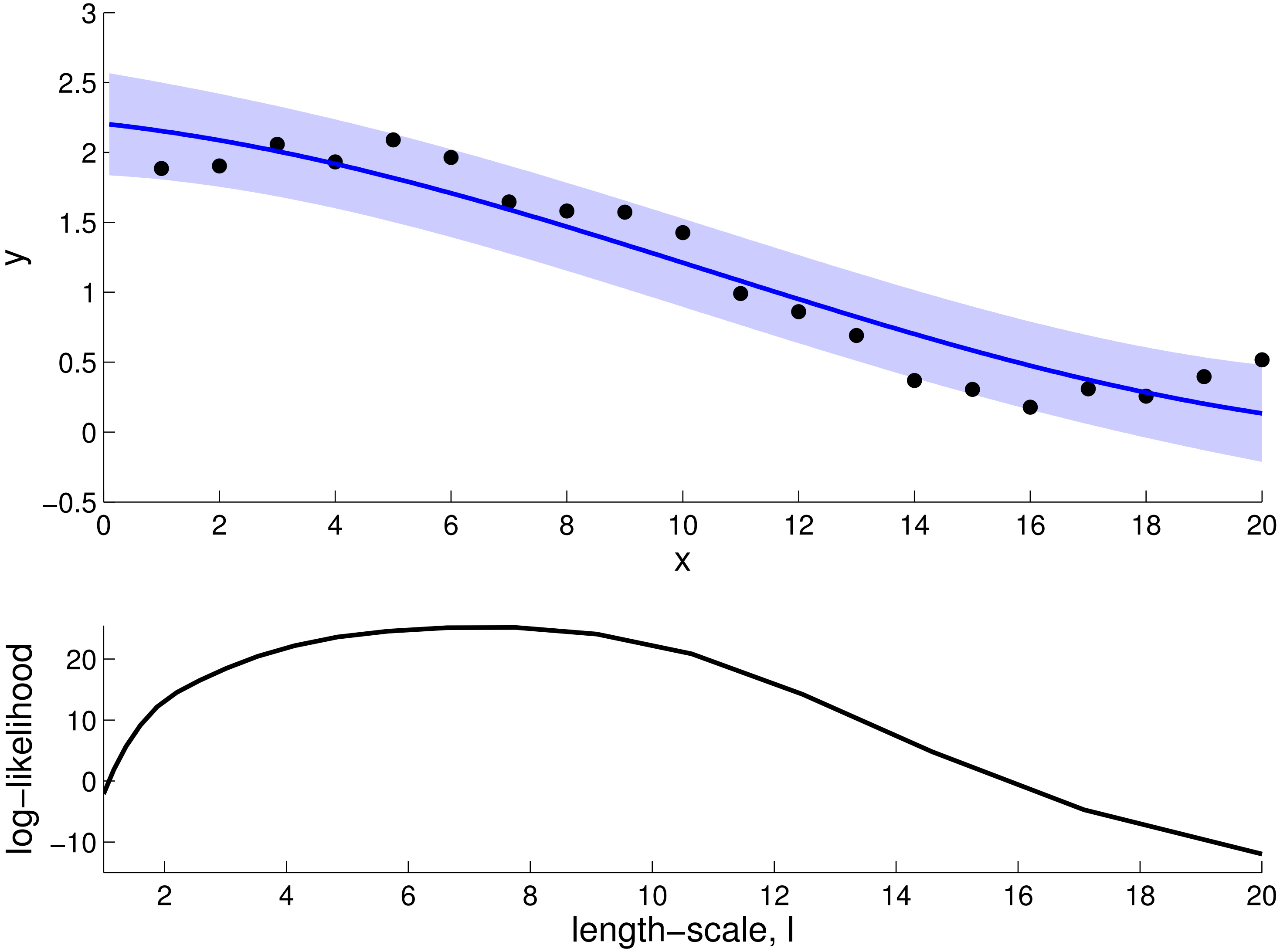

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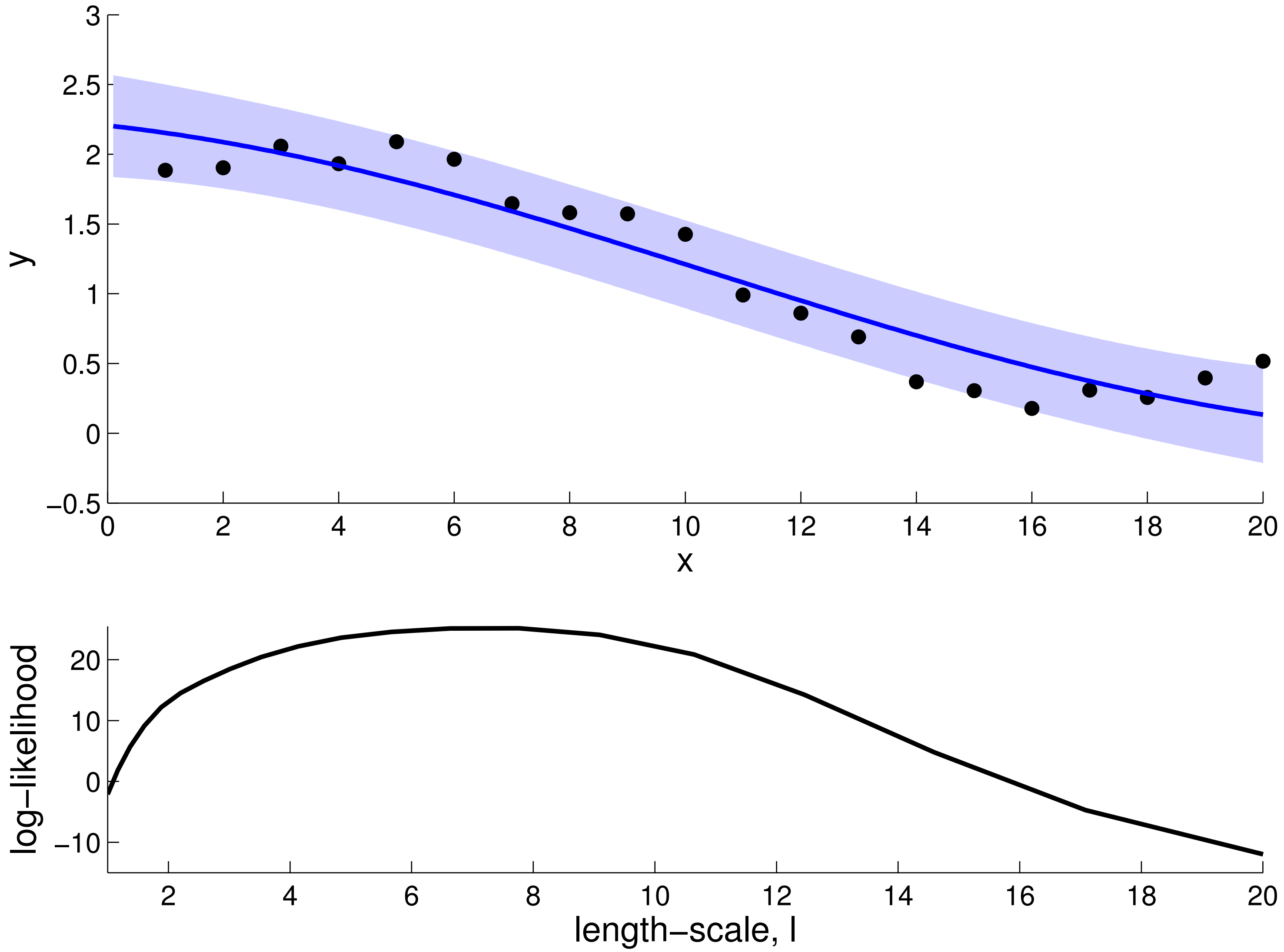

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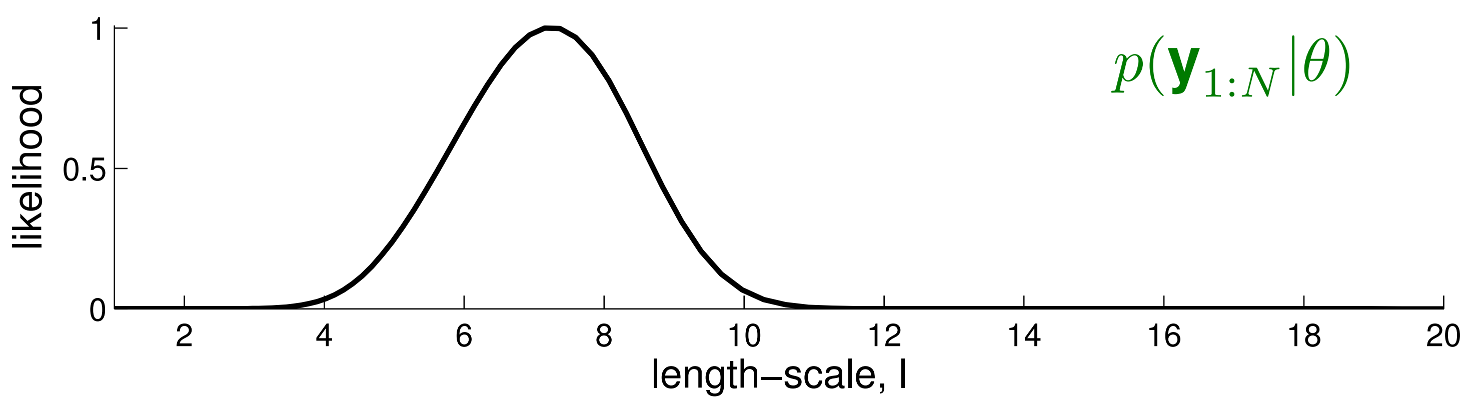

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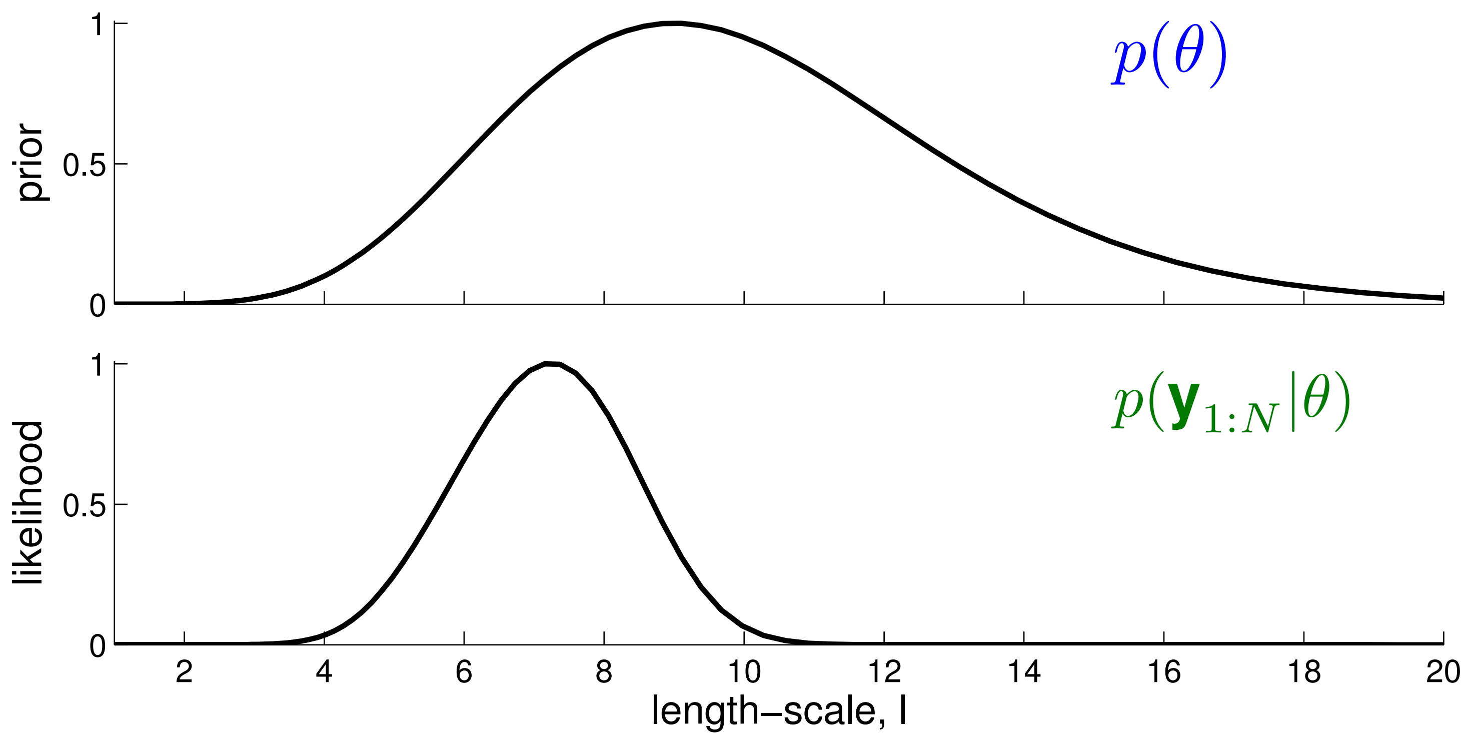

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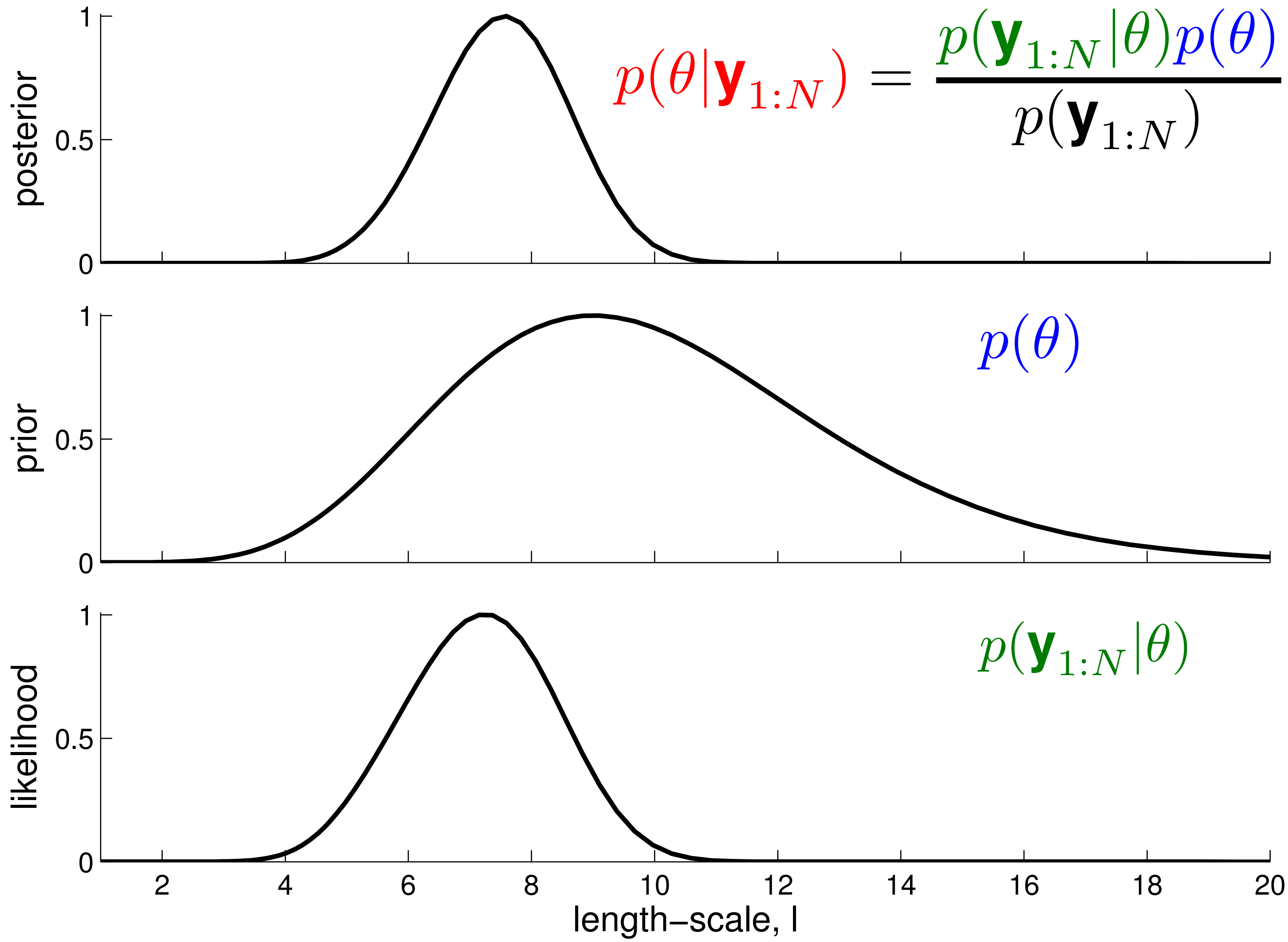

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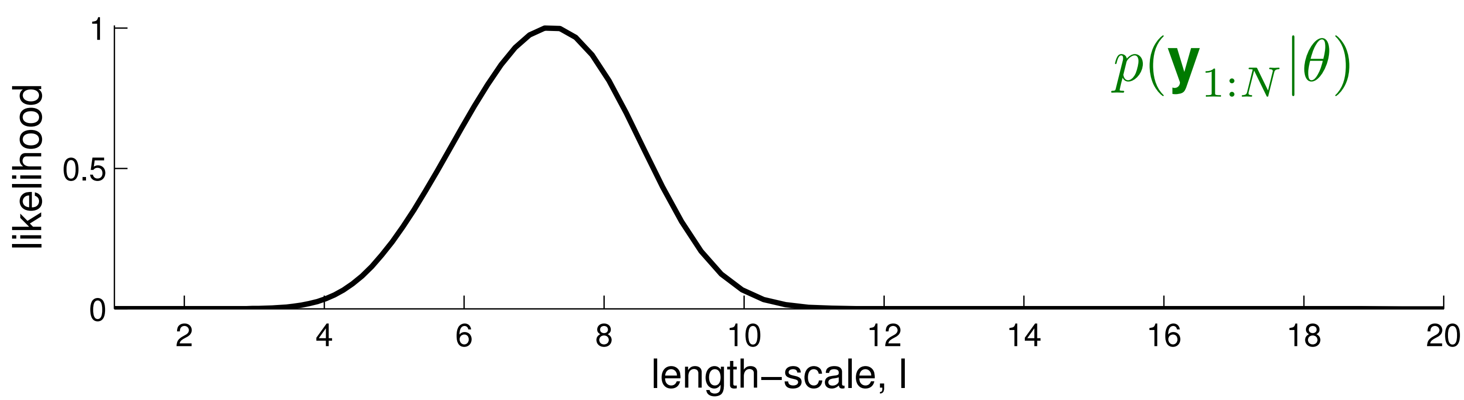

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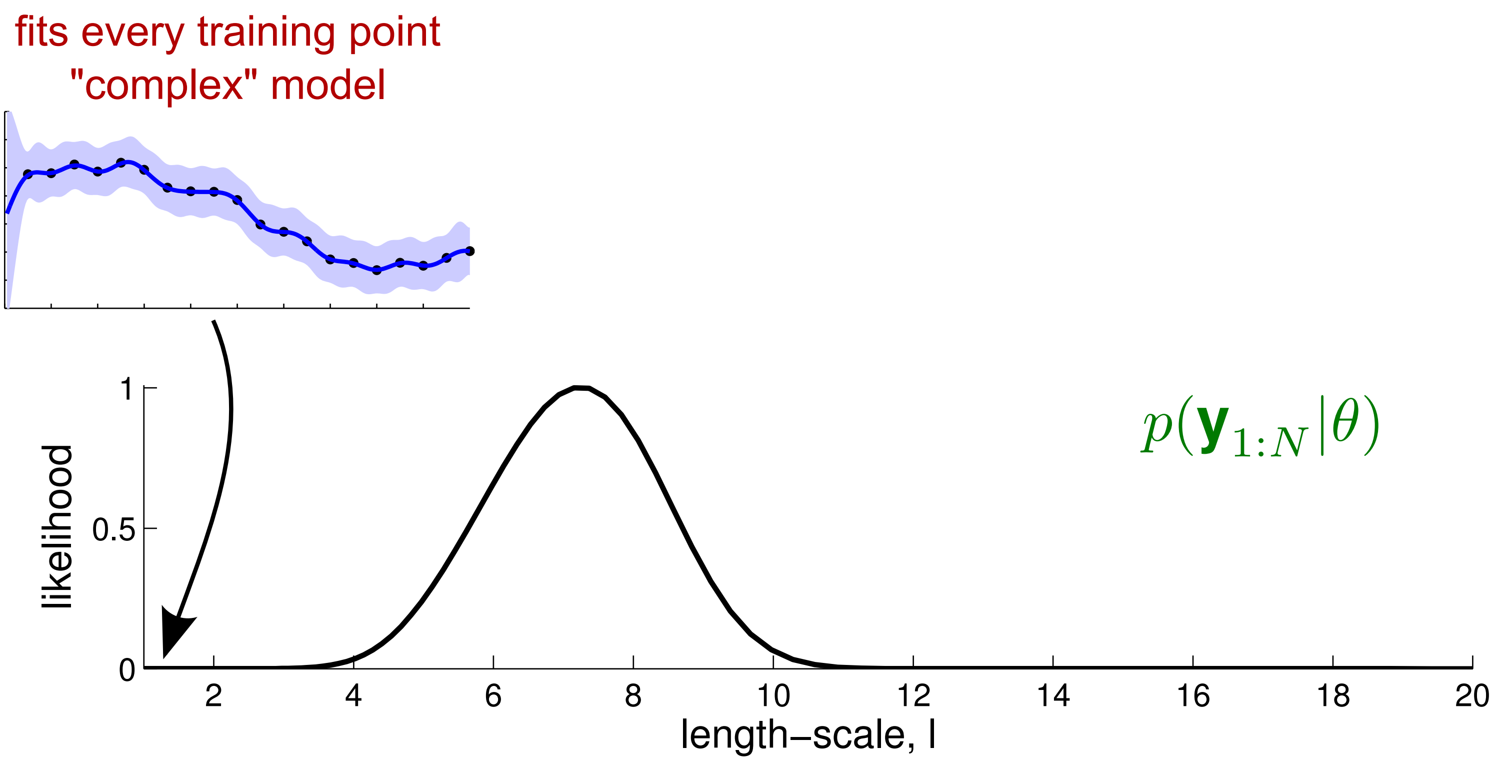

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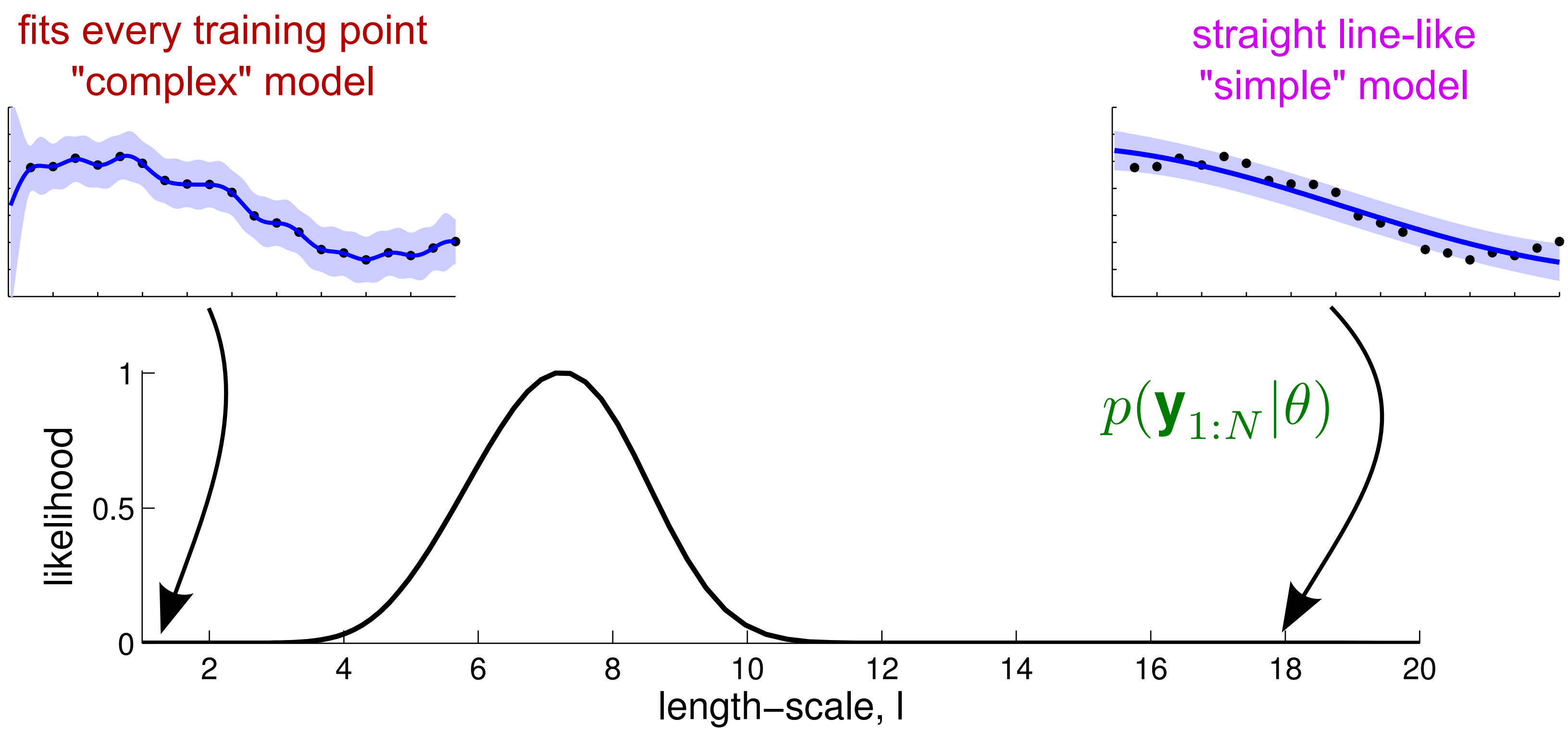

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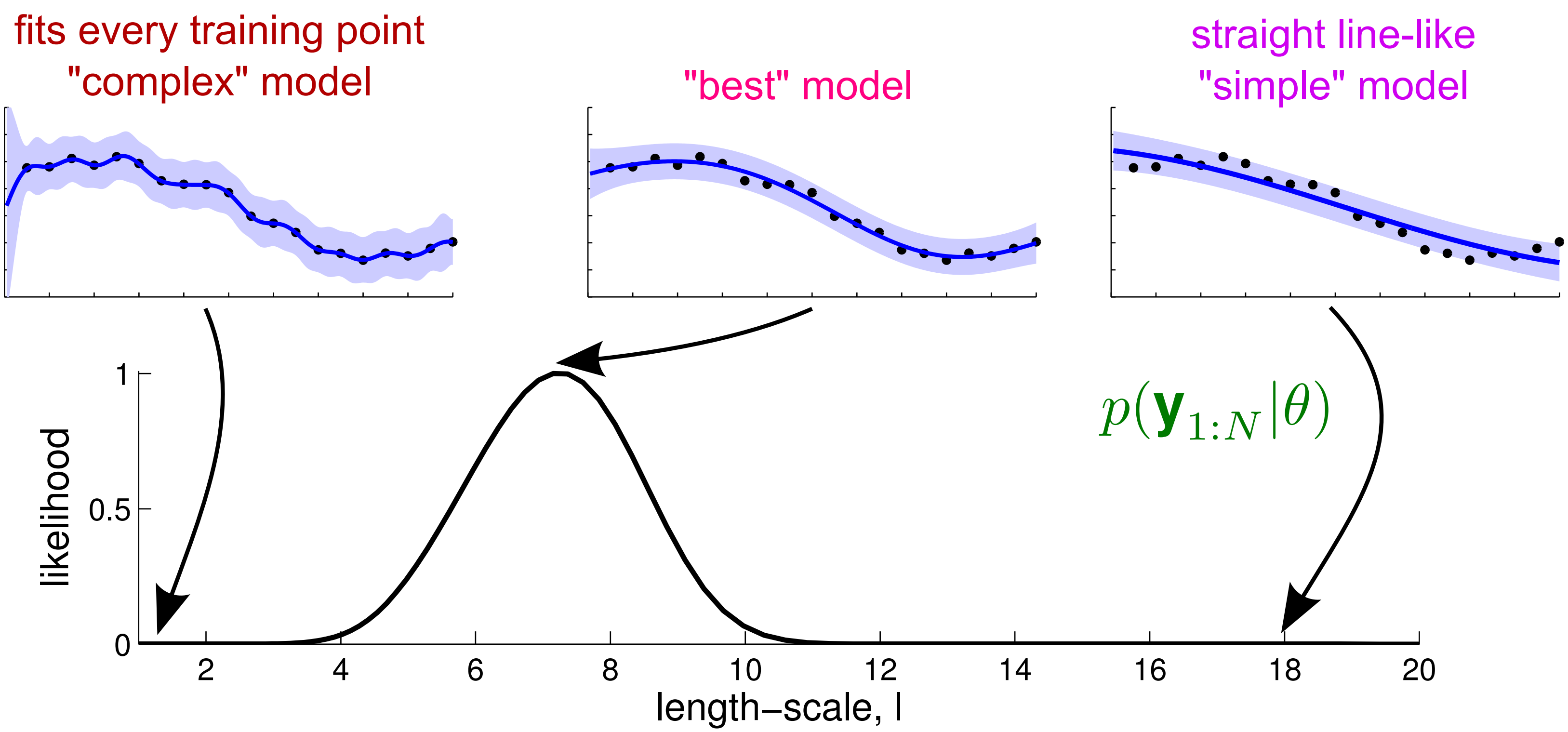

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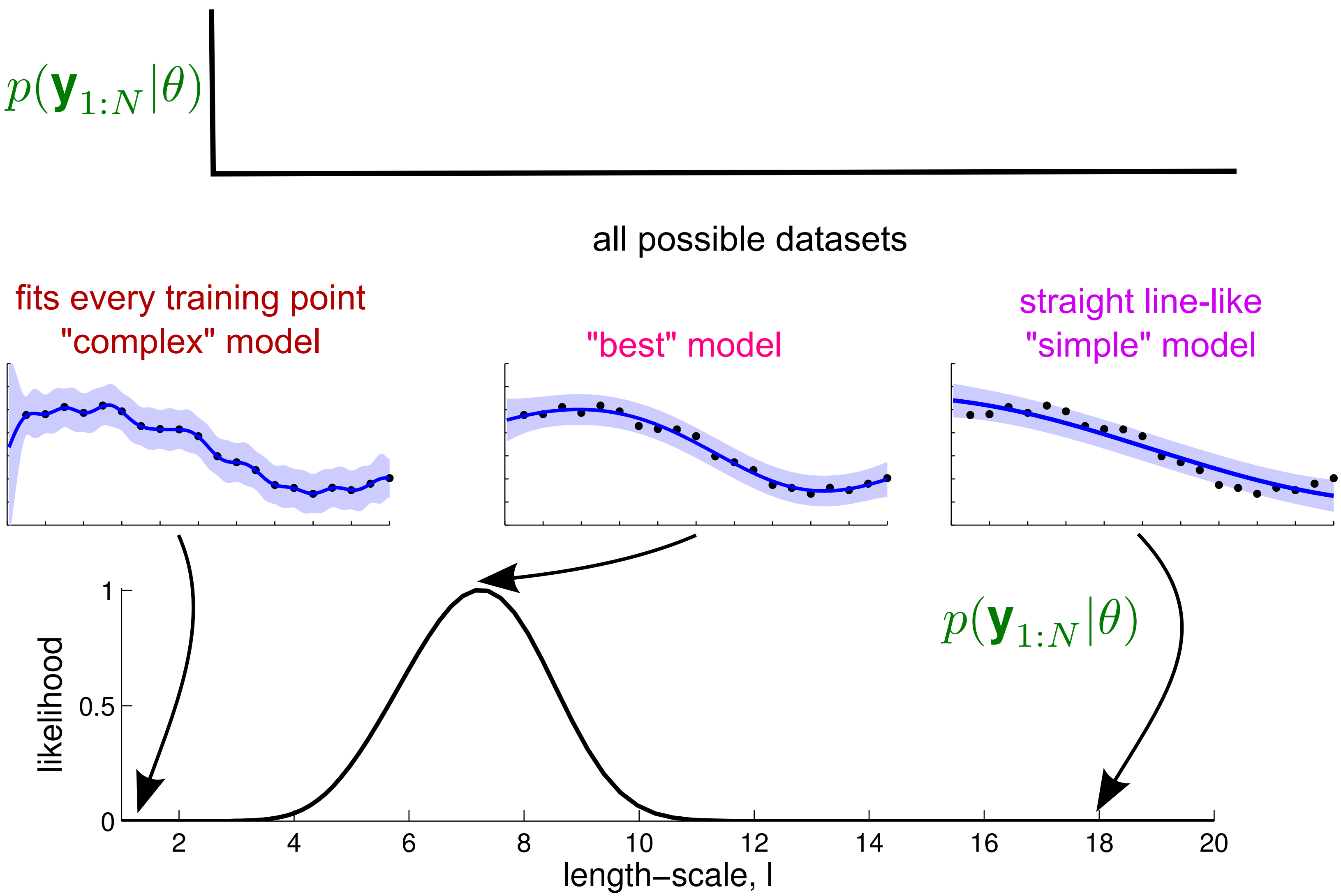

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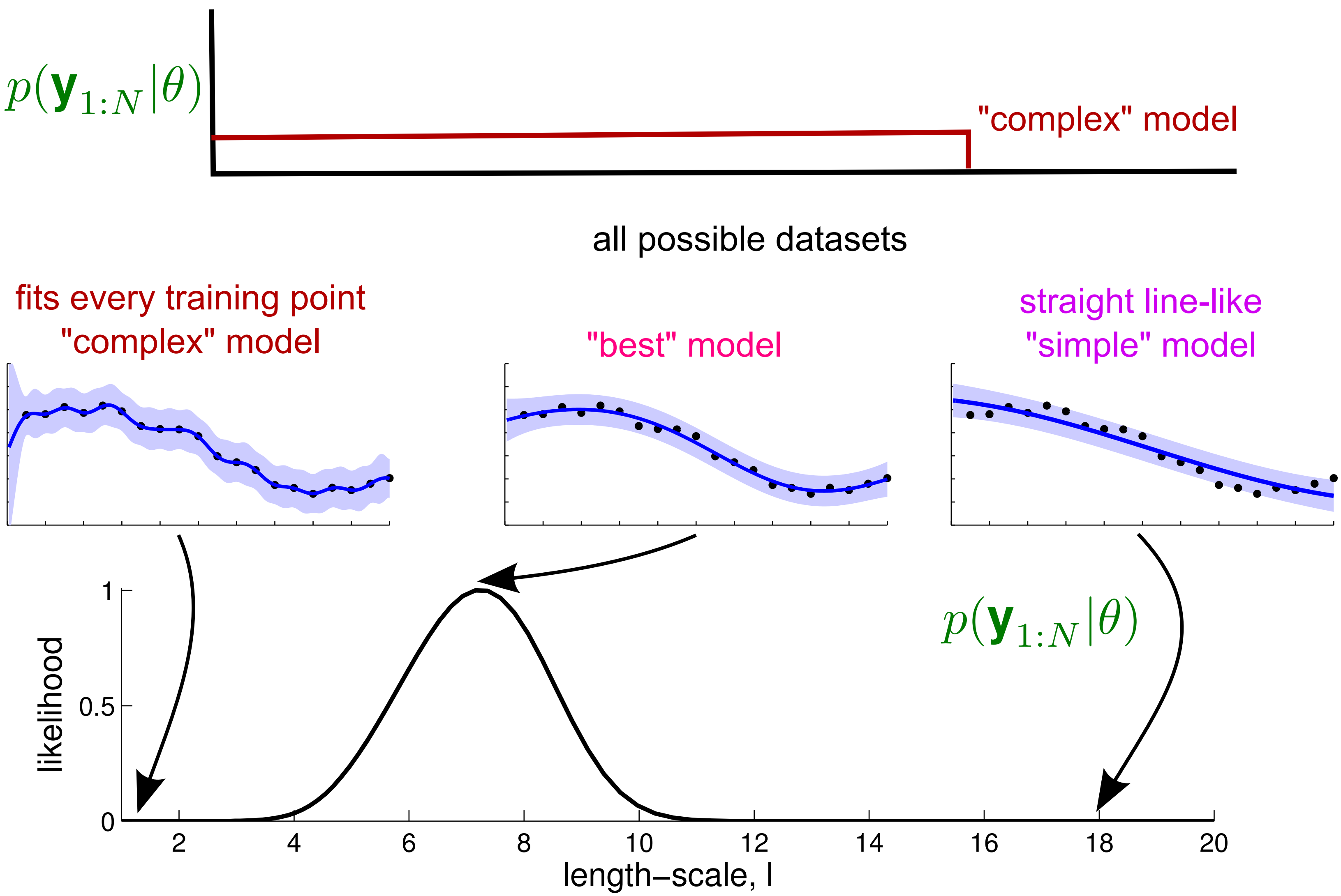

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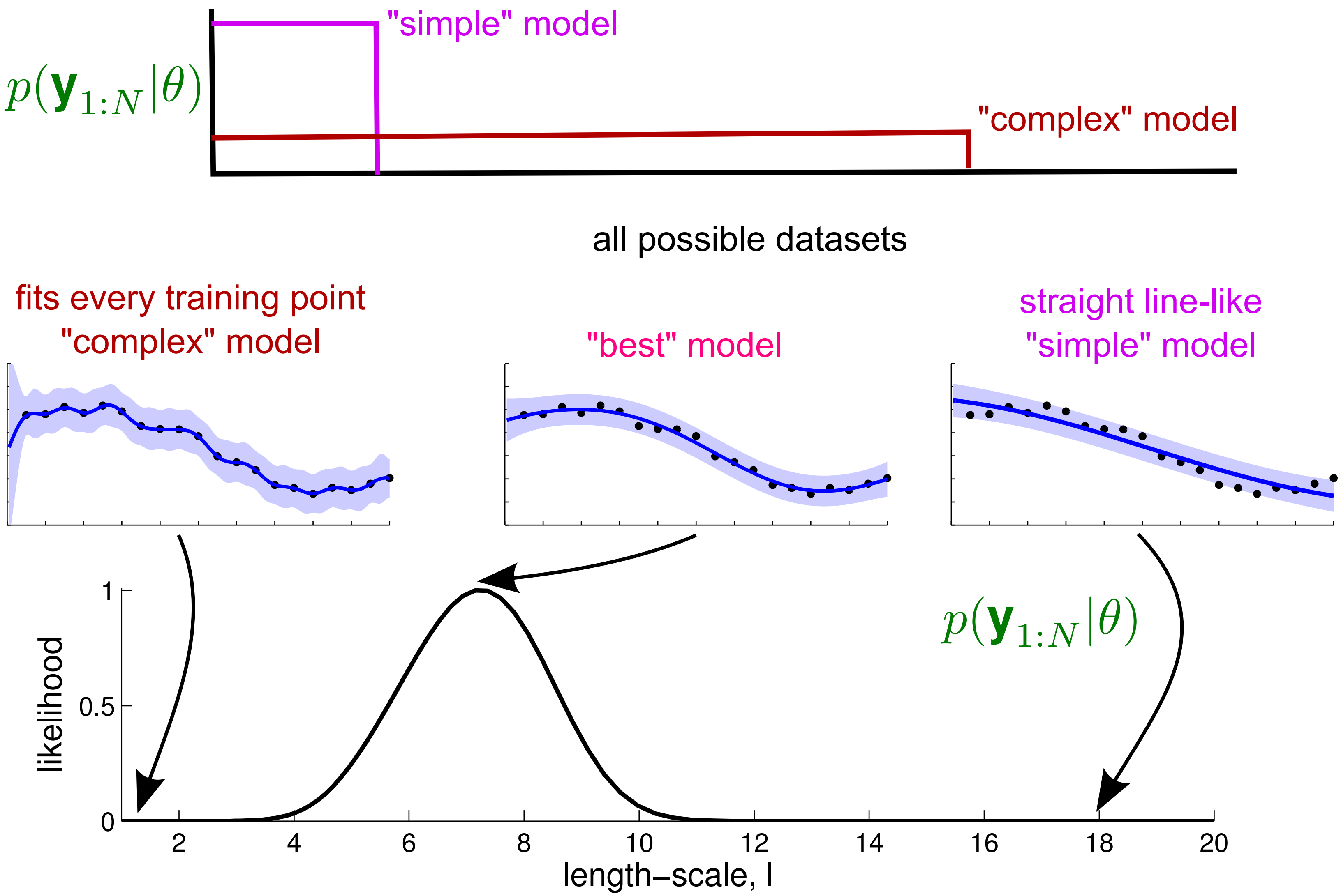

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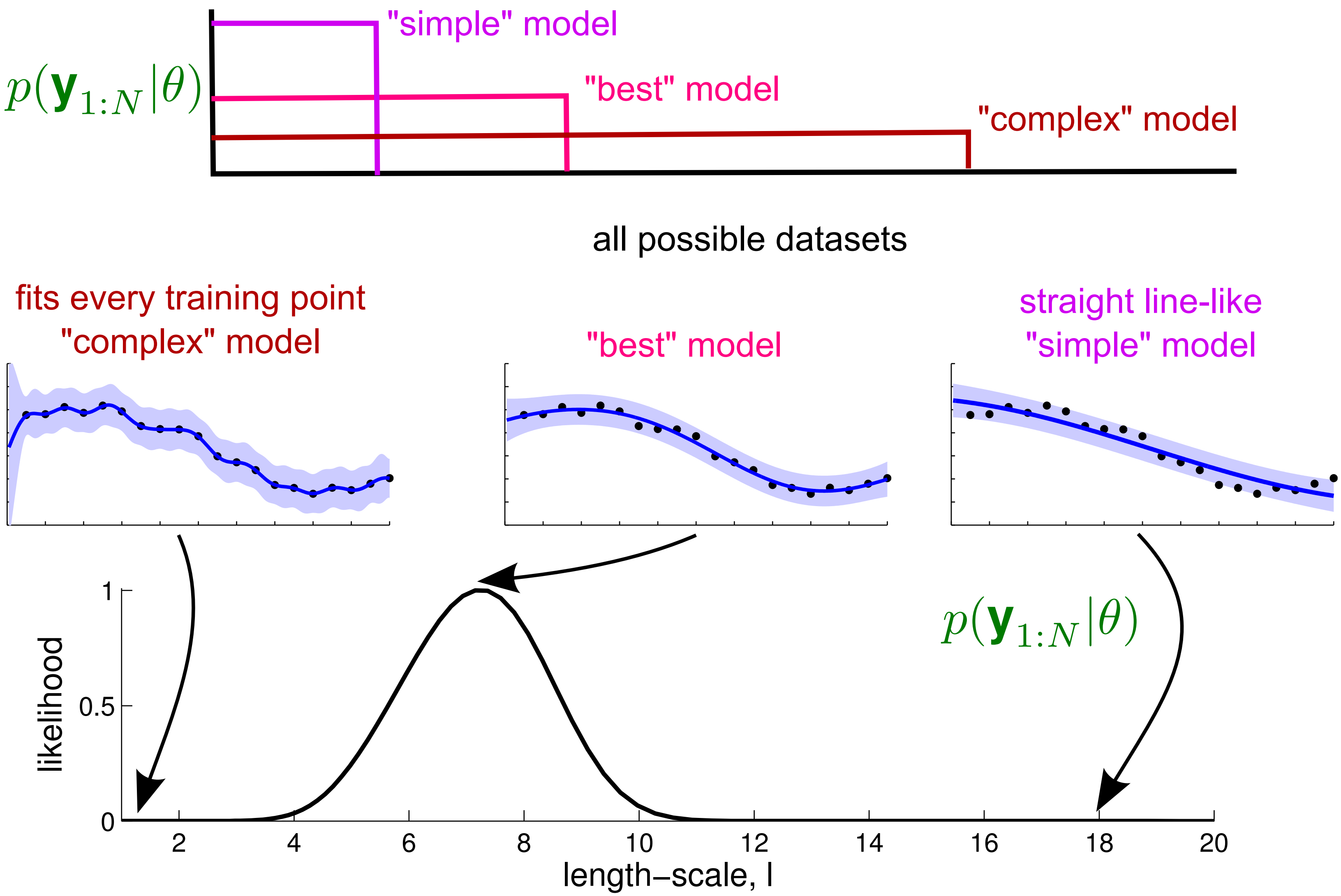
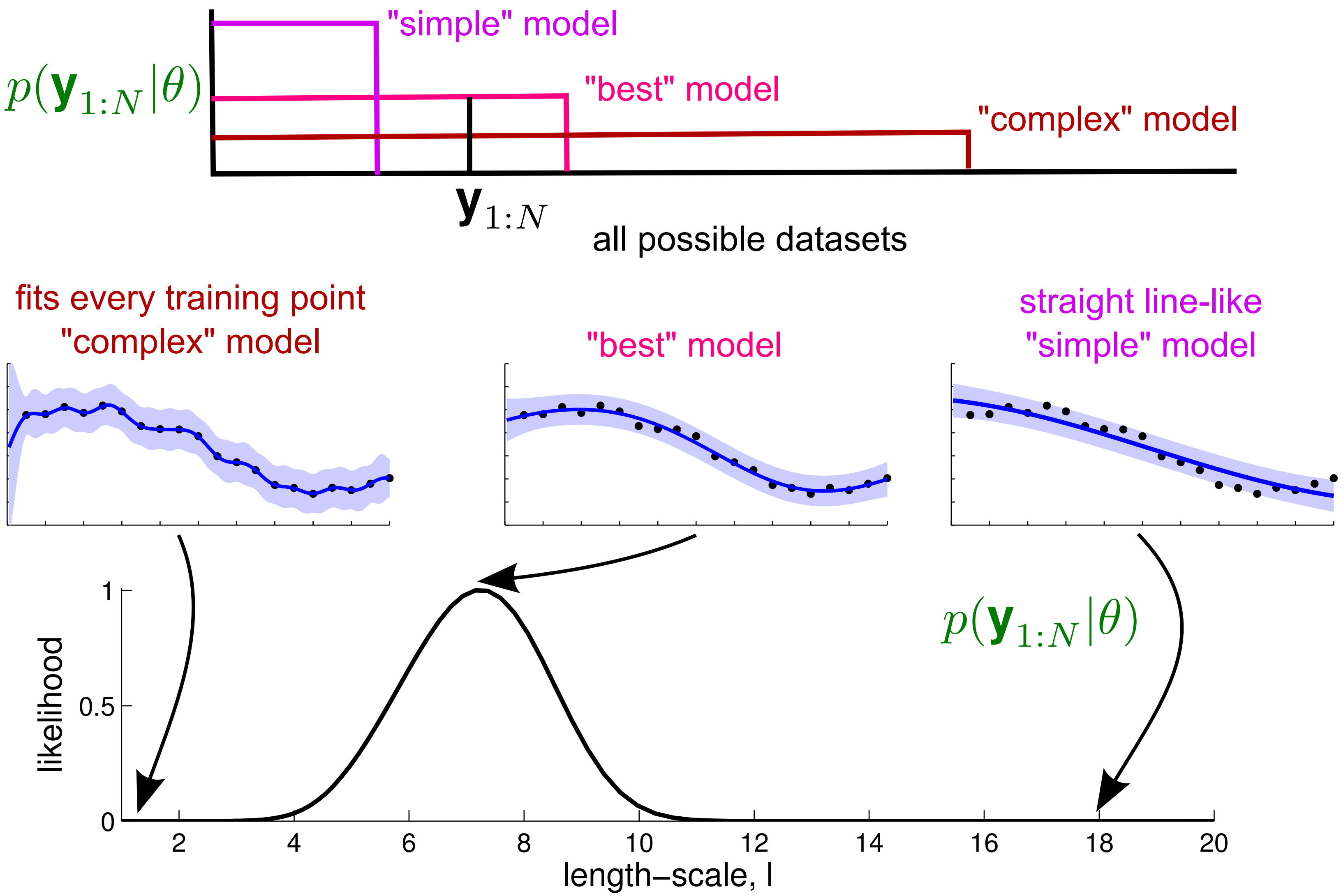


Why does Bayesian inference work? Occam's Razor.



How do we make predictions now?

$$p(\mathbf{y}'|\mathbf{y}_{1:N}, M) = \int \mathrm{d}\theta \;\; p(\mathbf{y}'|\mathbf{y}_{1:N}, \theta, M) p(\theta|\mathbf{y}_{1:N}, M)$$

- for every setting of the parameters...
- make a prediction for the testing points (as before) $p(\mathbf{y}'|\mathbf{y}_{1:N}, \theta, M)$
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Only need two rules for Bayesian computation: product and sum rules

$$p(\mathsf{x}, \mathsf{y}) = p(\mathsf{x}|\mathsf{y})p(\mathsf{y}) = p(\mathsf{y}|\mathsf{x})p(\mathsf{x}) \qquad\qquad p(\mathsf{x}) = \sum_{\mathsf{y}} p(\mathsf{x}, \mathsf{y})$$

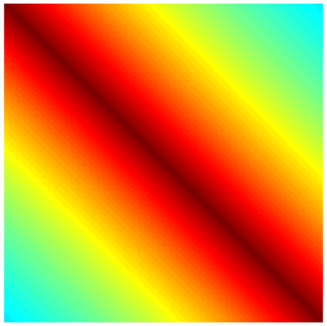
What effect does the form of the covariance function have?

