GAUSSIAN PROCESS FOR REGRESSION

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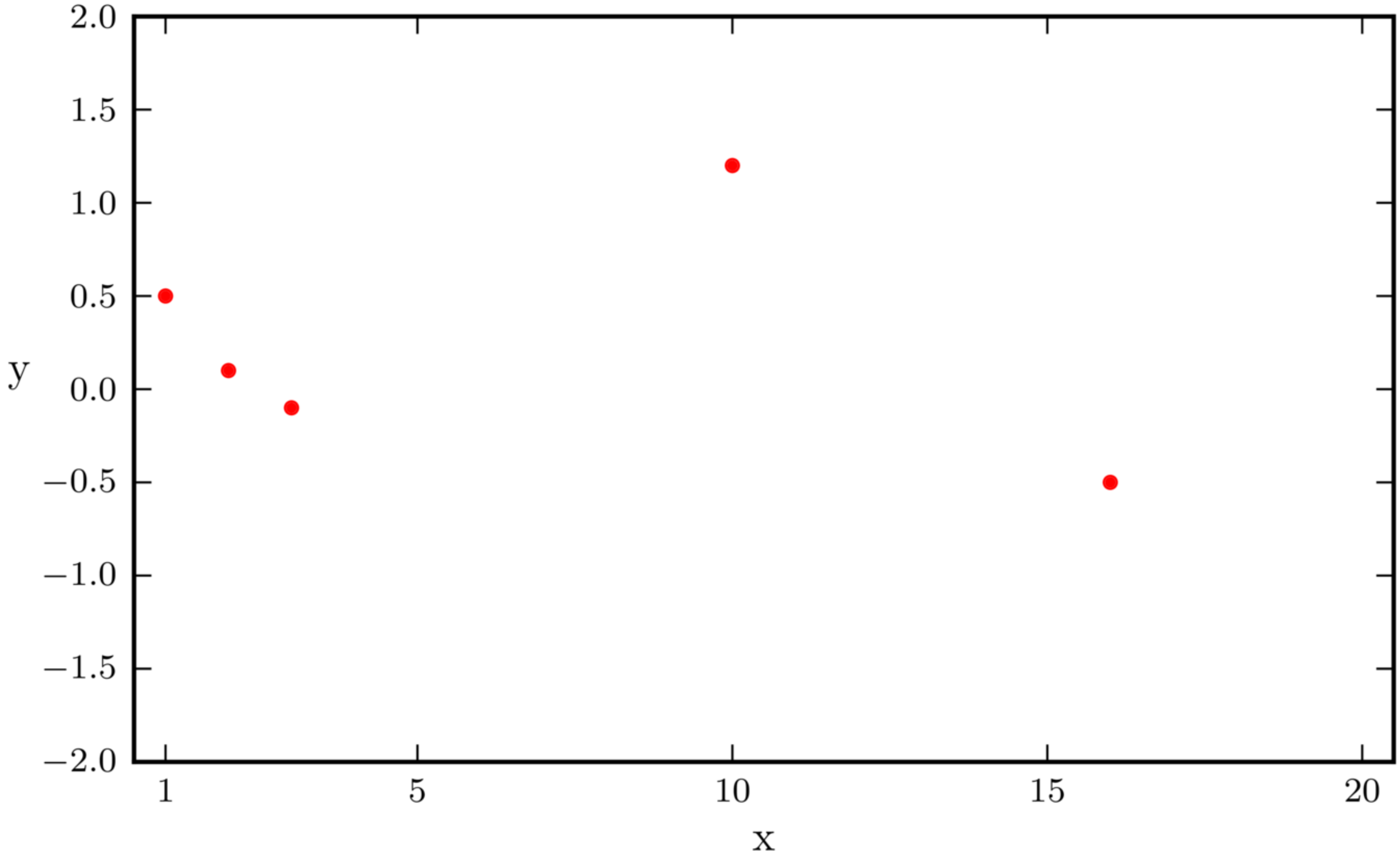
Majority of slides were borrowed from Dr. Richard E. Turner

Gaussian Processes

- Gaussian processes (GPs) provide a principled, practical, probabilistic approach to learning in kernel machines.
- The “kernel” plays the role of covariance matrix in GPs.
- Can be used to learn nonlinear regression and classification problems.
- GPs are nonparametric models!
- We will start with the nonlinear regression problems.

- Note: Gaussian Process Regression (GPR) is not Linear Regression or Ridge Regression. GPR is a nonlinear model. It is more close to support vector regressions than to linear regressions.

Nonlinear Regression Problem



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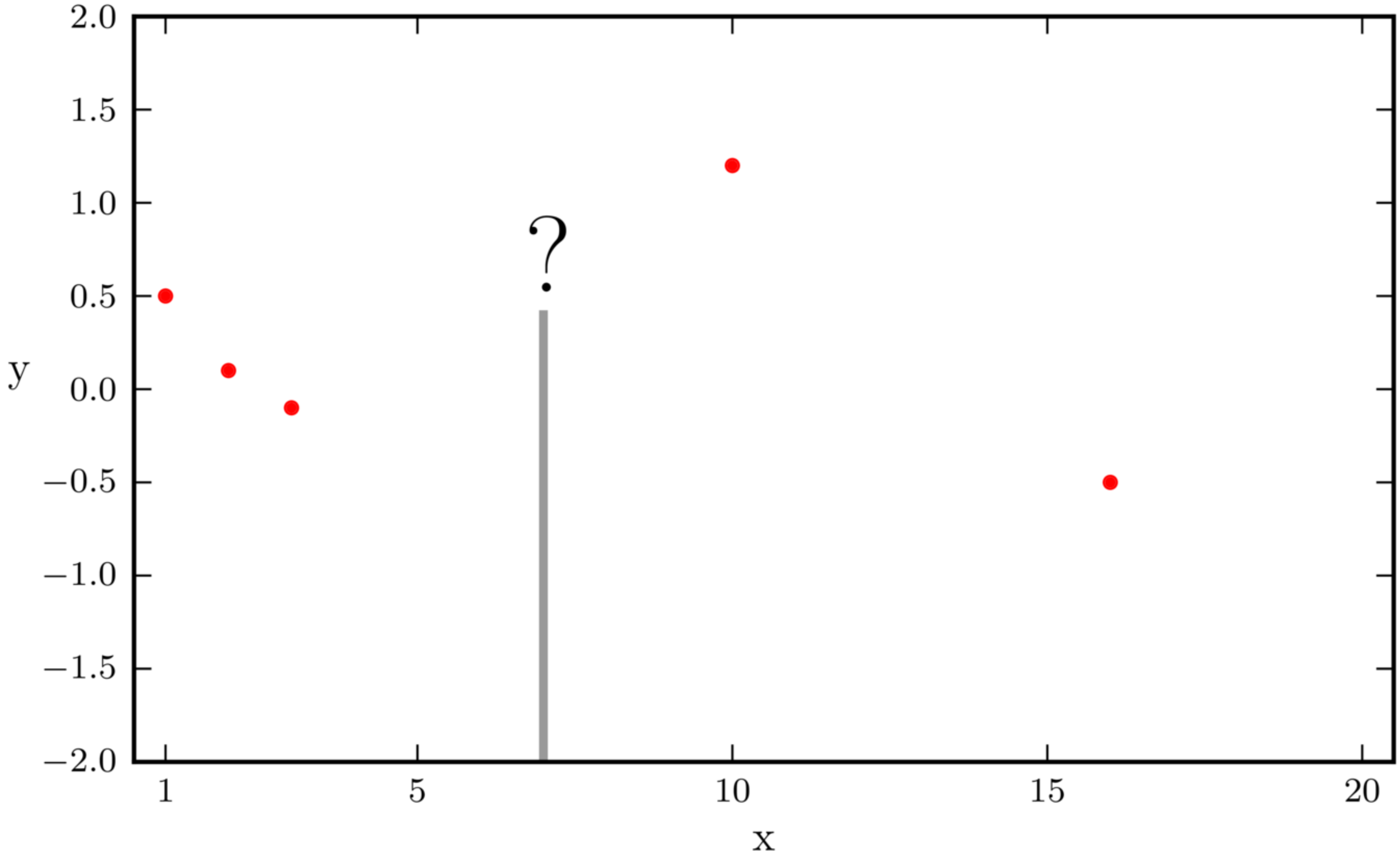