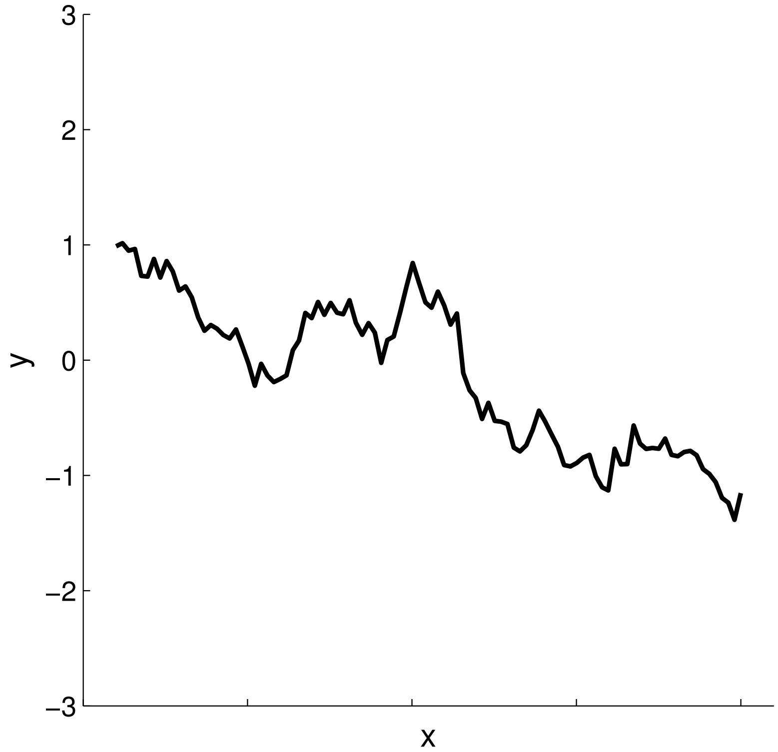
$$K(x_1, x_2) = \sigma^2 \exp\left(-\frac{1}{2l^2}|x_1 - x_2|\right)$$

Laplacian covariance function

Browninan motion

Ornstein-Uhlenbeck

$\Sigma =$ 



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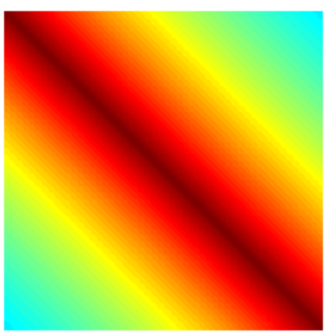
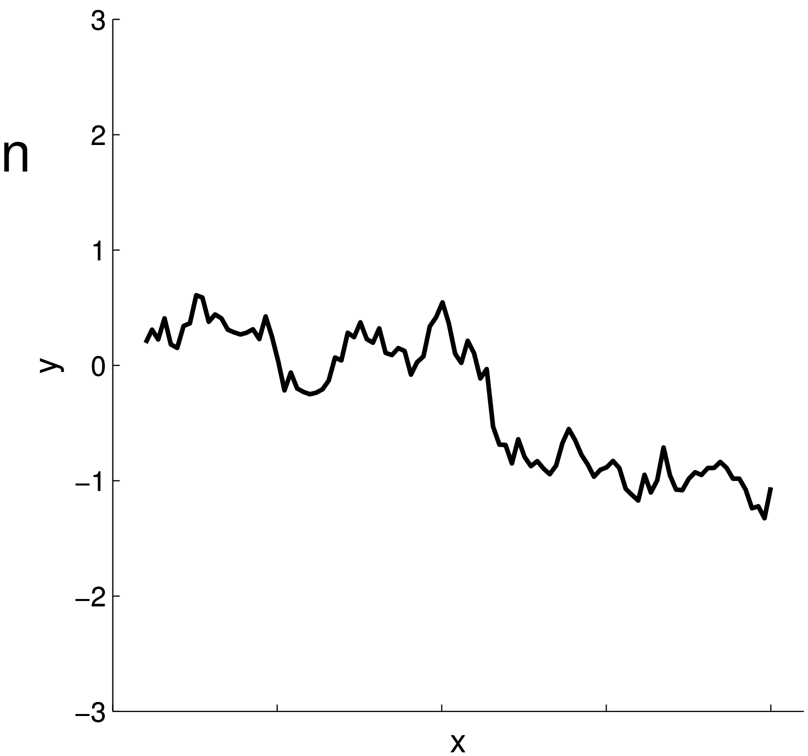
$\Sigma =$ 



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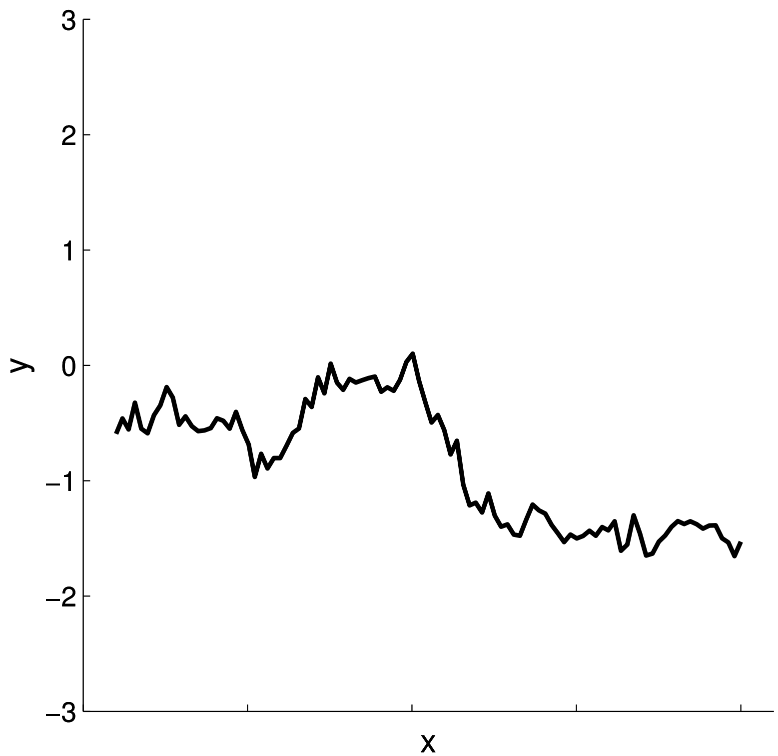

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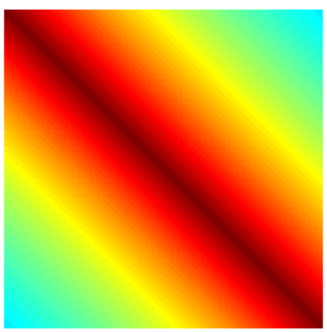

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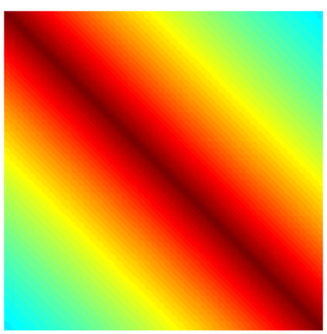

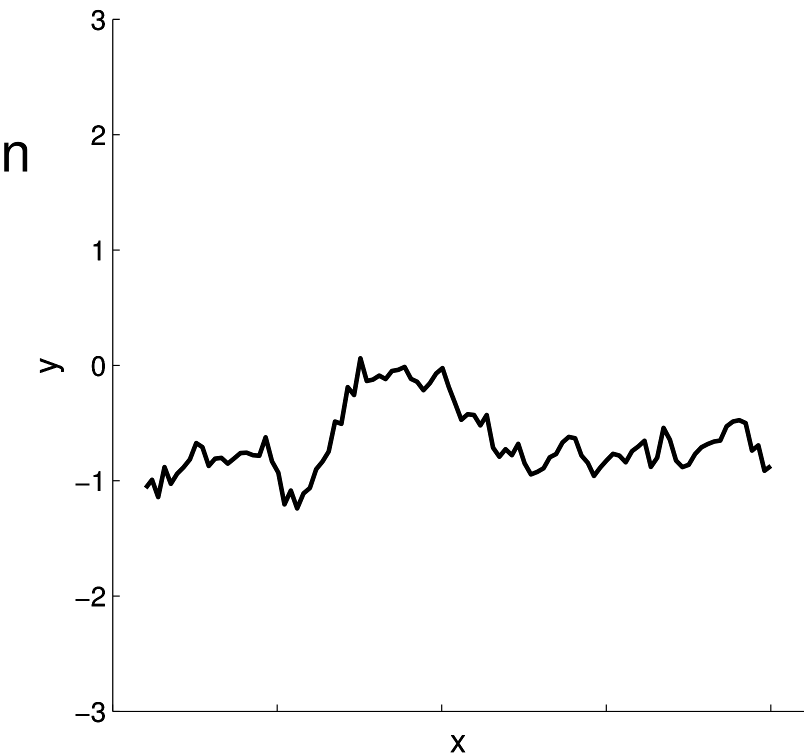

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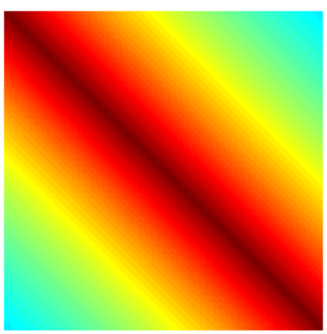
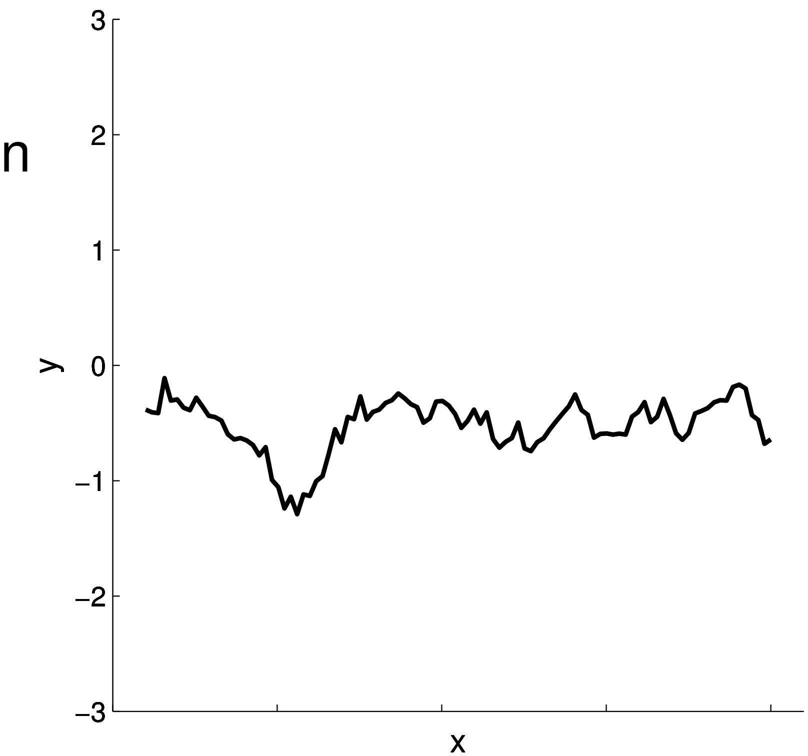
$\Sigma =$ 



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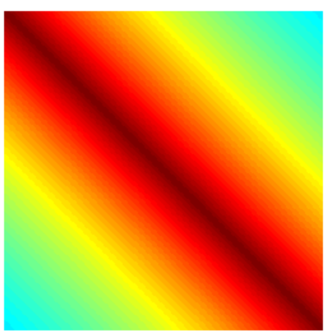

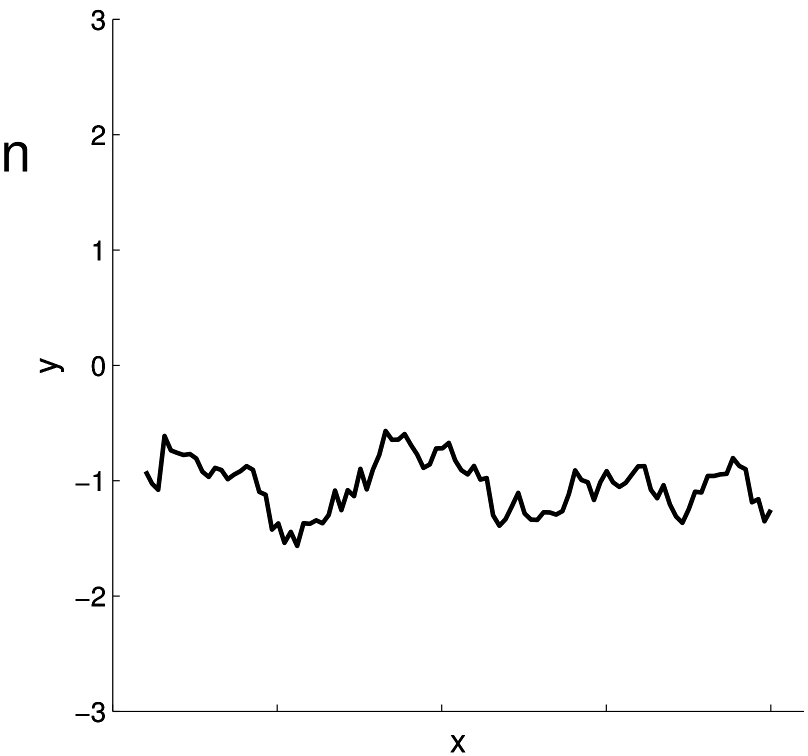

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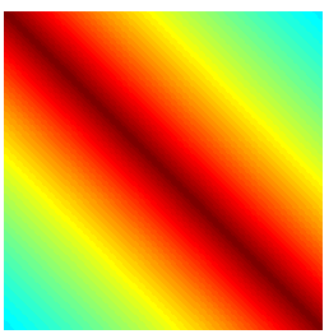
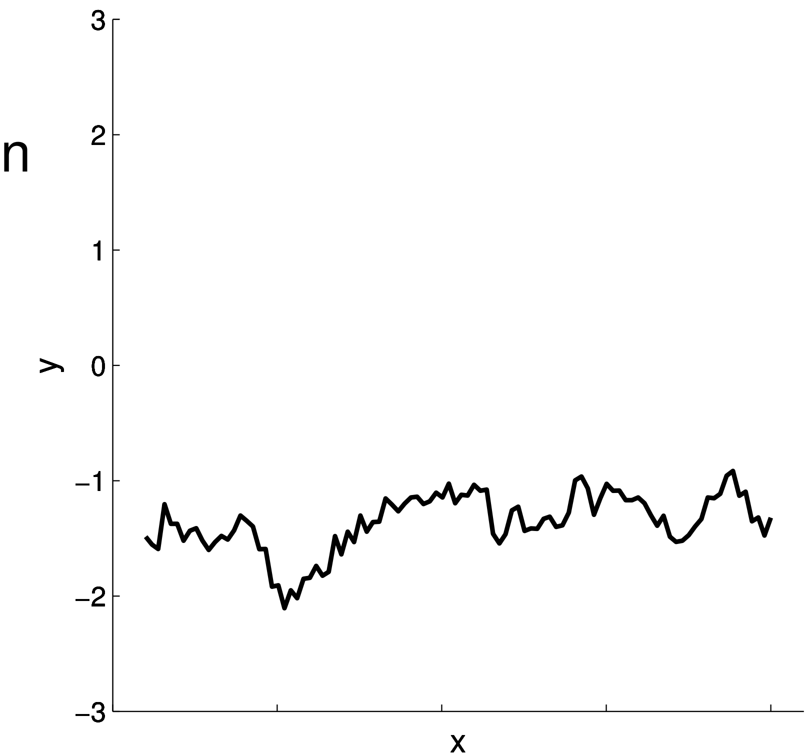
$\Sigma =$ 



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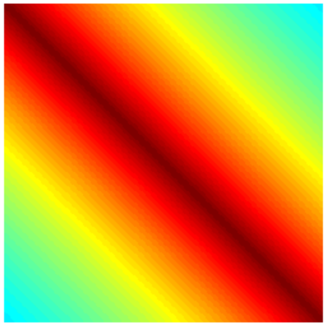
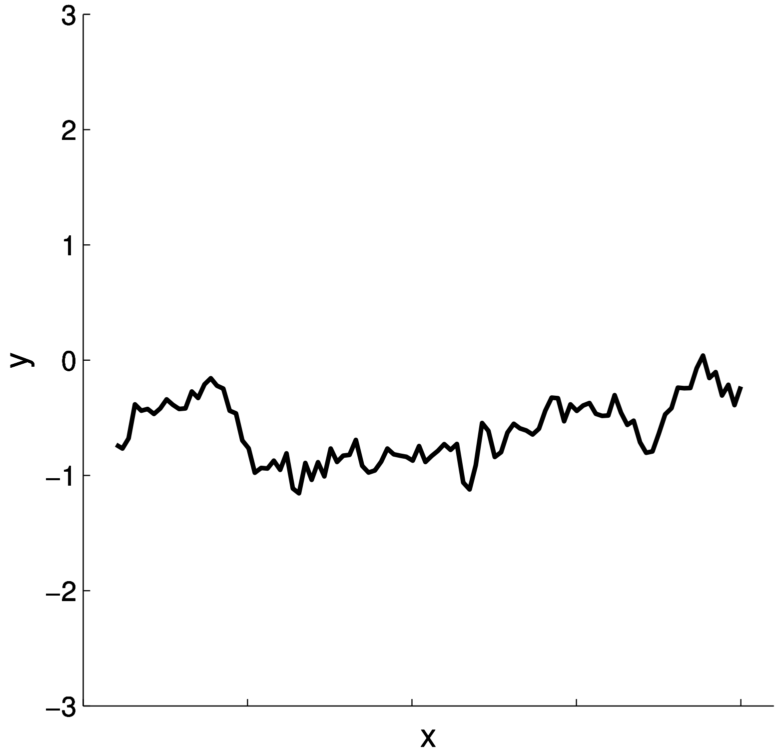
$\Sigma =$ 



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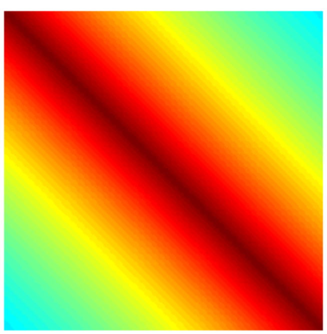
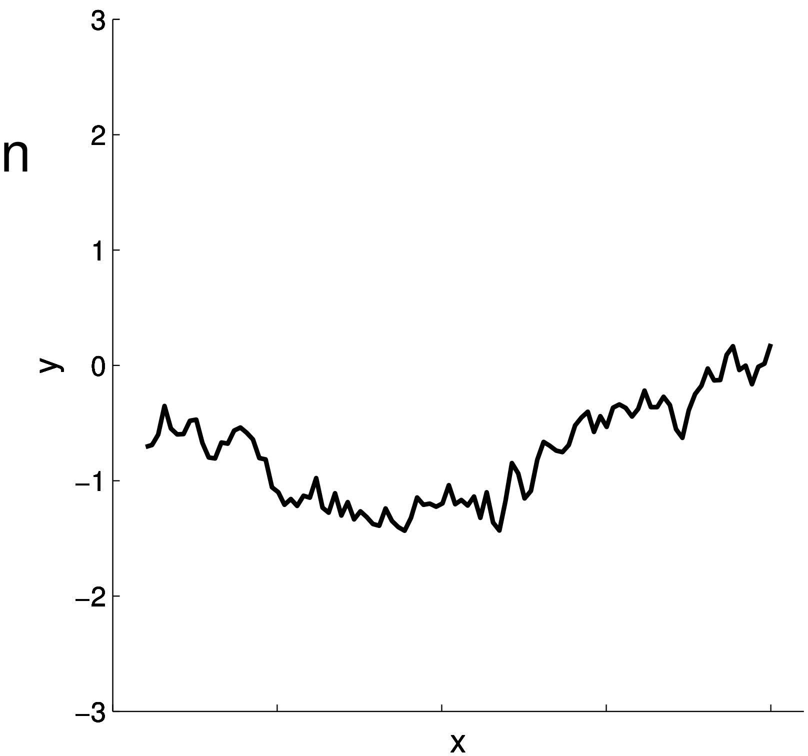
$\Sigma =$ 



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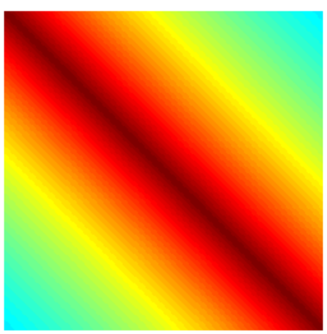

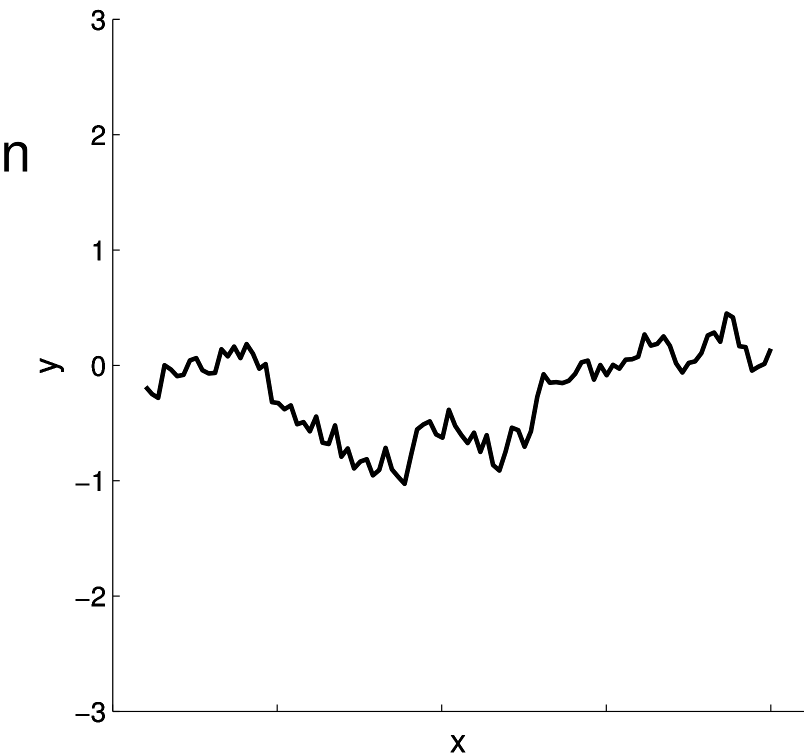

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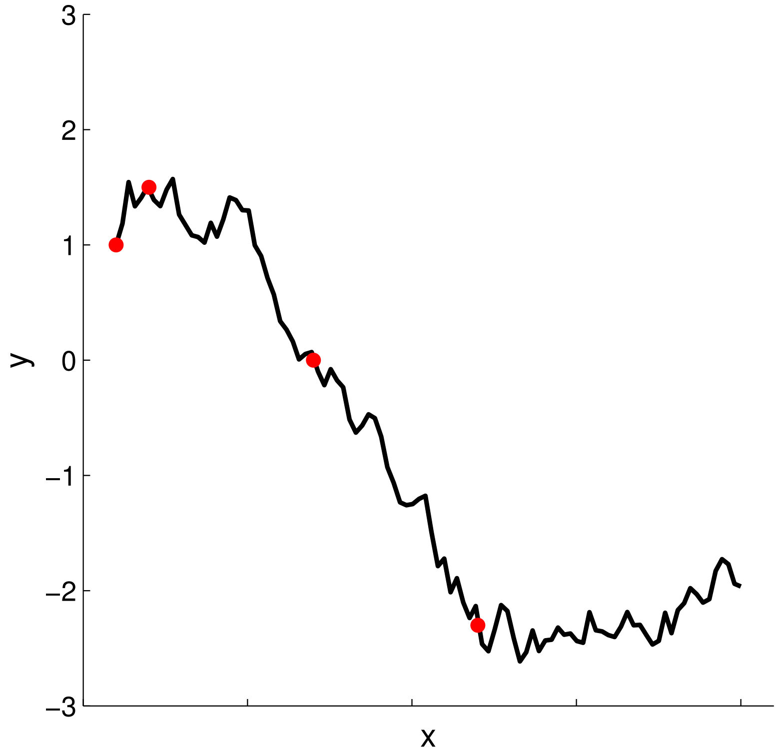
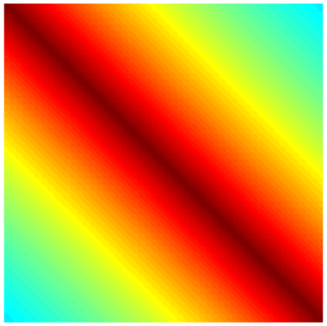


$\Sigma =$ 

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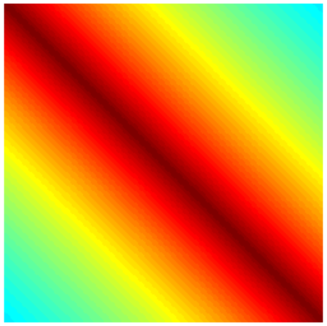
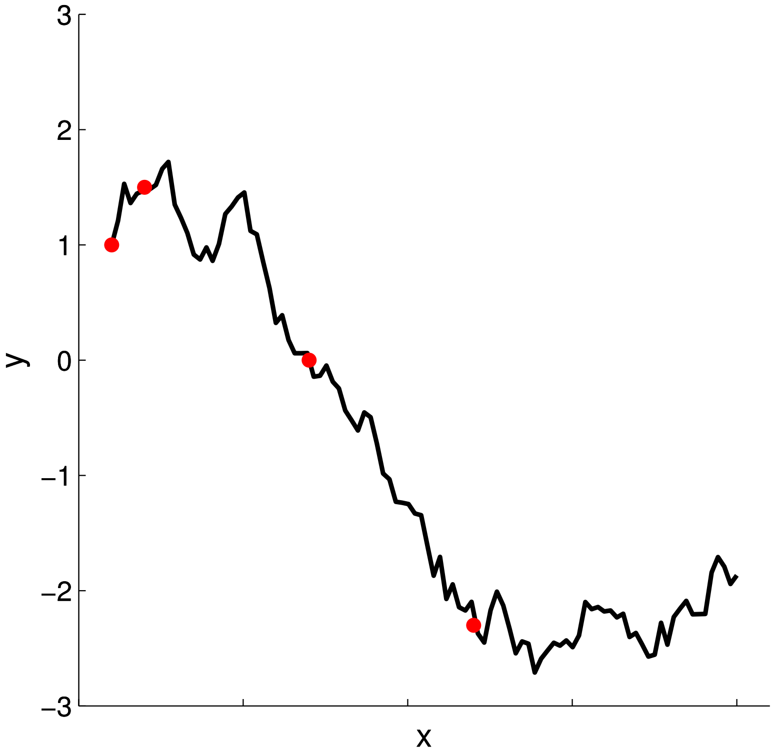
$\Sigma =$ 



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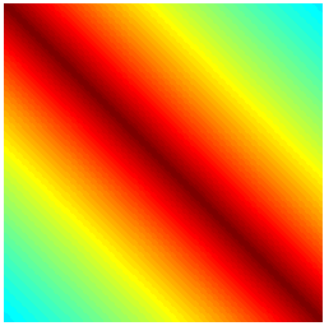
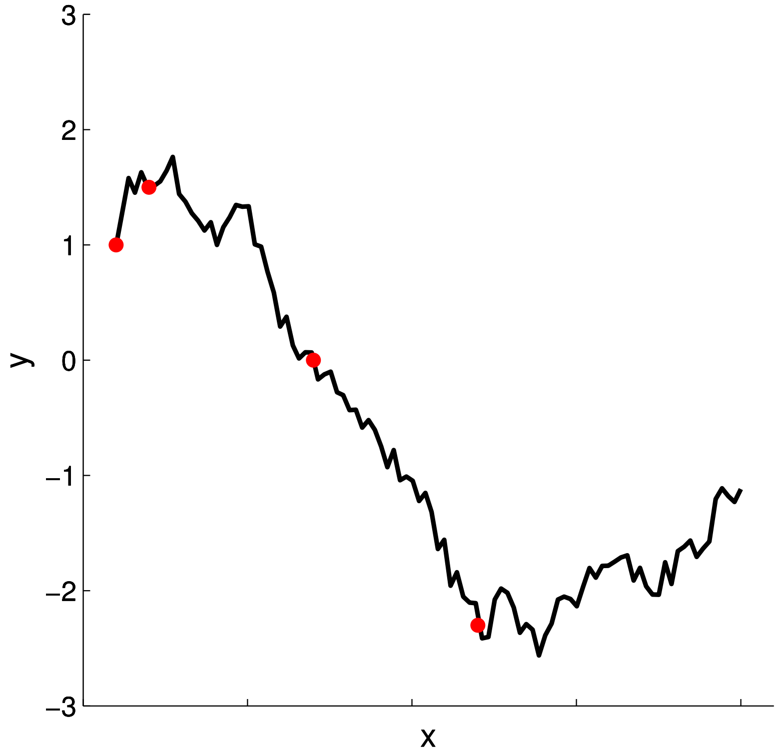
$\Sigma =$ 



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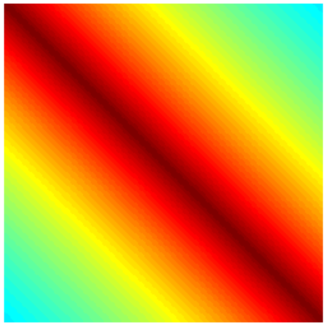
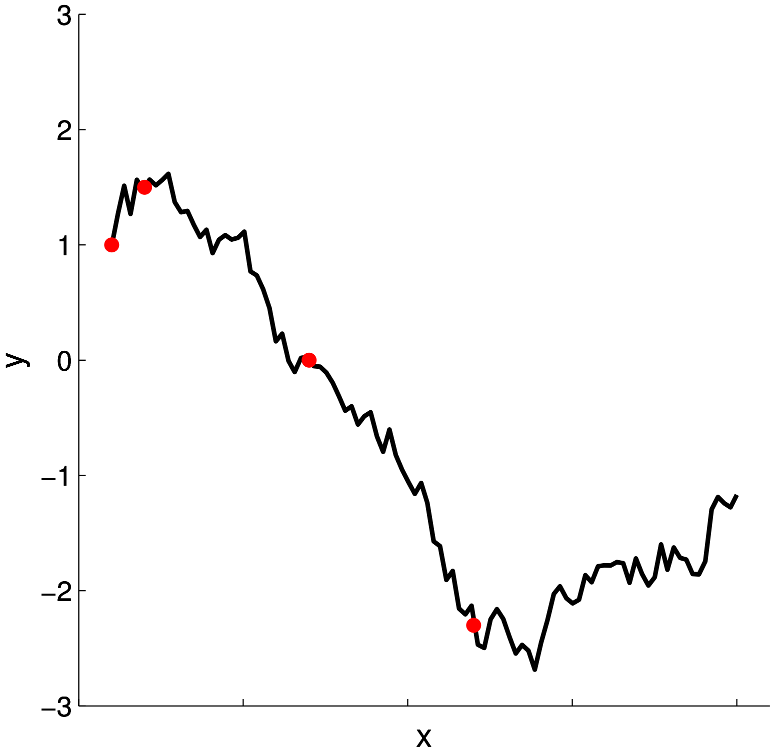
$\Sigma =$ 



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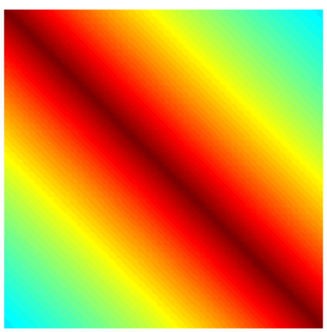
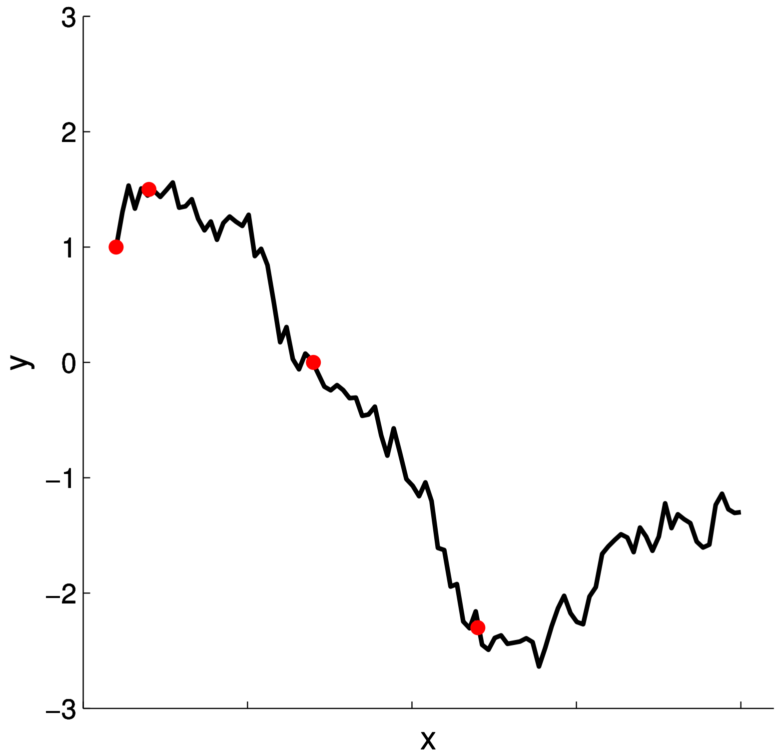
$\Sigma =$ 



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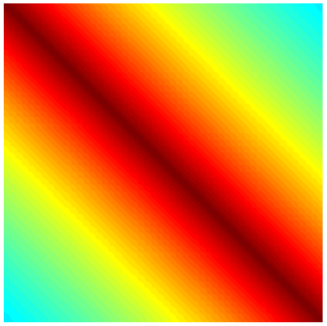

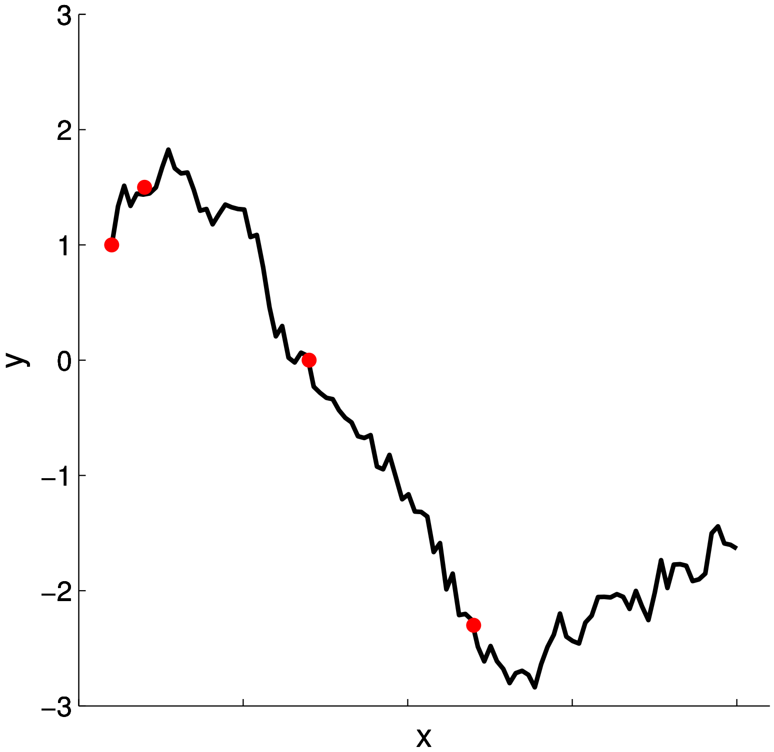

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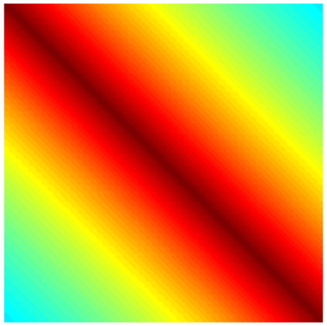

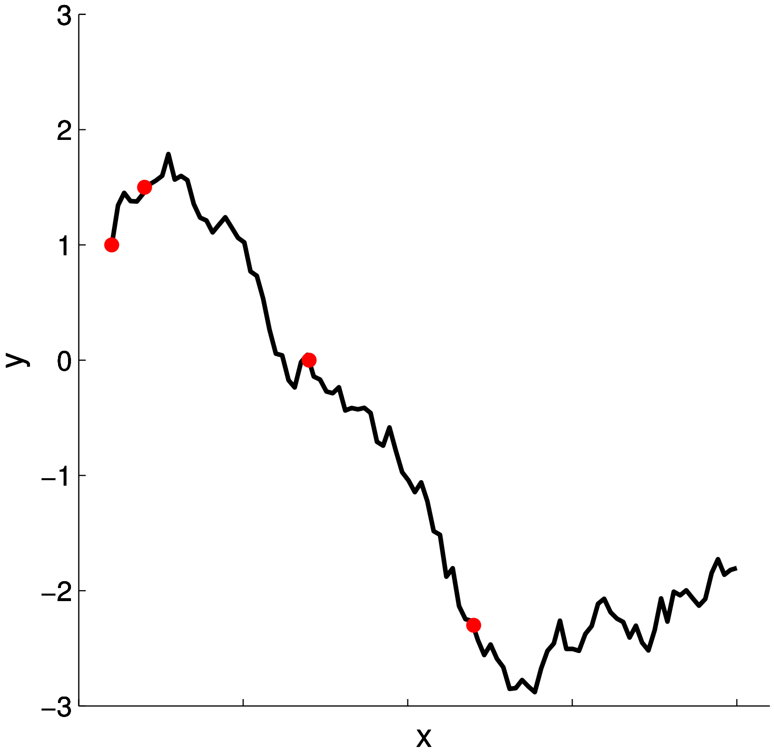

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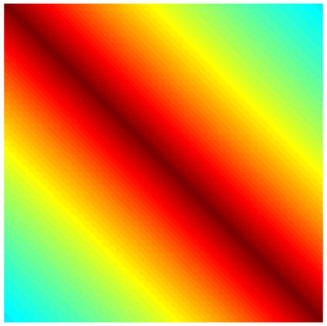

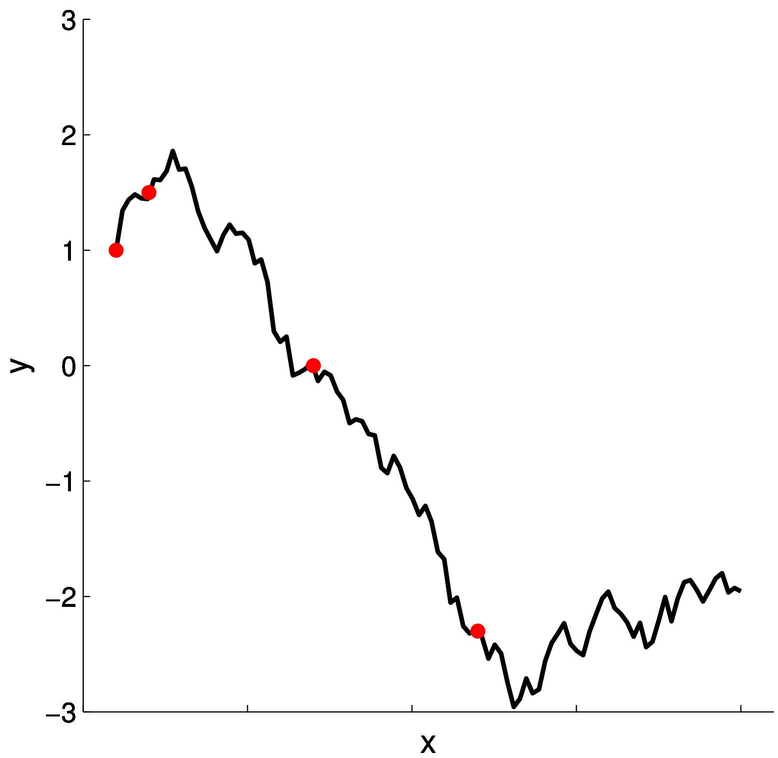

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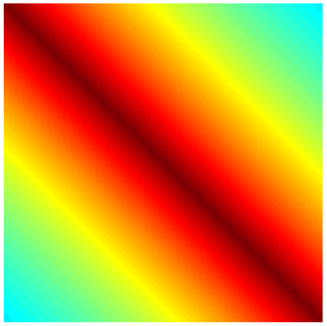
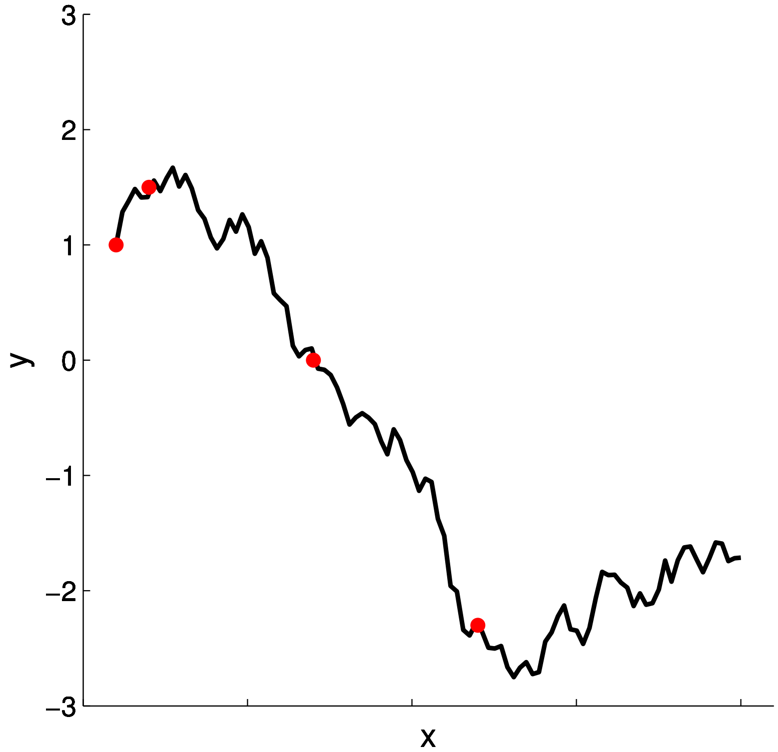
Laplacian covariance function

Browninan motion

Ornstein-Uhlenbeck

$\Sigma =$ 



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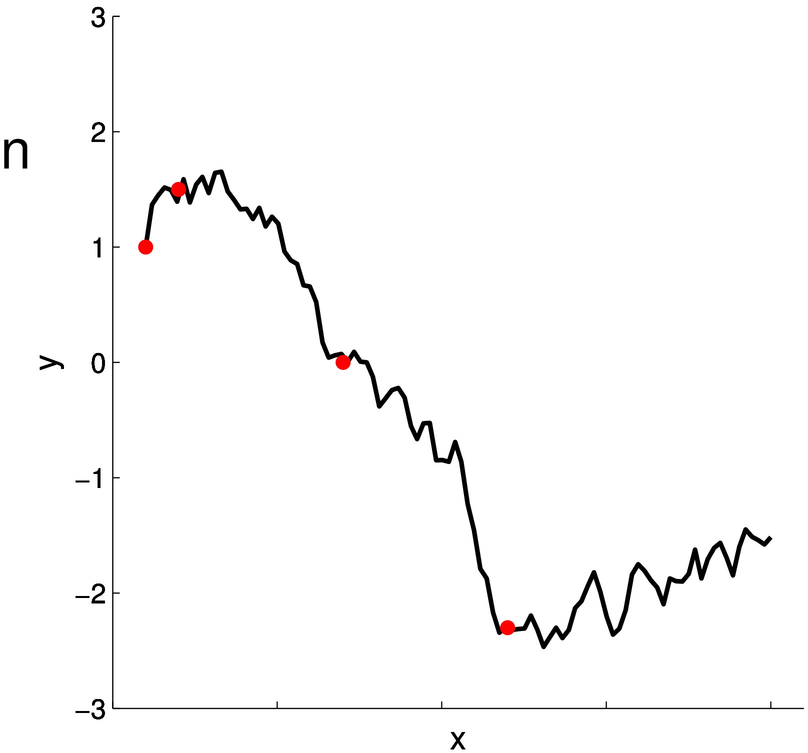
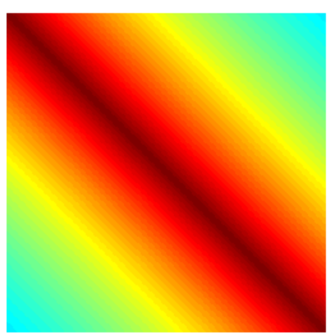


$\Sigma =$ 

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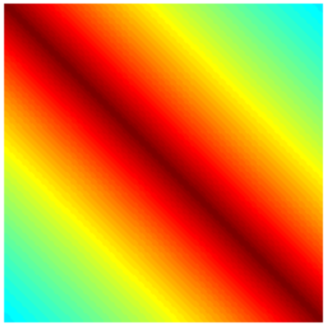
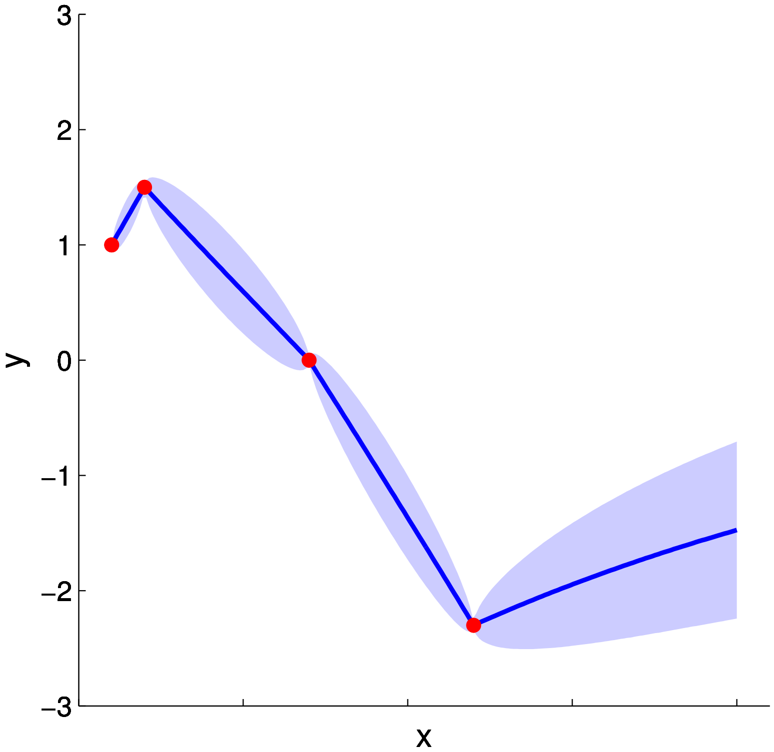
$\Sigma =$ 



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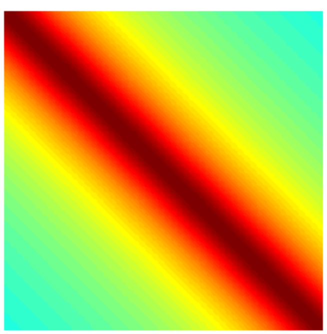

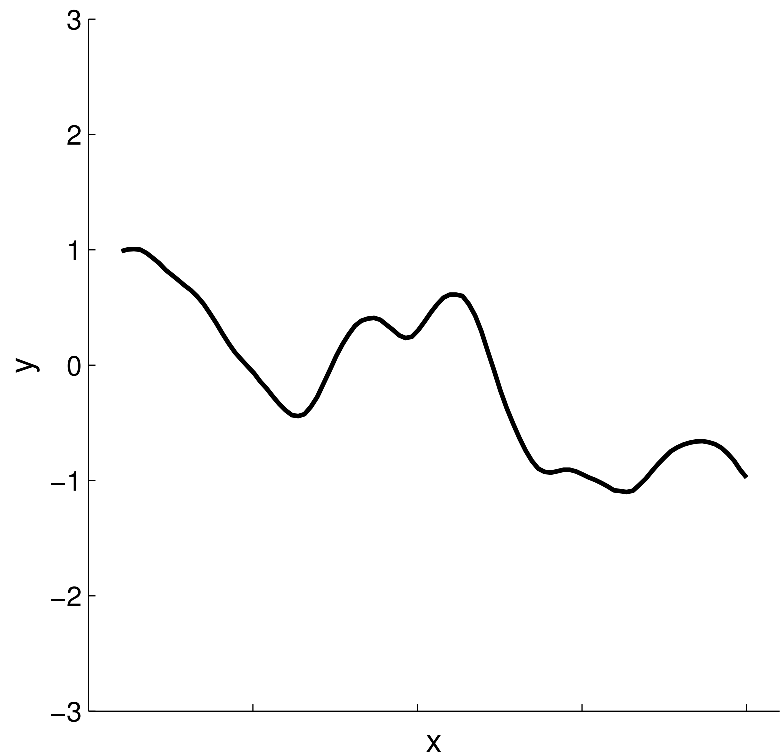

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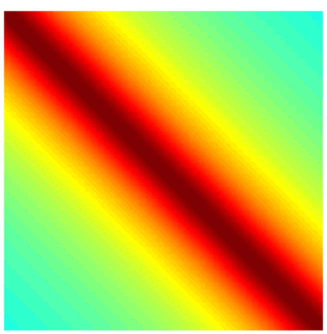

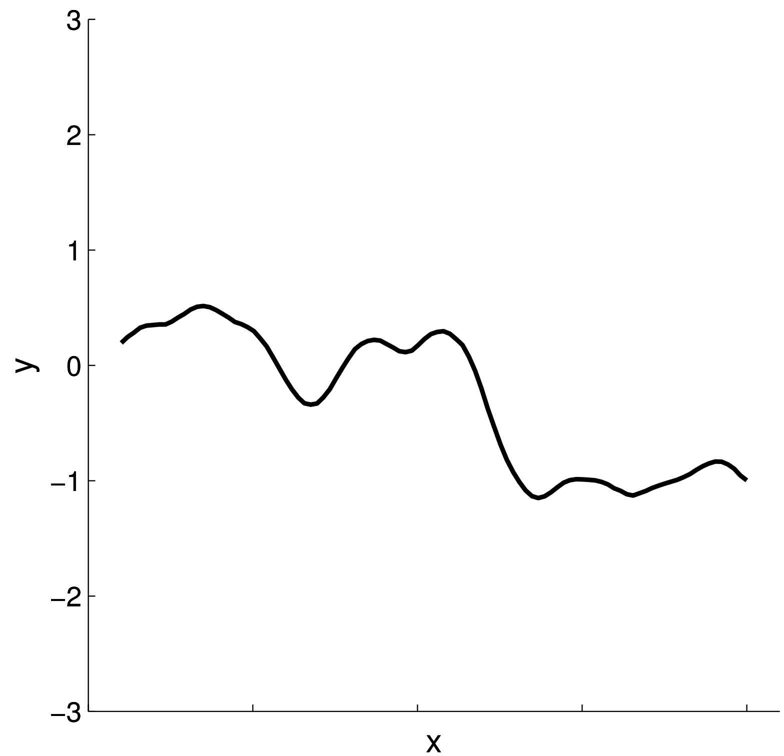

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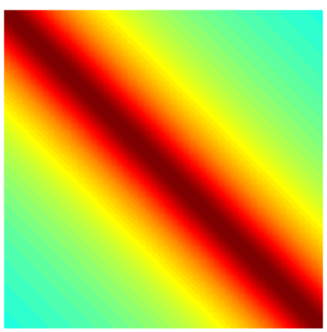
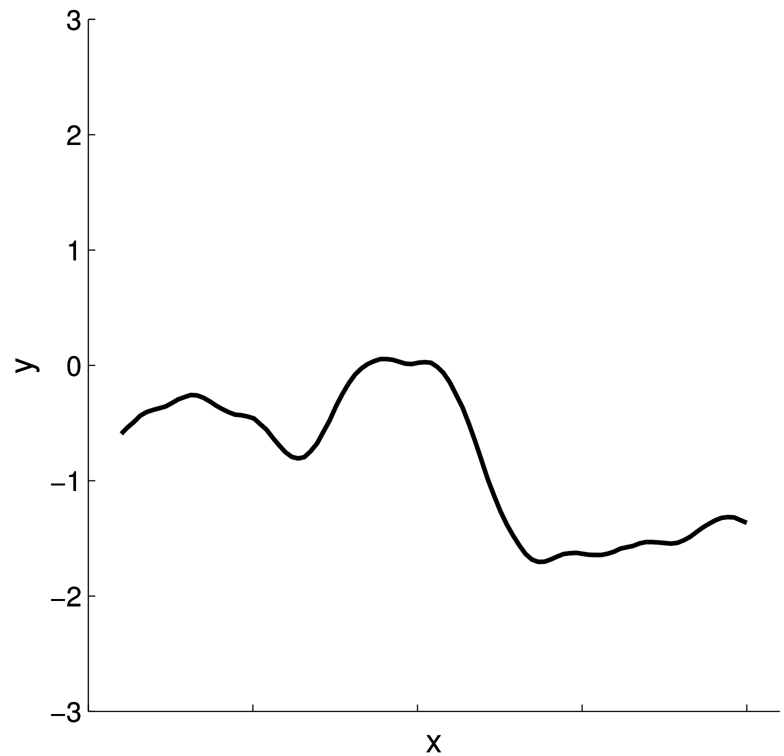
$\Sigma =$ 



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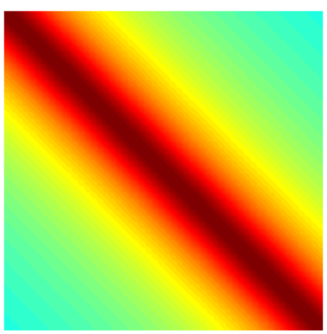
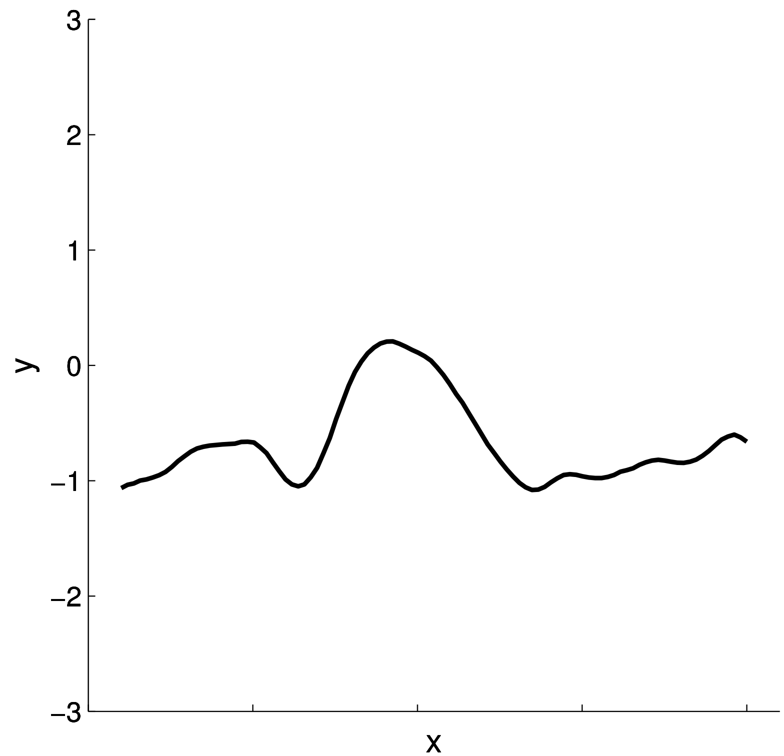
$\Sigma =$ 