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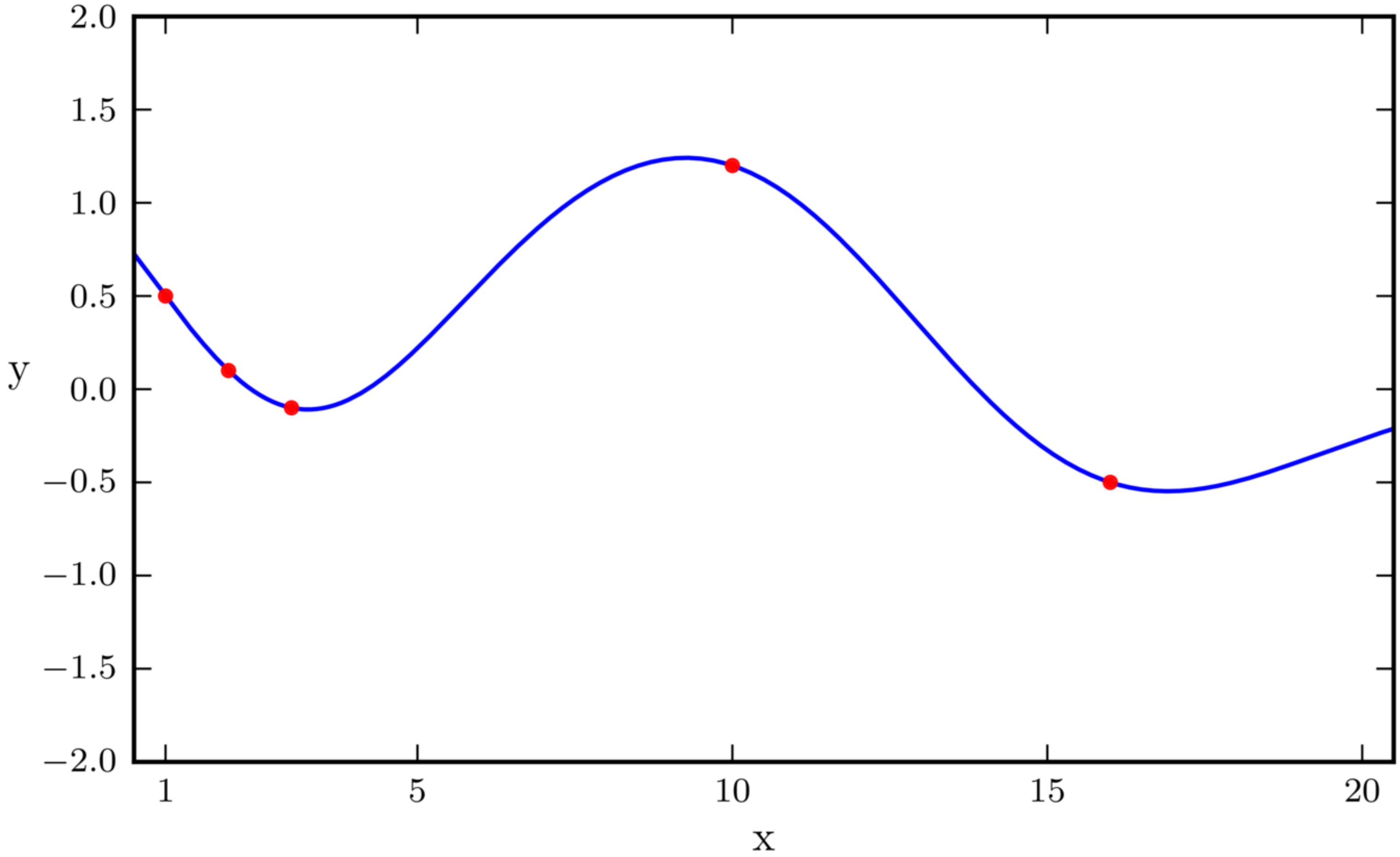