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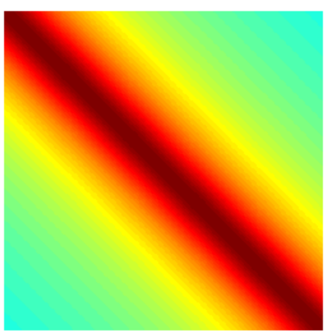
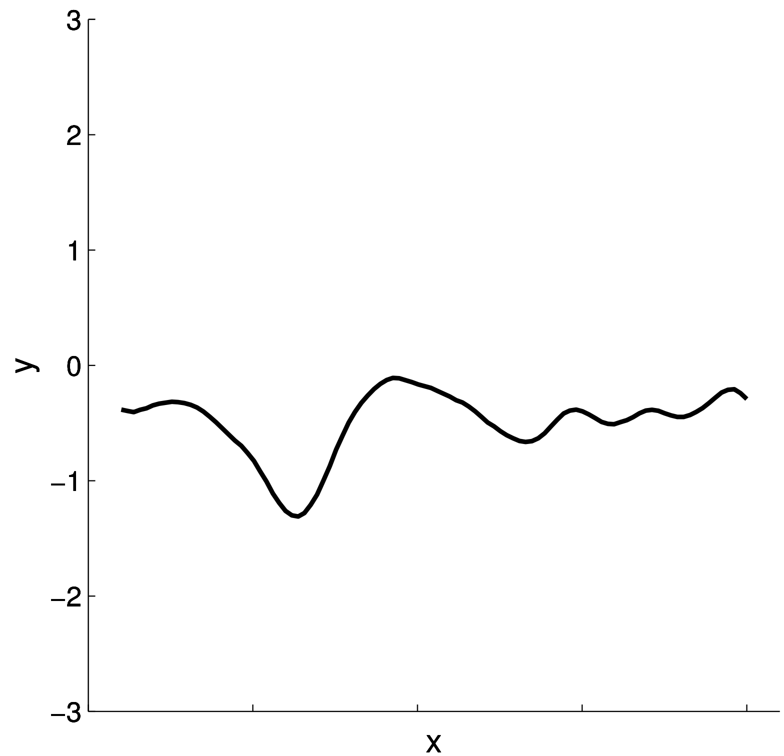
$\Sigma =$ 



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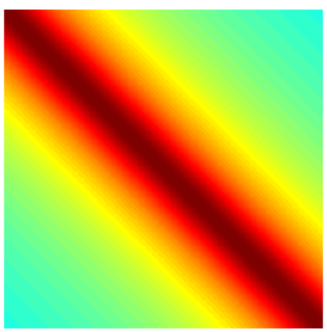
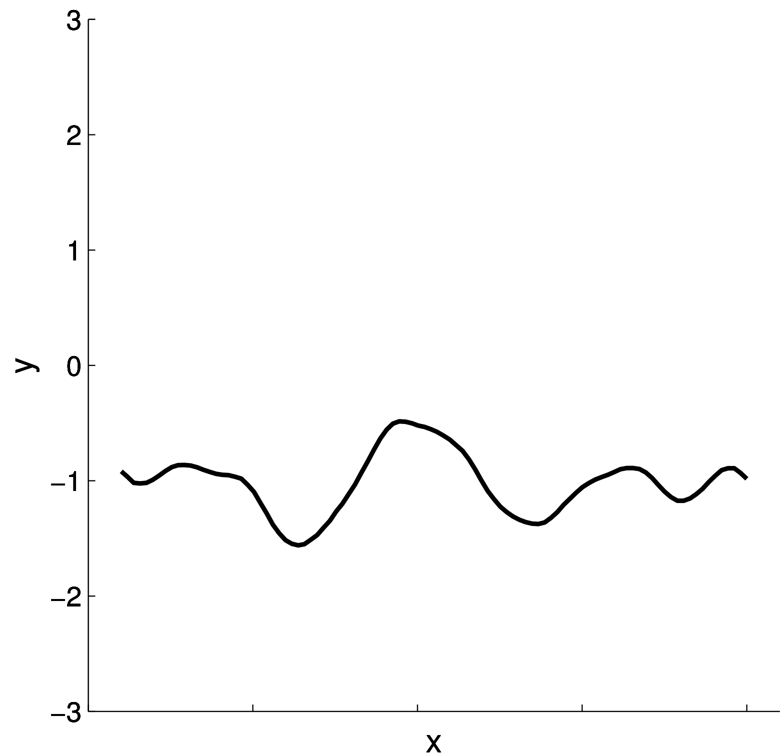
$\Sigma =$ 



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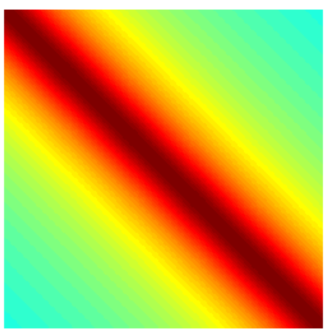

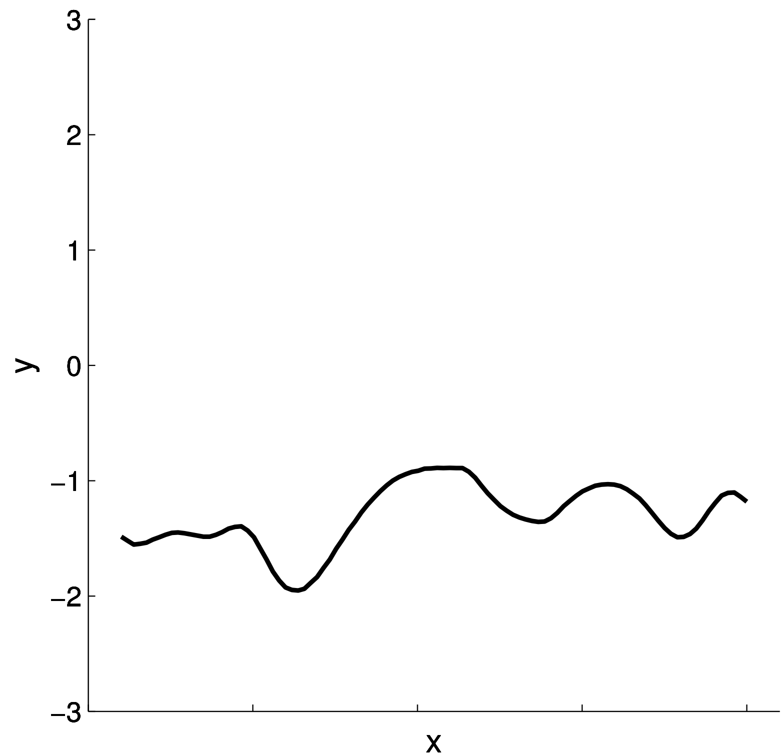

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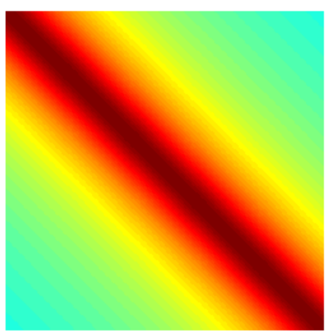

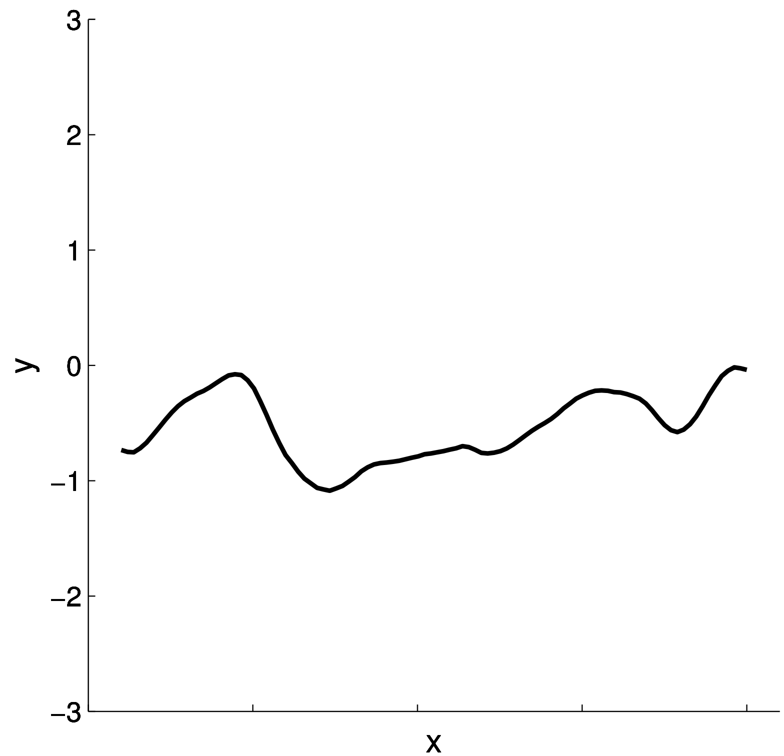

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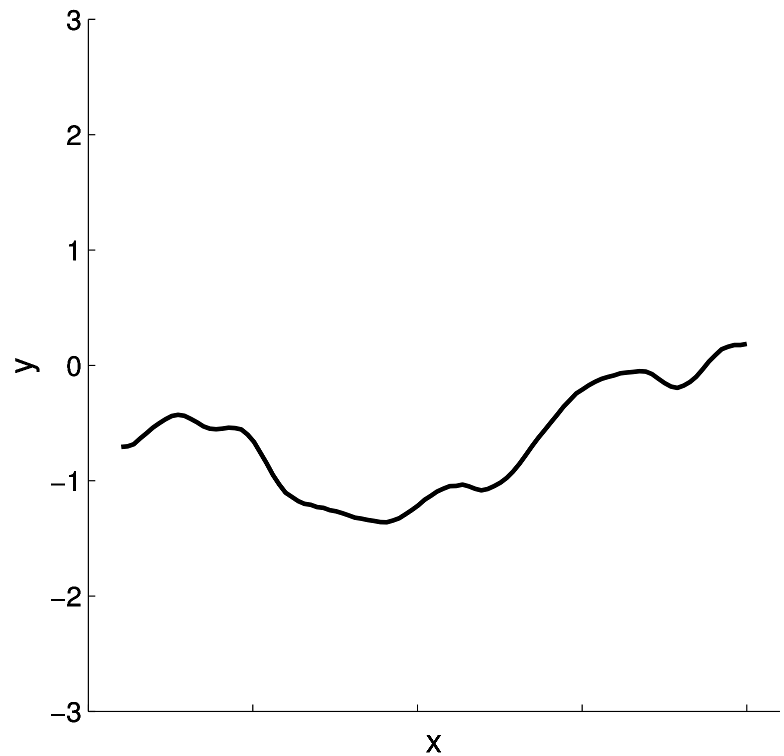

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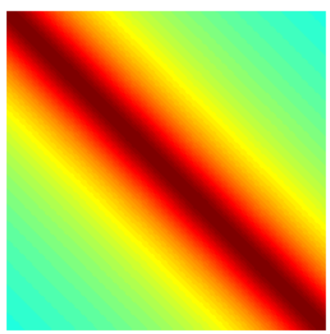

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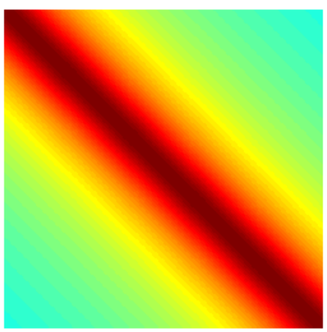
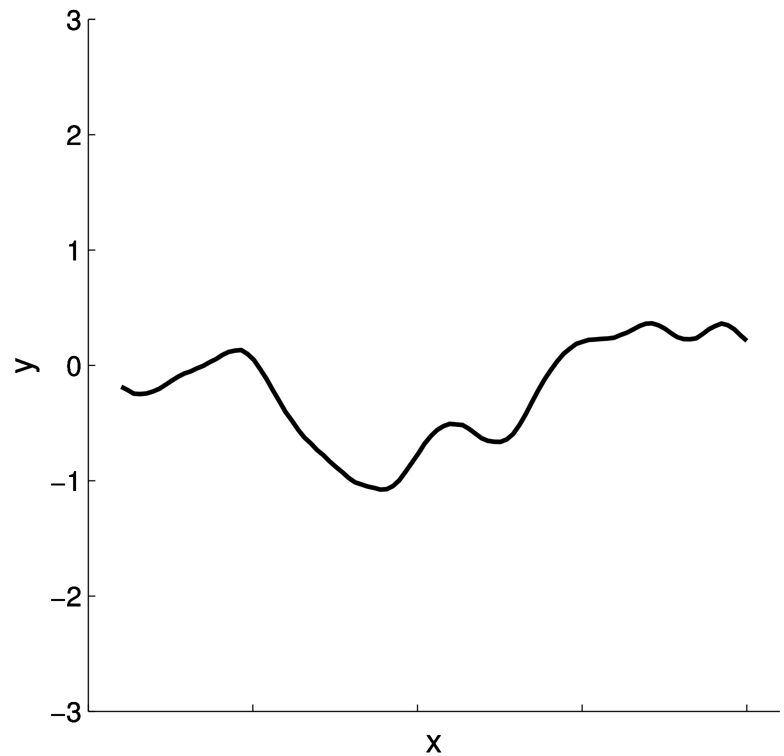
$\Sigma =$ 



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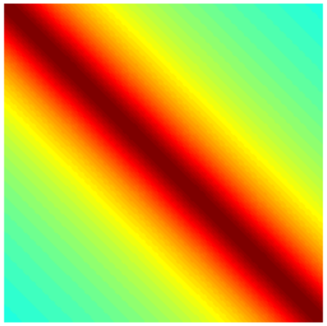
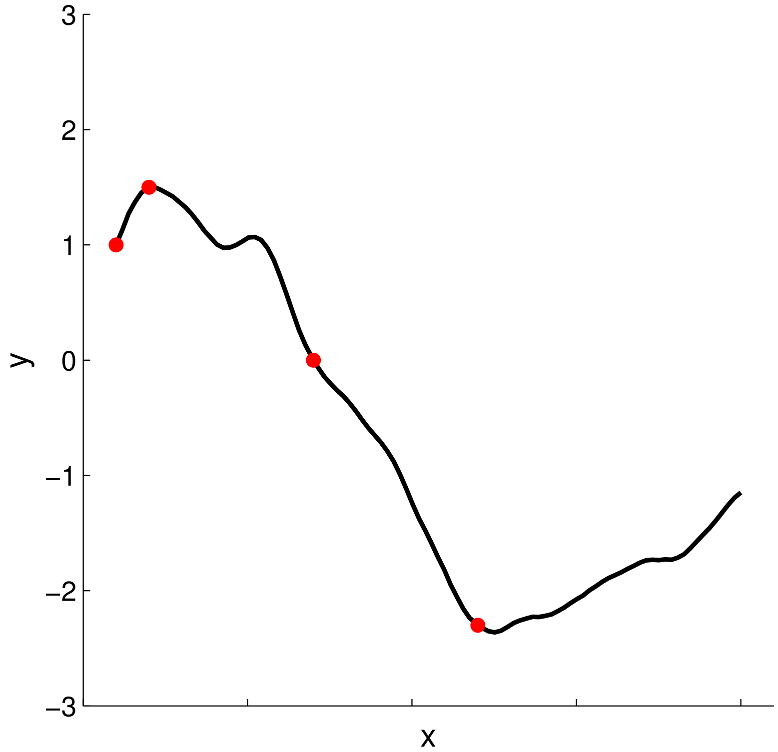
$\Sigma =$ 



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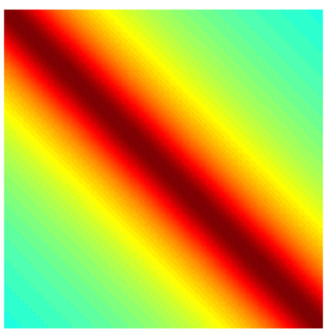
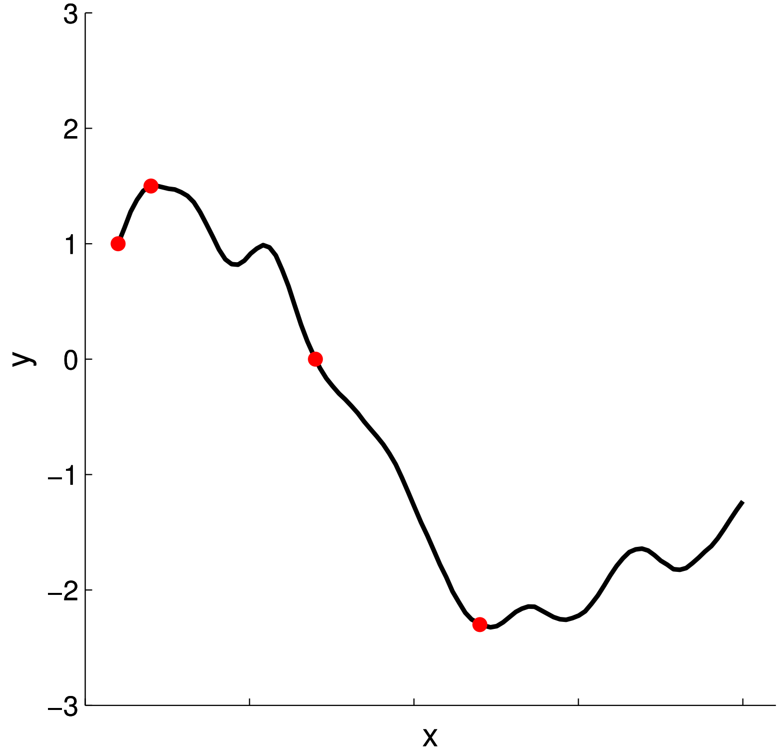
$\Sigma =$ 



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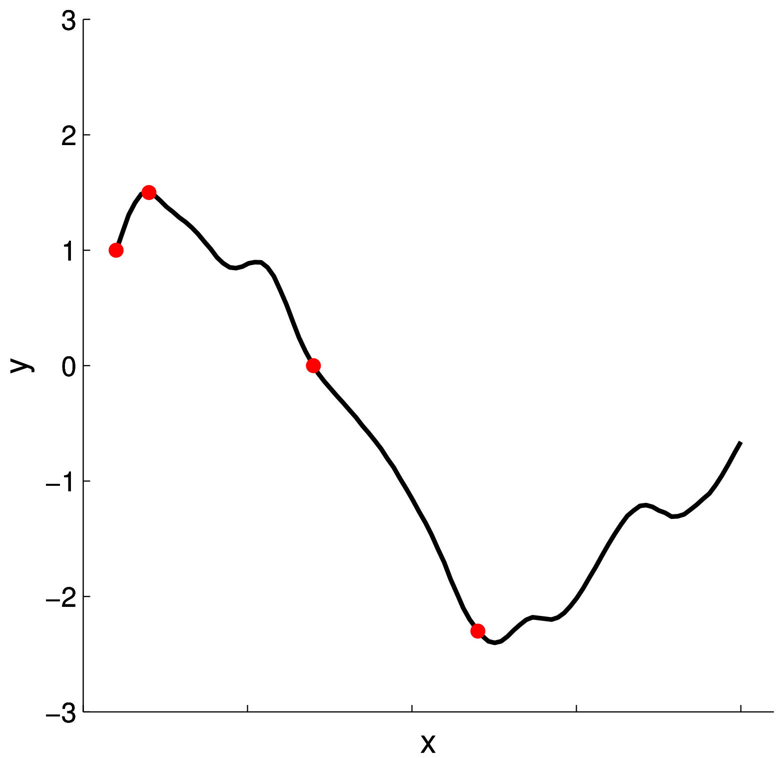

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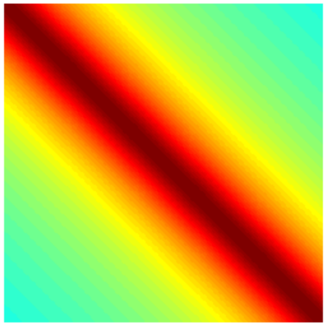

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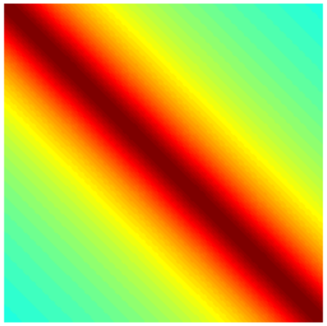

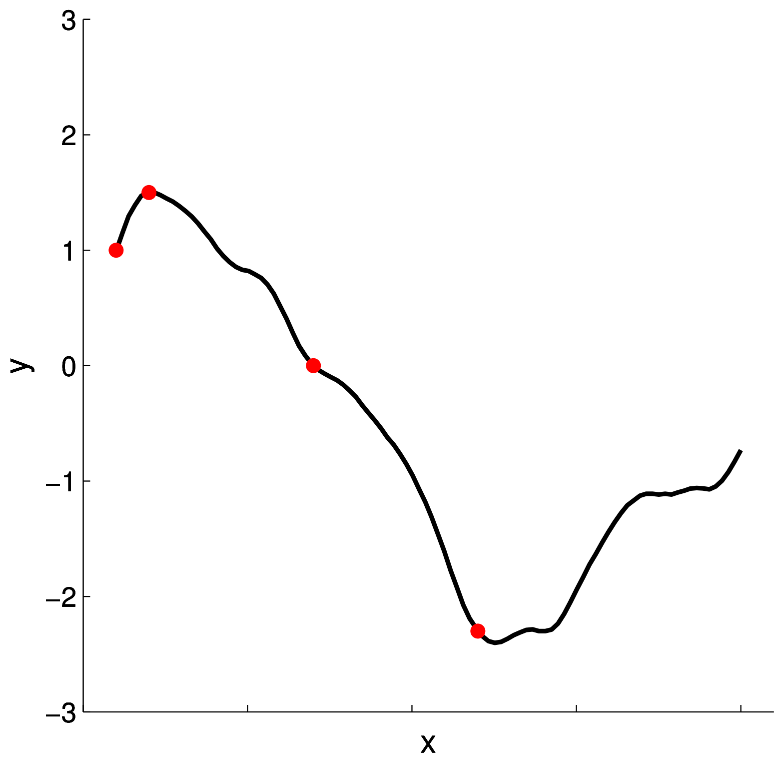

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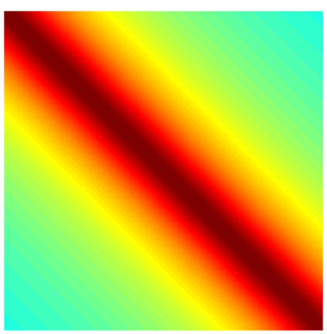
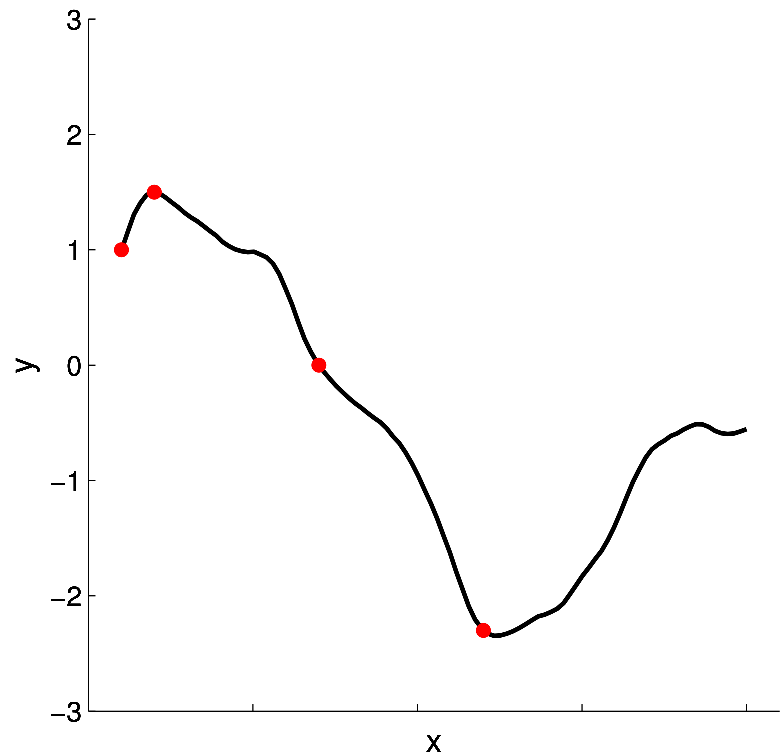
$\Sigma =$ 



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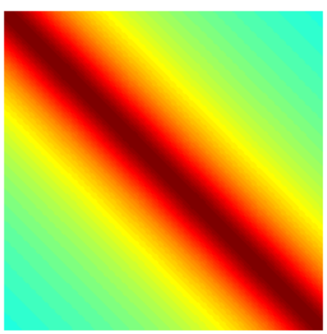
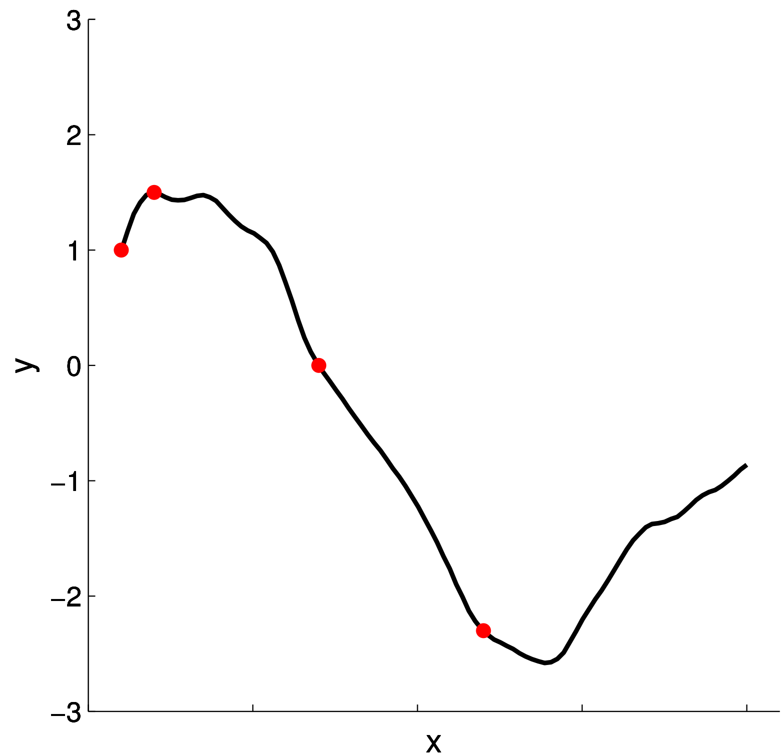
$\Sigma =$ 



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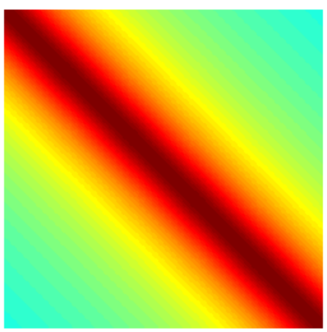
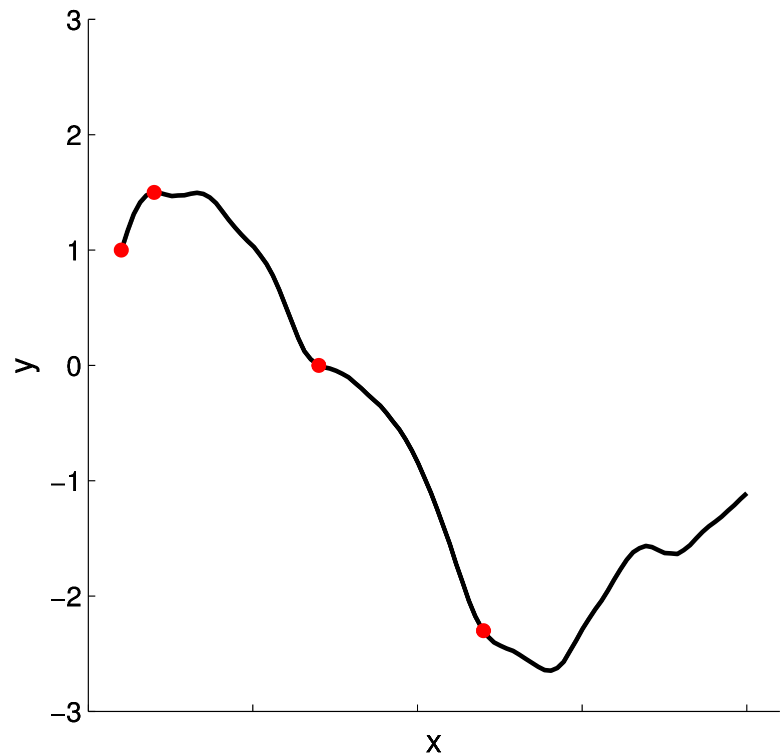
$\Sigma =$ 



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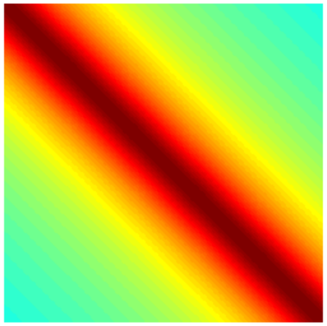

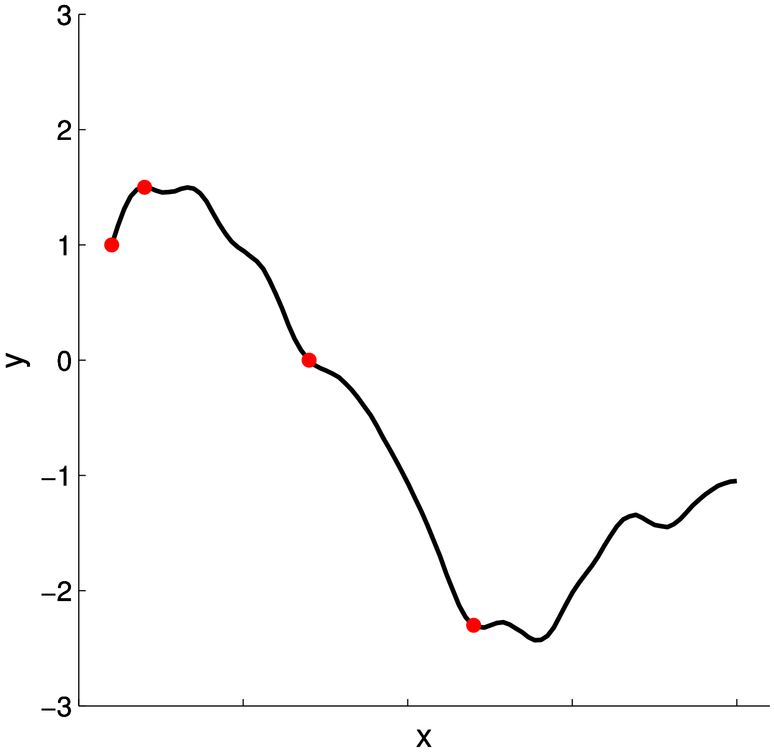

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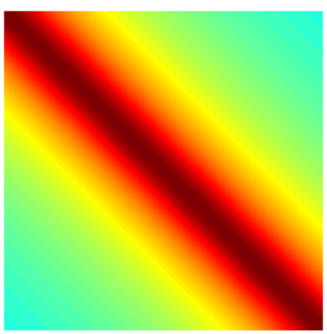
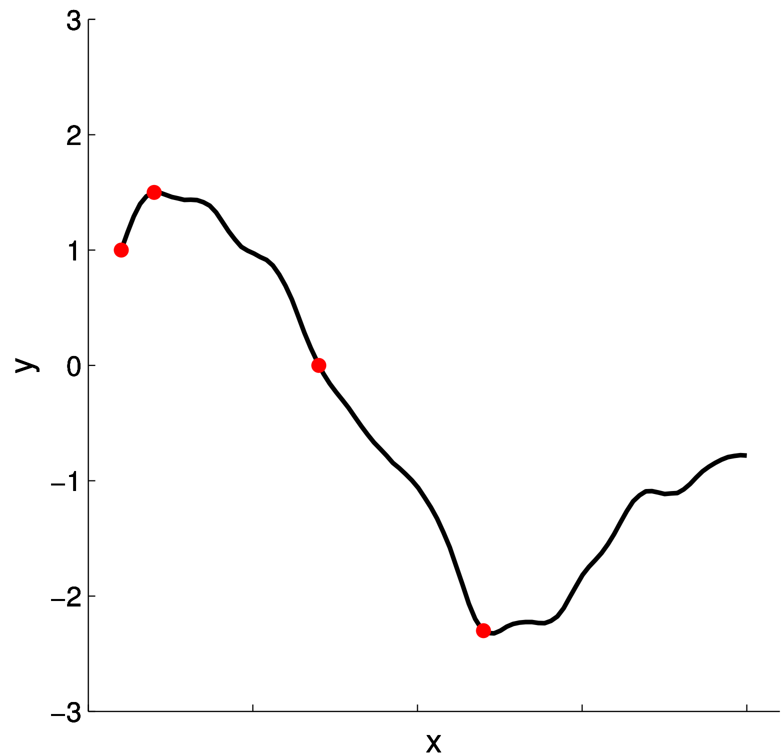
$\Sigma =$ 



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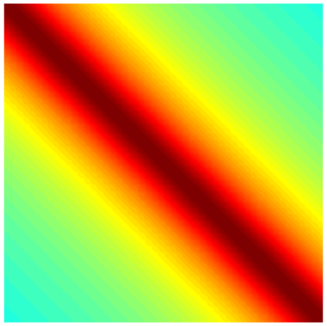

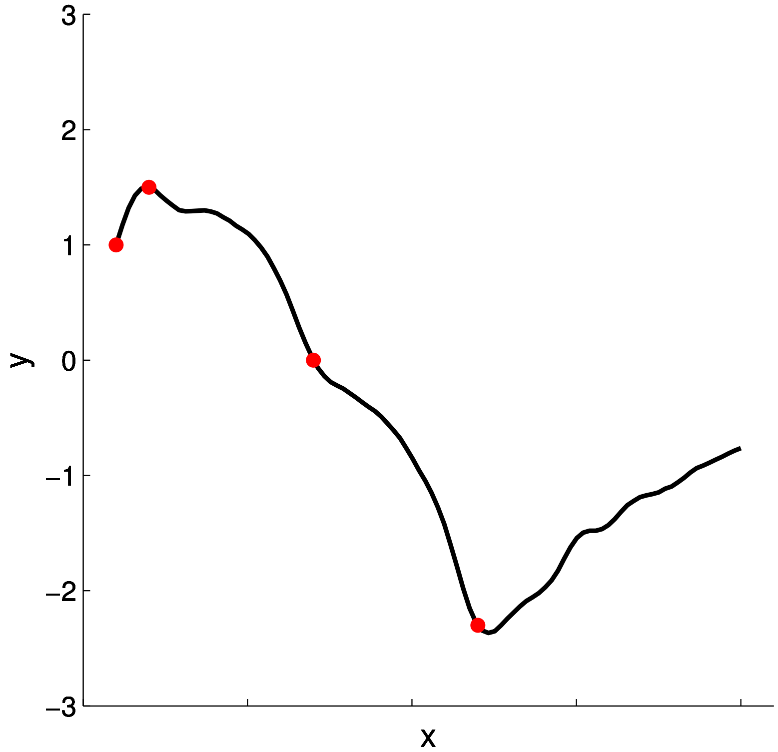

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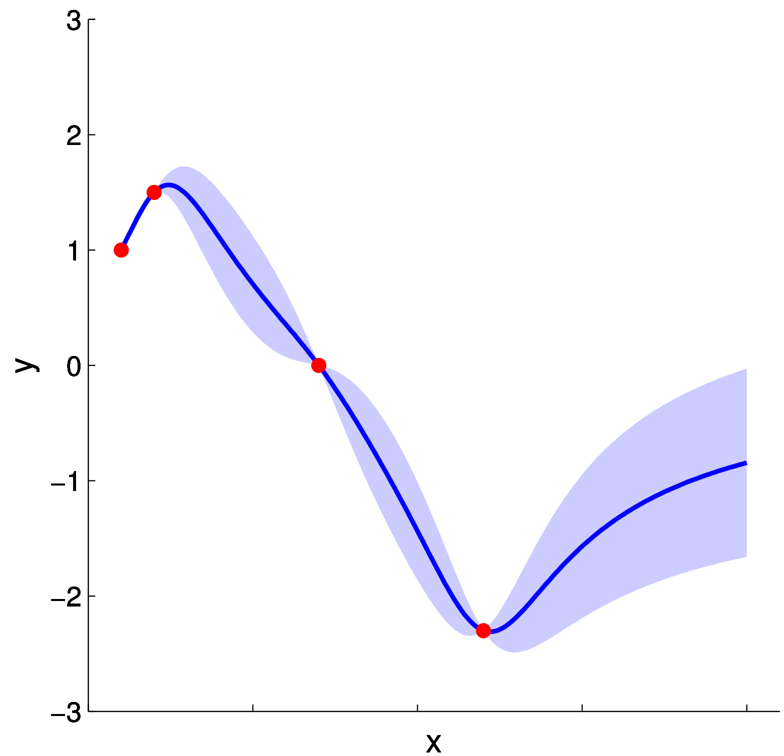

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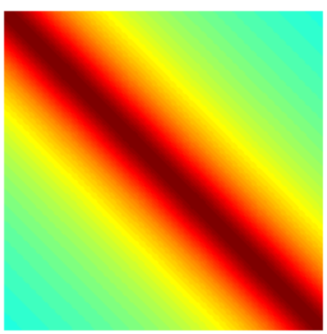

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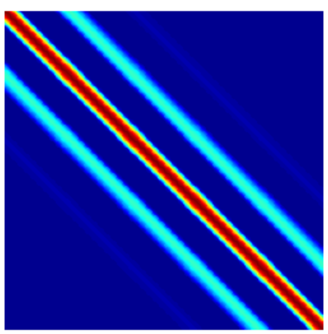
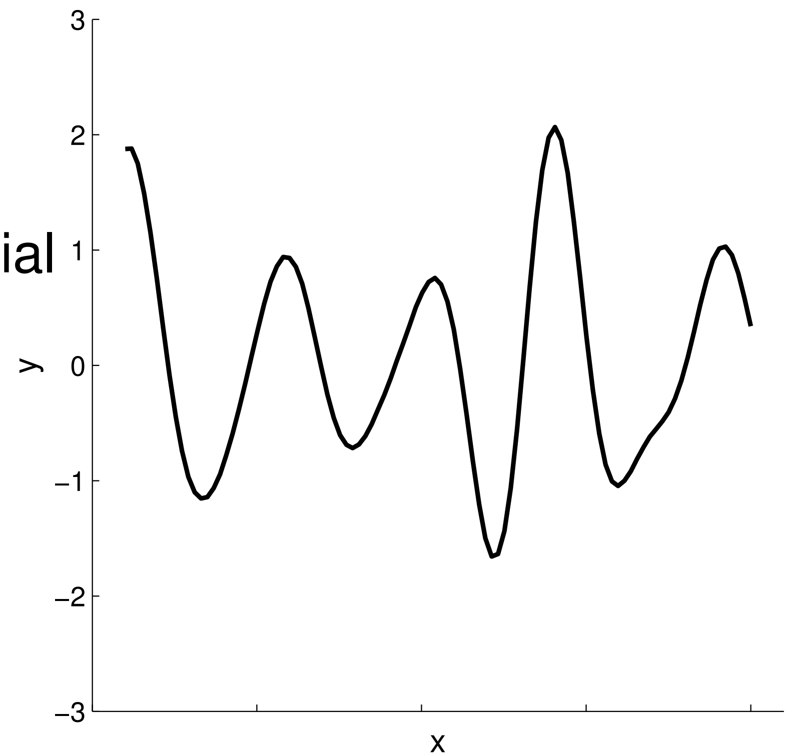
sinusoid $\times$ squared exponential

$\Sigma =$ 



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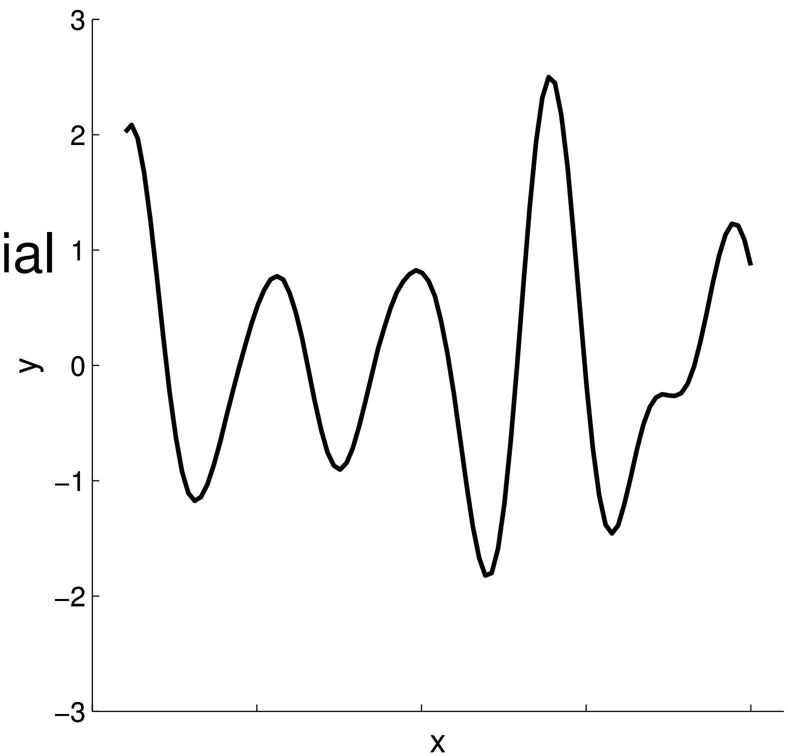
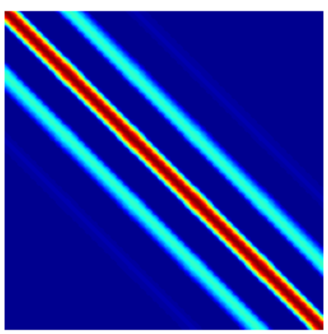


$\Sigma =$ 

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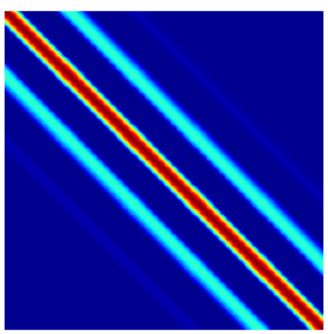
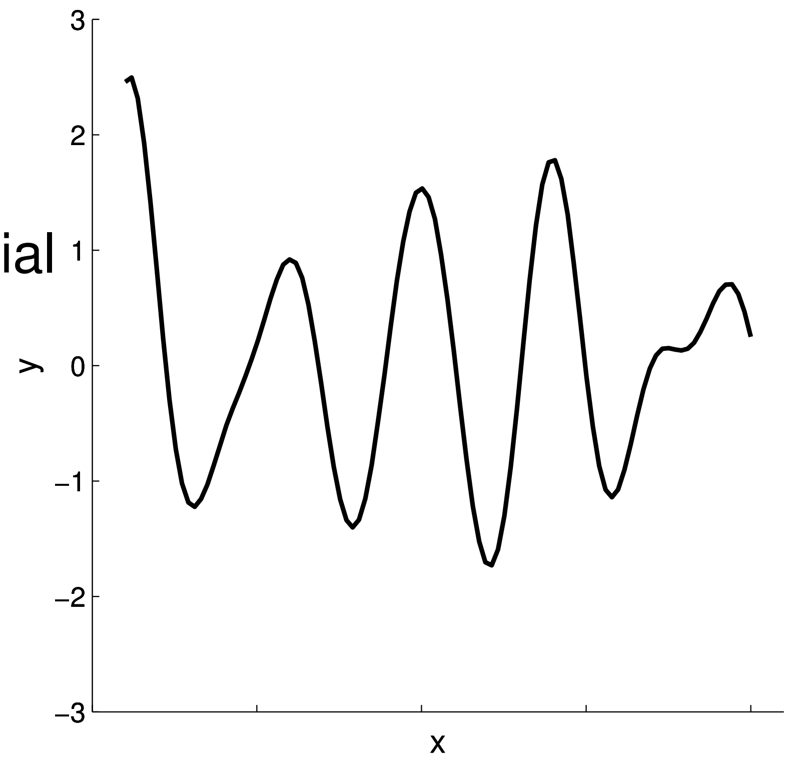
$\Sigma =$ 



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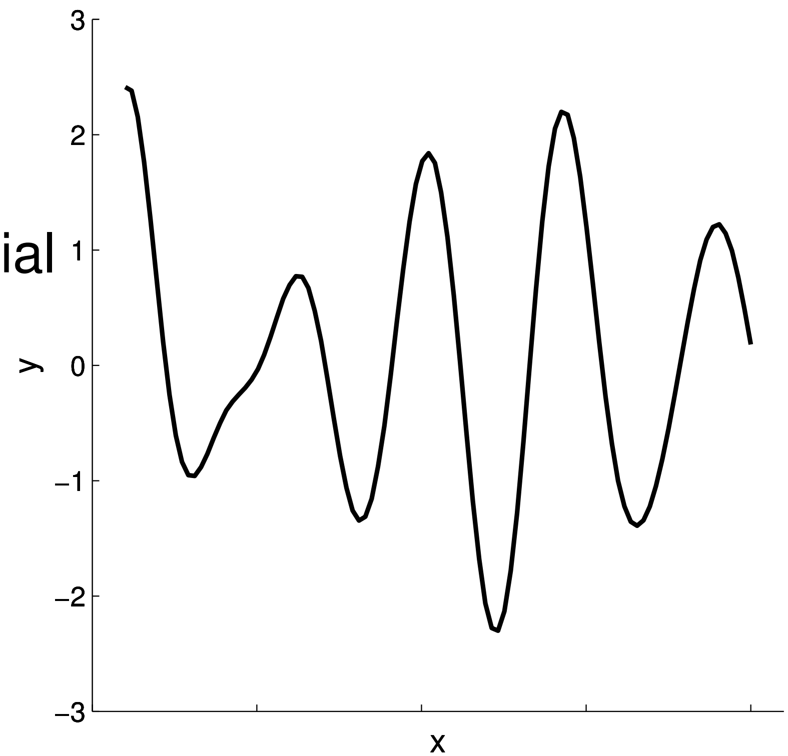
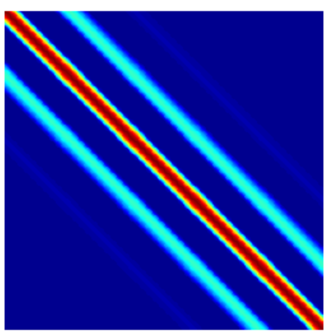


$\Sigma =$ 

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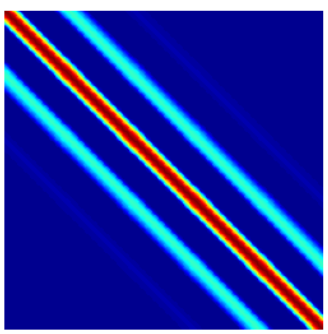
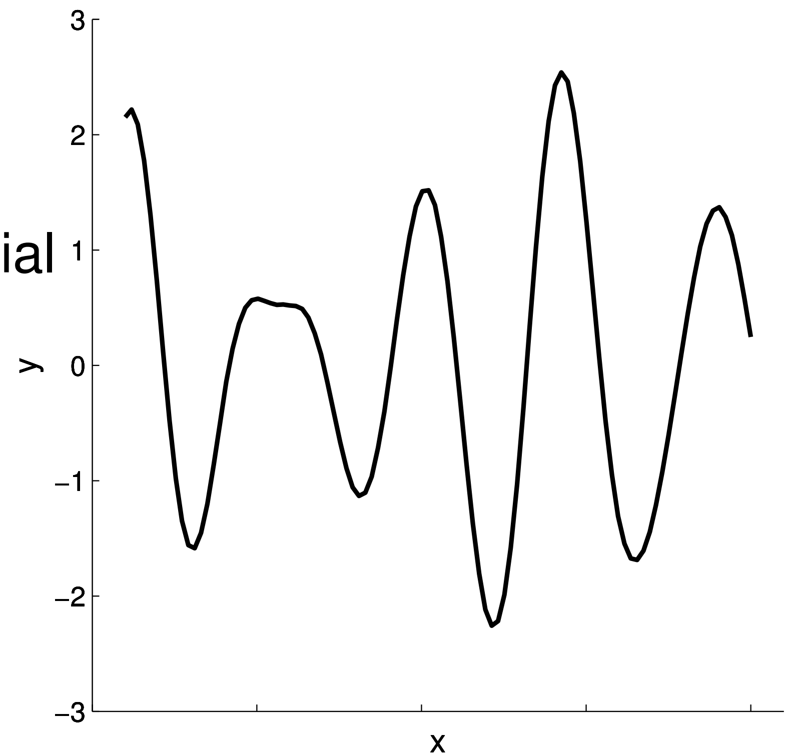
Periodic

sinusoid $\times$ squared exponential

$\Sigma =$ 



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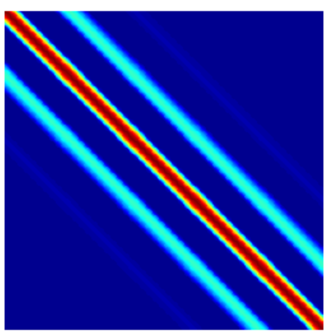
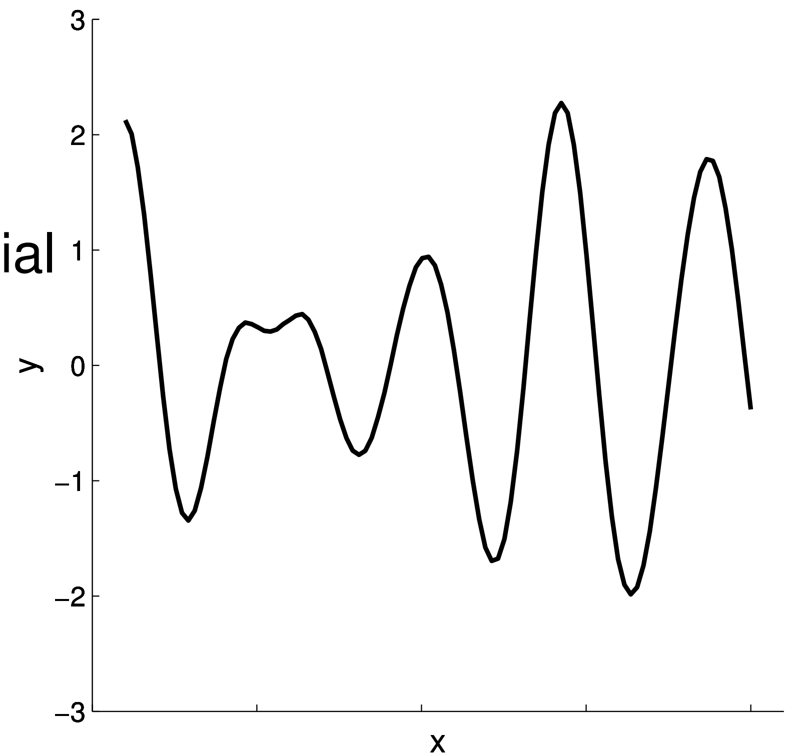
$\Sigma =$ 



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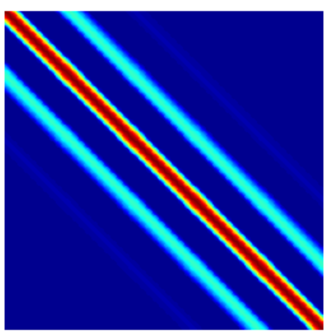
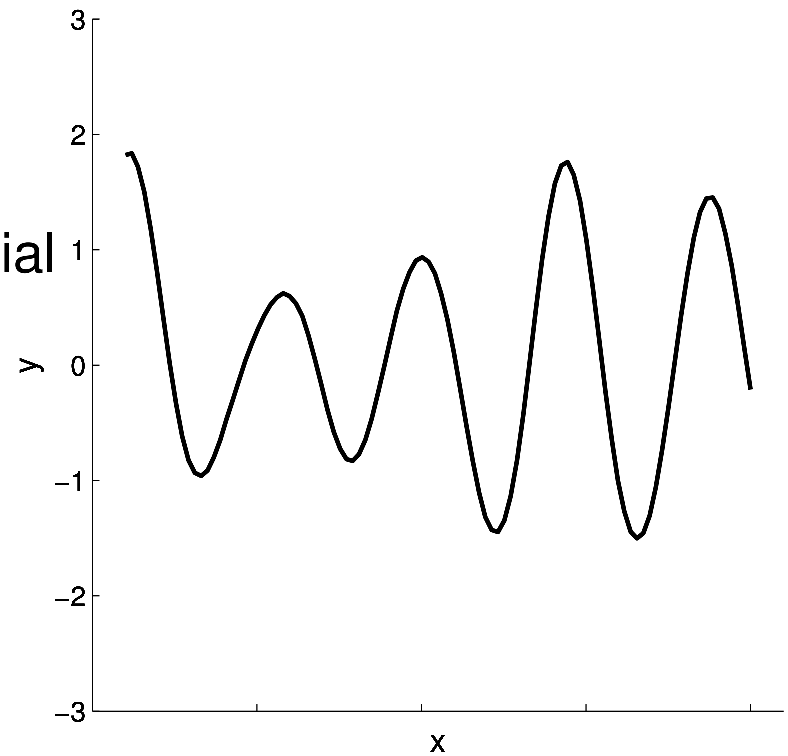
$\Sigma =$ 



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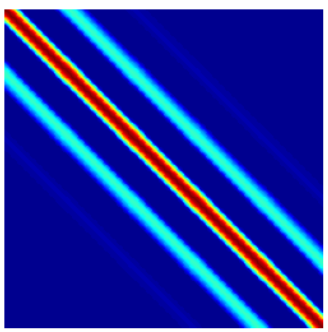
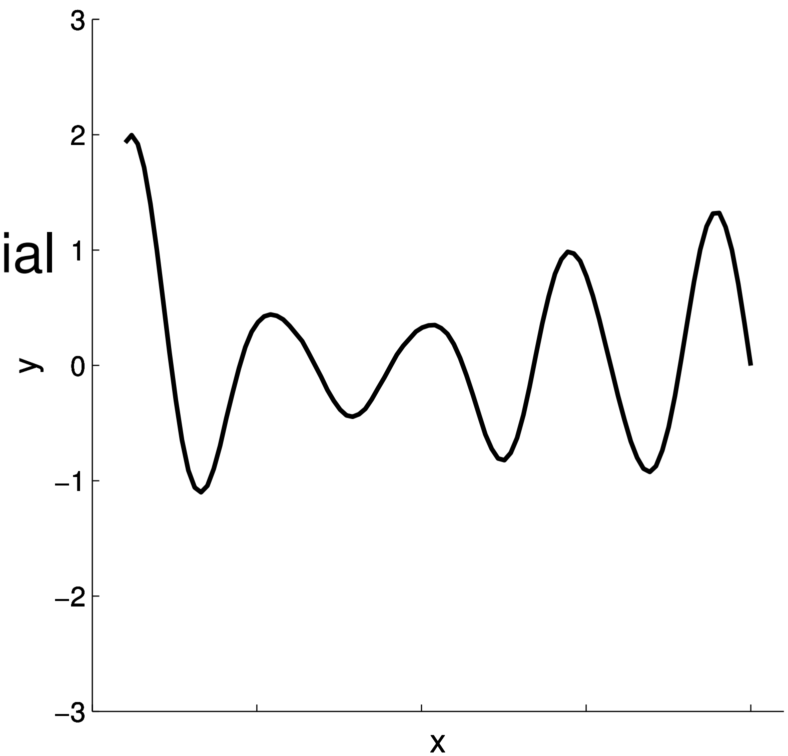
$\Sigma =$ 



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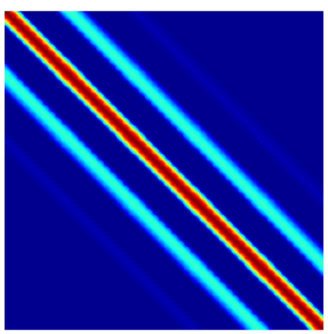
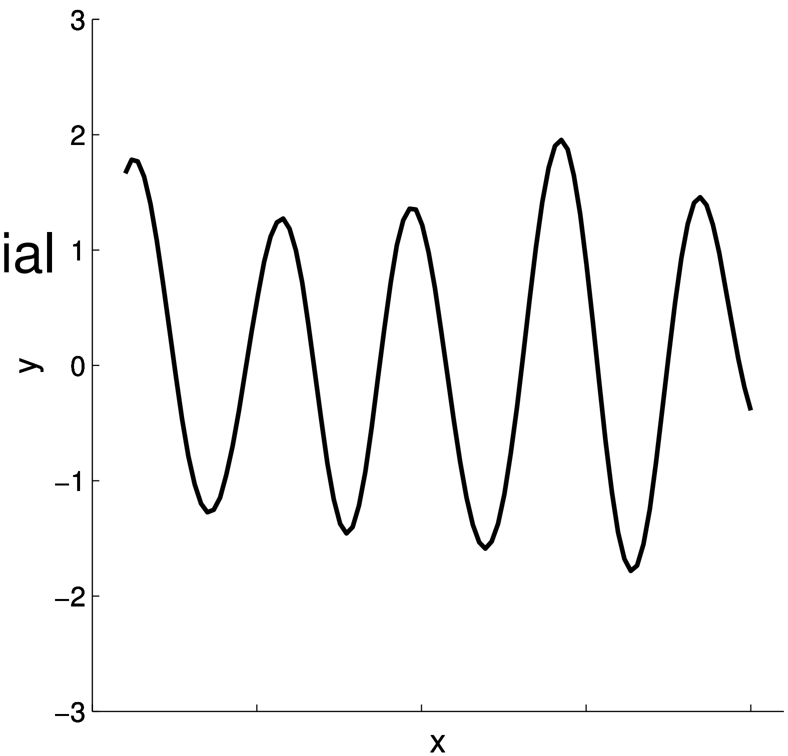
$\Sigma =$ 



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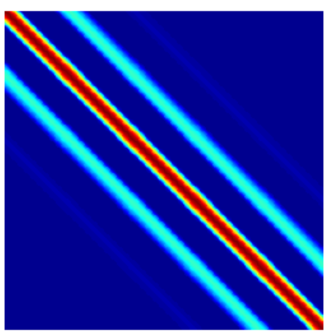
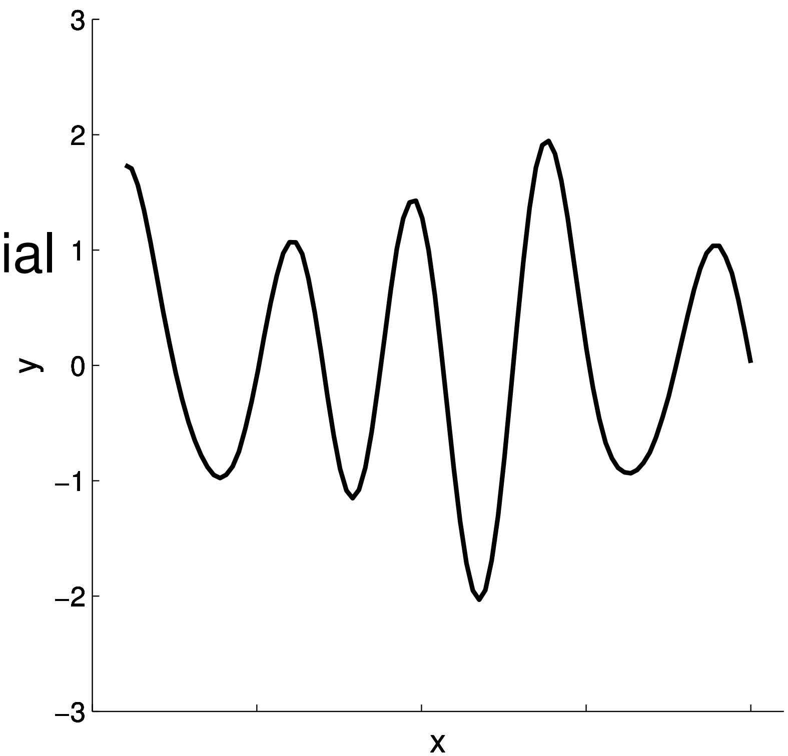
$\Sigma =$ 



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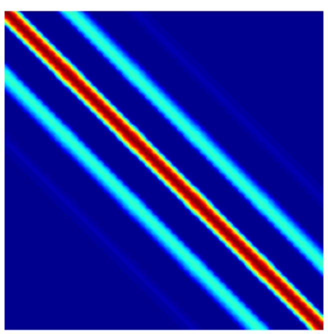
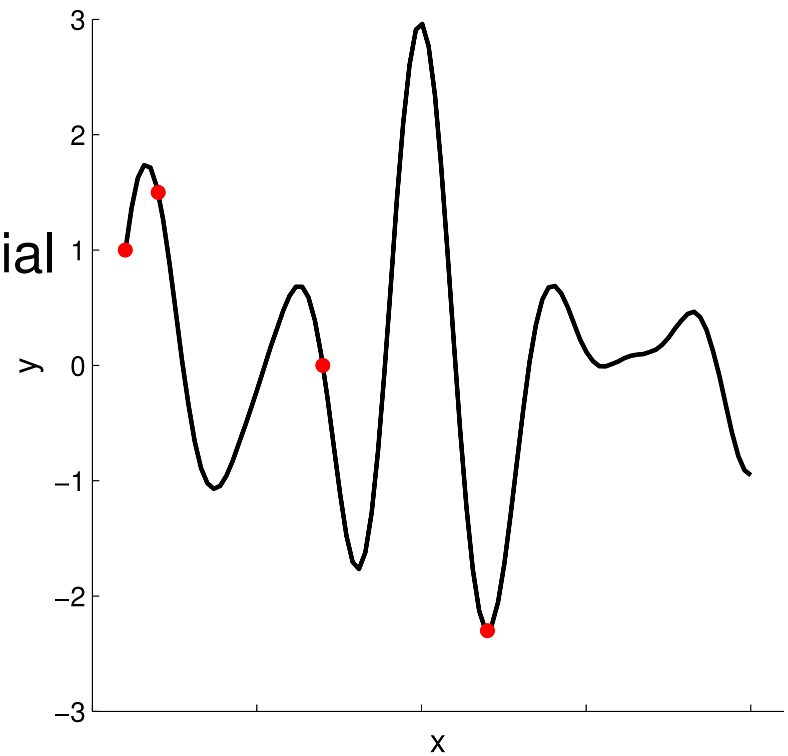
$\Sigma =$ 



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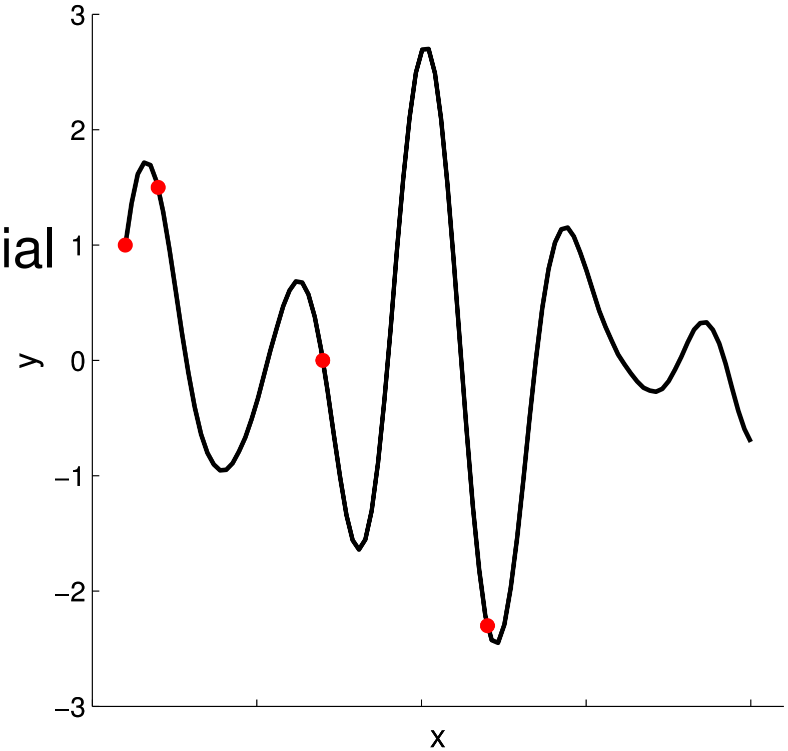
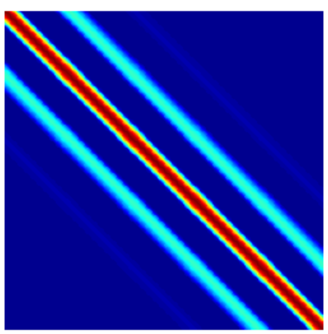


$\Sigma =$ 

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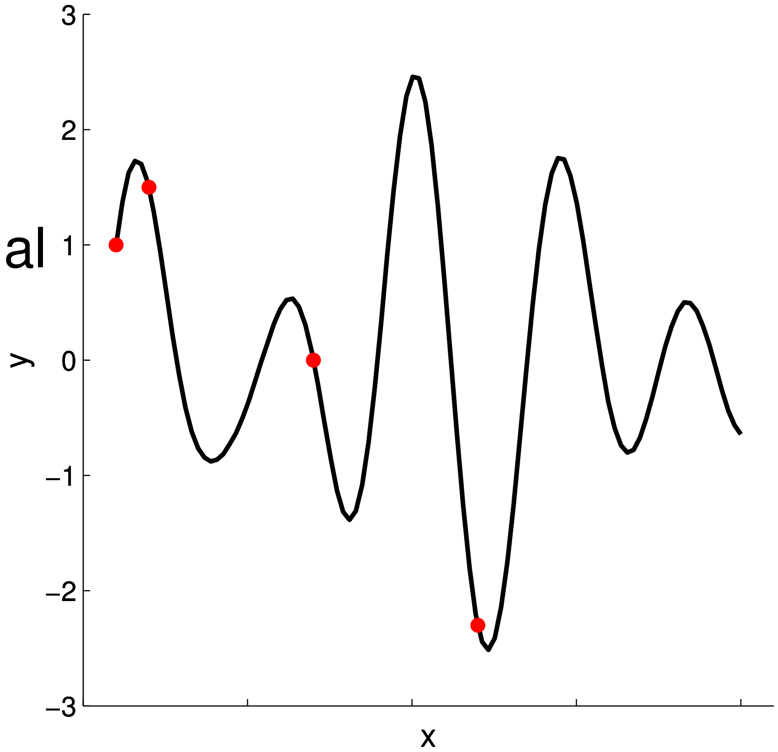
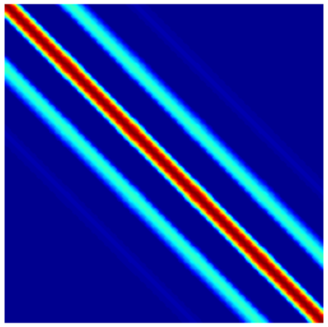


$\Sigma =$ 

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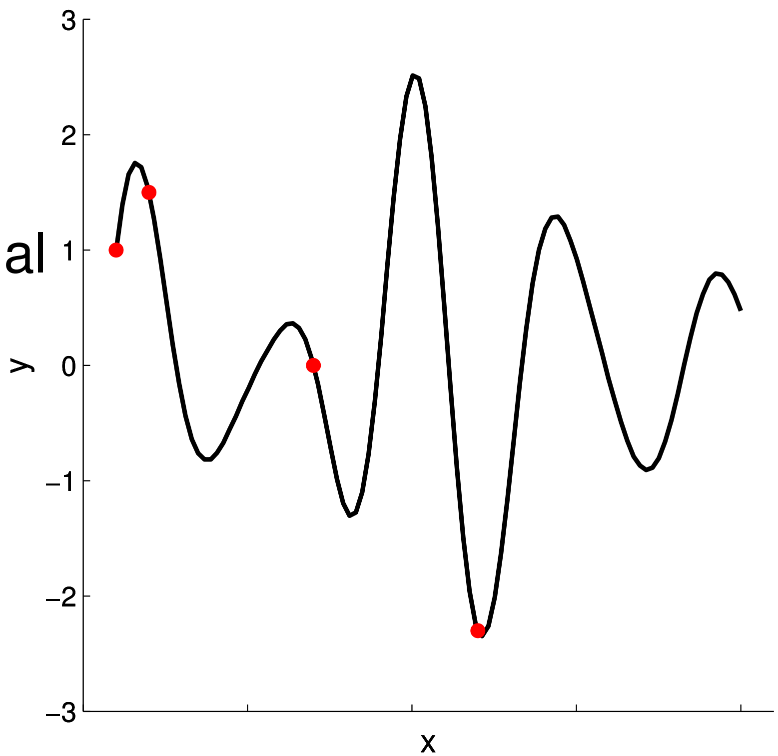
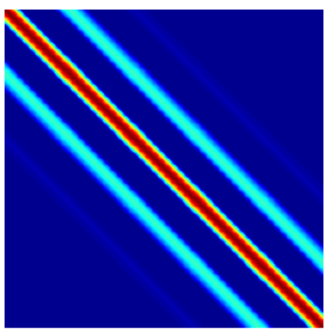


$\Sigma =$ 

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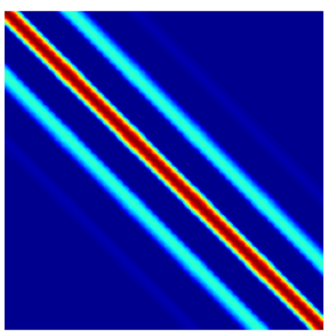
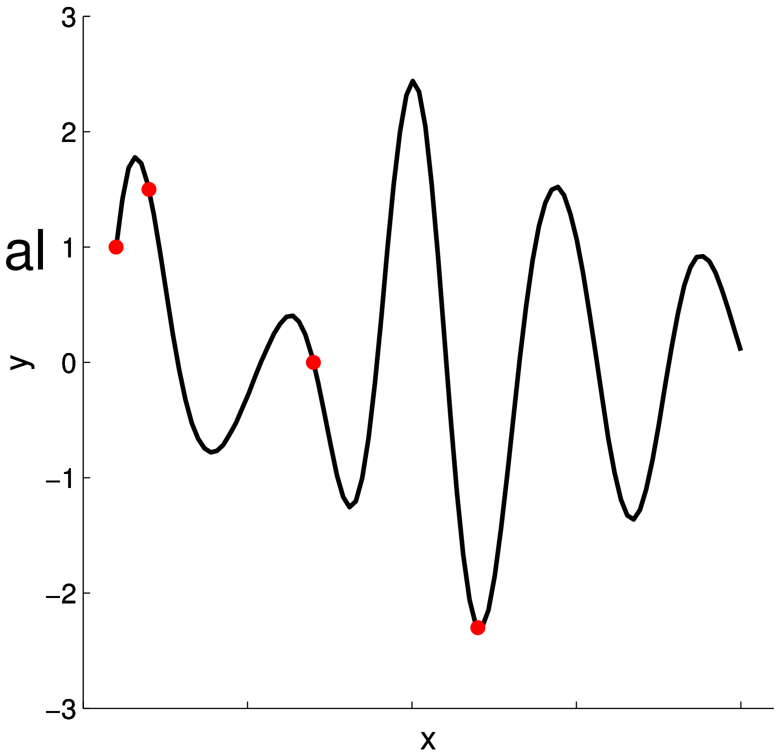
$\Sigma =$ 



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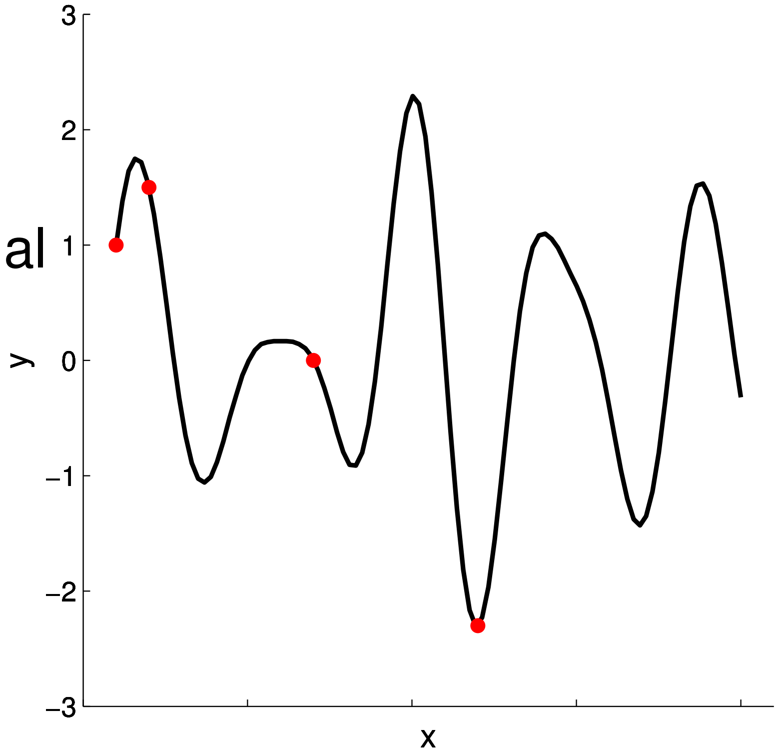
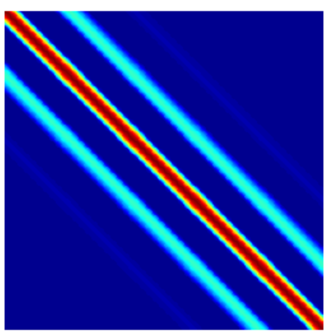


$\Sigma =$ 

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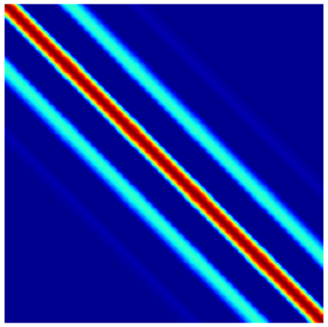

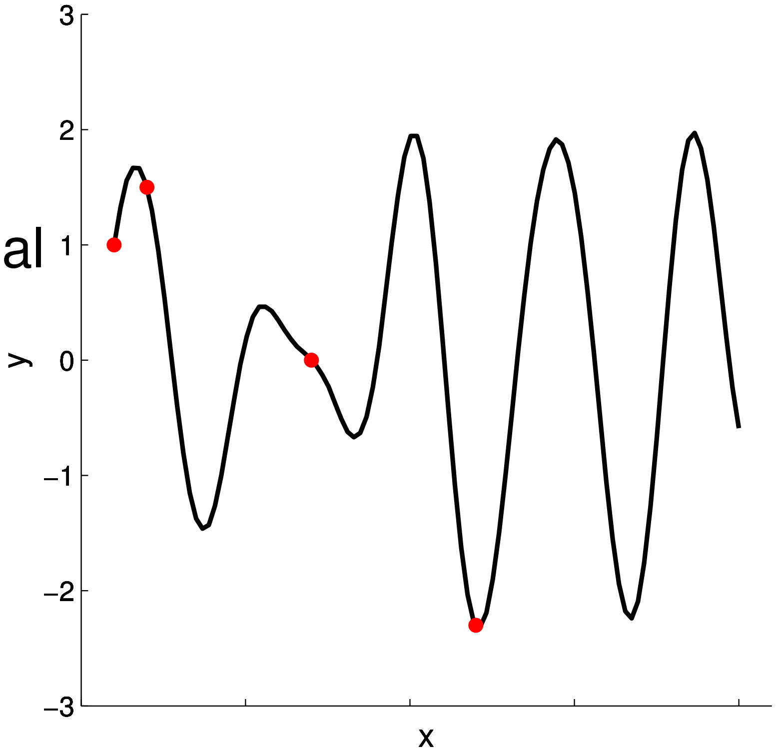

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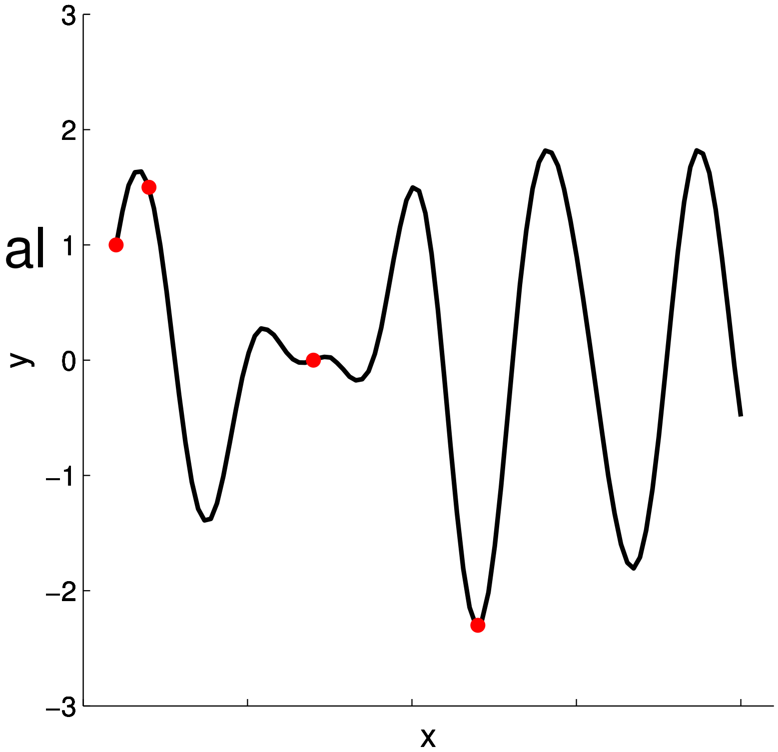
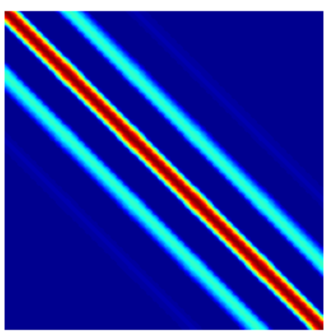


$\Sigma =$ 

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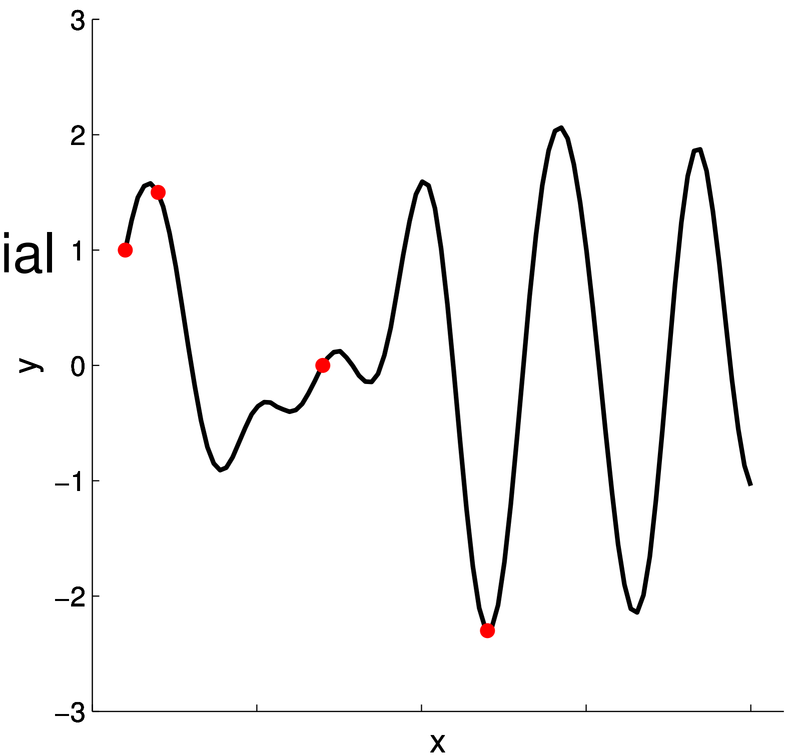

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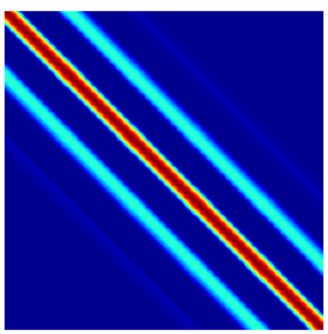

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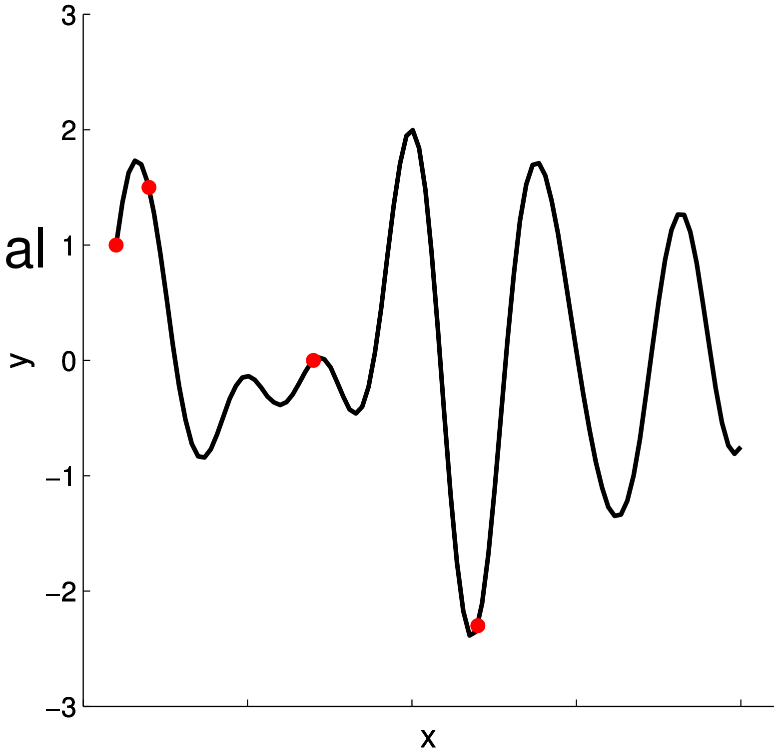
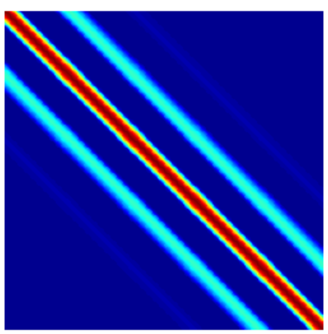


$\Sigma =$ 

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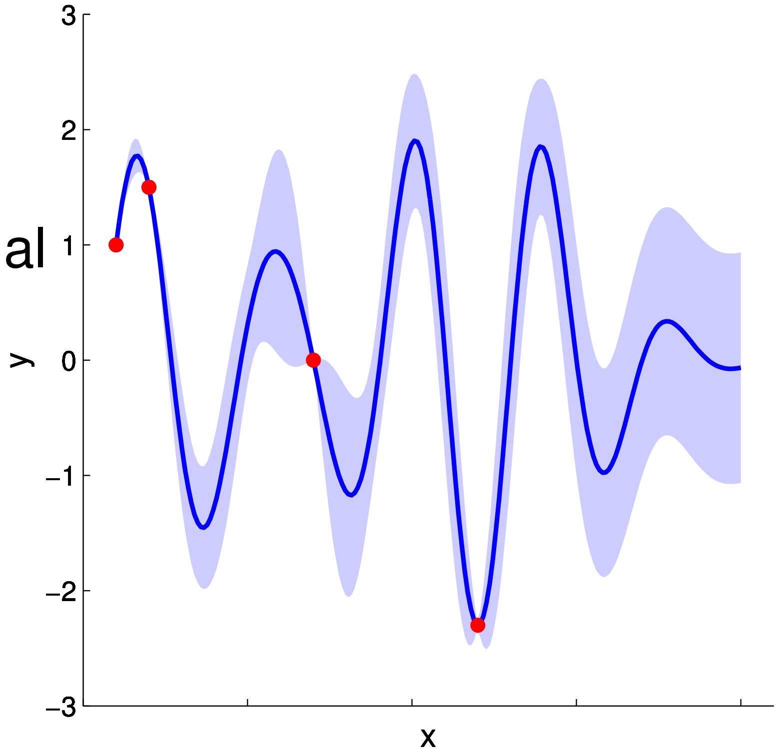

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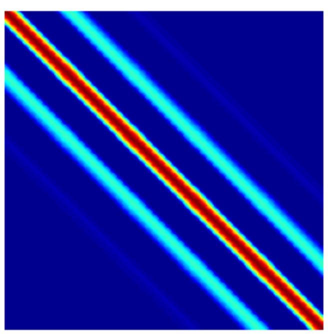
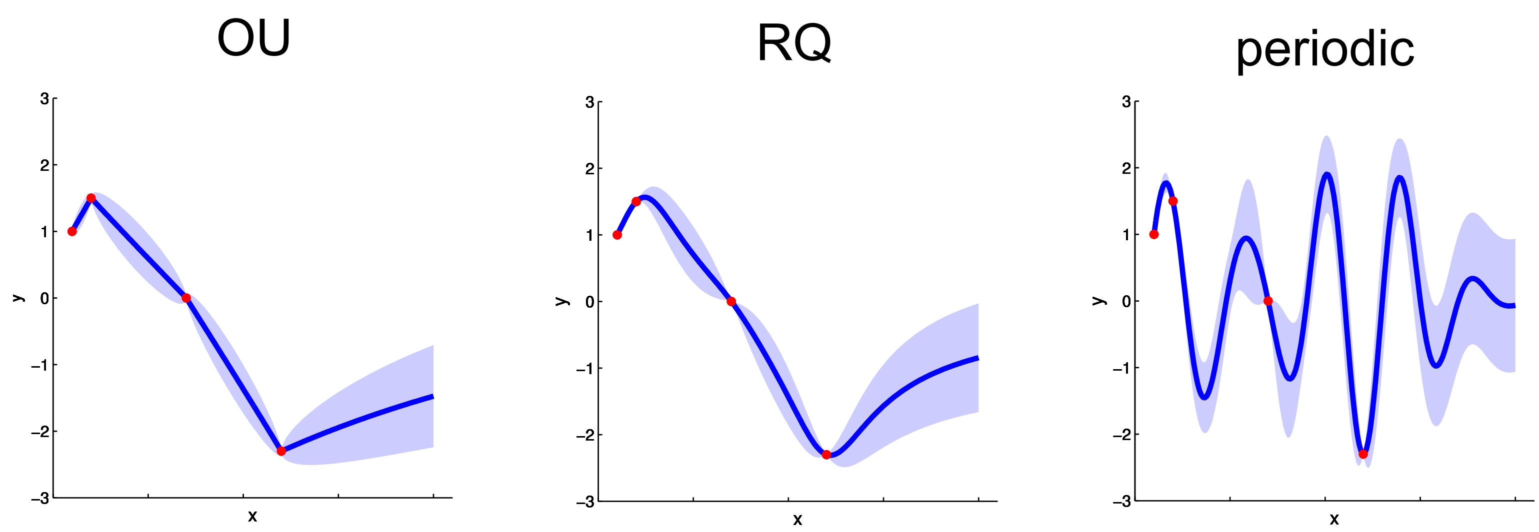


The covariance function has a large effect



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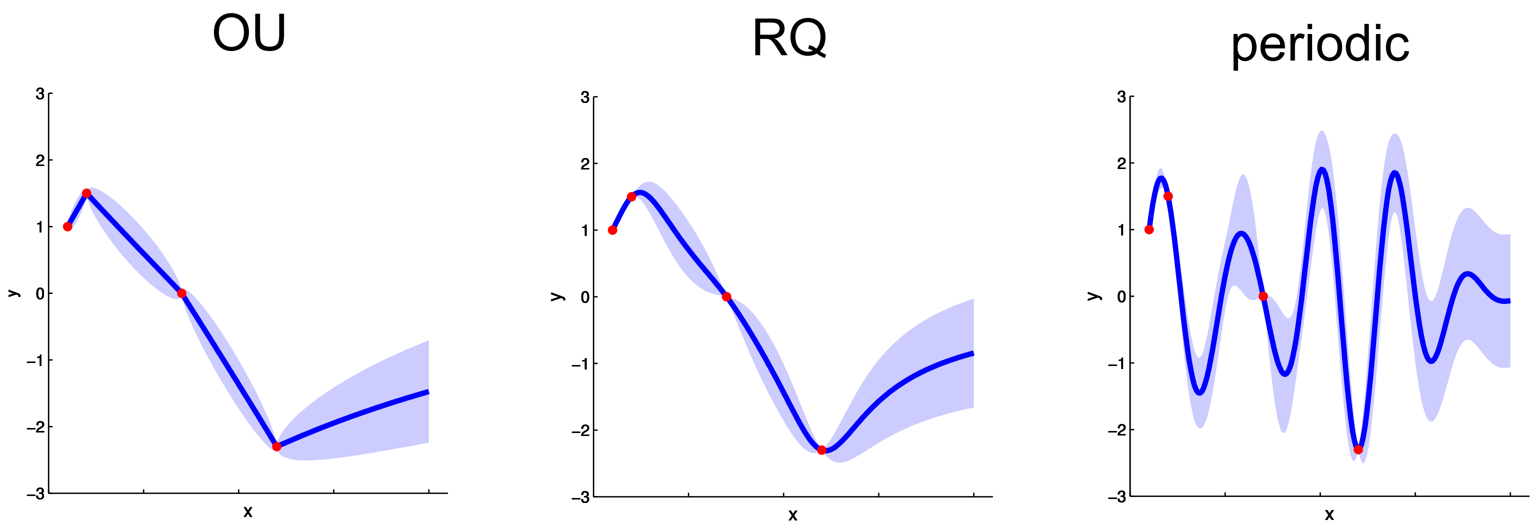

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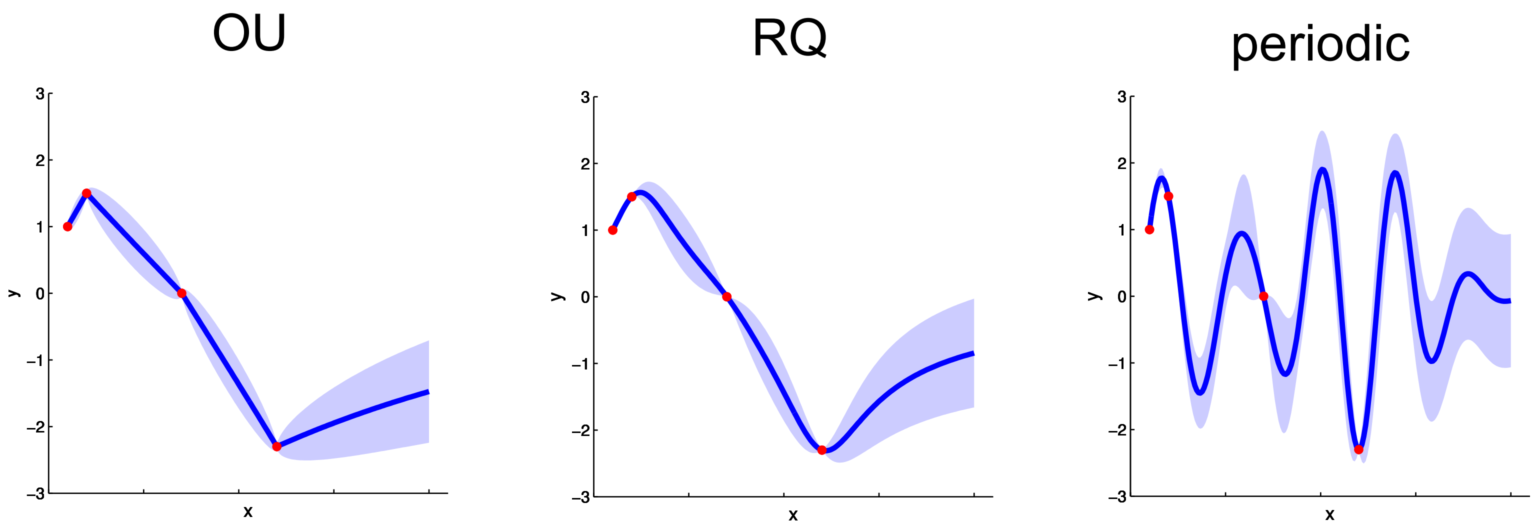

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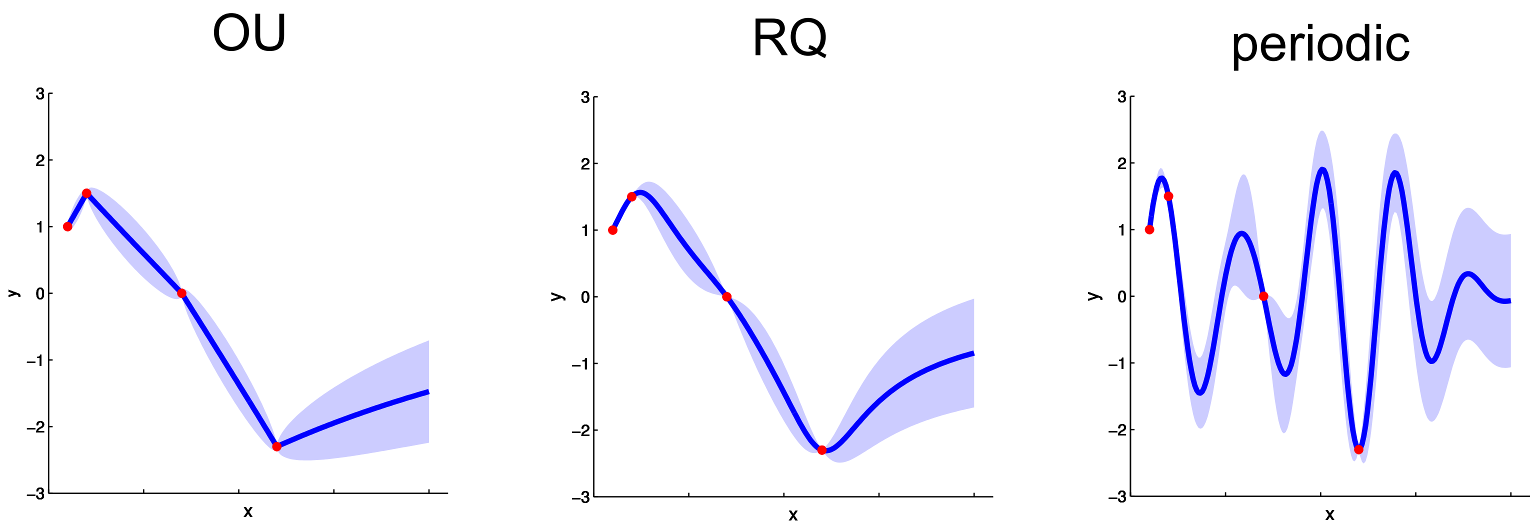

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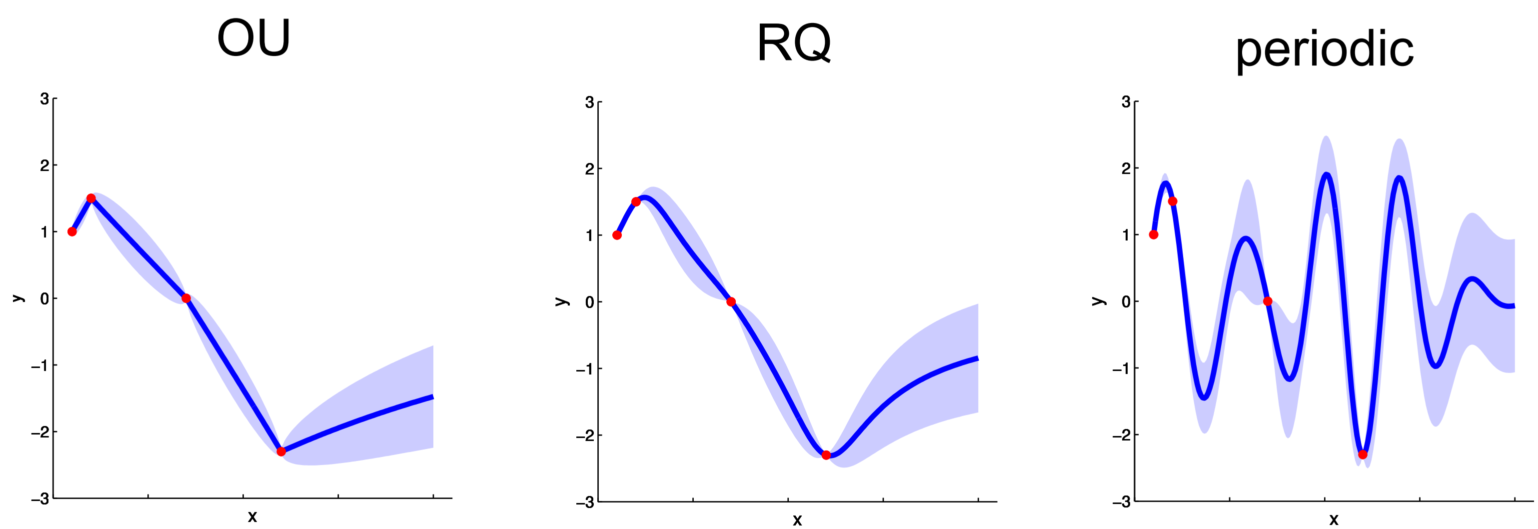

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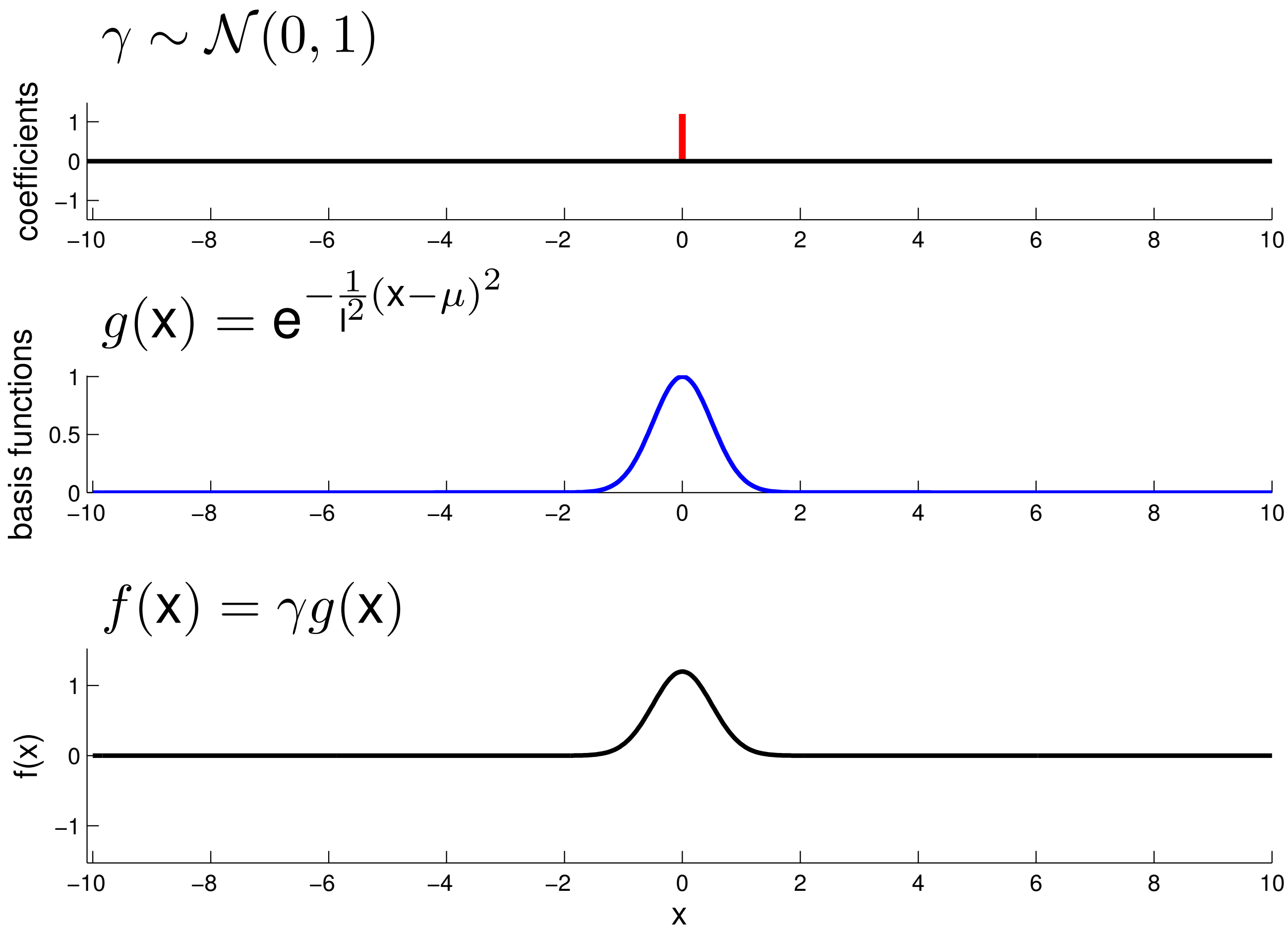
Health warnings: Hard to compute (need approximations)