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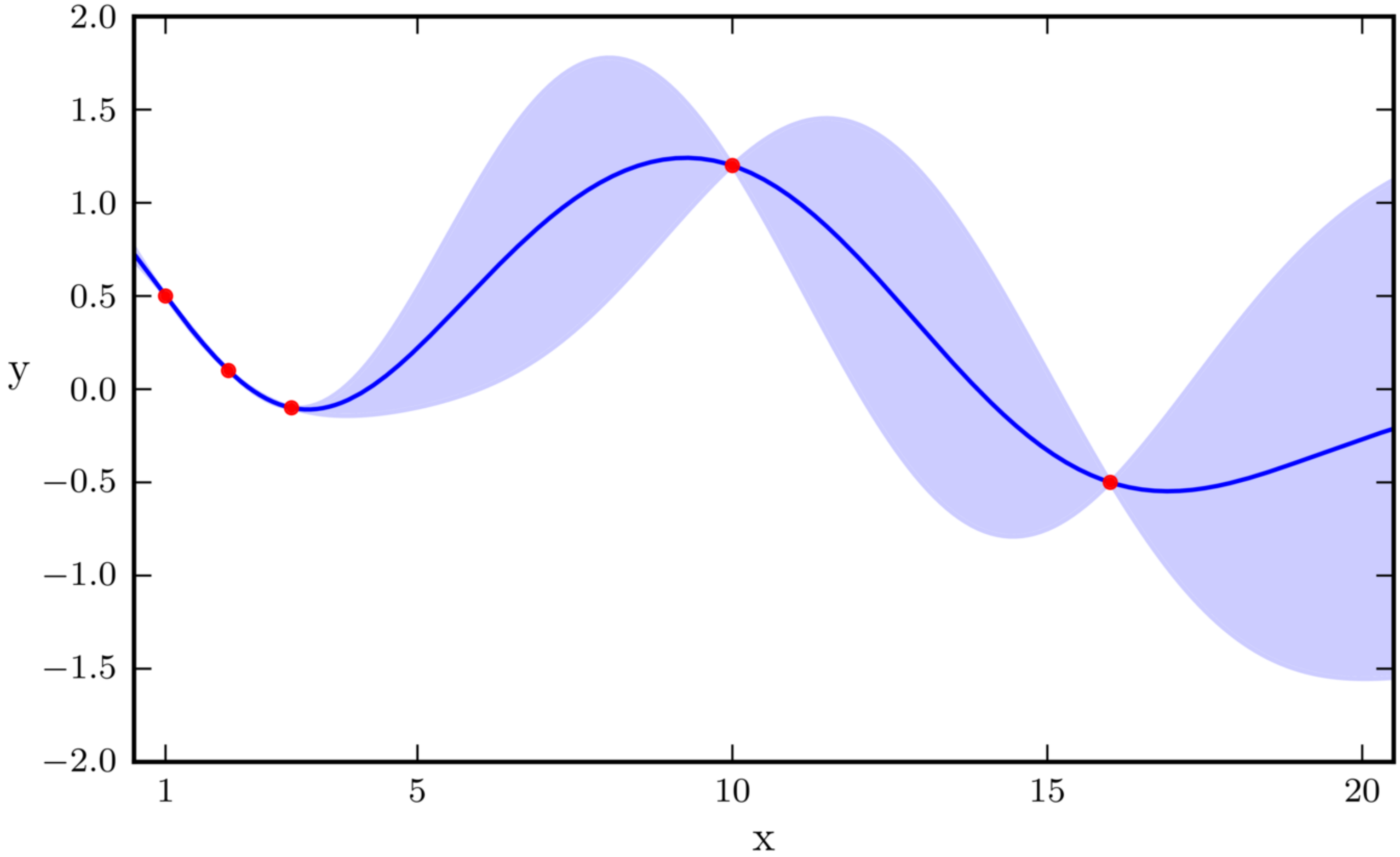