Often results are very sensitive to the priors $p(\theta|M)$

Basis function view of Gaussian processes



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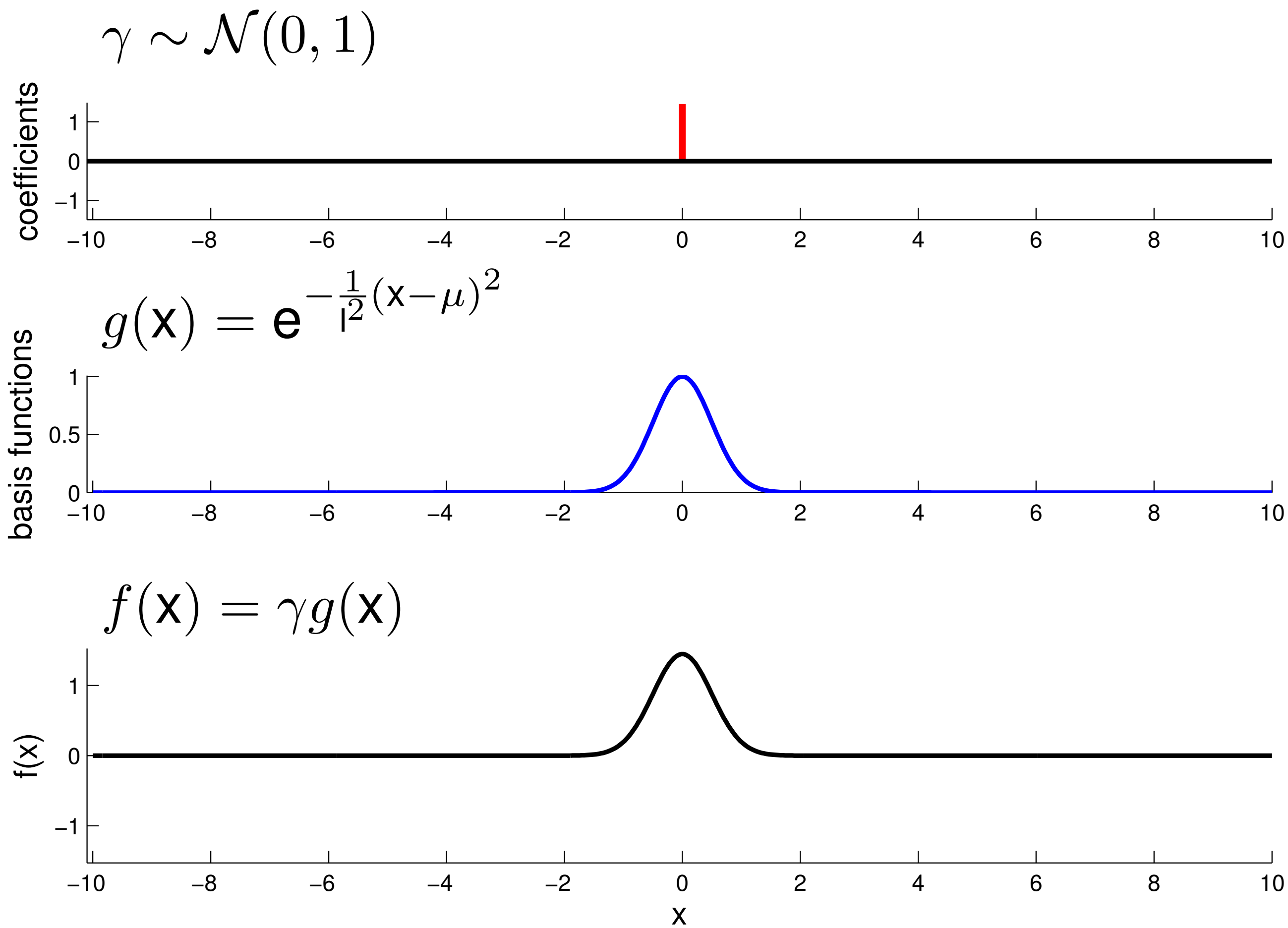

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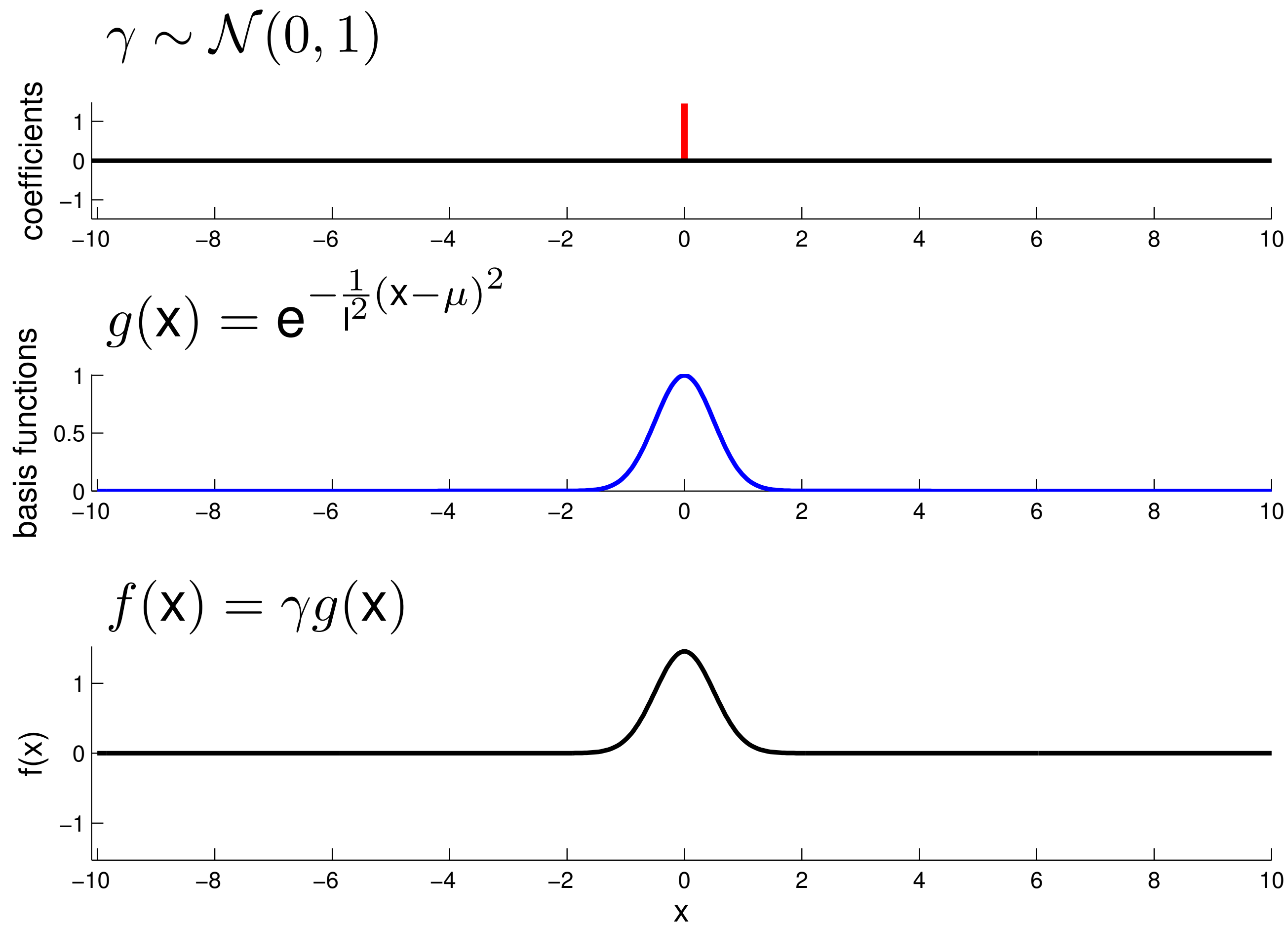

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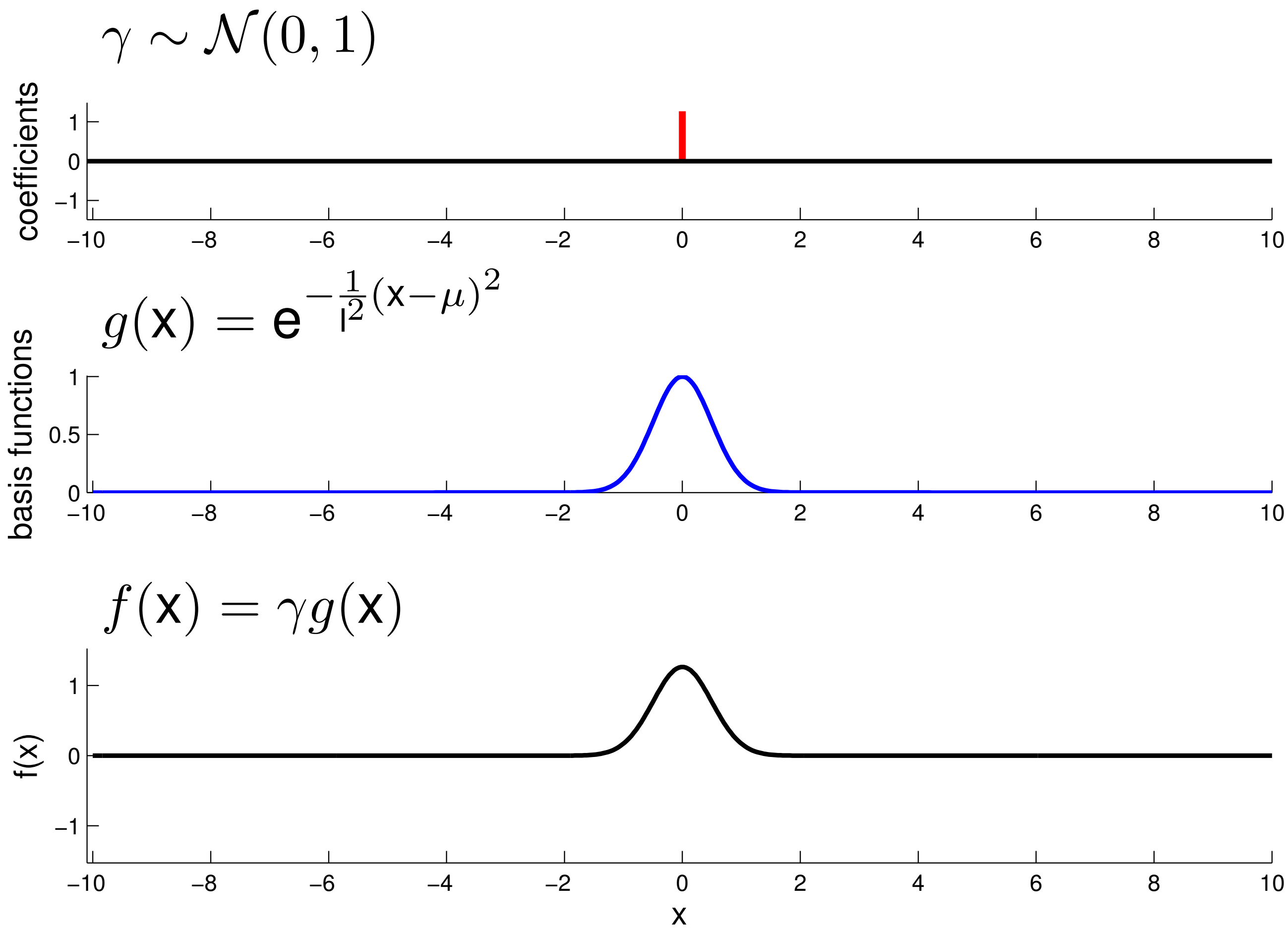

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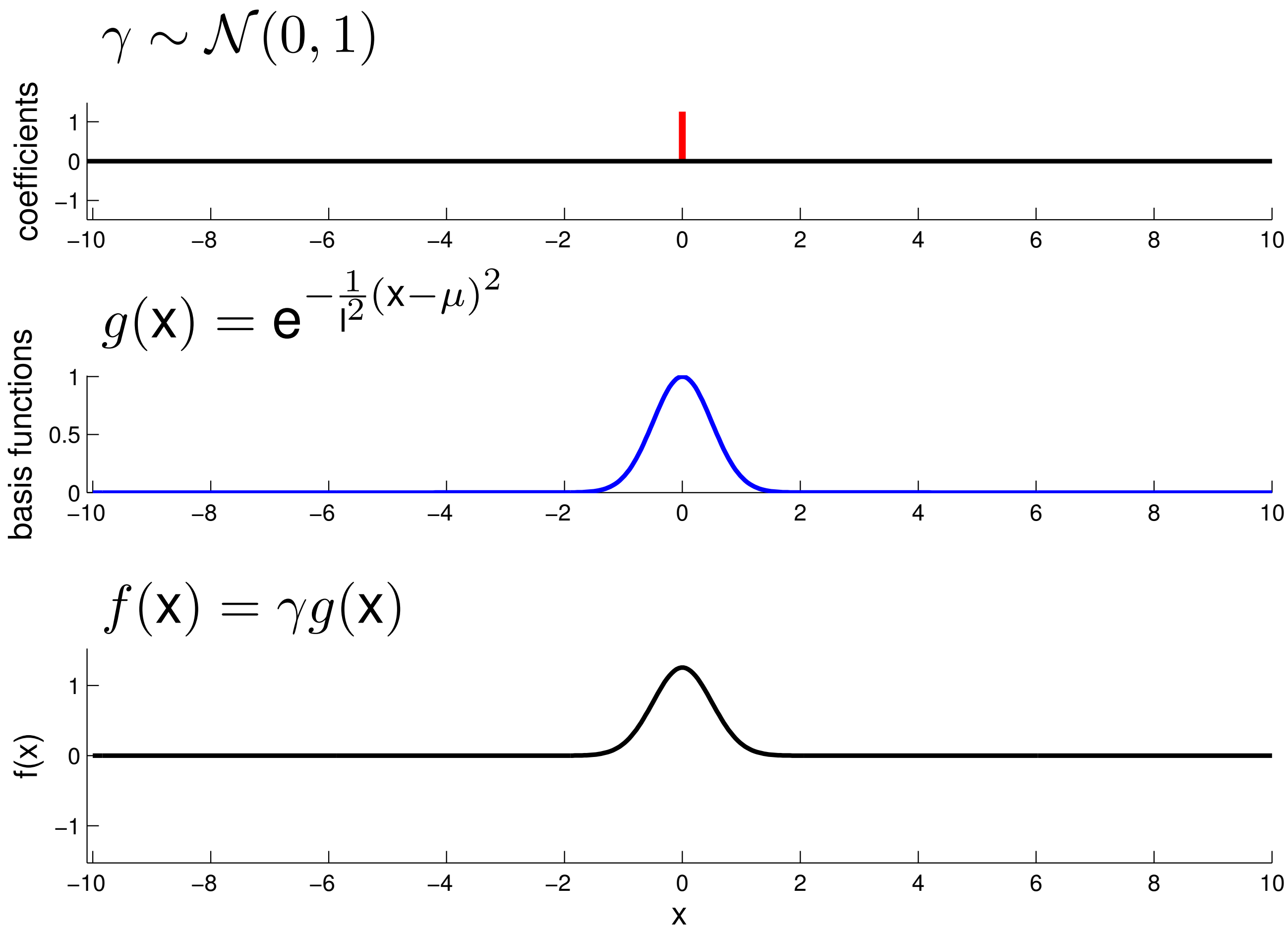

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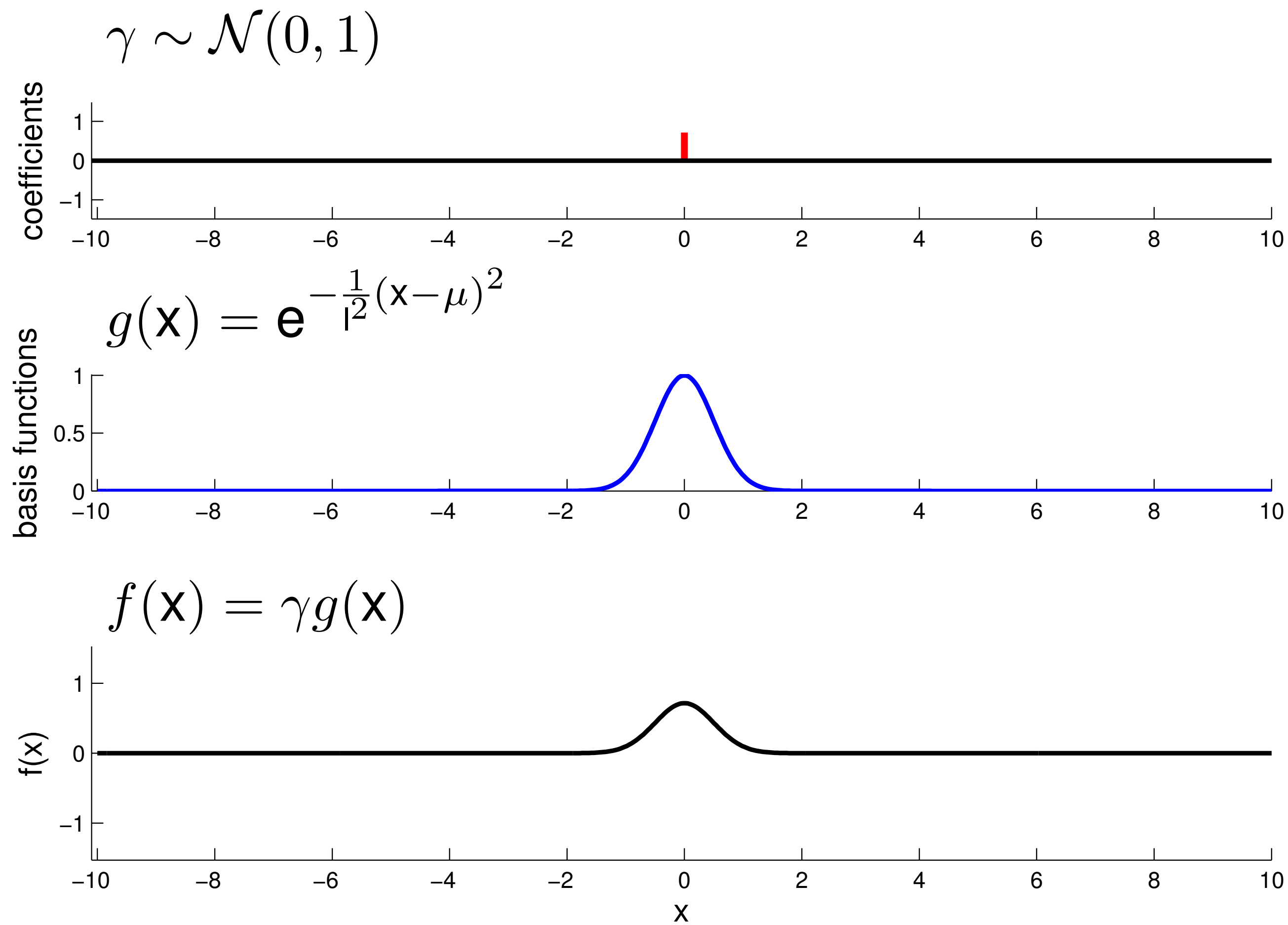

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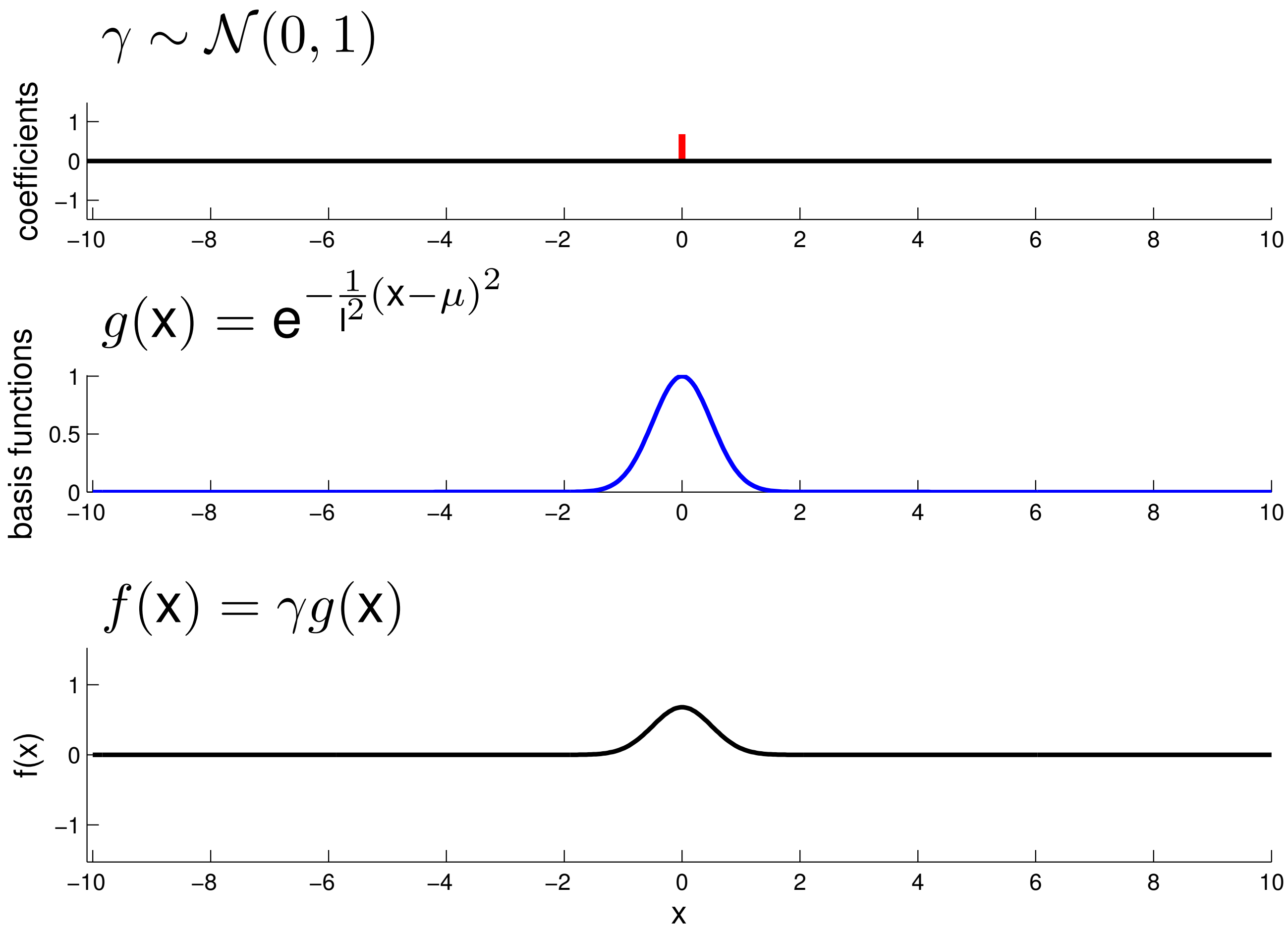

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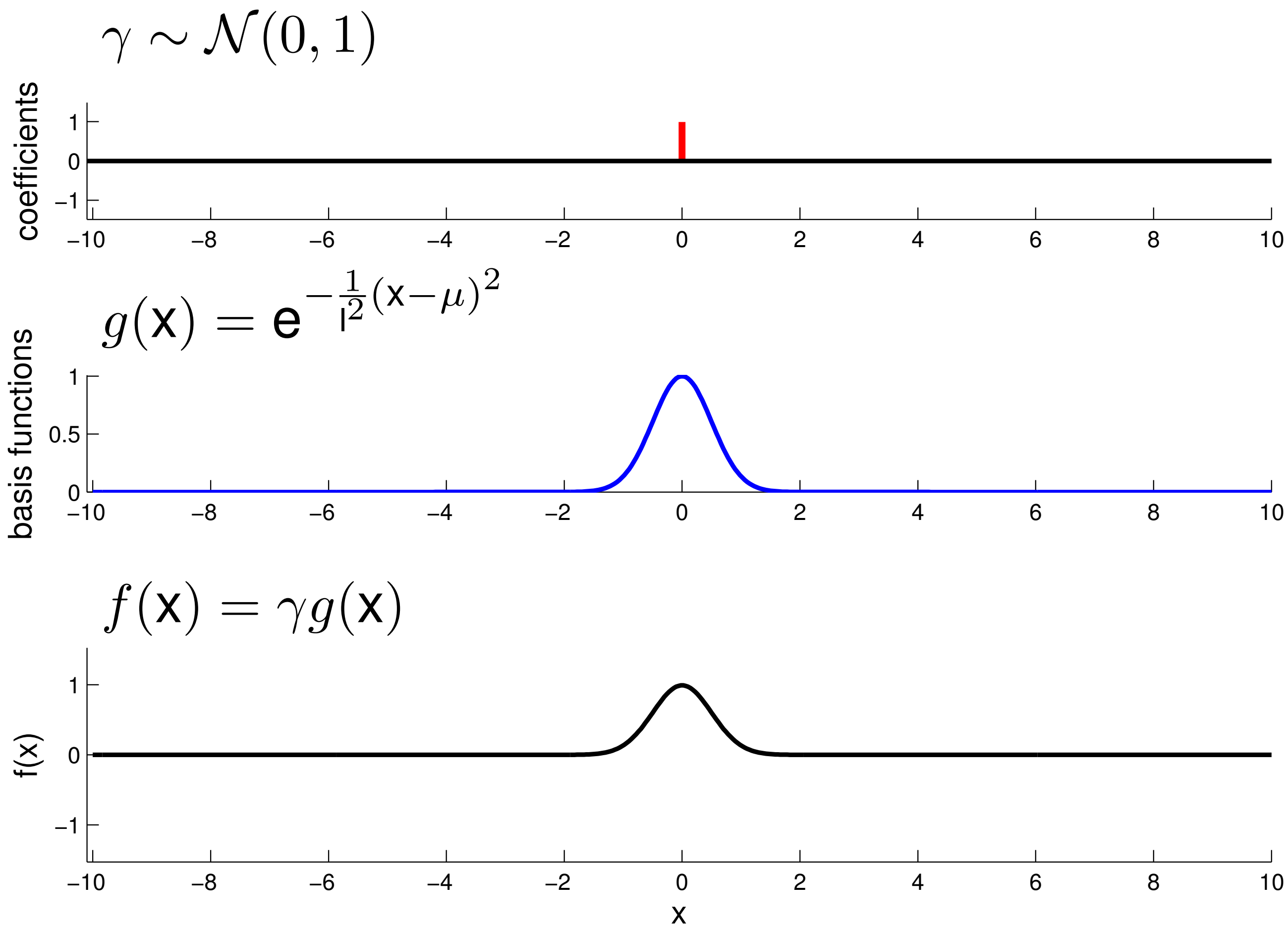

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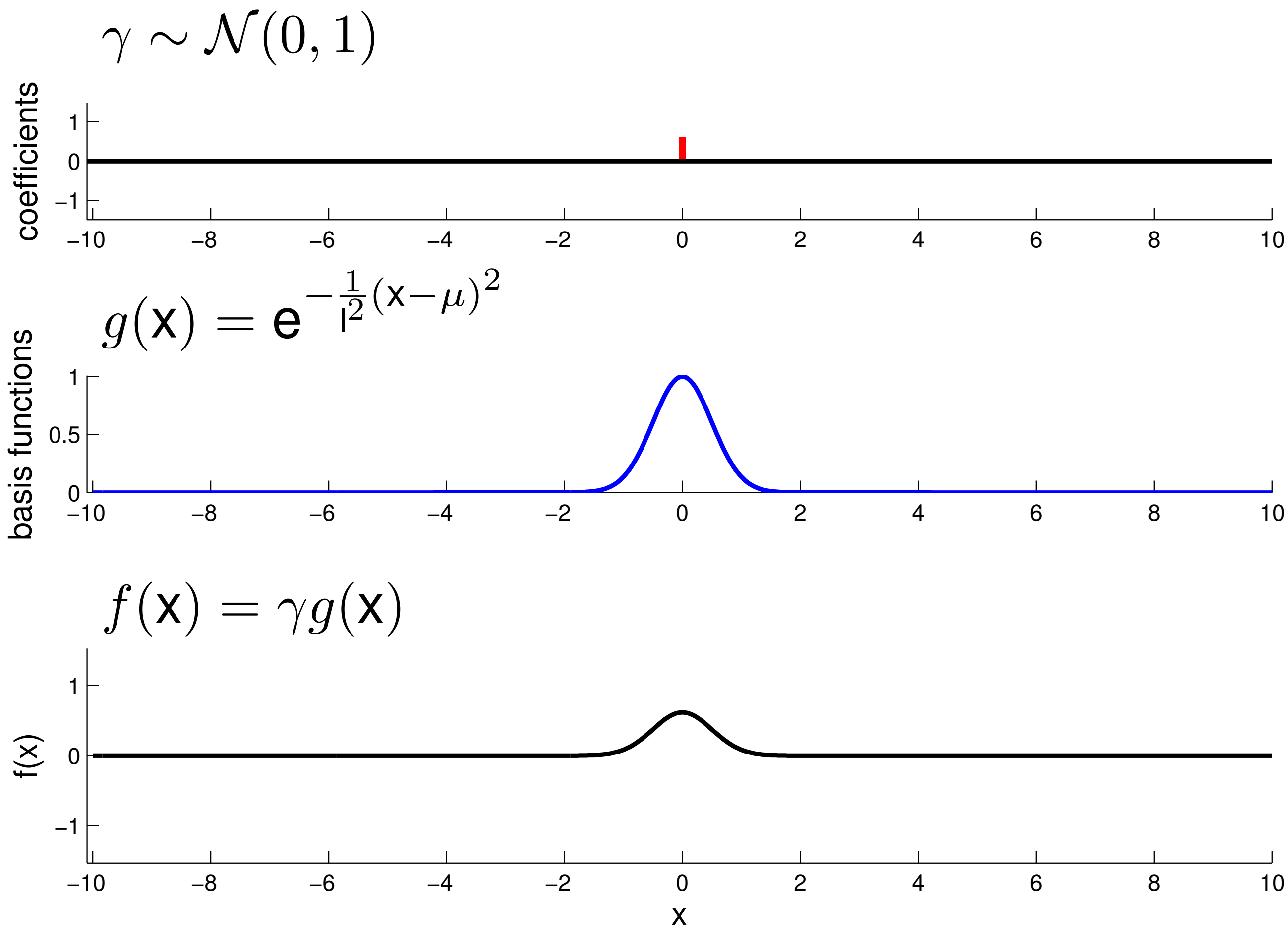

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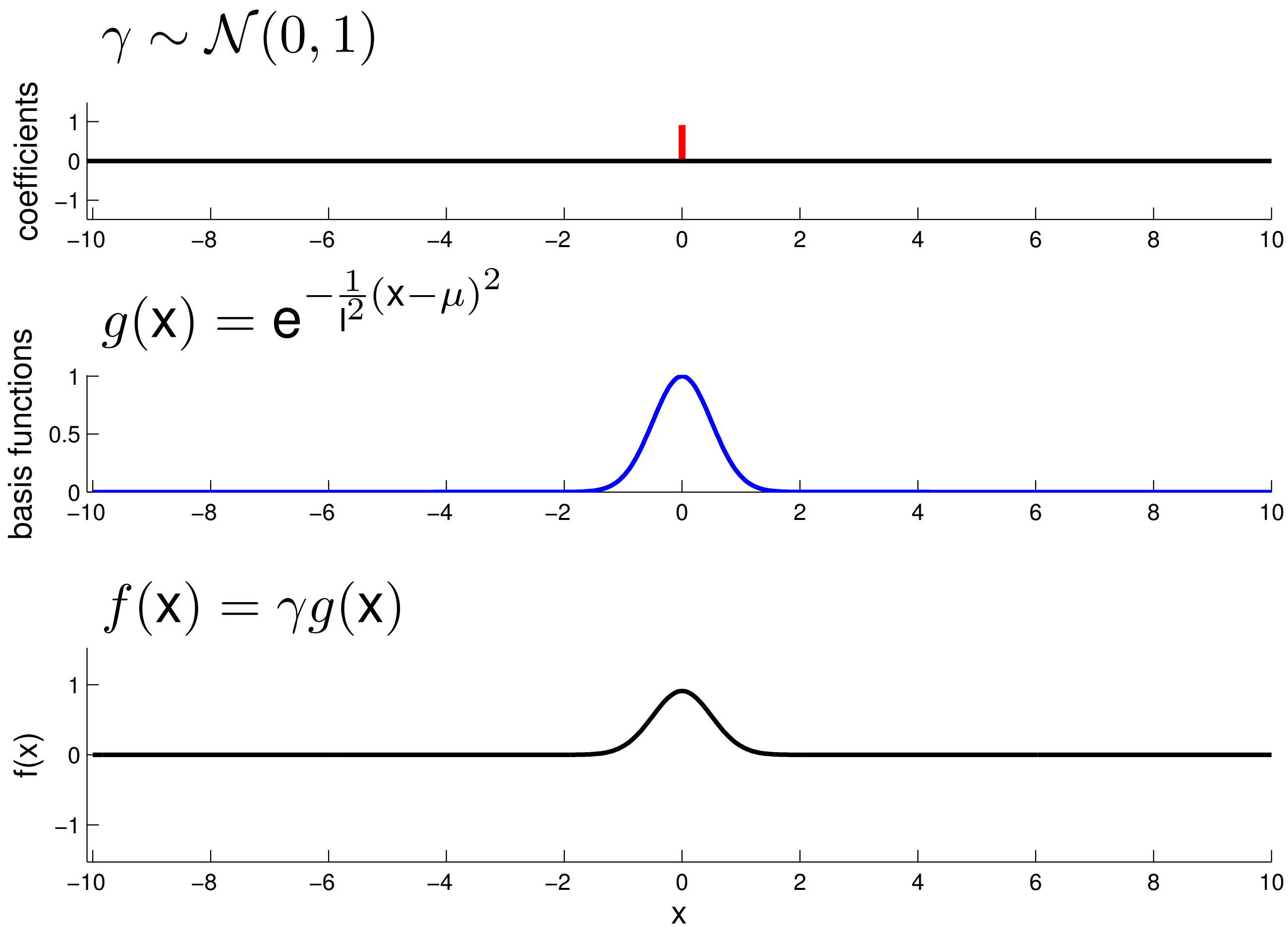

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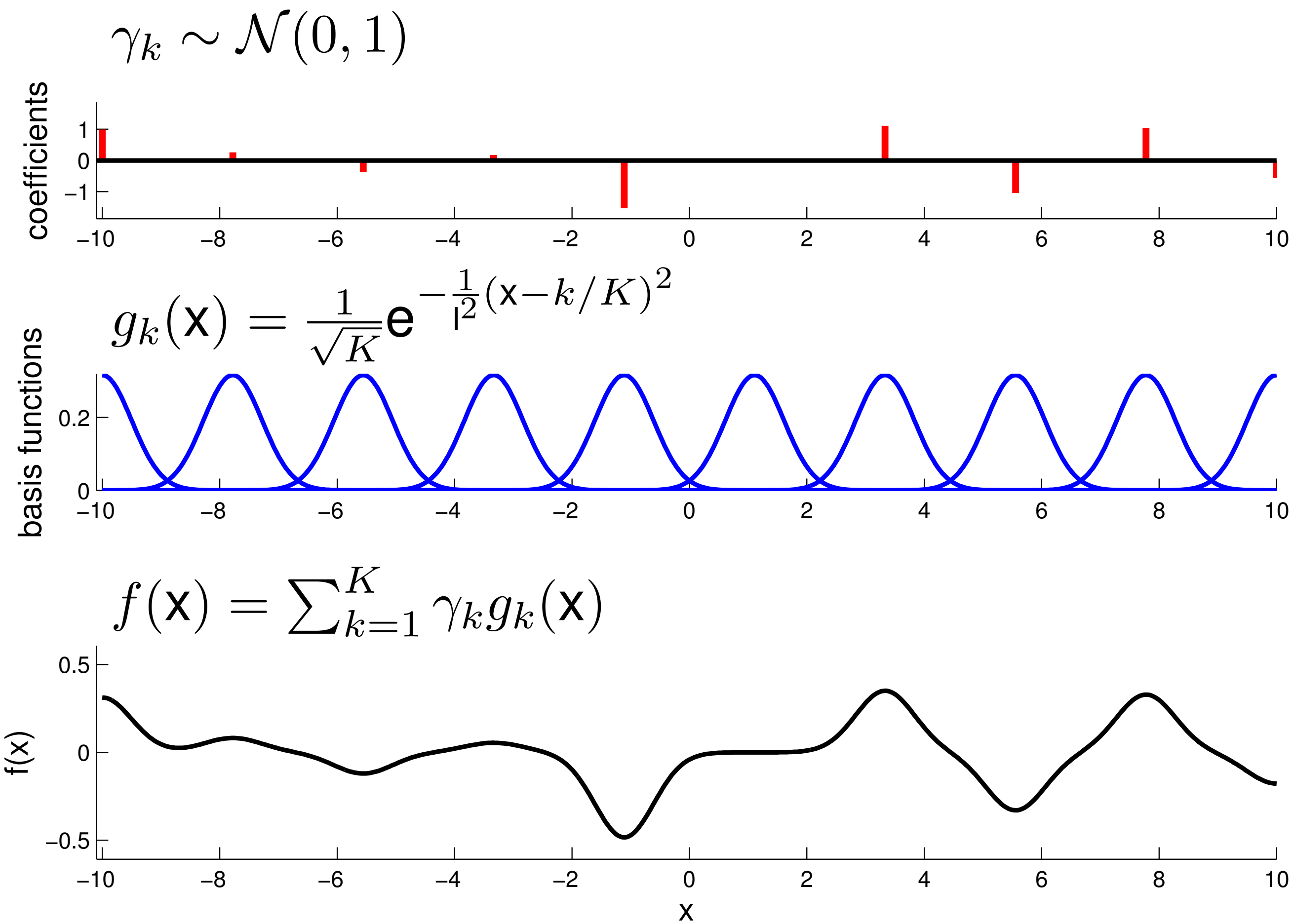

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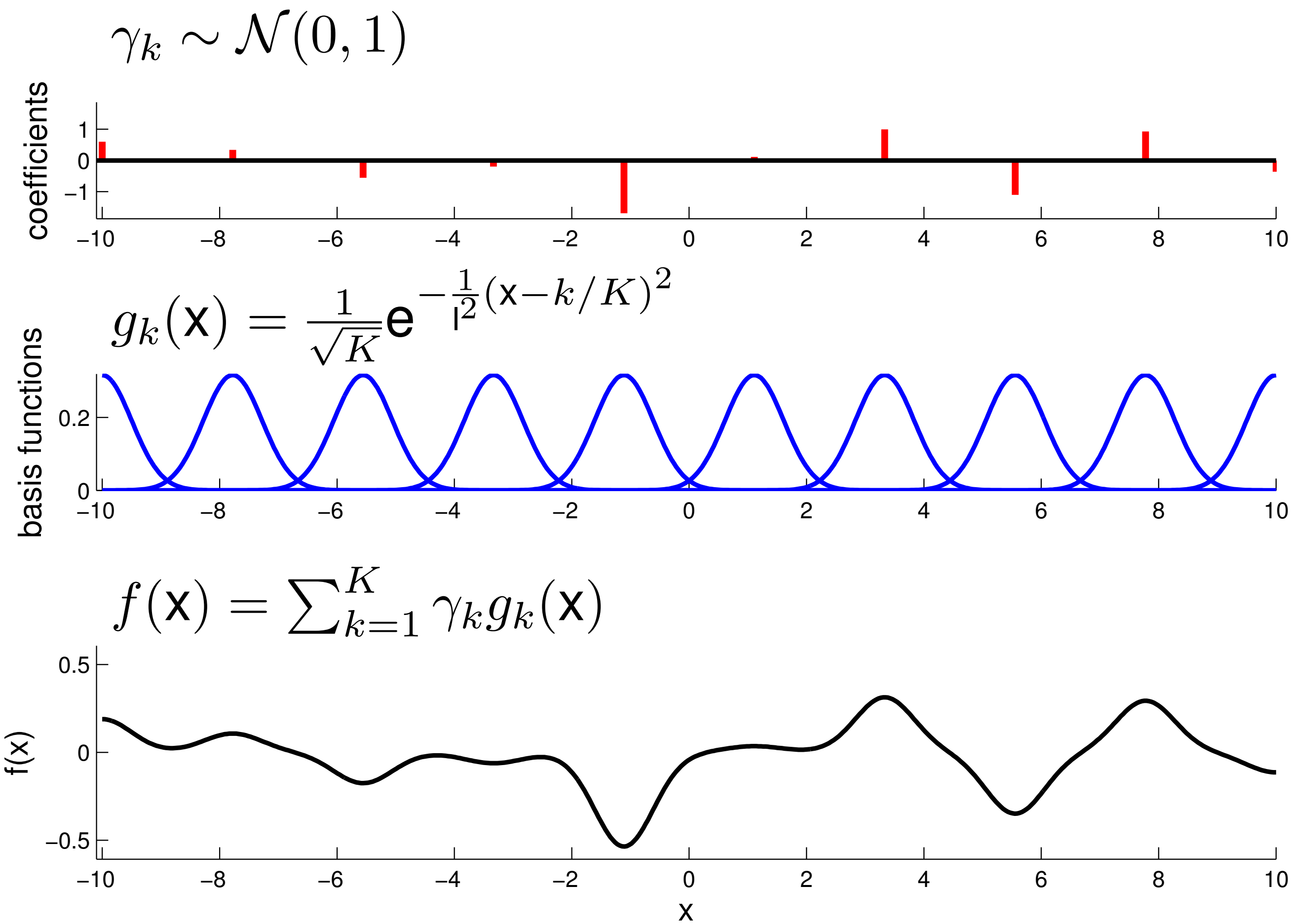

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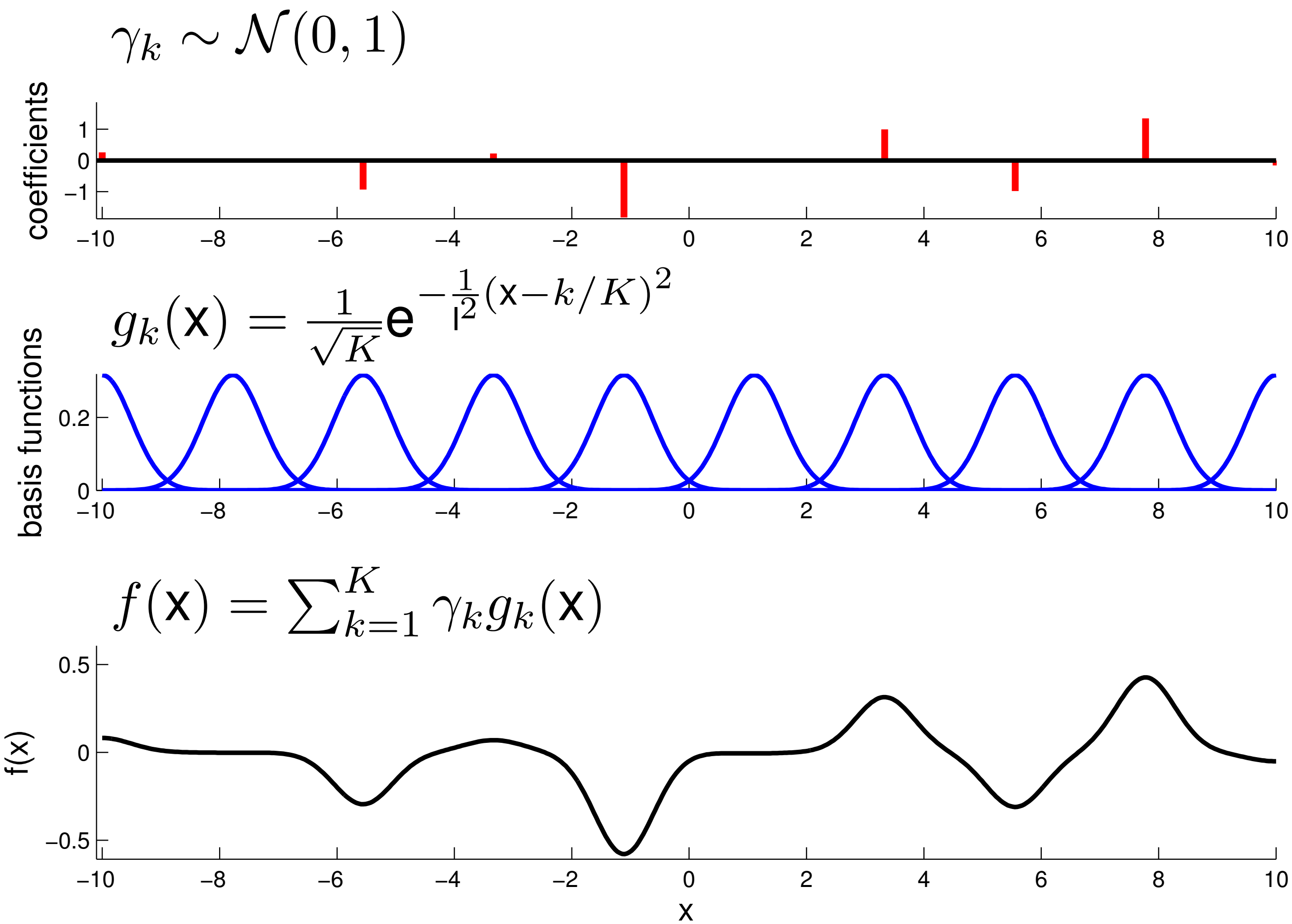

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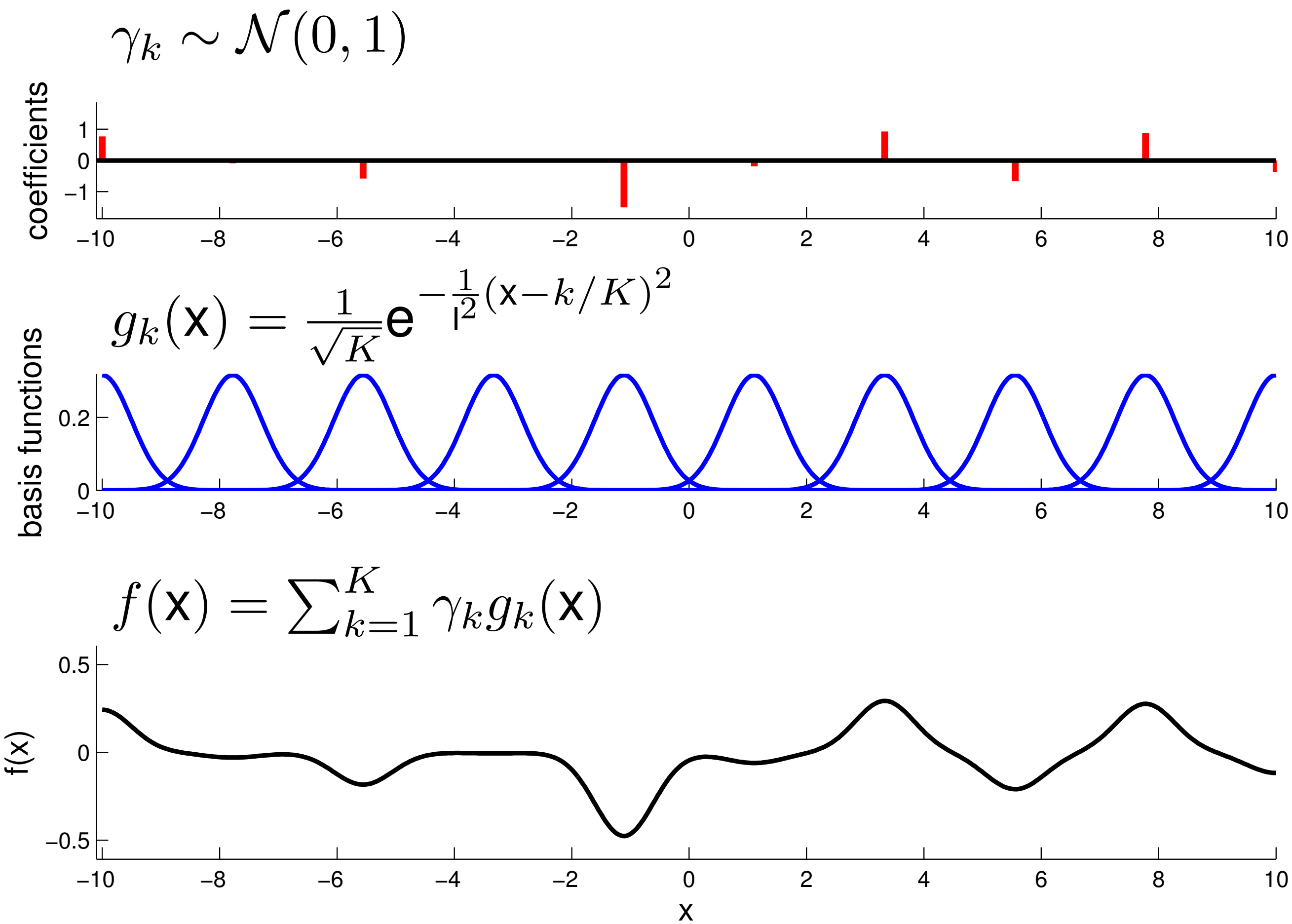

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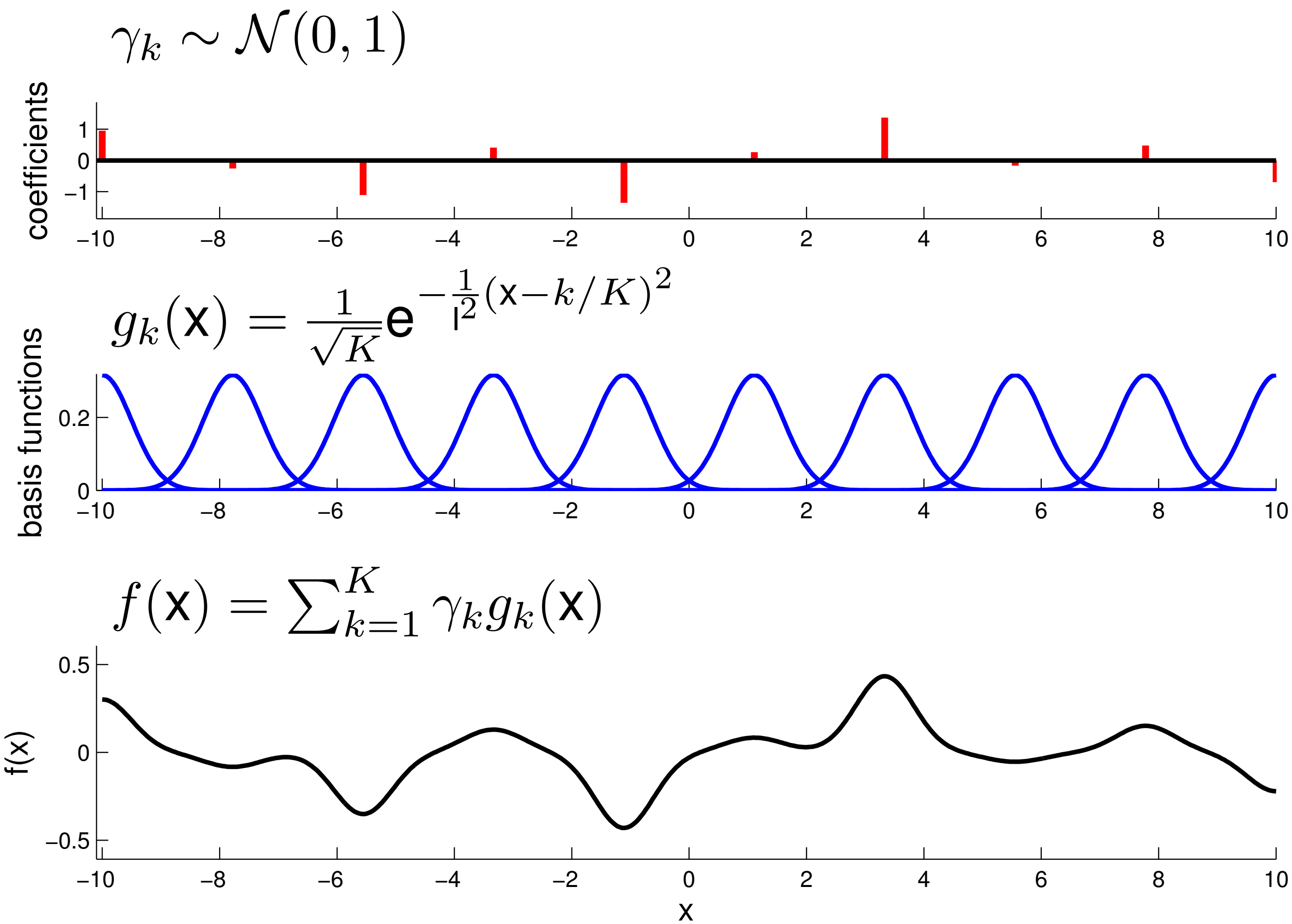

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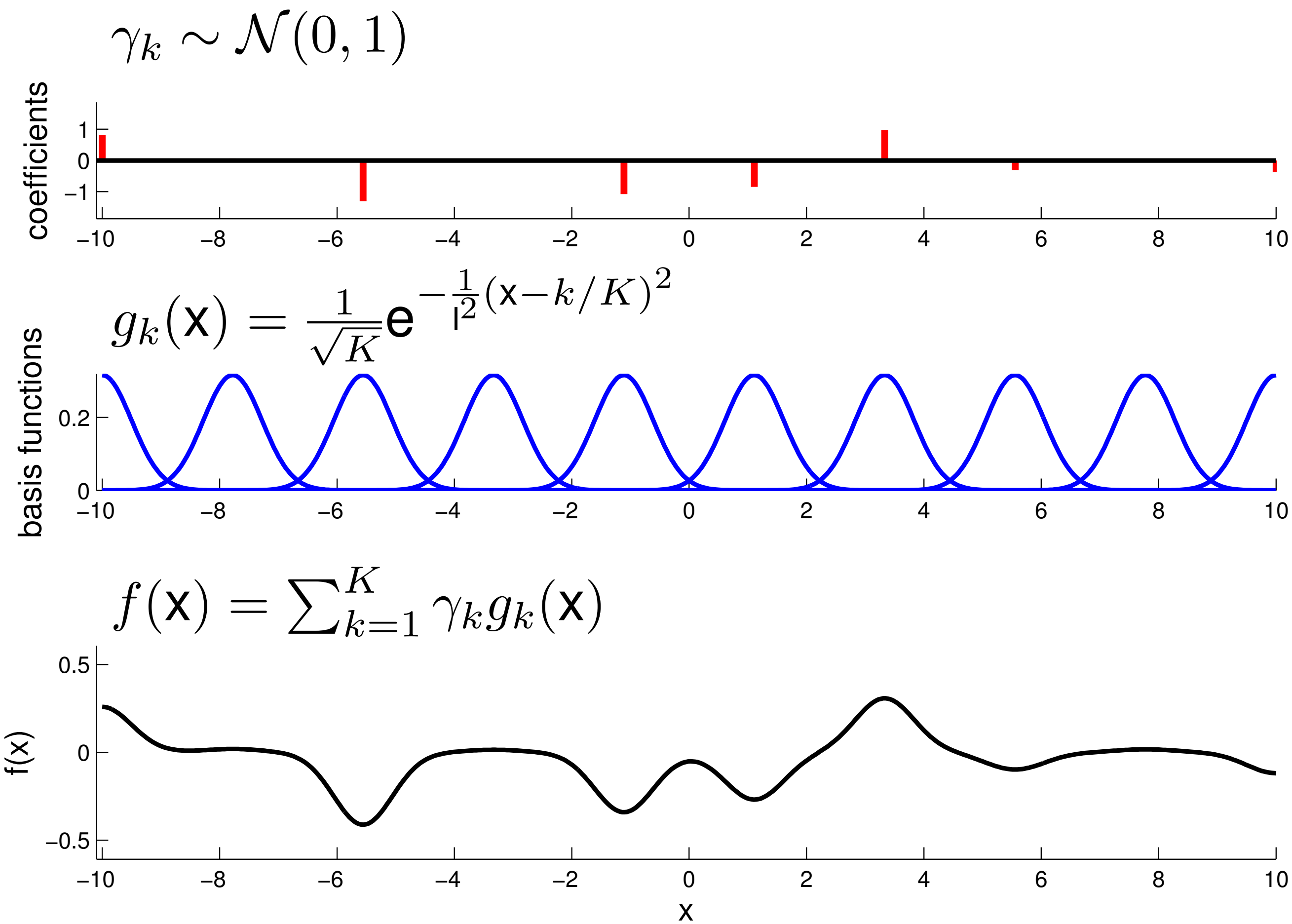

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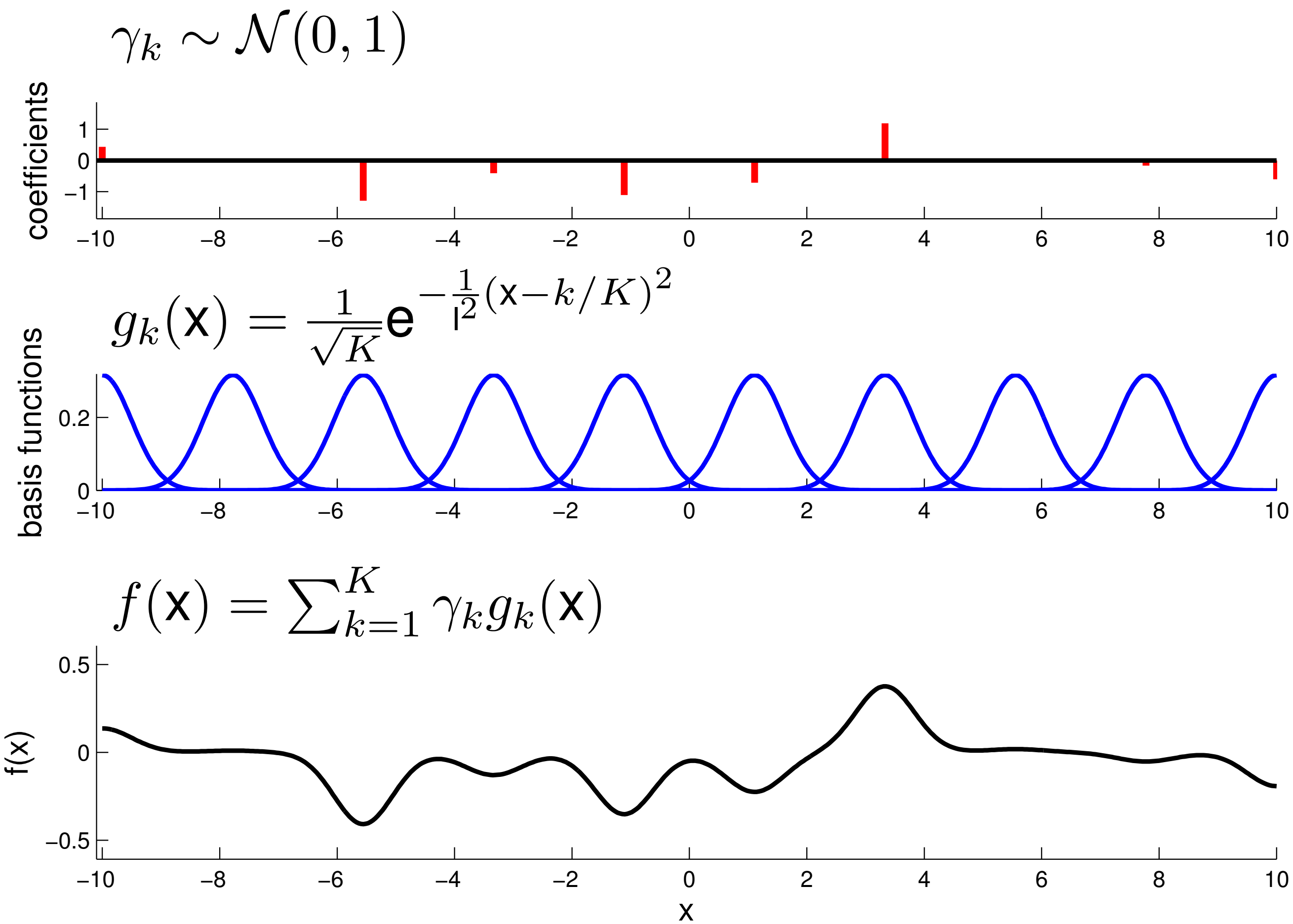

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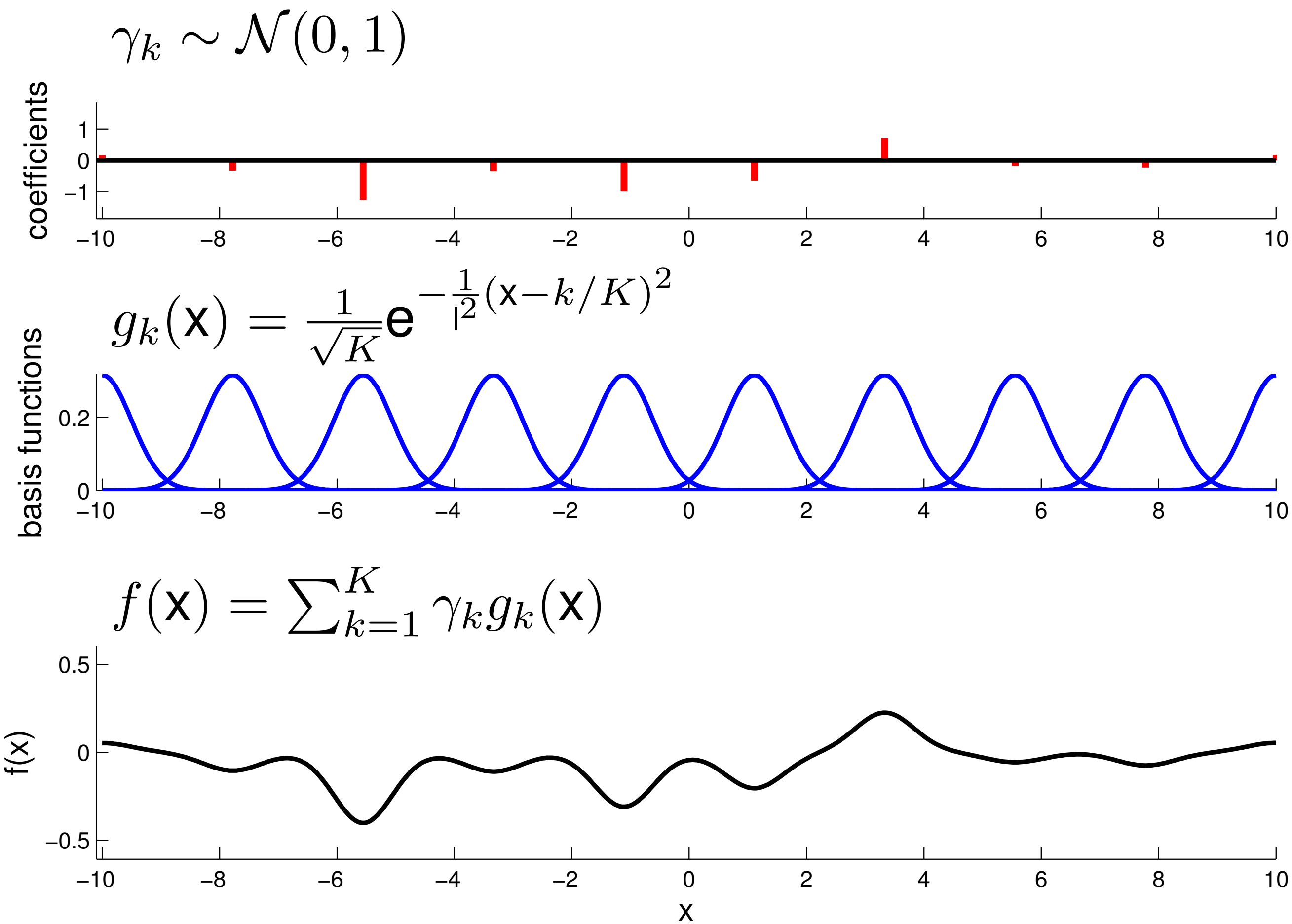
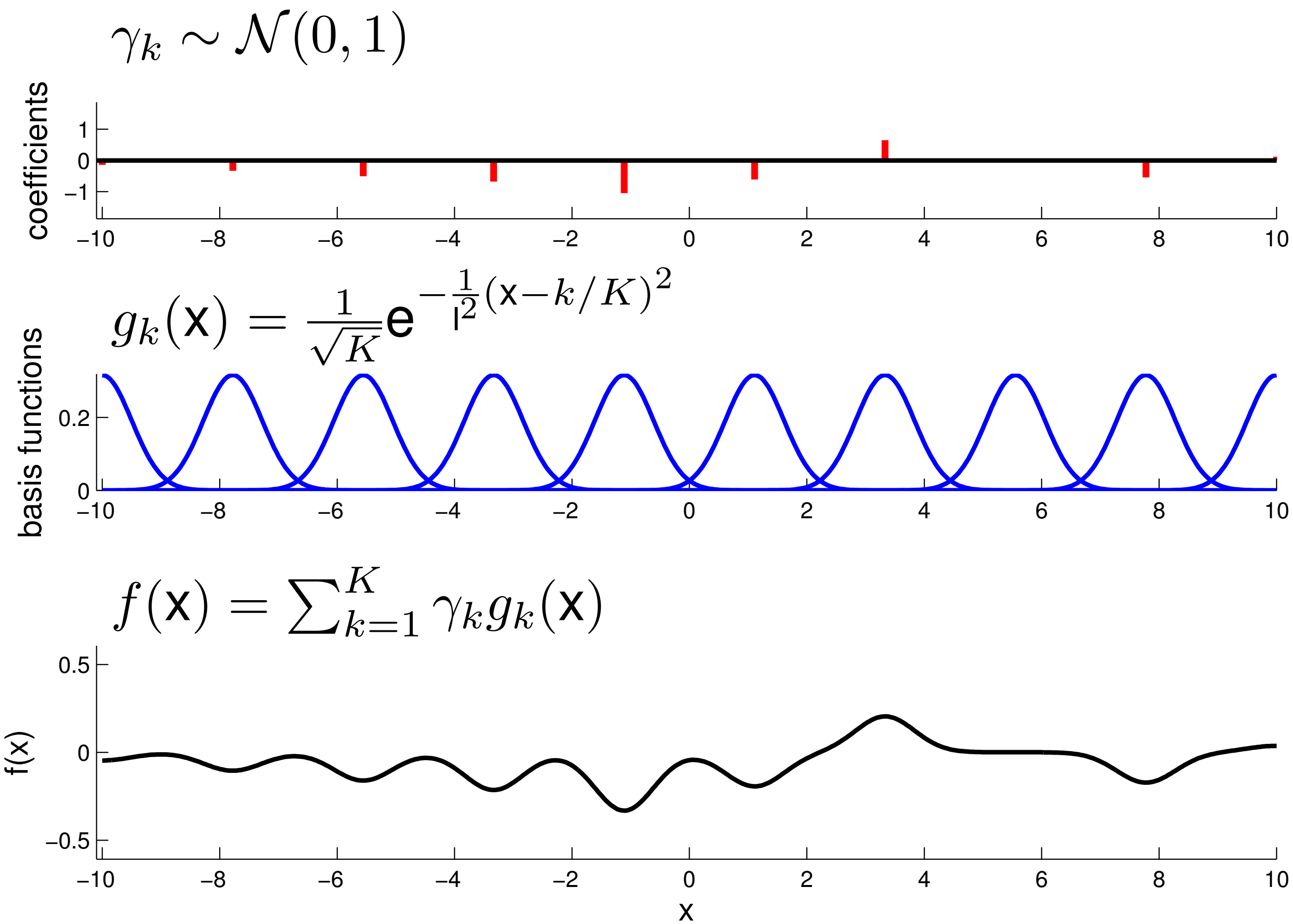
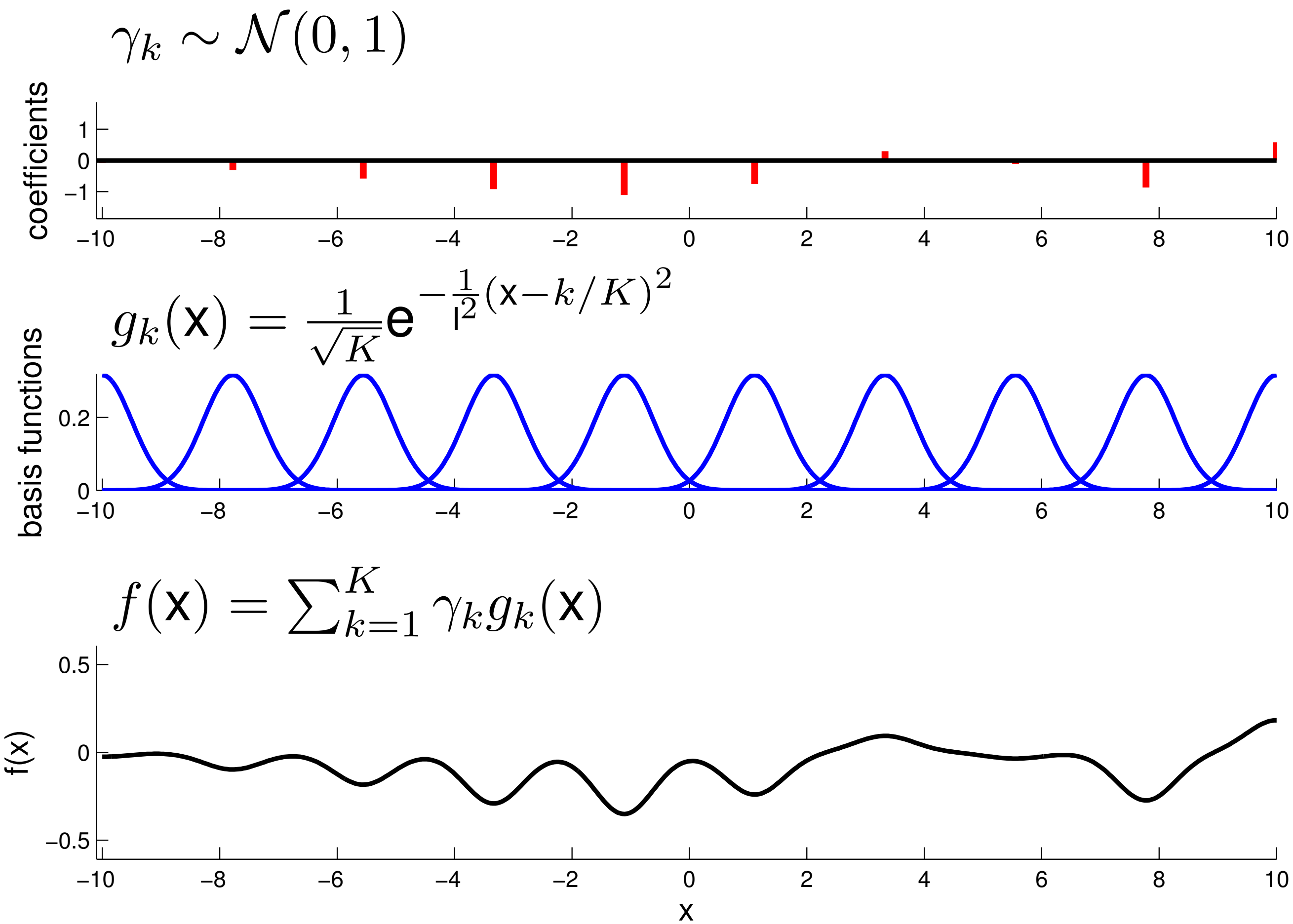


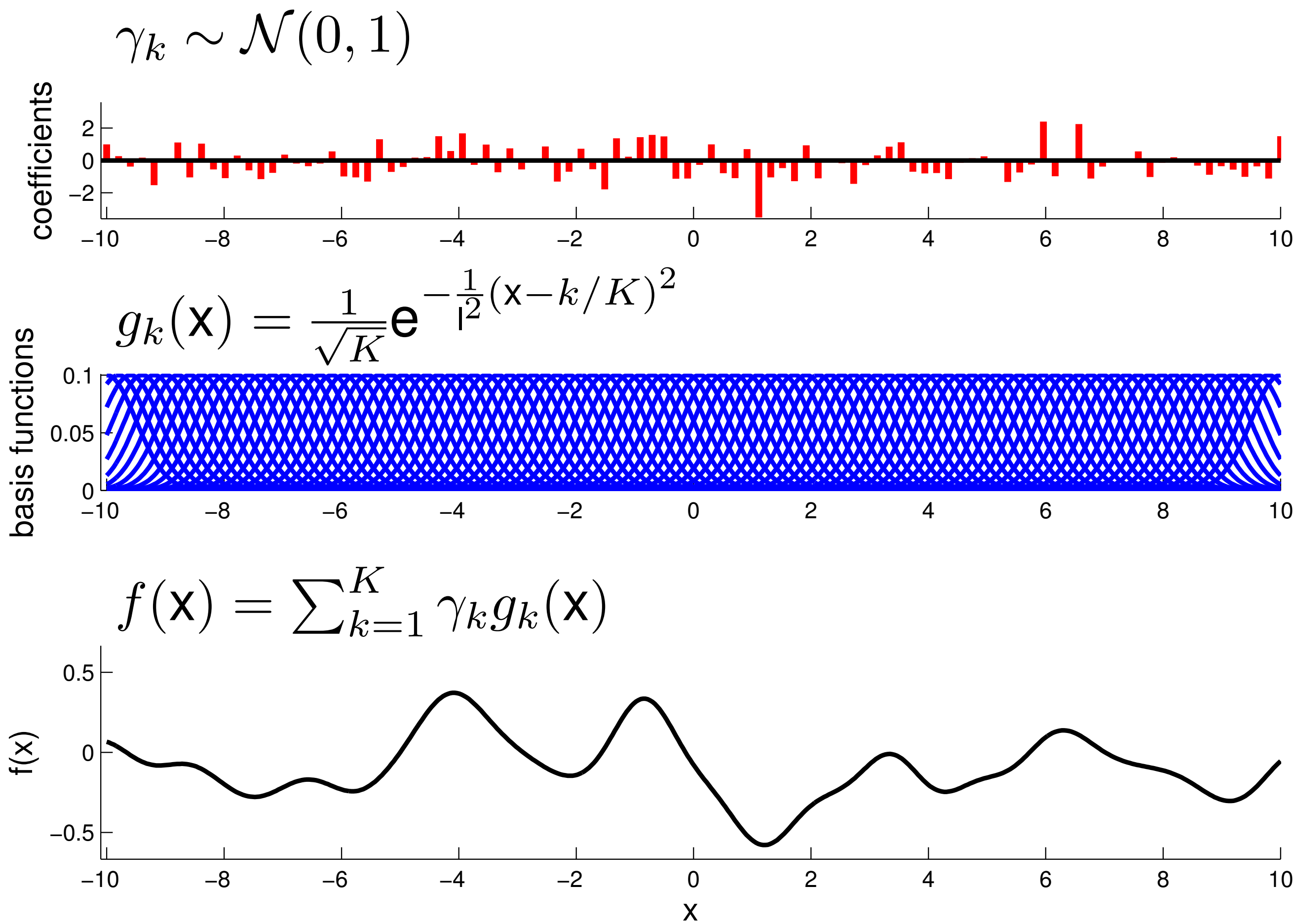
Basis function view of Gaussian processes



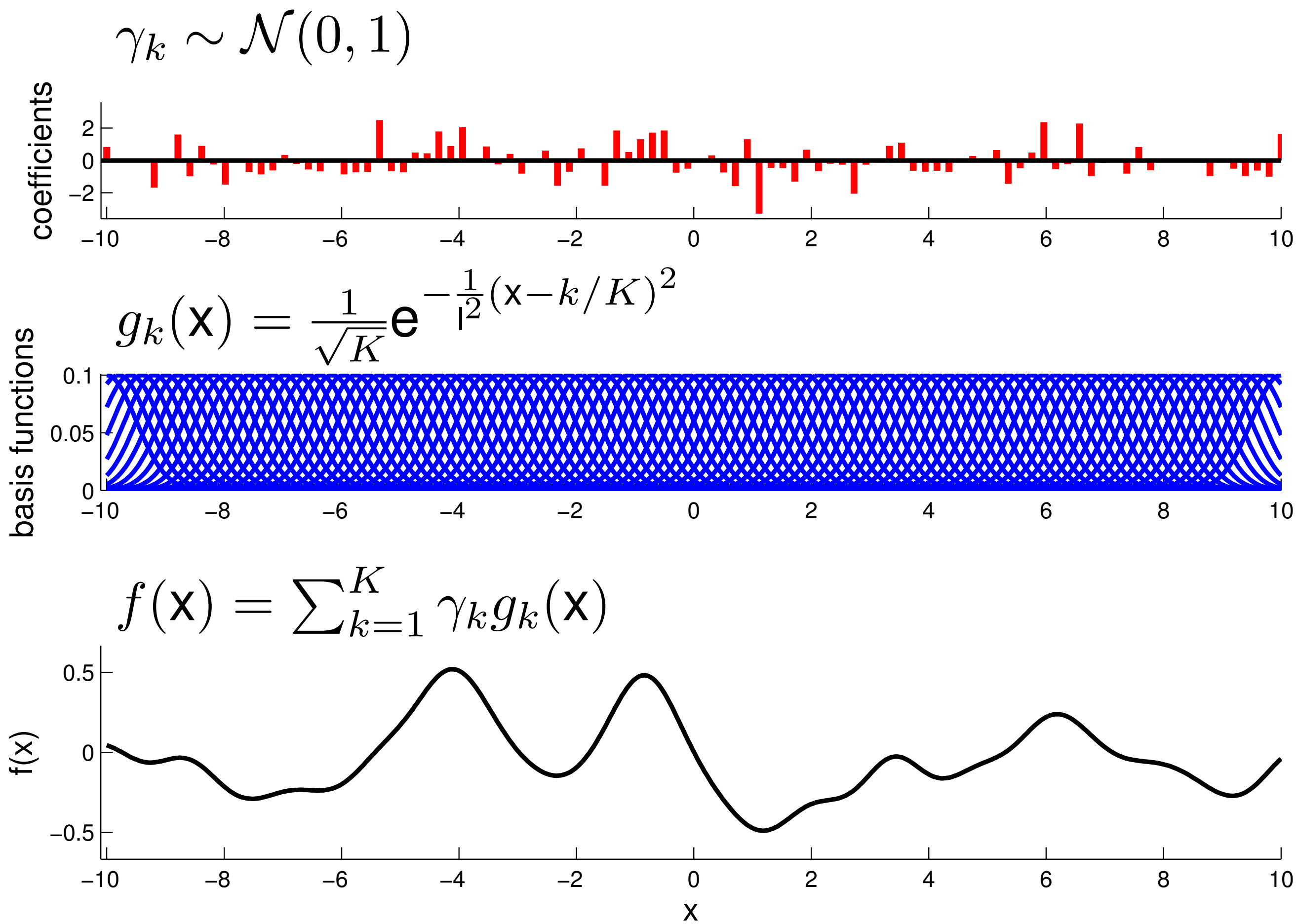
Basis function view of Gaussian processes



Basis function view of Gaussian processes



Basis function view of Gaussian processes



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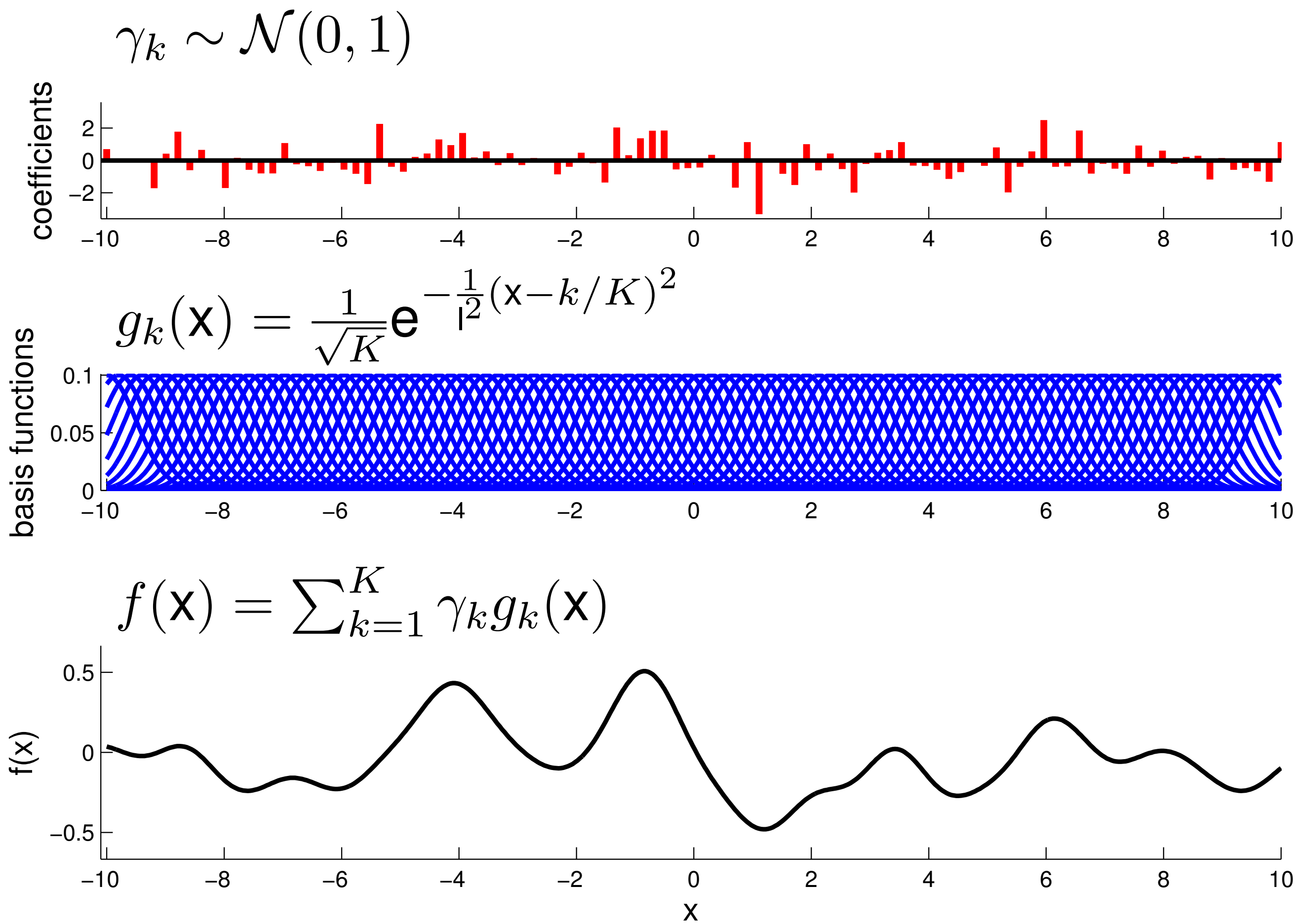

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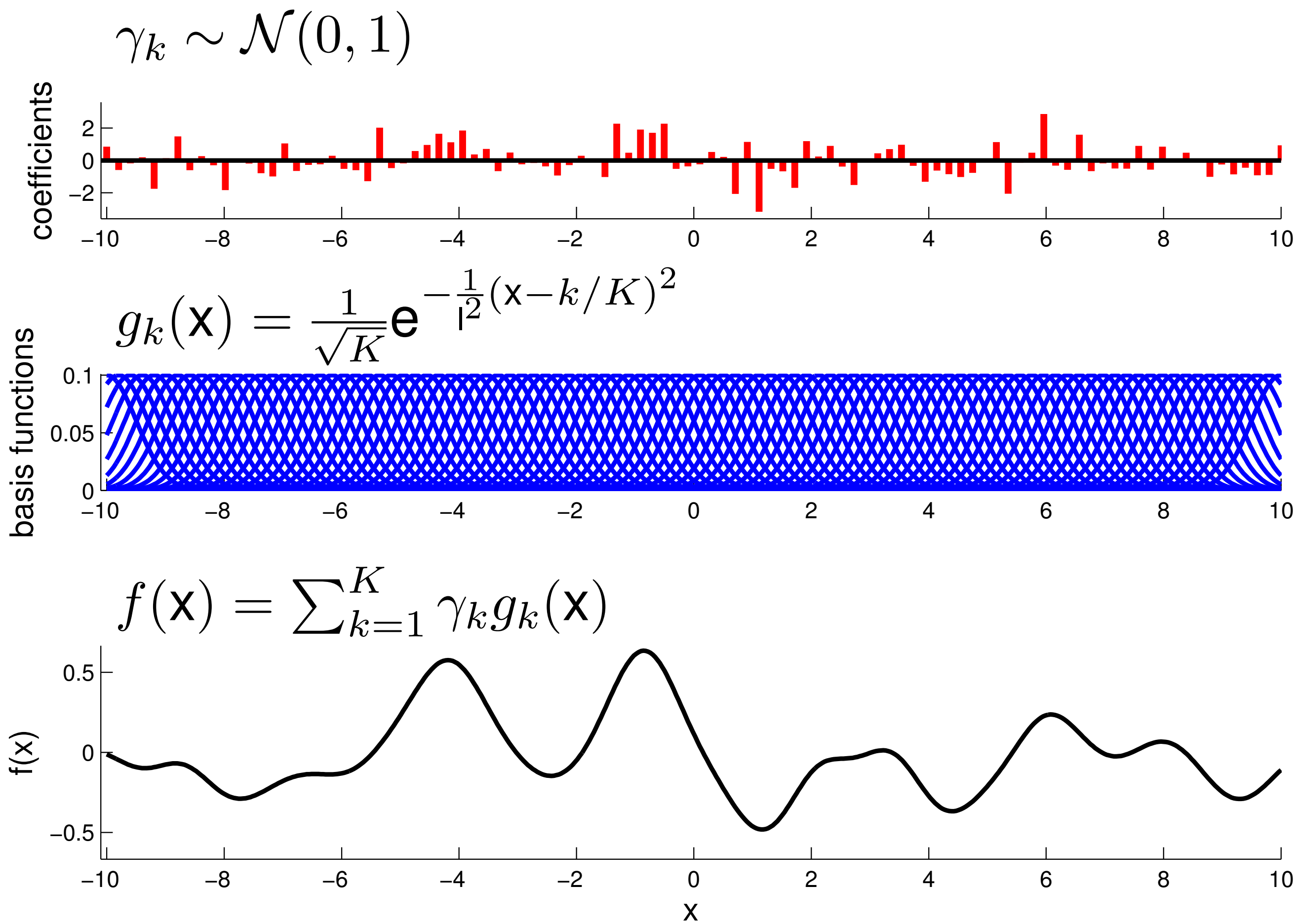

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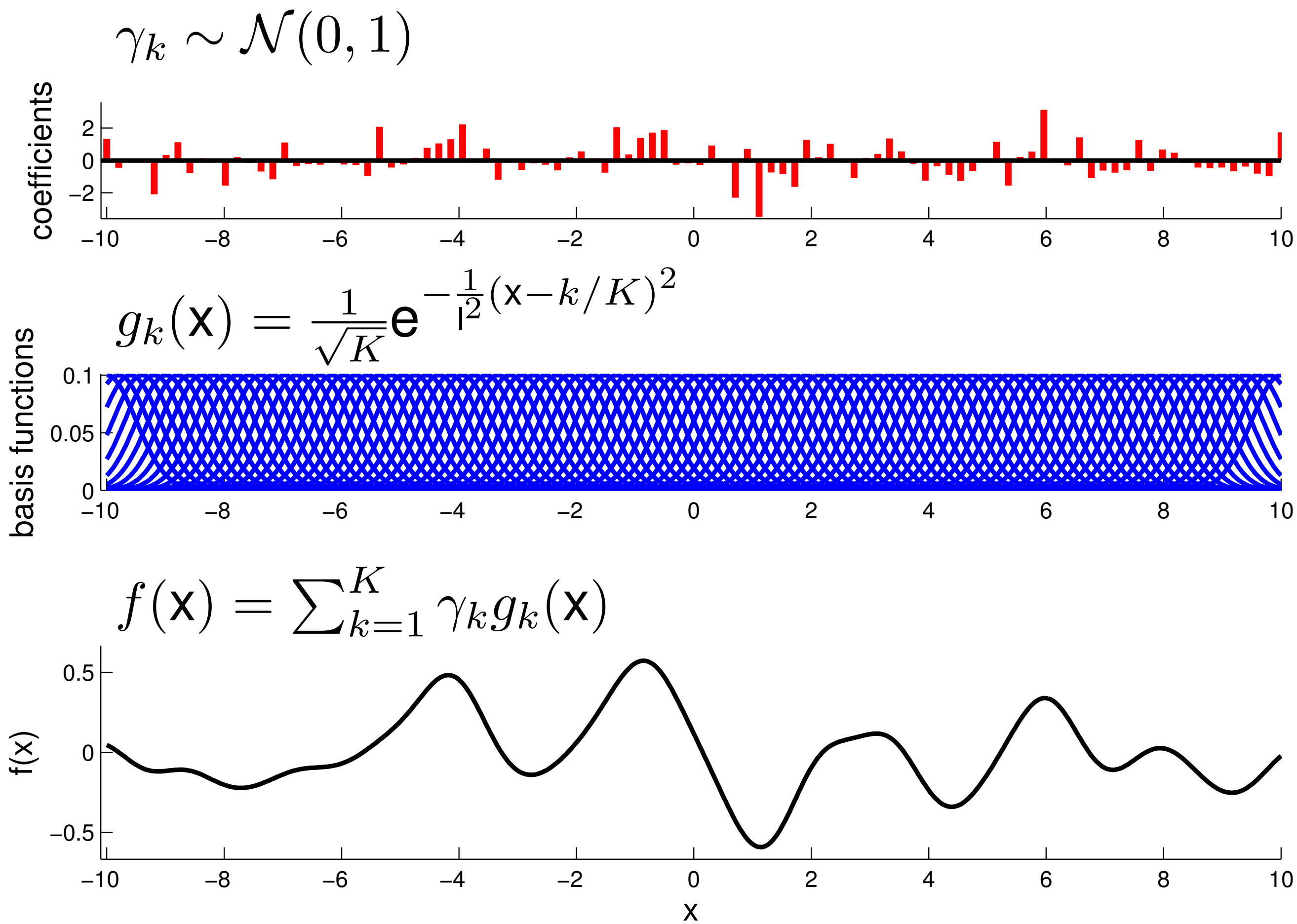

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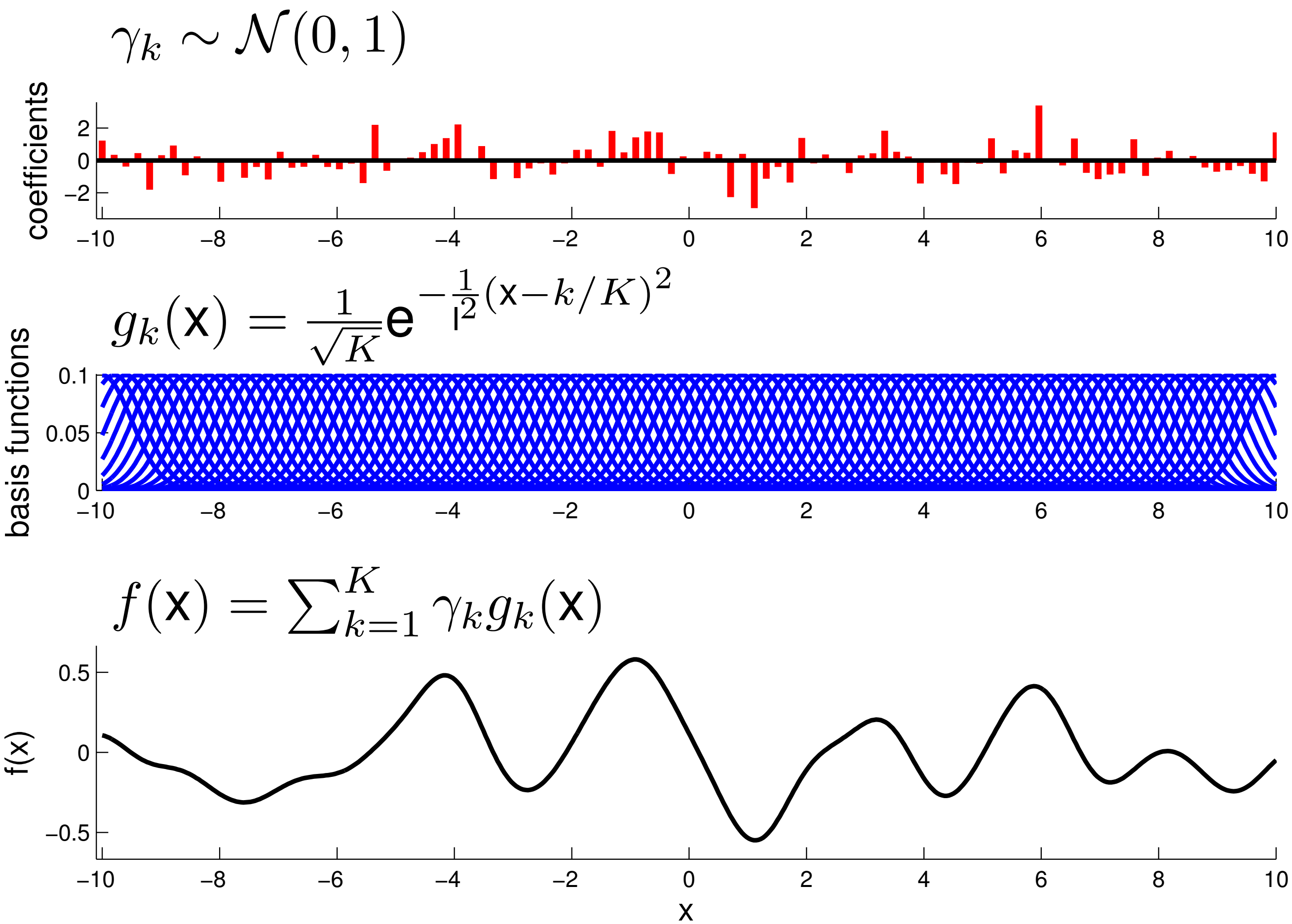

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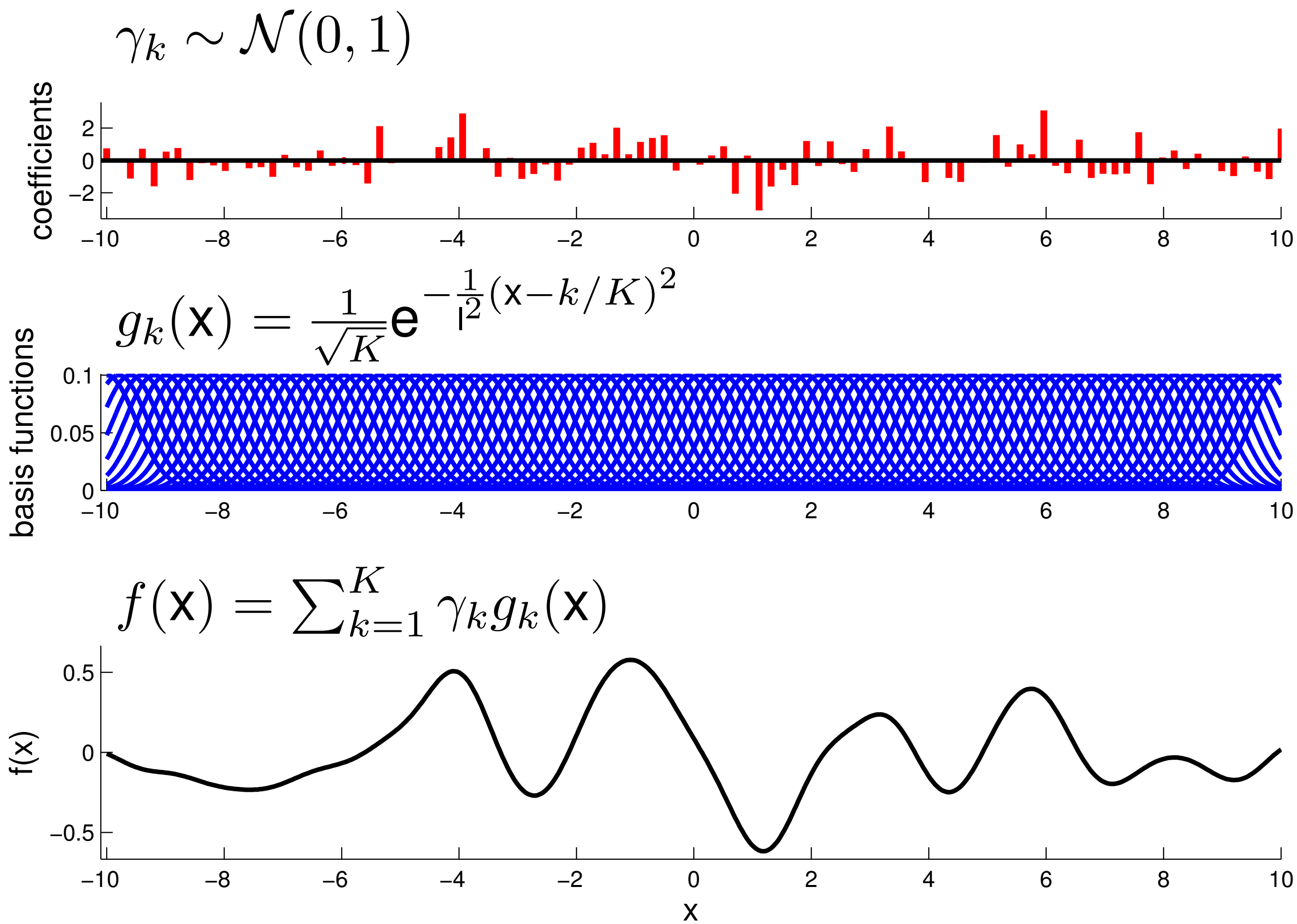

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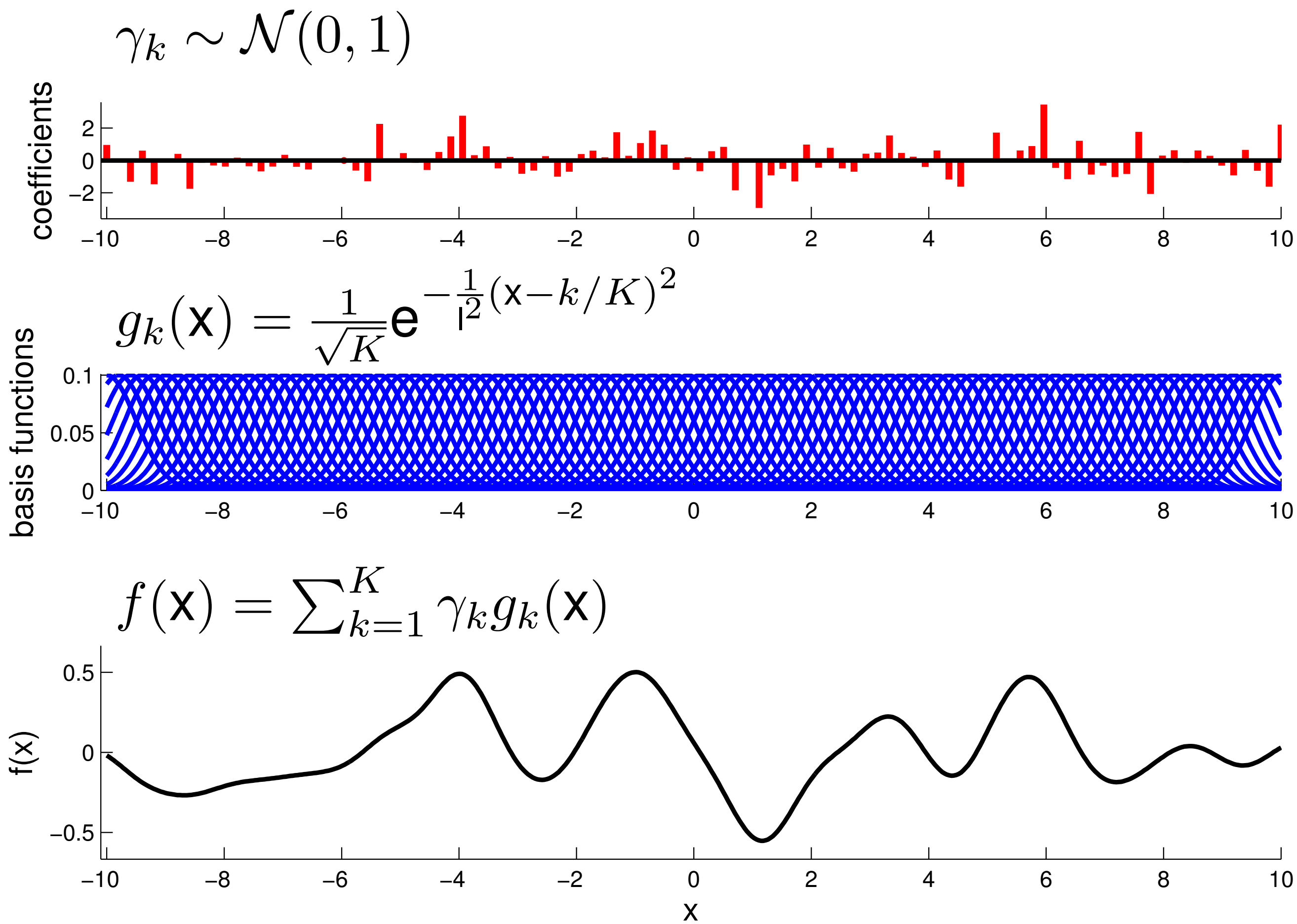

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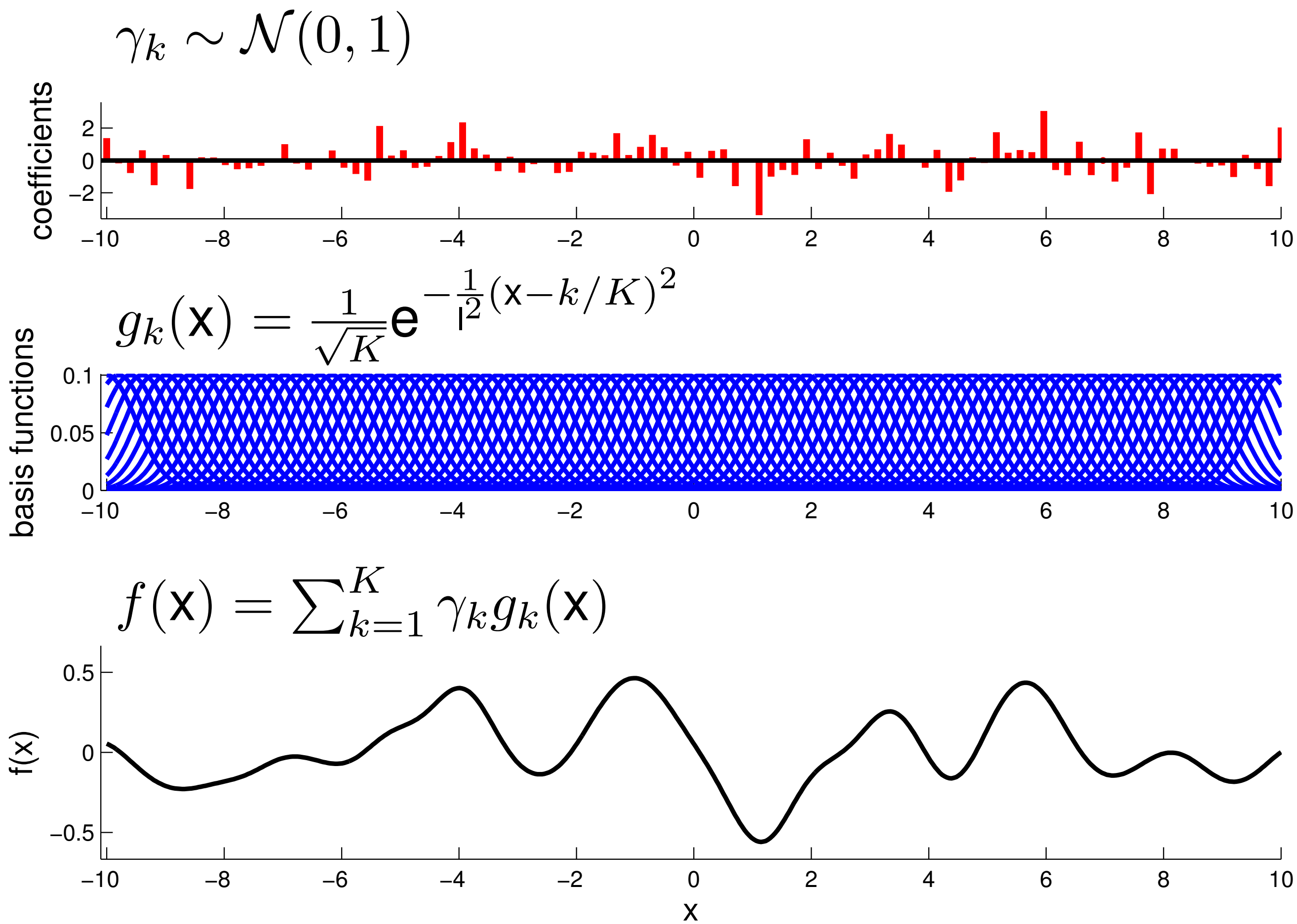
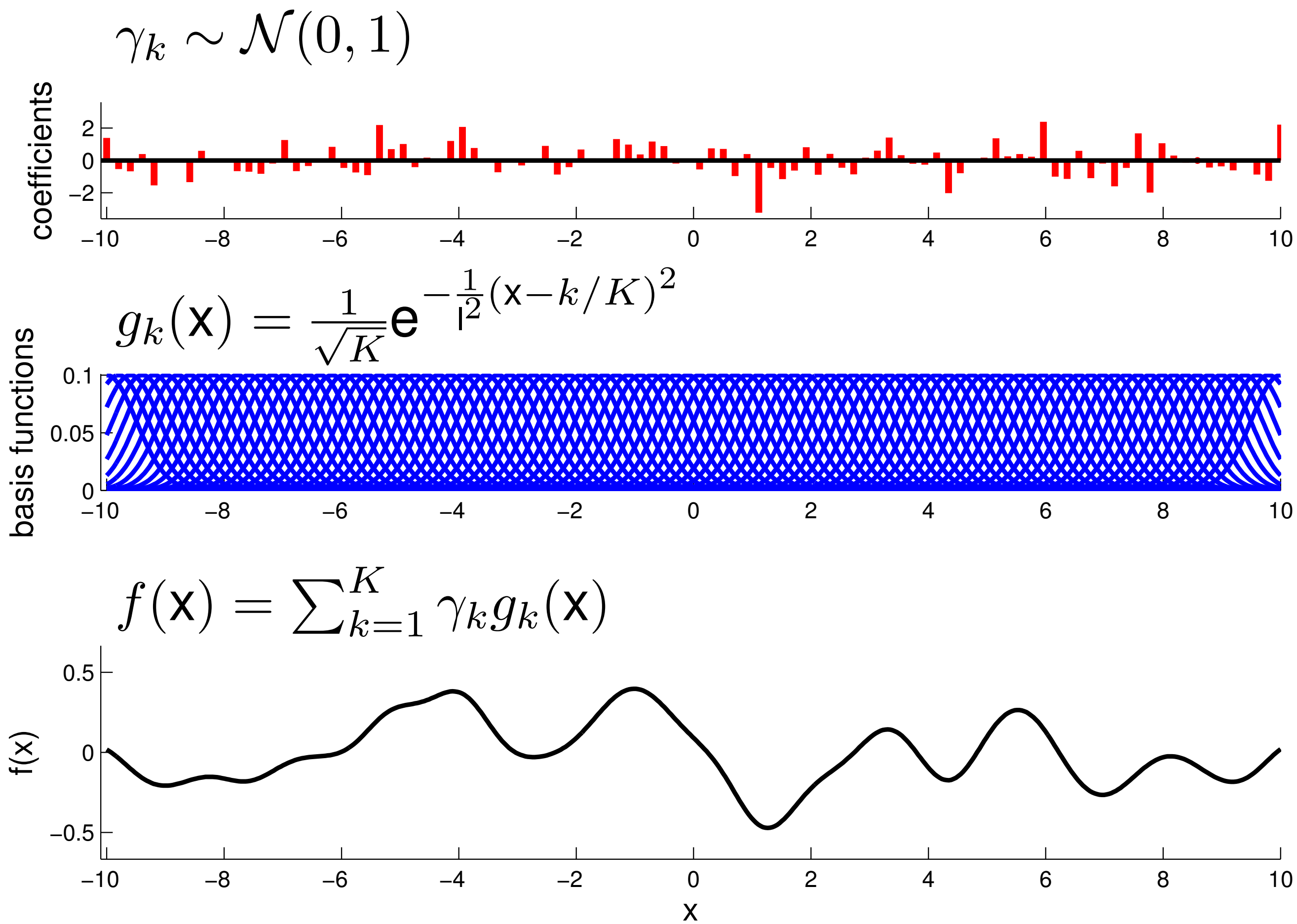


Basis function view of Gaussian processes



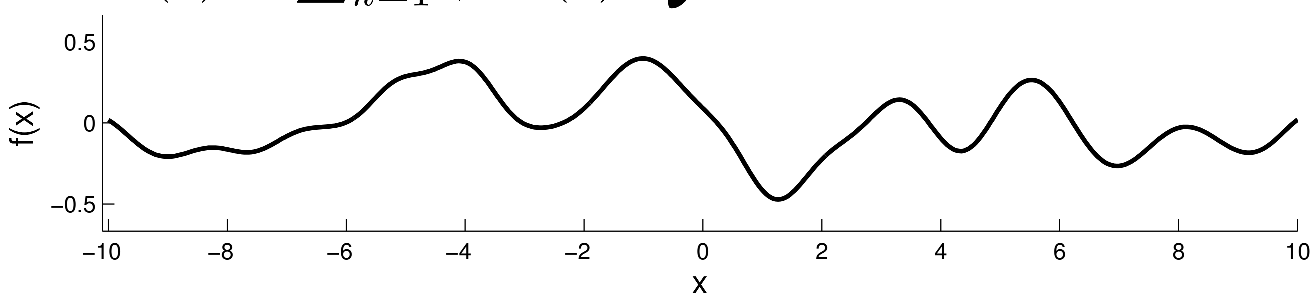
Basis function view of Gaussian processes

$$\gamma_k \sim \mathcal{N}(0,1)$$

$$g_k(\mathsf{x}) = \frac{1}{\sqrt{K}} \mathsf{e}^{-\frac{1}{\mathsf{l}^2}(\mathsf{x}-k/K)^2}$$

$$f(\mathsf{x}) = \sum_{k=1}^{K} \gamma_k g_k(\mathsf{x})$$

$$m(\mathsf{x}) = \langle f(\mathsf{x}) \rangle$$



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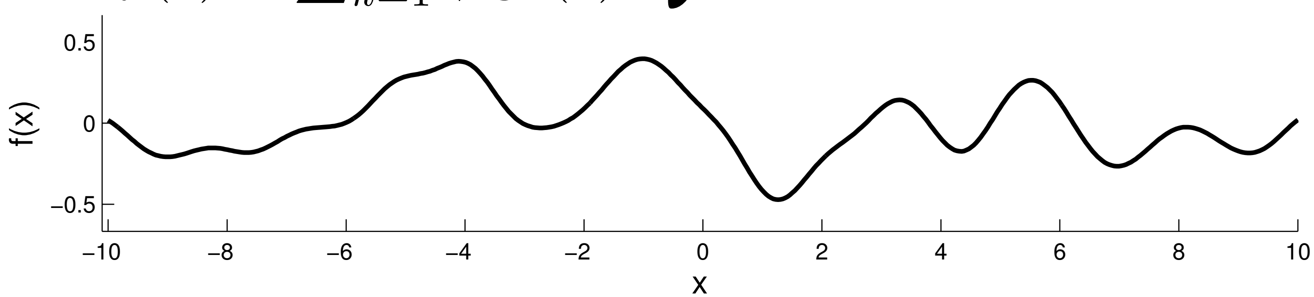

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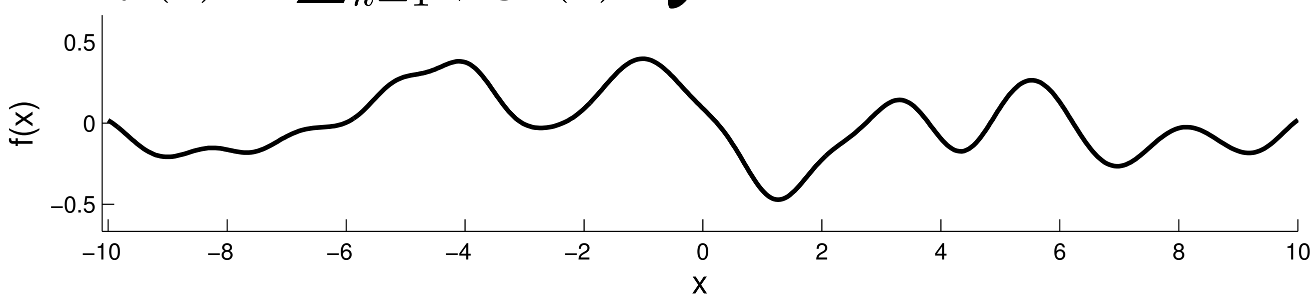

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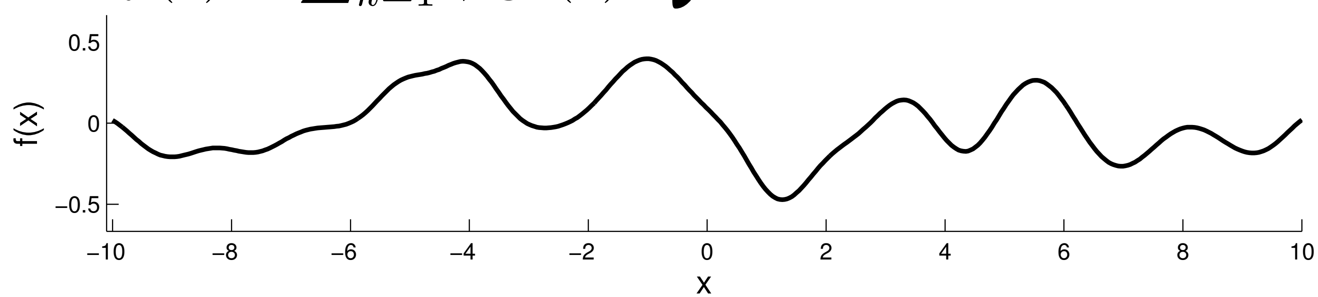

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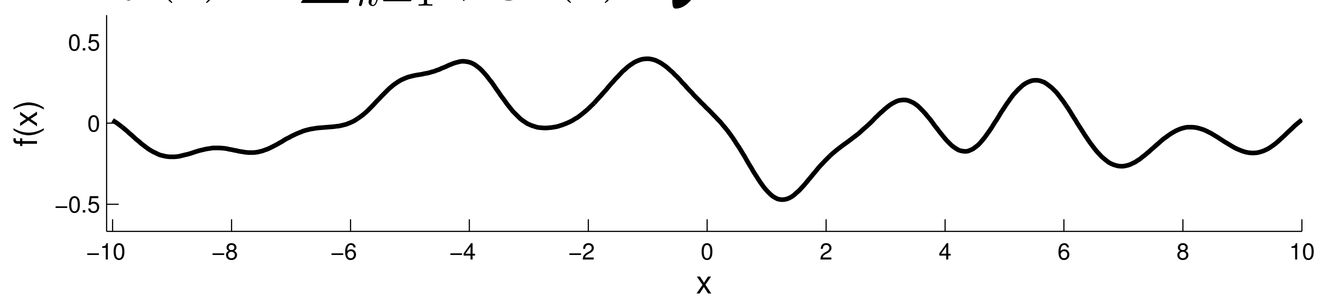

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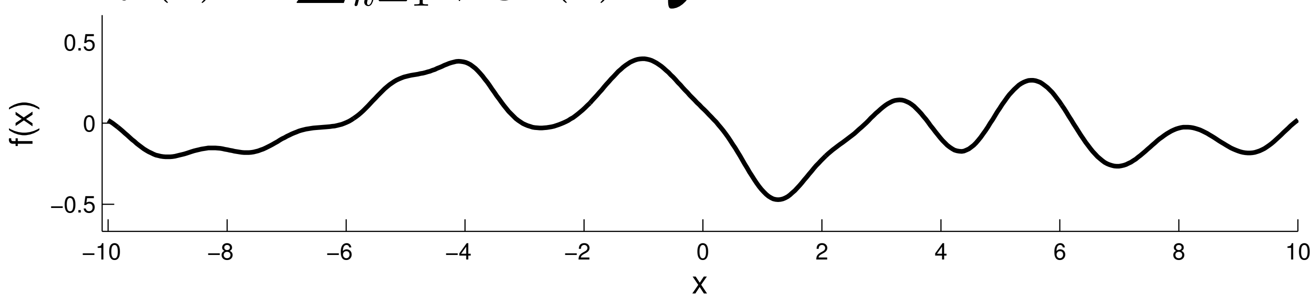

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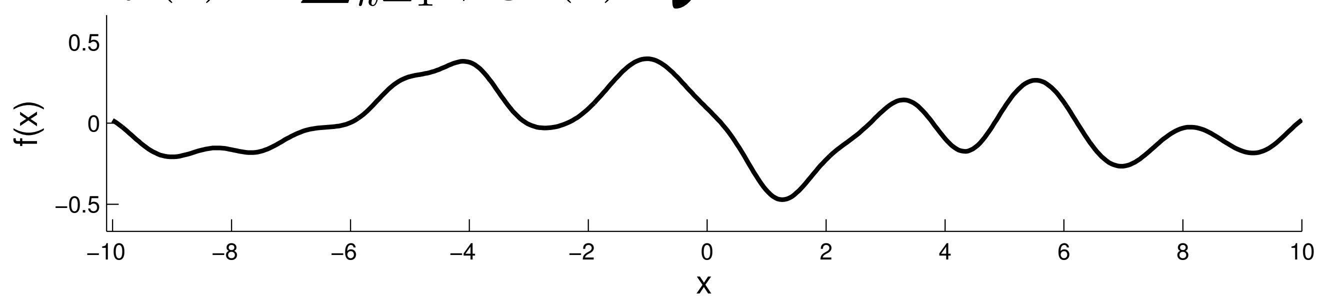

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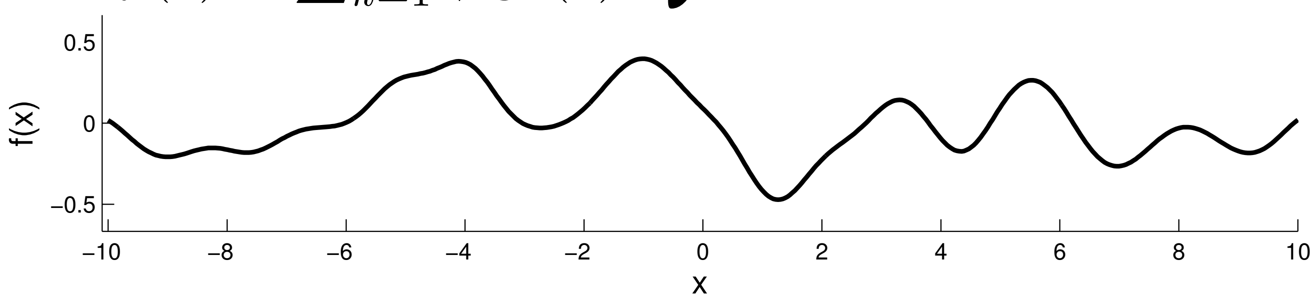

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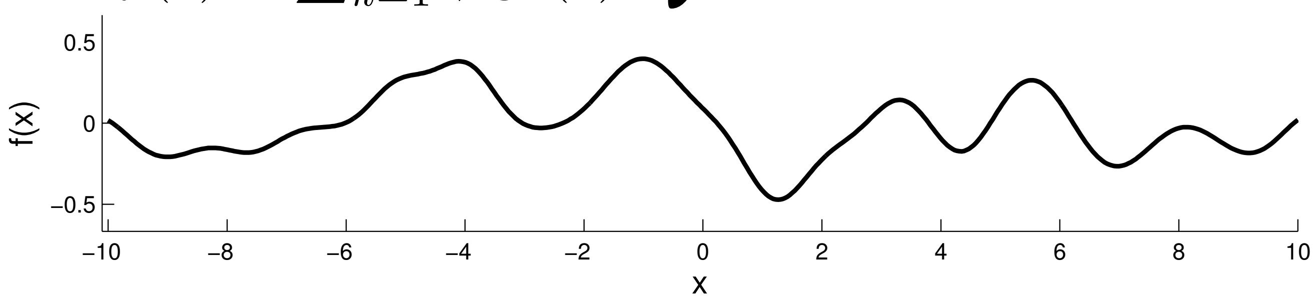

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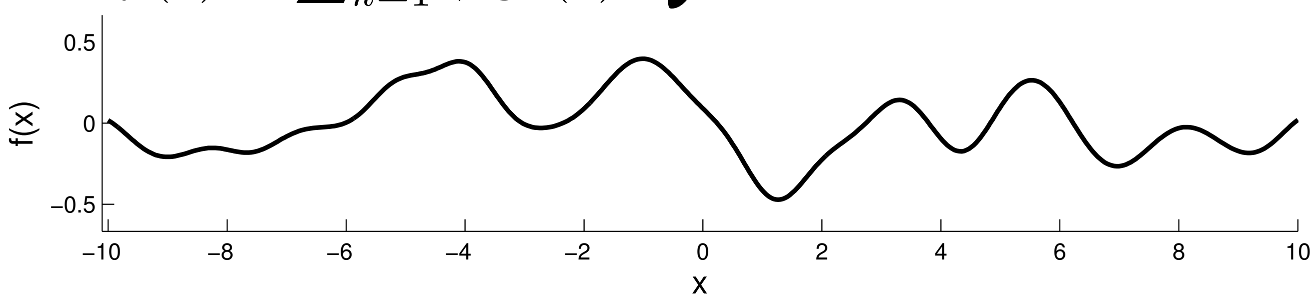

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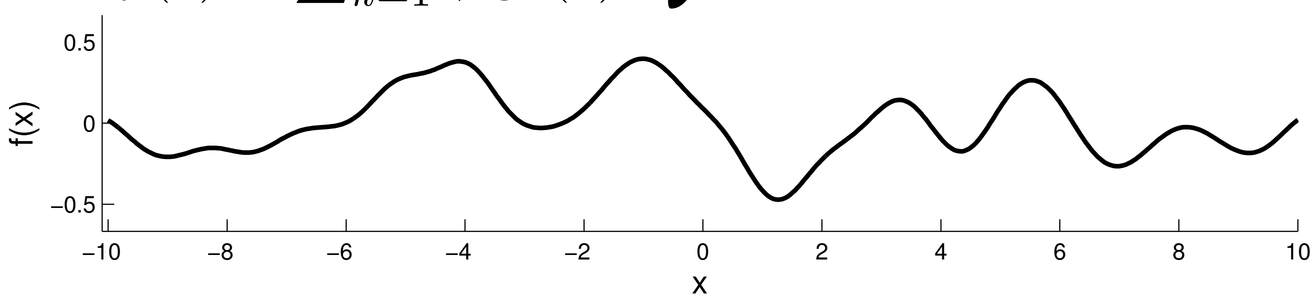
$$\underset{K \to \infty}{\longrightarrow} \quad \int du \;\; \mathsf{e}^{-\frac{1}{\mathsf{l}^2}(\mathsf{x}-u)^2 - \frac{1}{\mathsf{l}^2}(\mathsf{x}'-u)^2}$$



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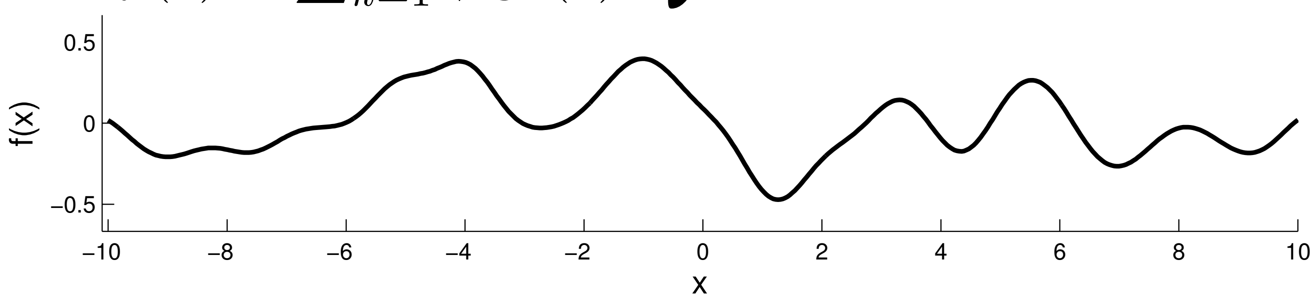

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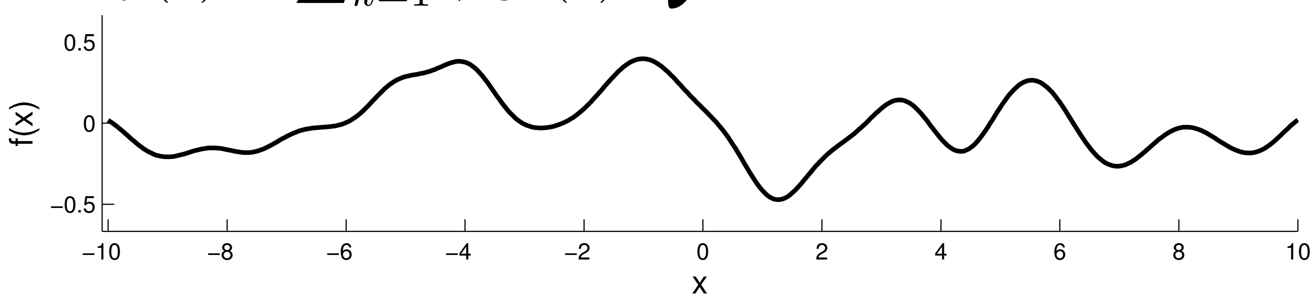
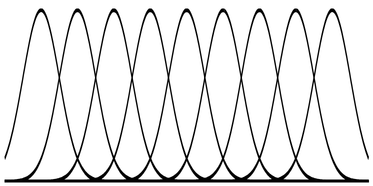


Gaussian processes $\equiv$ models with ∞ parameters

Basis function view of Gaussian Processes

$$\mathsf{y} = \sum_k \gamma_k g_k(\mathsf{x}) \qquad \gamma_k \sim \mathcal{N}(0, \Gamma_k)$$

basis function



$g_k(\mathsf{x})$

$$\exp\left(-\frac{1}{l}(\mathsf{x} - \mu_k)^2\right)$$

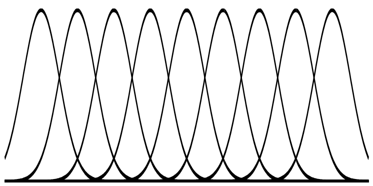
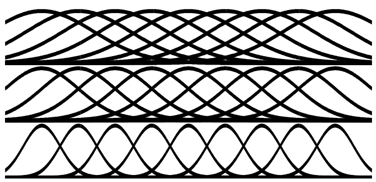
$\mathsf{K}(\mathsf{x}, \mathsf{x}')$

$$\exp\left(-\frac{1}{2l}(\mathsf{x} - \mathsf{x}')^2\right)$$

squared exponential

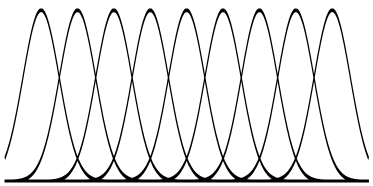
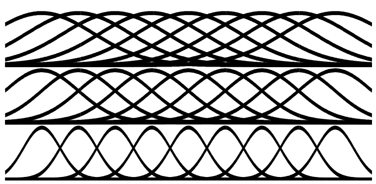
Basis function view of Gaussian Processes

$$\mathsf{y} = \sum_k \gamma_k g_k(\mathsf{x}) \qquad \gamma_k \sim \mathcal{N}(0, \Gamma_k)$$

basis function	$g_k(\mathsf{x})$	$\mathsf{K}(\mathsf{x}, \mathsf{x}')$	
	$\exp\left(-\frac{1}{l}(\mathsf{x} - \mu_k)^2\right)$	$\exp\left(-\frac{1}{2l}(\mathsf{x} - \mathsf{x}')^2\right)$	squared exponential
	$\exp\left(-\frac{1}{l_k}(\mathsf{x} - \mu_k)^2\right)$	$\left(1 + \frac{1}{2\alpha \mathsf{l}^2}\lvert\mathsf{x} - \mathsf{x}'\rvert\right)^{-\alpha}$	rational quadratic $\Gamma_k = \mathsf{invGam}(\mathsf{l})$

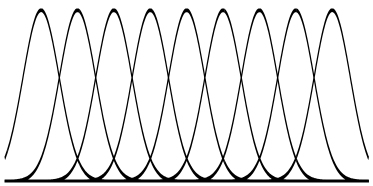
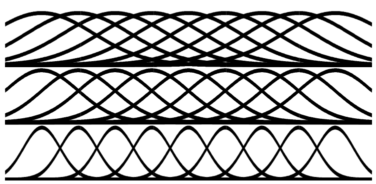
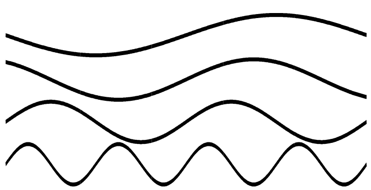
Basis function view of Gaussian Processes

$$\mathsf{y} = \sum_k \gamma_k g_k(\mathsf{x}) \qquad \gamma_k \sim \mathcal{N}(0, \Gamma_k)$$

basis function	$g_k(\mathsf{x})$	$\mathsf{K}(\mathsf{x}, \mathsf{x}')$	
	$\exp\left(-\frac{1}{l}(\mathsf{x} - \mu_k)^2\right)$	$\exp\left(-\frac{1}{2l}(\mathsf{x} - \mathsf{x}')^2\right)$	squared exponential
	$\exp\left(-\frac{1}{l_k}(\mathsf{x} - \mu_k)^2\right)$	mixture of SEs: $\left(1 + \frac{1}{2\alpha \mathsf{l}^2}\lvert\mathsf{x} - \mathsf{x}'\rvert\right)^{-\alpha}$	rational quadratic $\Gamma_k = \mathsf{invGam(l)}$

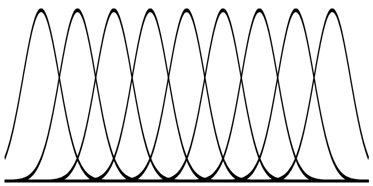
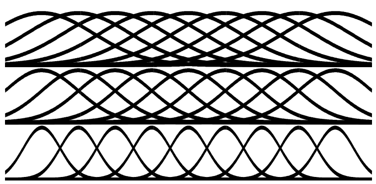
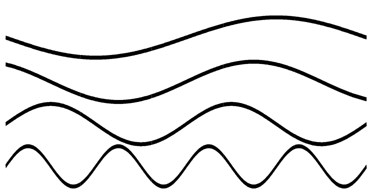
Basis function view of Gaussian Processes

$$\mathsf{y} = \sum_k \gamma_k g_k(\mathsf{x}) \qquad \gamma_k \sim \mathcal{N}(0, \Gamma_k)$$

basis function	$g_k(\mathsf{x})$	$\mathsf{K}(\mathsf{x}, \mathsf{x}')$	
	$\exp\left(-\frac{1}{l}(\mathsf{x} - \mu_k)^2\right)$	$\exp\left(-\frac{1}{2l}(\mathsf{x} - \mathsf{x}')^2\right)$	squared exponential
	$\exp\left(-\frac{1}{l_k}(\mathsf{x} - \mu_k)^2\right)$	mixture of SEs: $\left(1 + \frac{1}{2\alpha \mathsf{l}^2}\lvert\mathsf{x} - \mathsf{x}'\rvert\right)^{-\alpha}$	rational quadratic $\Gamma_k = \text{invGam}(\mathsf{l})$
	$\sin(\omega_k \mathsf{x})$ & $\cos(\omega_k \mathsf{x})$	$\sum_k \Gamma_k \cos(\omega_k(\mathsf{x} - \mathsf{x}'))$	any stationary covariance (Fourier basis)

Basis function view of Gaussian Processes

$$\mathsf{y} = \sum_k \gamma_k g_k(\mathsf{x}) \qquad \gamma_k \sim \mathcal{N}(0, \Gamma_k)$$

basis function	$g_k(\mathsf{x})$	$\mathsf{K}(\mathsf{x},\mathsf{x}')$	
	$\exp\left(-\frac{1}{l}(\mathsf{x}-\mu_k)^2\right)$	$\exp\left(-\frac{1}{2l}(\mathsf{x}-\mathsf{x}')^2\right)$	squared exponential
	$\exp\left(-\frac{1}{l_k}(\mathsf{x}-\mu_k)^2\right)$	mixture of SEs $\left(1+\frac{1}{2\alpha \mathsf{l}^2}\lvert\mathsf{x}-\mathsf{x}'\rvert\right)^{-\alpha}$	rational quadratic $\Gamma_k = \text{invGam}(\mathsf{l})$
	data = Fourier series with Gaussian coefficients $\sin(\omega_k \mathsf{x})$ & $\cos(\omega_k \mathsf{x})$	covariance even function $\sum_k \Gamma_k \cos(\omega_k(\mathsf{x}-\mathsf{x}'))$	any stationary covariance (Fourier basis)

Basis function view of Gaussian Processes

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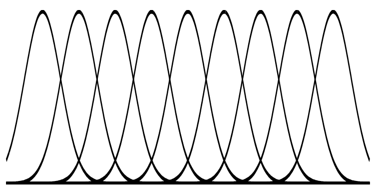
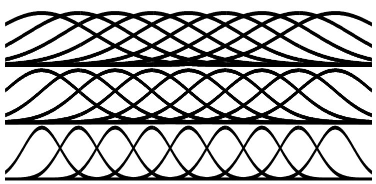
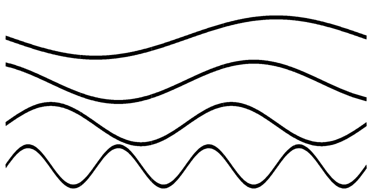
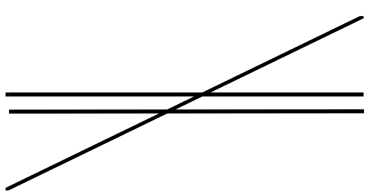
basis function	$g_k(\mathsf{x})$	$\mathsf{K}(\mathsf{x}, \mathsf{x}')$	
	$\exp\left(-\frac{1}{l}(\mathsf{x} - \mu_k)^2\right)$	$\exp\left(-\frac{1}{2l}(\mathsf{x} - \mathsf{x}')^2\right)$	squared exponential
	$\exp\left(-\frac{1}{l_k}(\mathsf{x} - \mu_k)^2\right)$	mixture of SEs ↓ $\left(1 + \frac{1}{2\alpha \mathsf{l}^2}\lvert\mathsf{x} - \mathsf{x}'\rvert\right)^{-\alpha}$	rational quadratic $\Gamma_k = \text{invGam}(\mathsf{l})$
	data = Fourier series with Gaussian coefficients $\sin(\omega_k \mathsf{x})$ & $\cos(\omega_k \mathsf{x})$	covariance even function ↓ $\sum_k \Gamma_k \cos(\omega_k(\mathsf{x} - \mathsf{x}'))$	any stationary covariance (Fourier basis)
	x and 1	$\Gamma_1 \mathsf{x}\mathsf{x}' + \Gamma_2$	linear regression

Basis function view of Gaussian Processes

Basis function view useful because:

- **connects to classical approaches**

- **basis function generative model is useful theoretically**
  - Q: are draws from a SE continuous and differentiable?
  - A: they are (almost surely, almost everywhere) as the basis functions are

- **thinking about the basis function generative model is useful practically**
  - Q: how could I construct a periodic covariance?
  - A: use periodic basis functions with Gaussian weights

Making new covariance functions from old

(positive) linear combinations
of covariance functions

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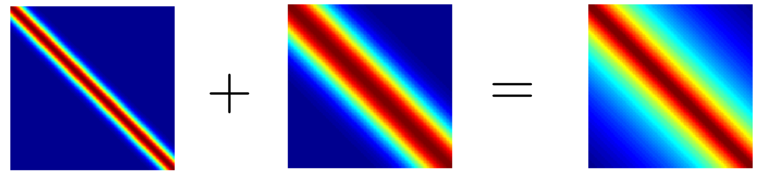

e.g. scale mixture of SE = rational quadratic

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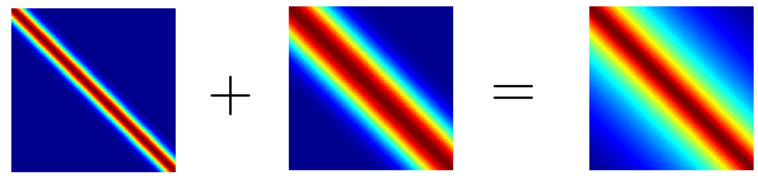

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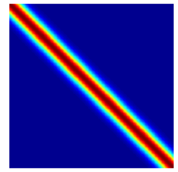
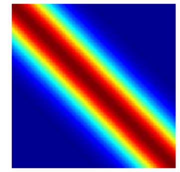
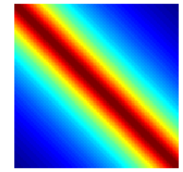
 $+$  $=$ 

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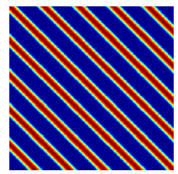
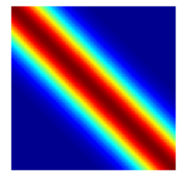
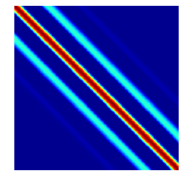
 $\times$  $=$ 

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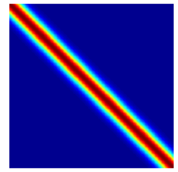
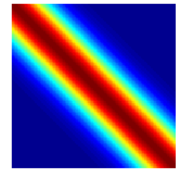
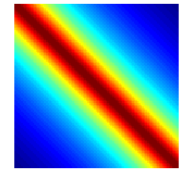
 +  = 

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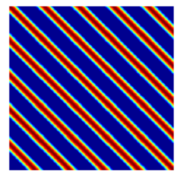
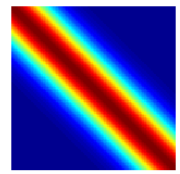
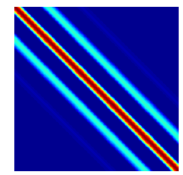
 $\times$  = 

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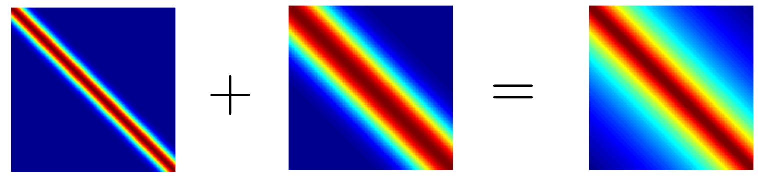

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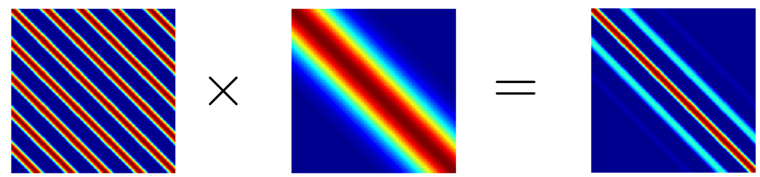

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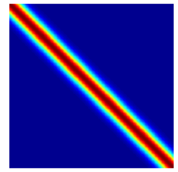
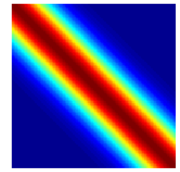
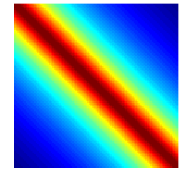
 $+$  $=$ 

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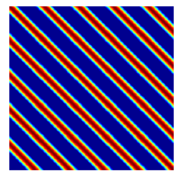
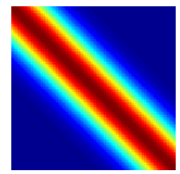
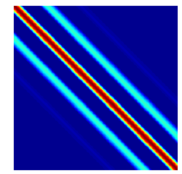
 $\times$  $=$ 

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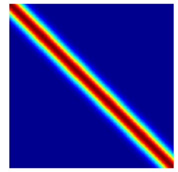
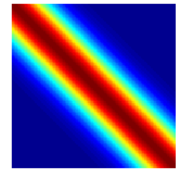
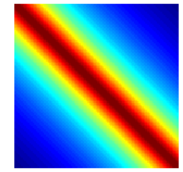
(positive) linear combinations of covariance functions

 $+$  $=$ 

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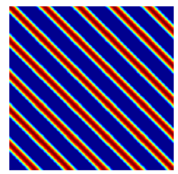
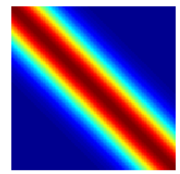
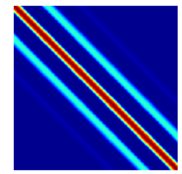
 $\times$  $=$ 

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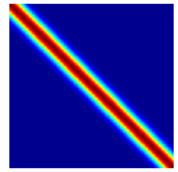
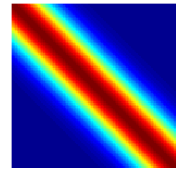
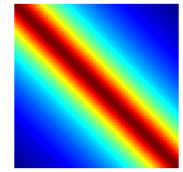
 $+$  $=$ 

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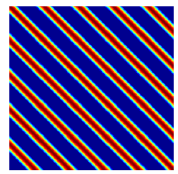
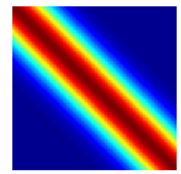
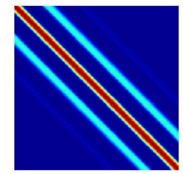
 $\times$  $=$ 

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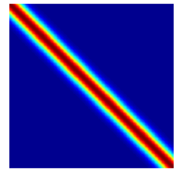
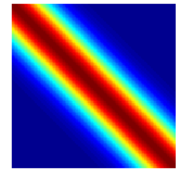
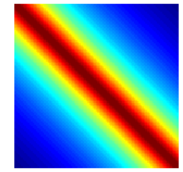
 $+$  $=$ 

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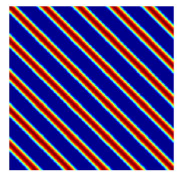
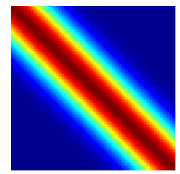
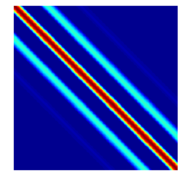
 $\times$  $=$ 

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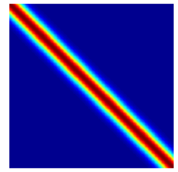
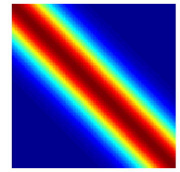
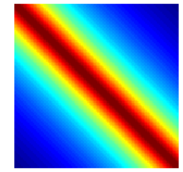
 $+$  $=$ 

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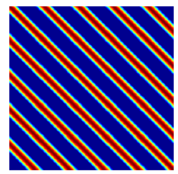
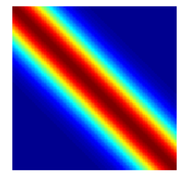
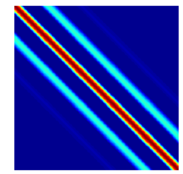
 $\times$  $=$ 

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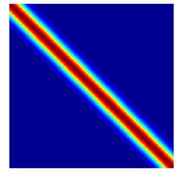
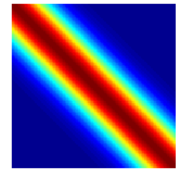
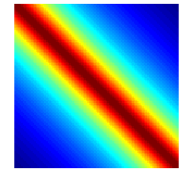
 $+$  $=$ 

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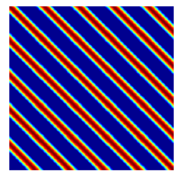
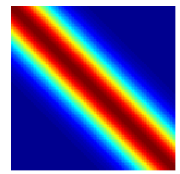
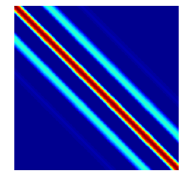
 $\times$  $=$ 

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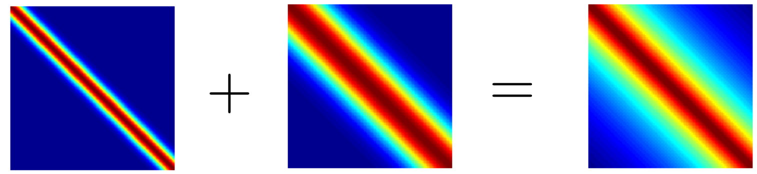

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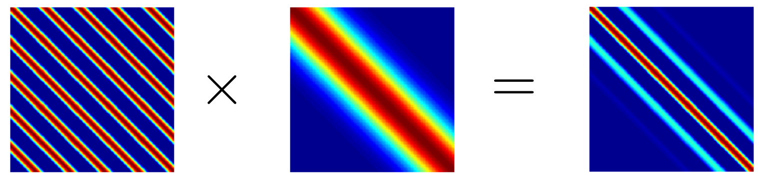


e.g. periodic × SE = $\cos(\omega \Delta \mathsf{x}) \exp(-\frac{1}{2l^2} \Delta \mathsf{x}^2)$

derivative of GP = GP

$$\frac{\mathrm{d}}{\mathrm{dx}} y(x) = \frac{\mathrm{d}}{\mathrm{dx}} \sum_{k=1}^{\infty} \gamma_k g_k(x) = \sum_{k=1}^{\infty} \gamma_k \frac{\mathrm{d}}{\mathrm{dx}} g_k(x)$$

new basis: $g'_k(x) = \frac{\mathrm{d}}{\mathrm{dx}} g_k(x)$

new covariance: $K'(x, x') = \frac{\mathrm{d}}{\mathrm{dx}} \frac{\mathrm{d}}{\mathrm{dx}'} K(x, x')$

integral of GP = GP

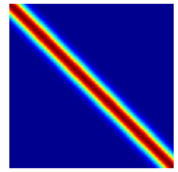
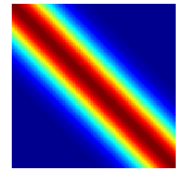
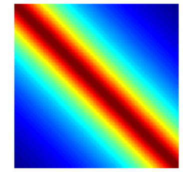
$$\int \mathrm{dx}\, y(x) = \sum_{k=1}^{\infty} \gamma_k \int \mathrm{dx}\, g_k(x)$$

new basis: $g'_k(x) = \int \mathrm{dx}\, g_k(x)$

new covariance: $K'(x, x') = \int \int \mathrm{dx dx}'\, K(x, x')$

Making new covariance functions from old

(positive) linear combinations of covariance functions

 $+$  $=$ 

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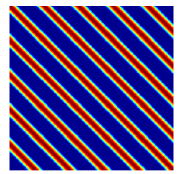
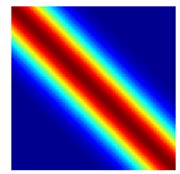
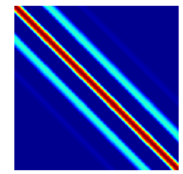
 $\times$  $=$ 

e.g. periodic × SE = $\cos(\omega \Delta \mathrm{x}) \exp(-\frac{1}{2l^2} \Delta \mathrm{x}^2)$

derivative of GP = GP

integral of GP = GP

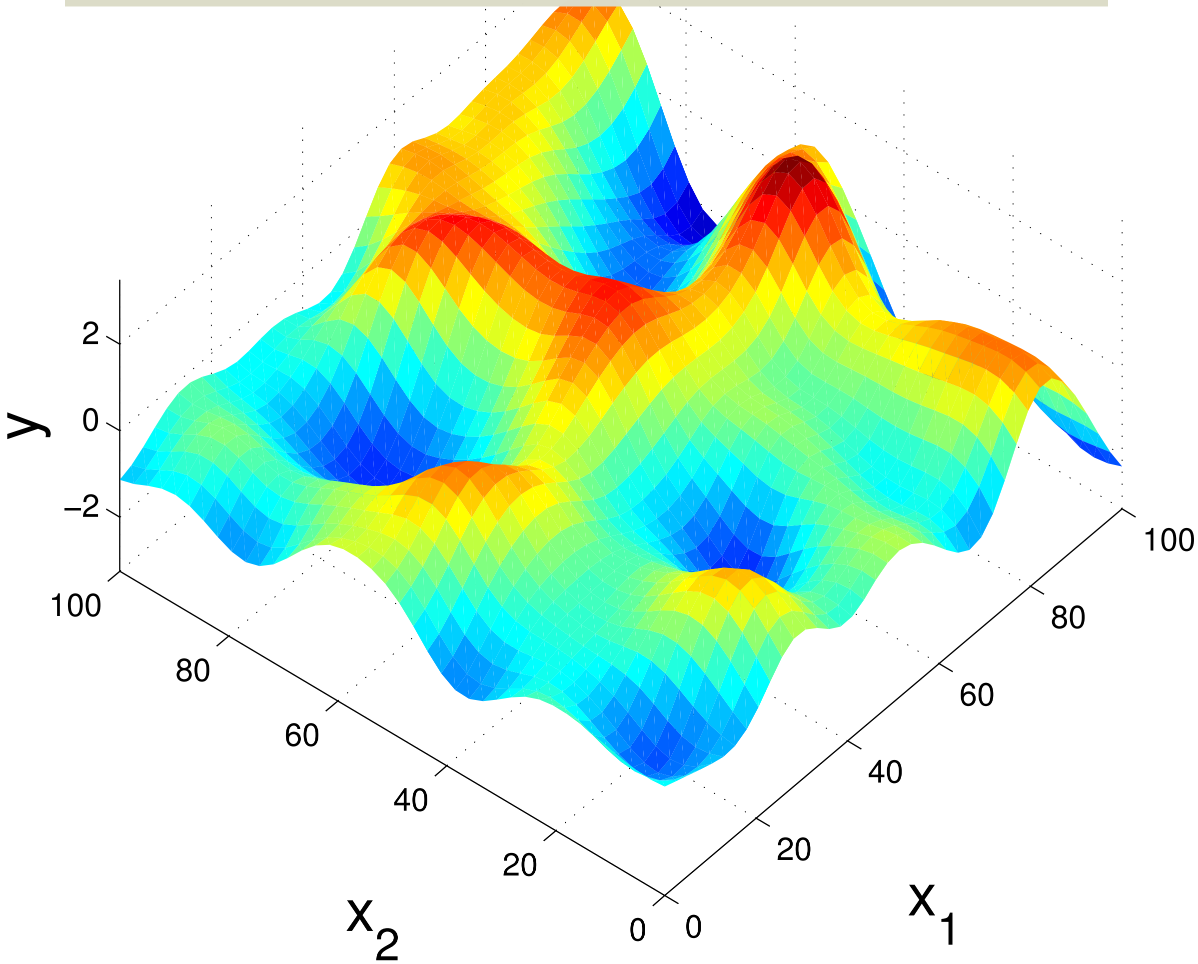
filtering a GP = GP

$\mathrm{V}(\mathrm{x}) \otimes \mathrm{y}(\mathrm{x})$

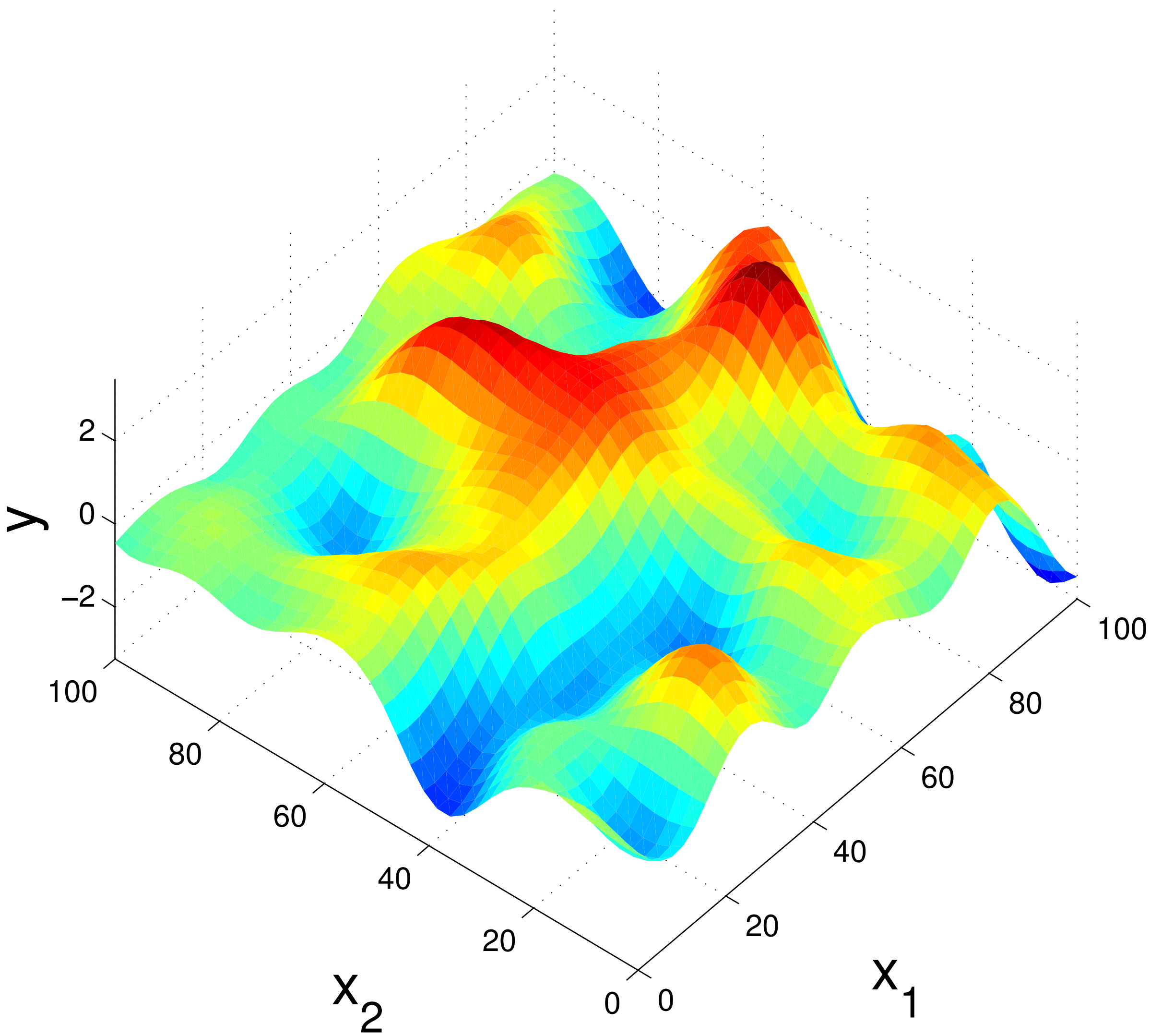
$\mathrm{K}'(\mathrm{x}, \mathrm{x}') = \mathrm{V}(\mathrm{x}) \otimes \mathrm{K}(\mathrm{x}, \mathrm{x}') \otimes \mathrm{V}(\mathrm{x}')$

Higher dimensional input spaces

$$K(\mathbf{x},\mathbf{x}') = \sigma^2 \exp\left(-\frac{1}{2l_1^2}(\mathsf{x}_1 - \mathsf{x}_1')^2 - \frac{1}{2l_2^2}(\mathsf{x}_2 - \mathsf{x}_2')^2\right)$$



Higher dimensional input spaces



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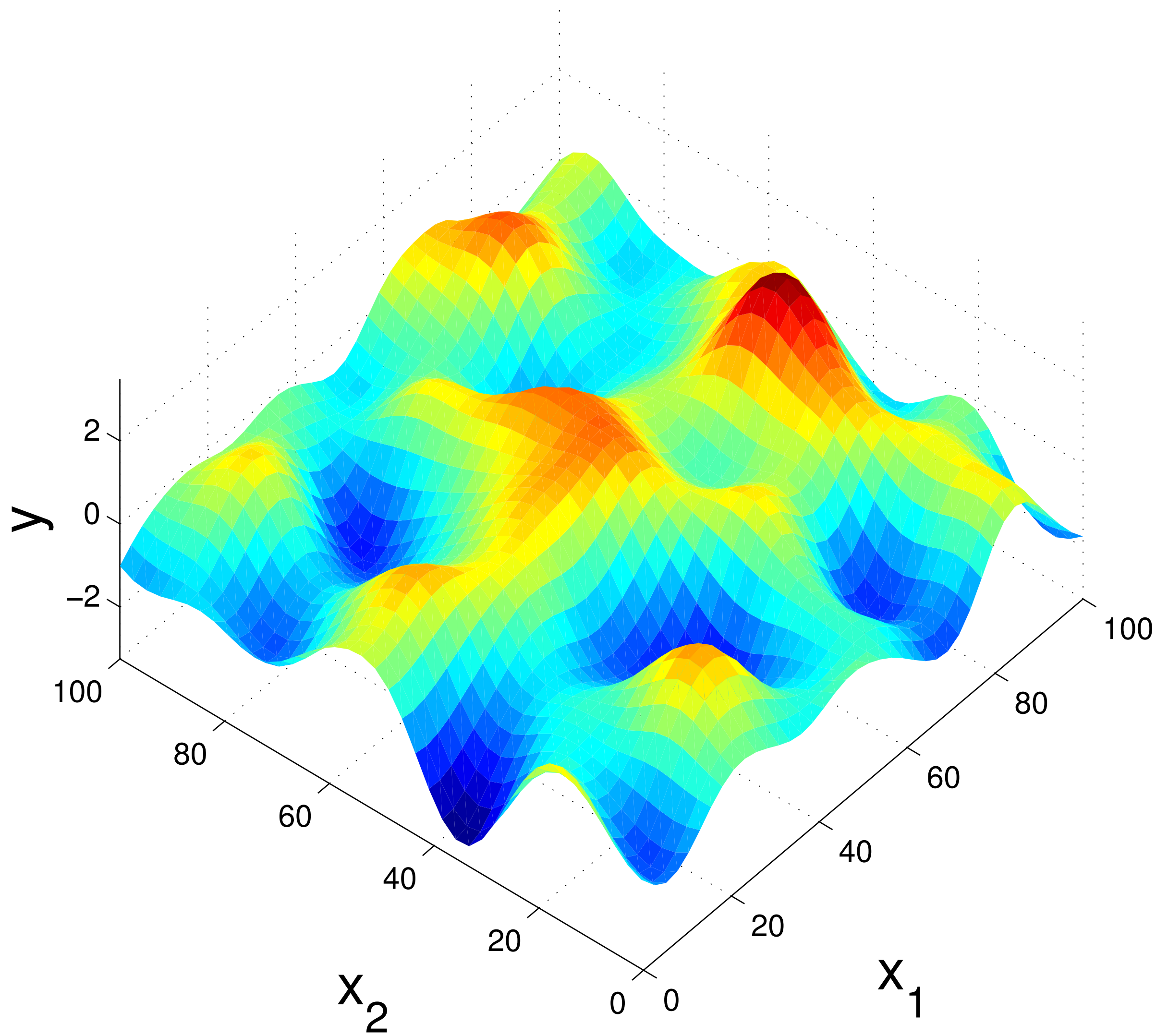
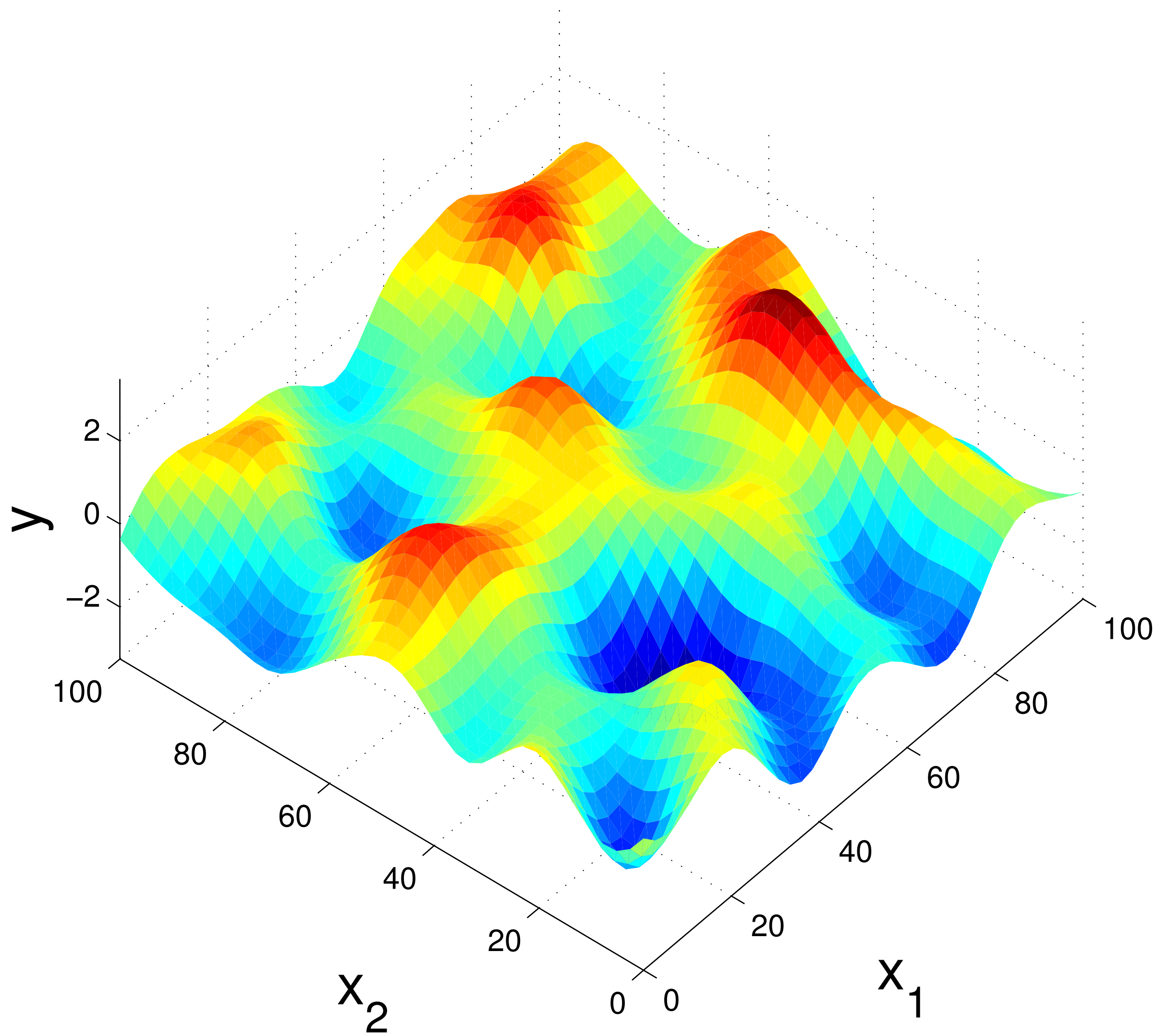


Higher dimensional input spaces



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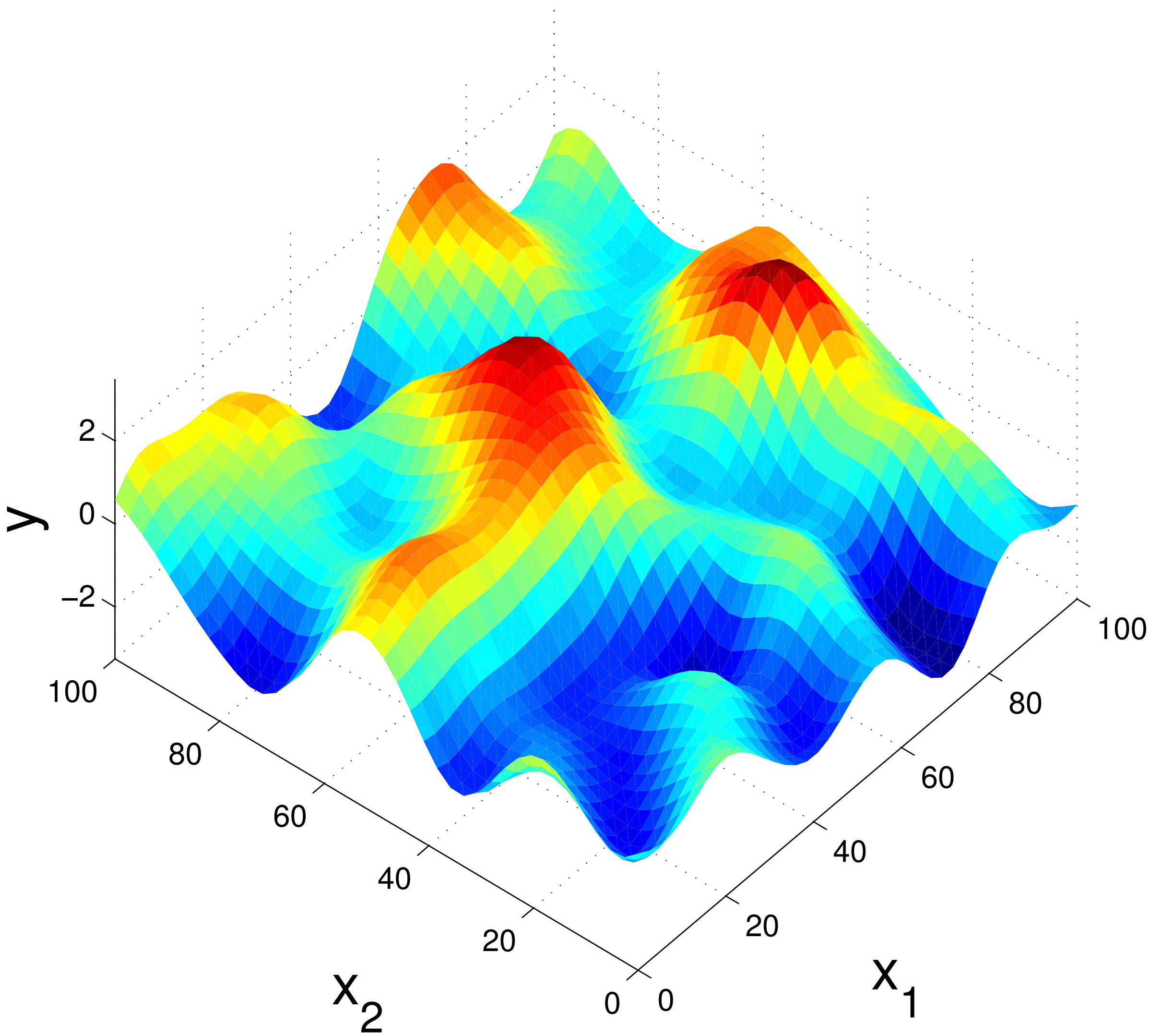

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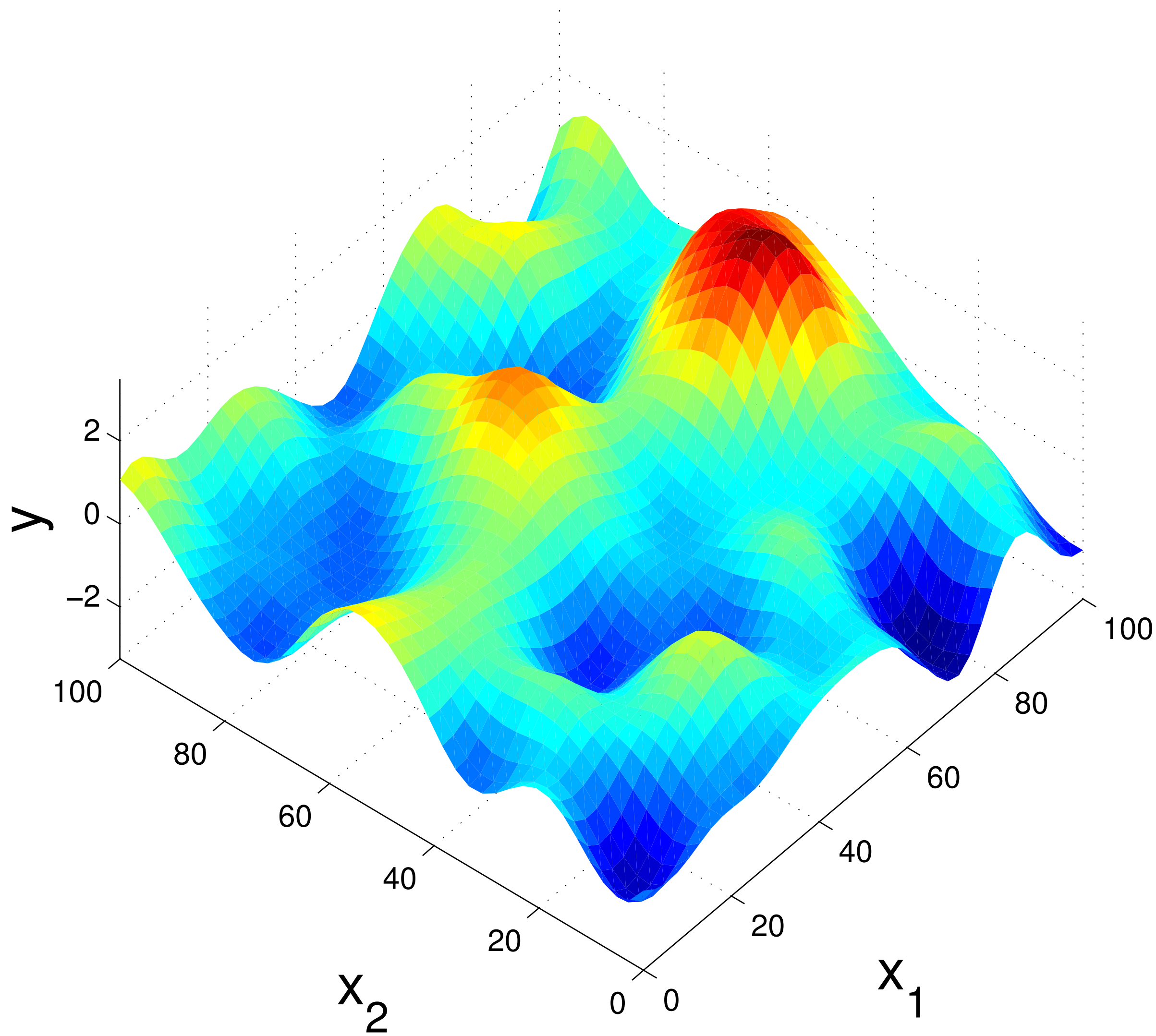

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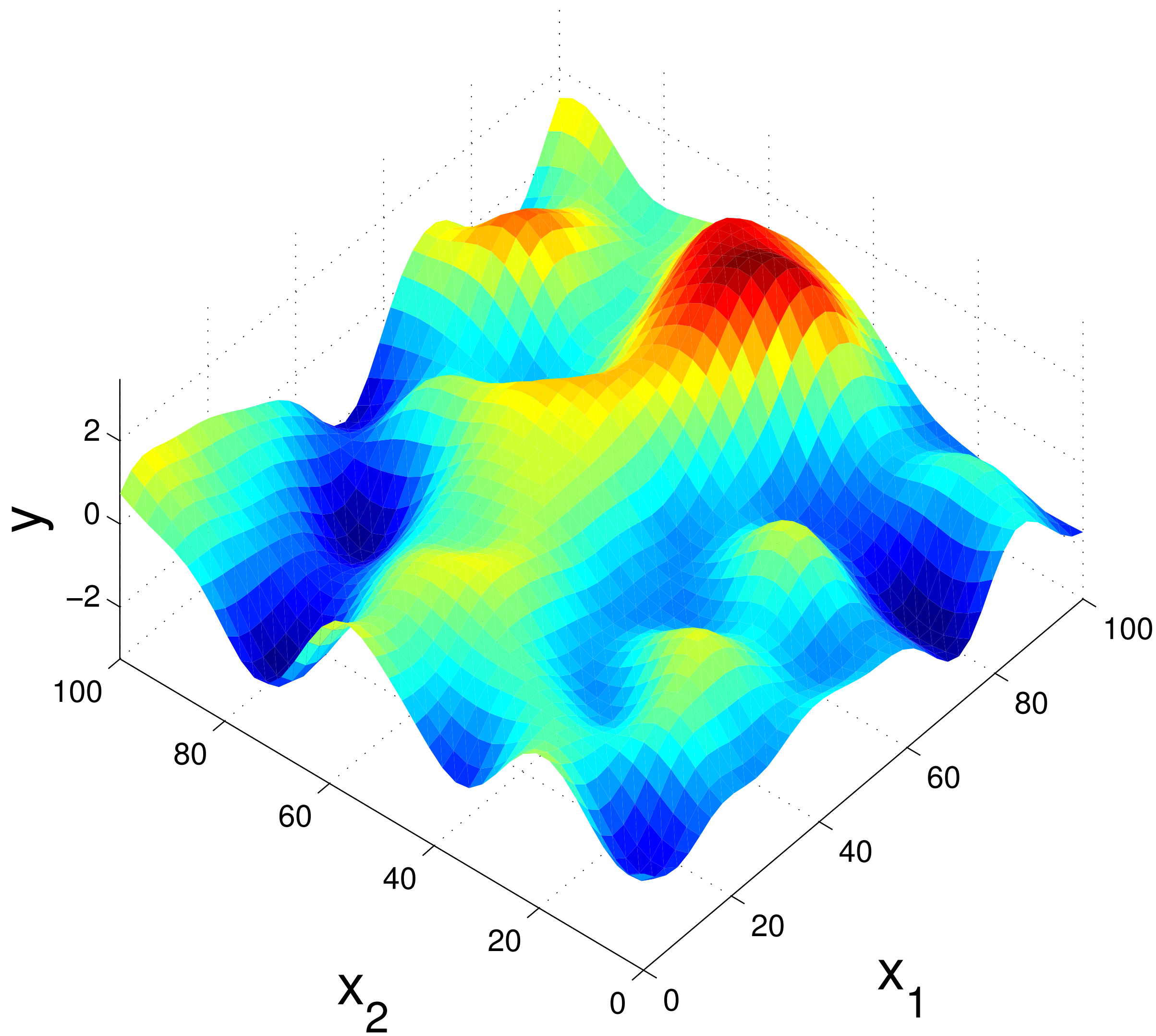

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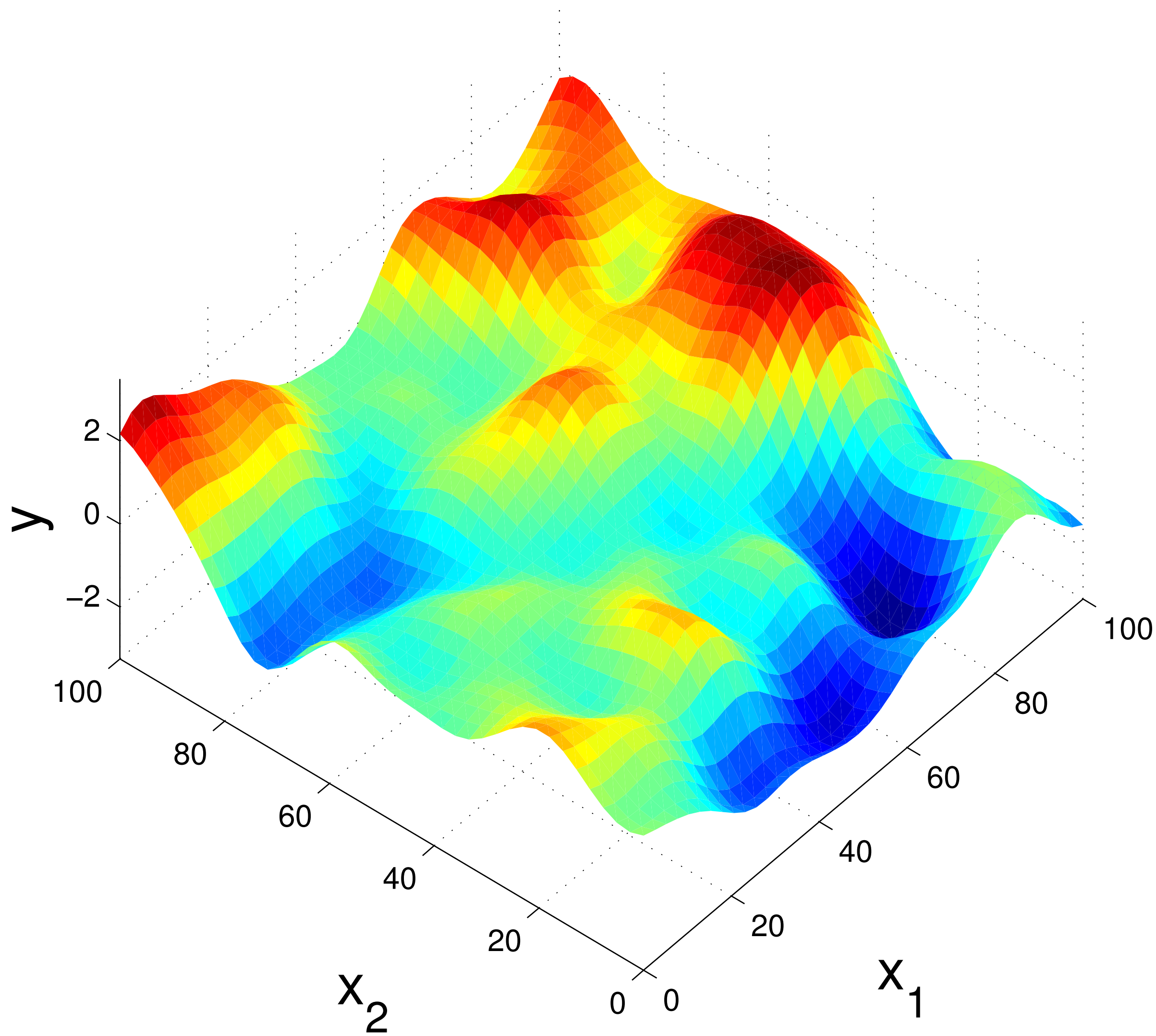

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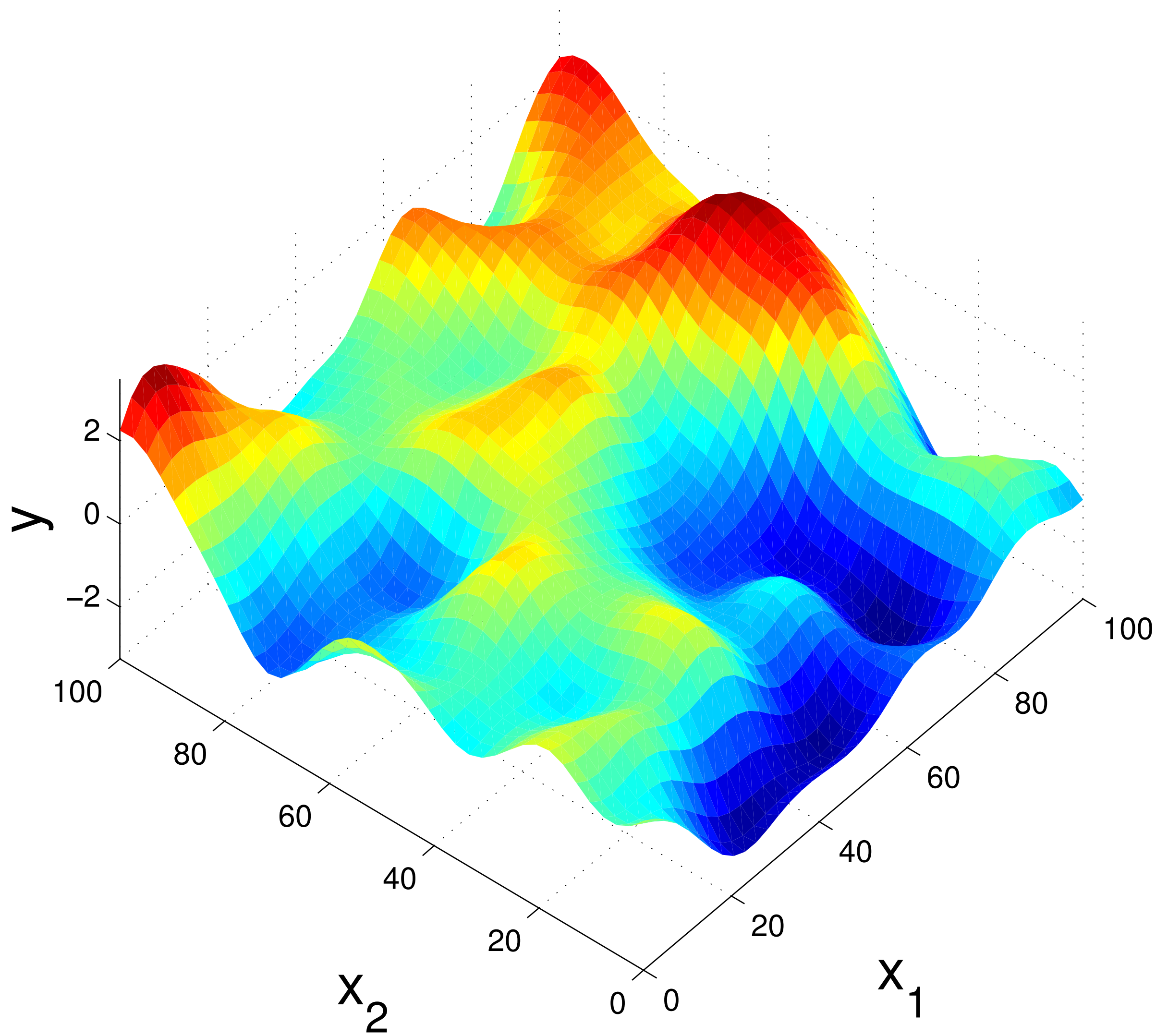

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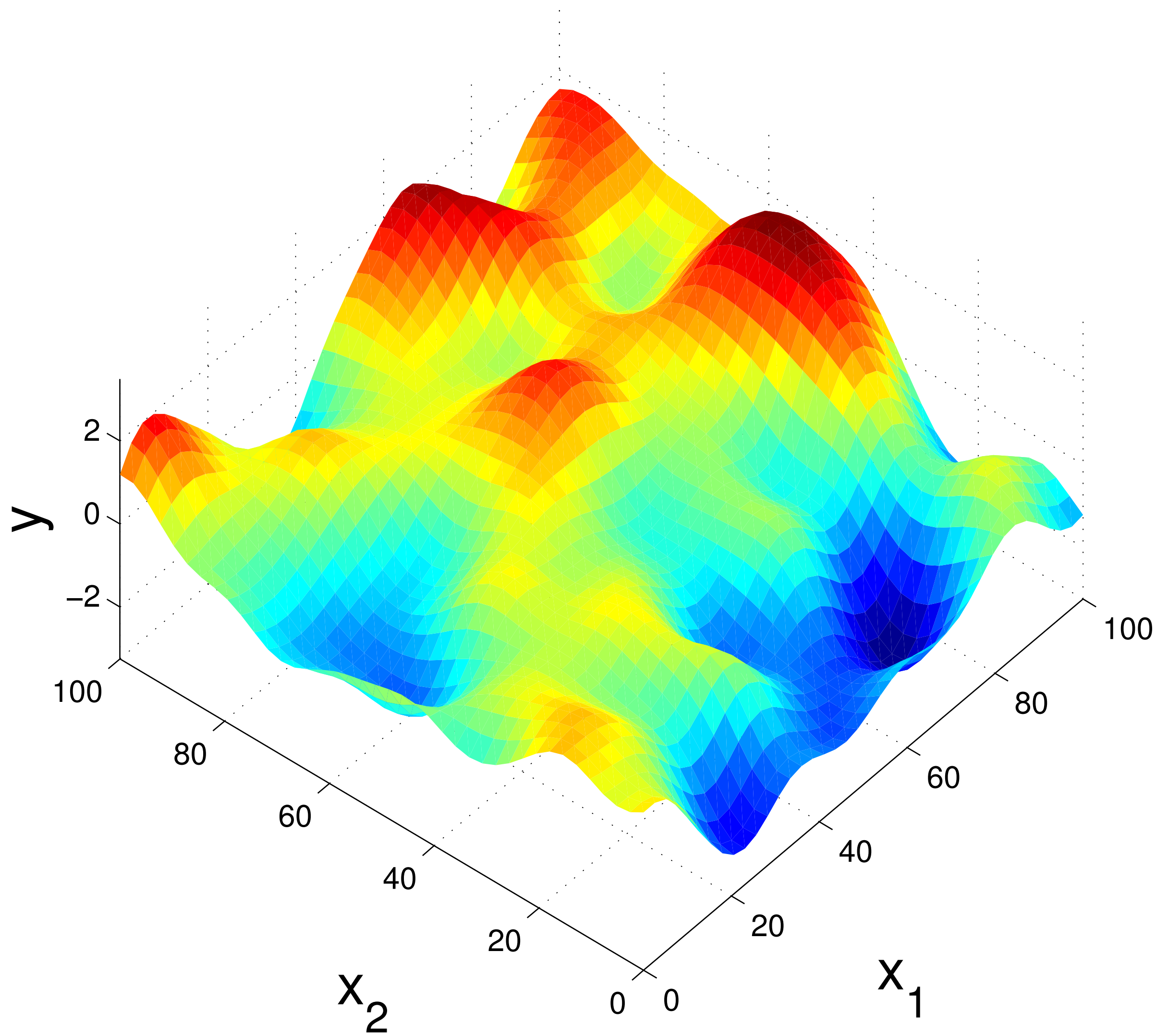

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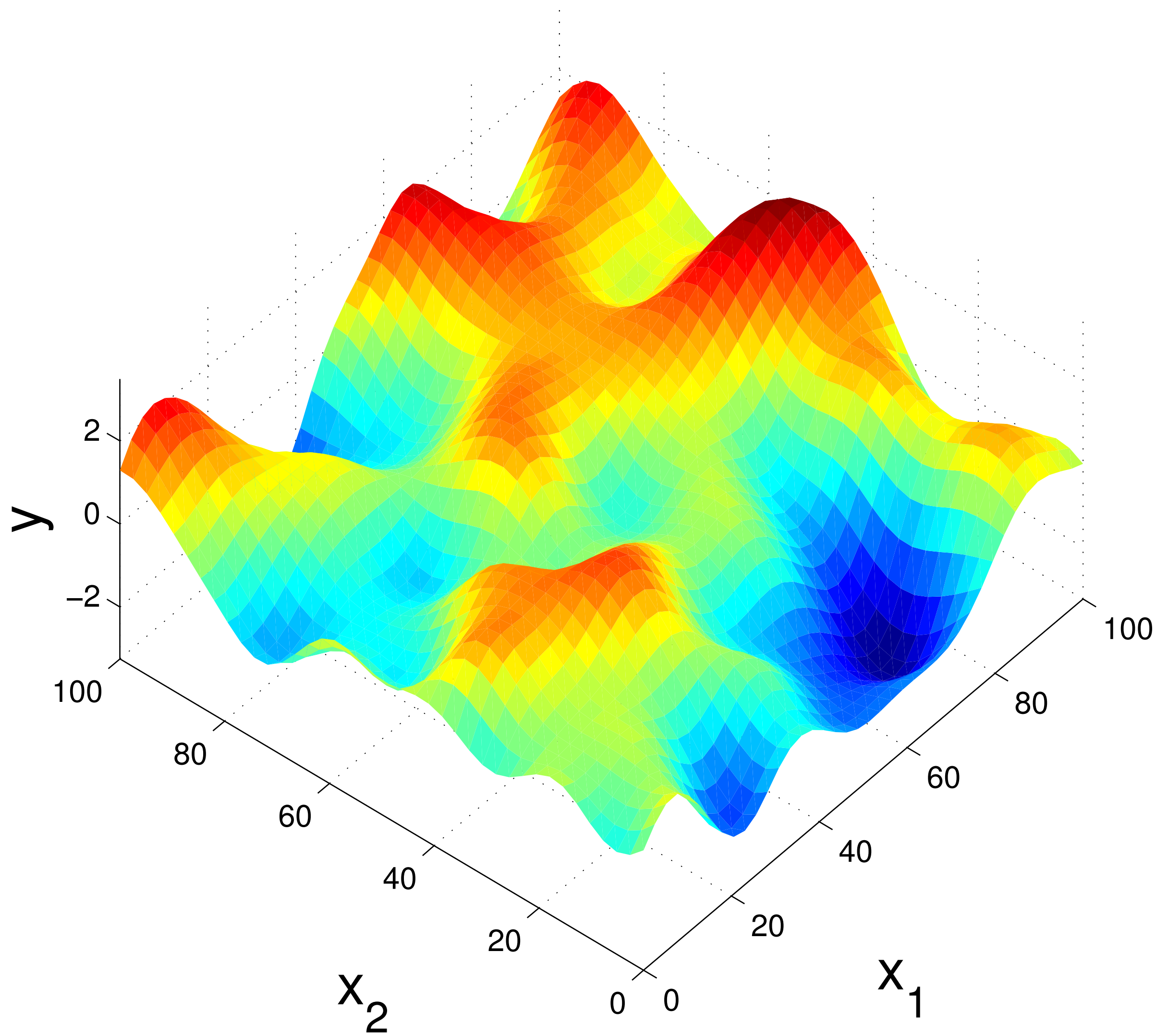

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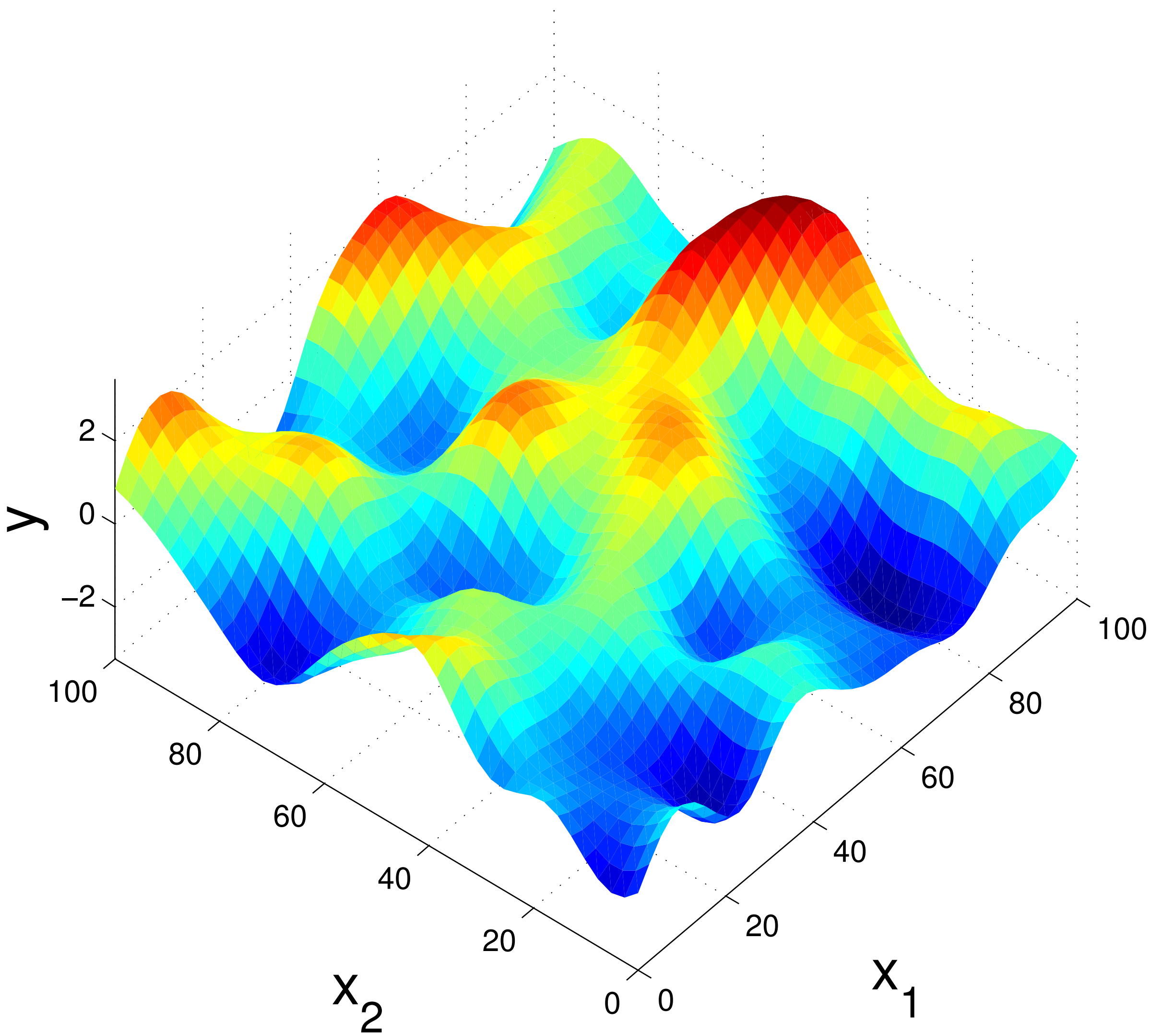

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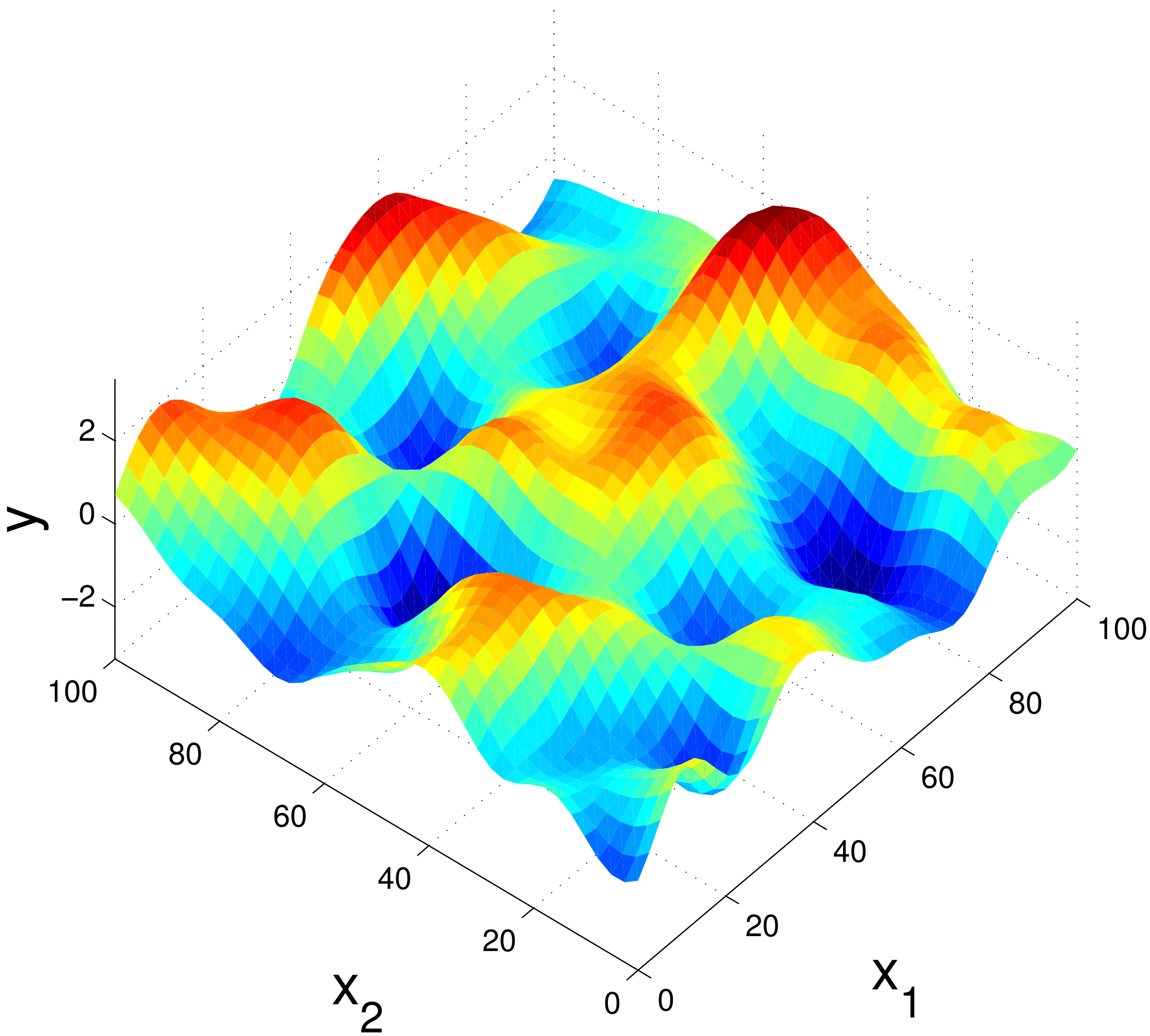

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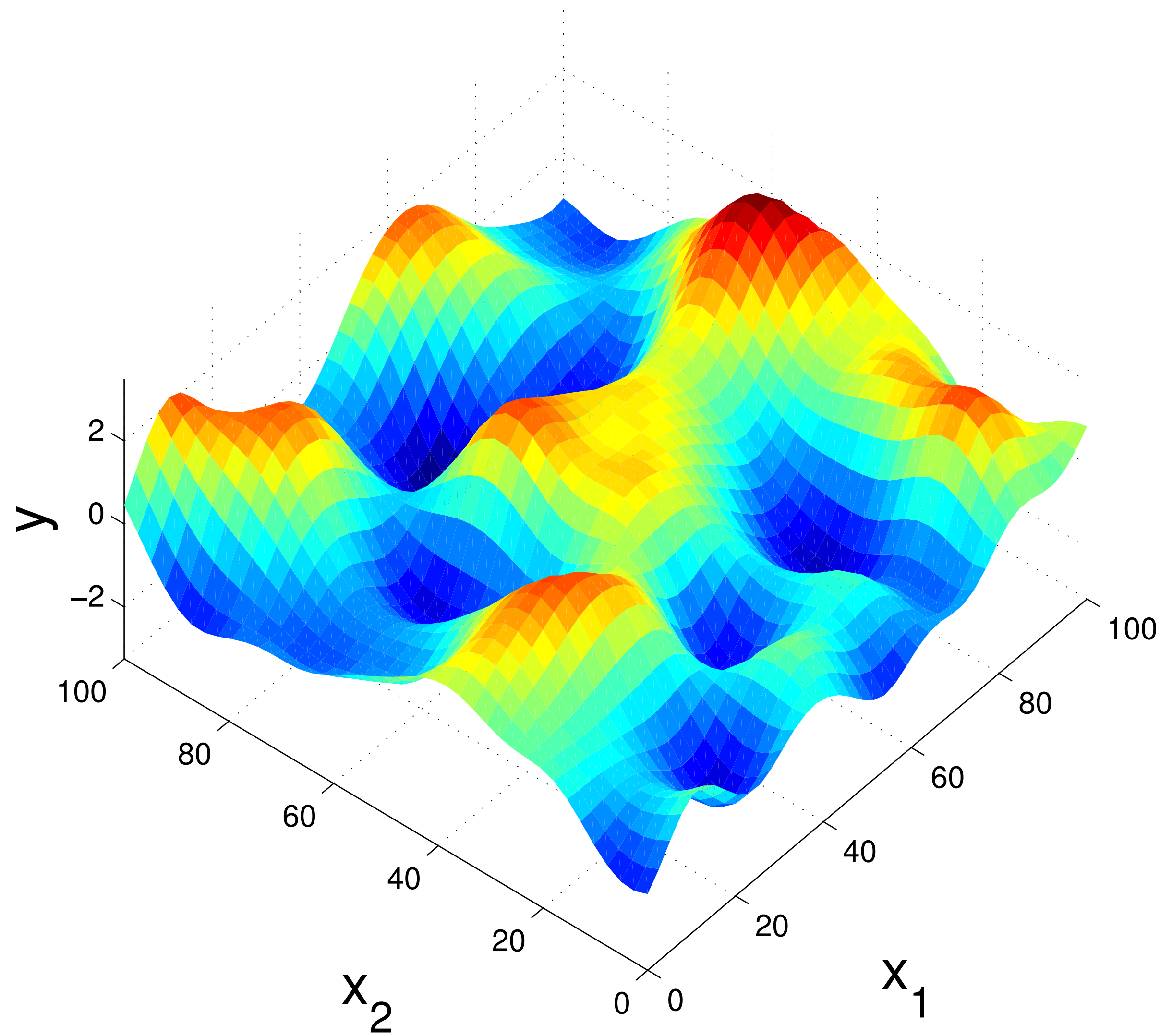

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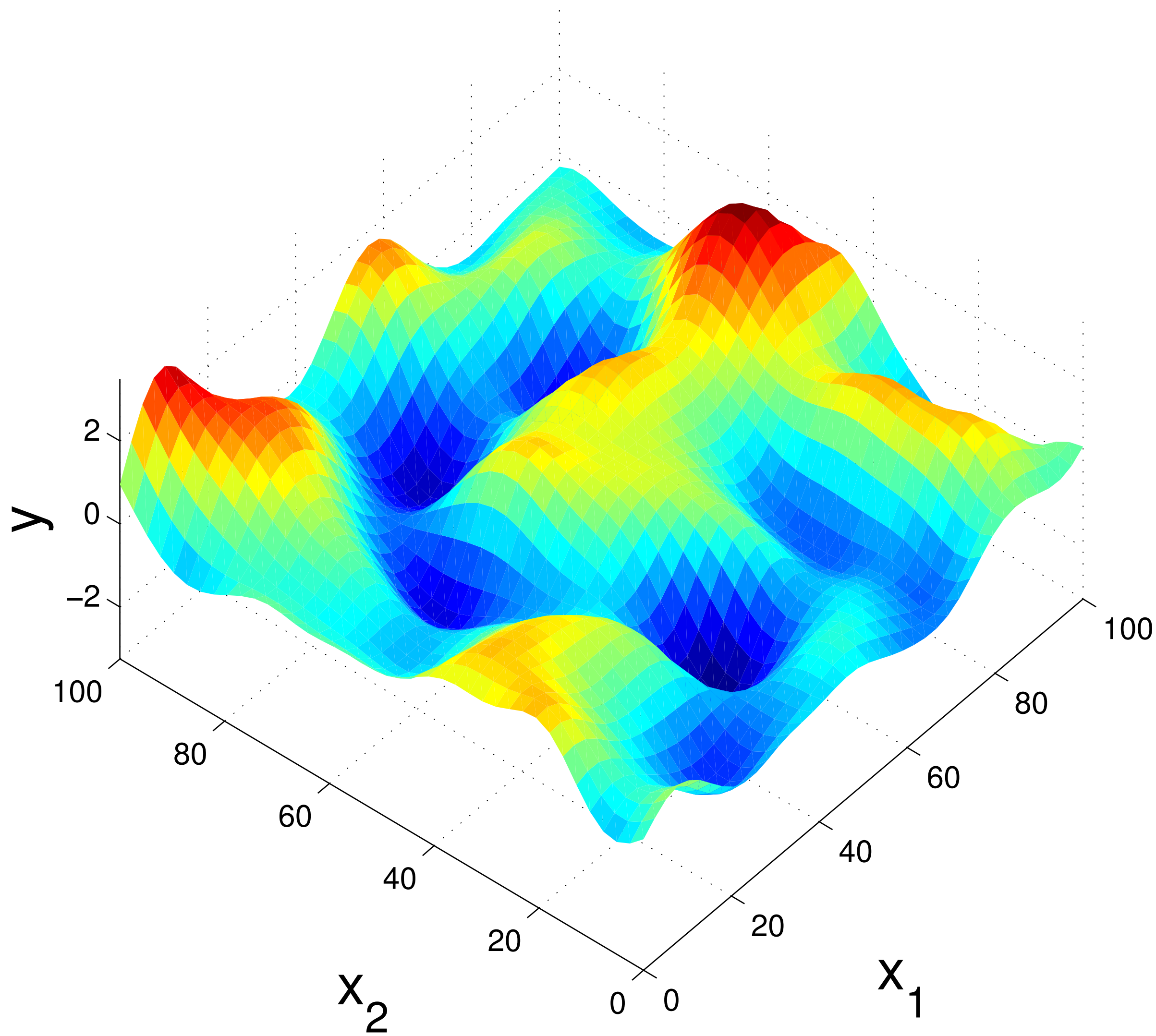


Computational cost

- prediction task
  - train on N points
  - test on M points

- prediction equations

$$\mu_M = \mathsf{K}_{MN}\mathsf{K}_{NN}^{-1}\mathsf{y}_N$$

$$\Sigma_{MM} = \mathsf{K}_{MM} - \mathsf{K}_{MN}\mathsf{K}_{NN}^{-1}\mathsf{K}_{NM}$$

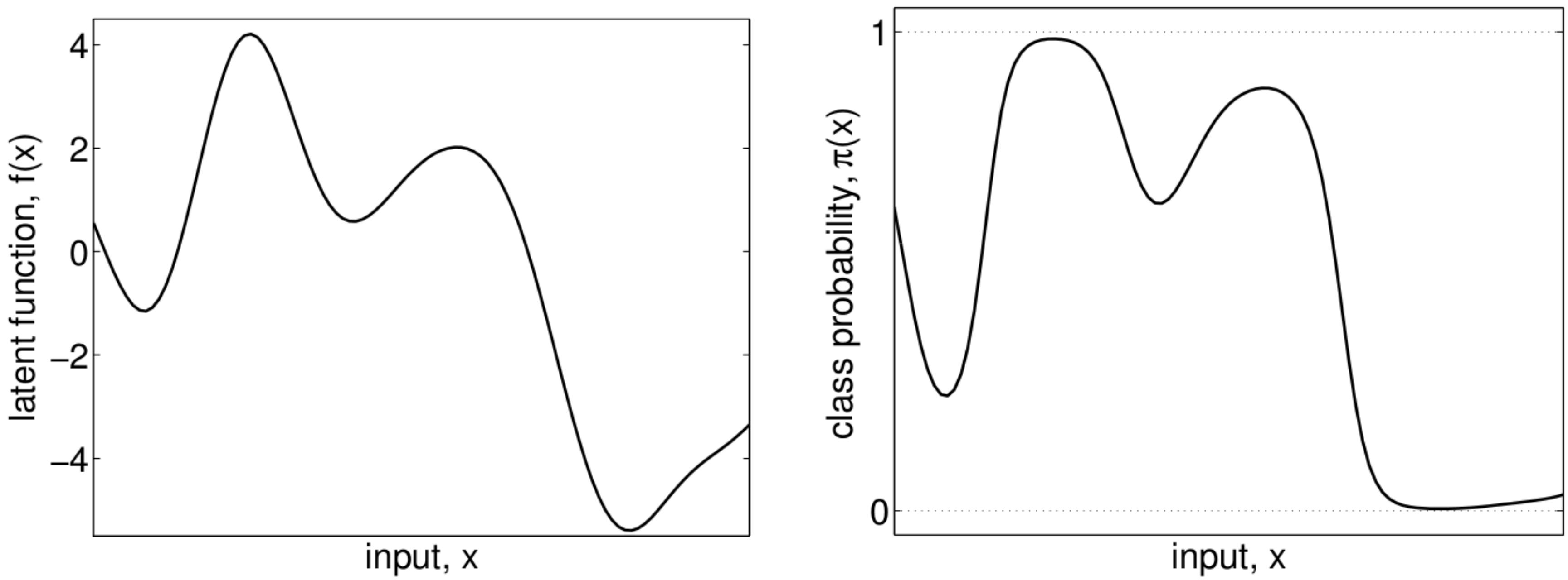
- Full cost $\mathcal{O}((N+M)^3)$ just variances $\mathcal{O}(N^2M)$

- Without special structure, computation is limited to $\mathcal{O}(1000)$ variables

$\Rightarrow$ Computational cost is a major limitation of GPs

Beyond regression: classification

Idea: points near each other in the input space tend to have similar labels



Class probability related to latent function:

$$\pi(\mathsf{x}) = p(\mathsf{y} = 1 | f(\mathsf{x})) = \Phi(f(\mathsf{x}))$$

Logistic link function a typical choice: $\Phi(f) = \frac{1}{1+\exp(-f)}$

Likelihood non-Gaussian $\Rightarrow$ prediction analytically intractable $\Rightarrow$ require approximations

Beyond regression

GPs useful when ever a prior over functions is required

- dimensionality reduction
- time-series models (Kalman filter)
- clustering
- active learning
- reinforcement learning
- ...

Summary

- Gaussian process: **collection of random variables, any finite subset of which are Gaussian distributed**
- Easy to use
  - Predictions correspond to models with infinite numbers of parameters
- GPs have many standard methods as special cases
- Problem: N^3 complexity
  - approximation methods for $N > 2000$ or special covariance functions
- **Great reference**: Rasmussen & Williams `www.gaussianprocess.org/`