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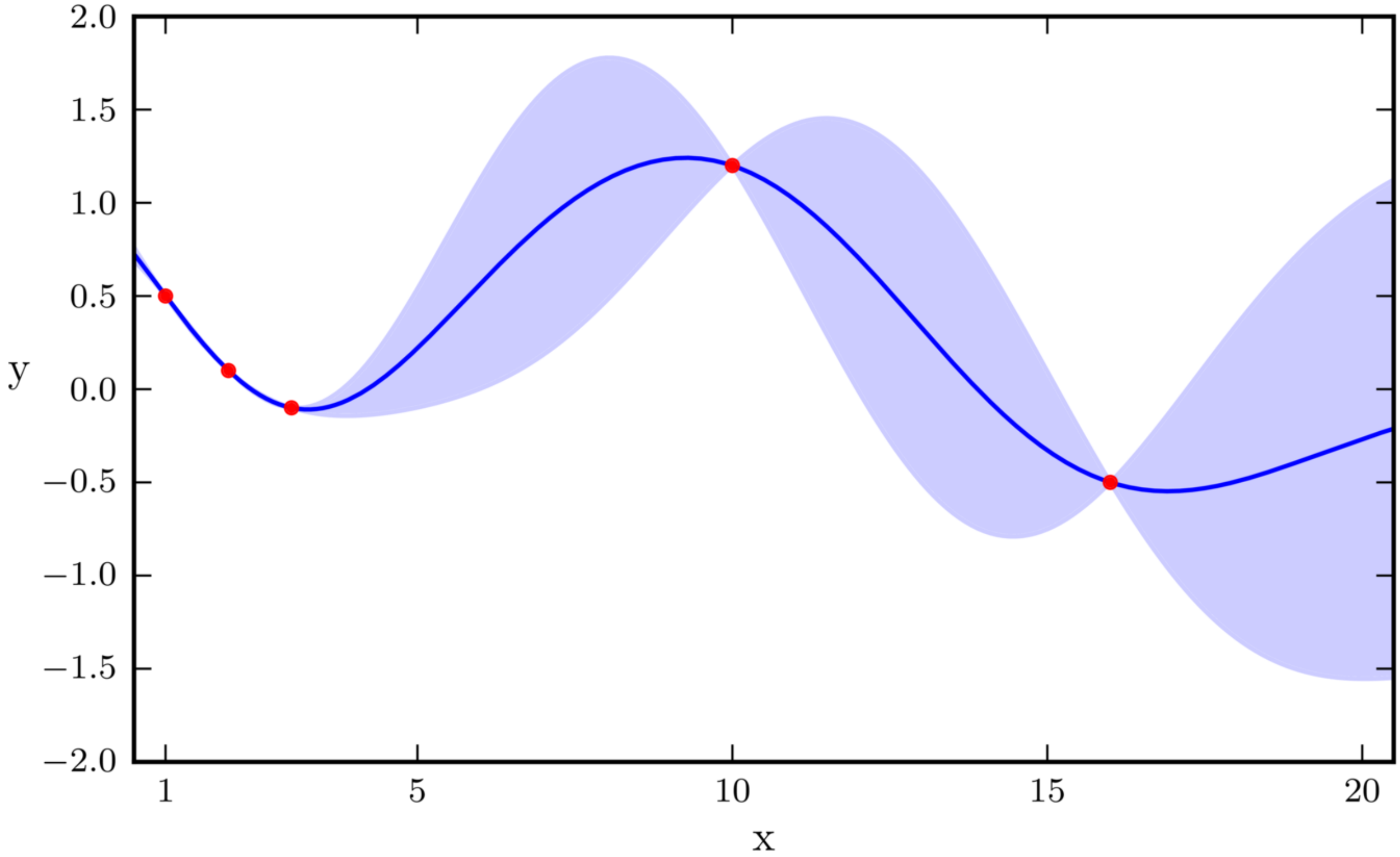
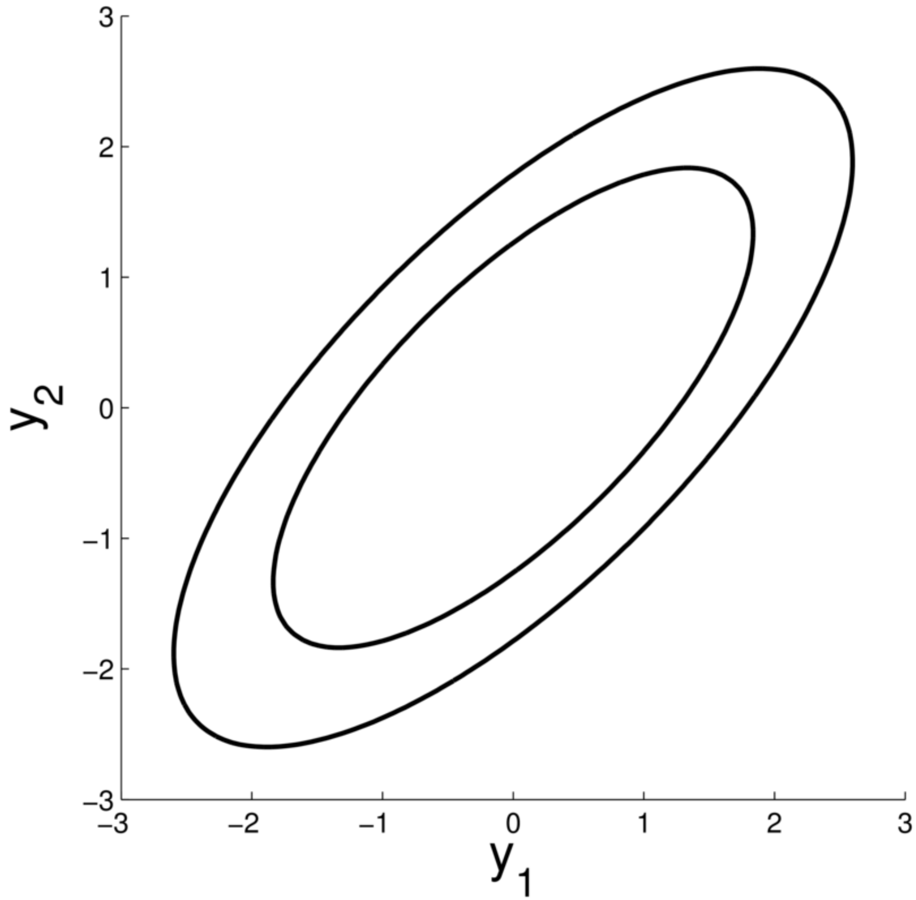


Can we do this with a plain old Gaussian?

Gaussian Distribution

$$f_{\mathbf{X}}(x_1,\ldots,x_k) = \frac{\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)}{\sqrt{(2\pi)^k|\boldsymbol{\Sigma}|}}$$

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



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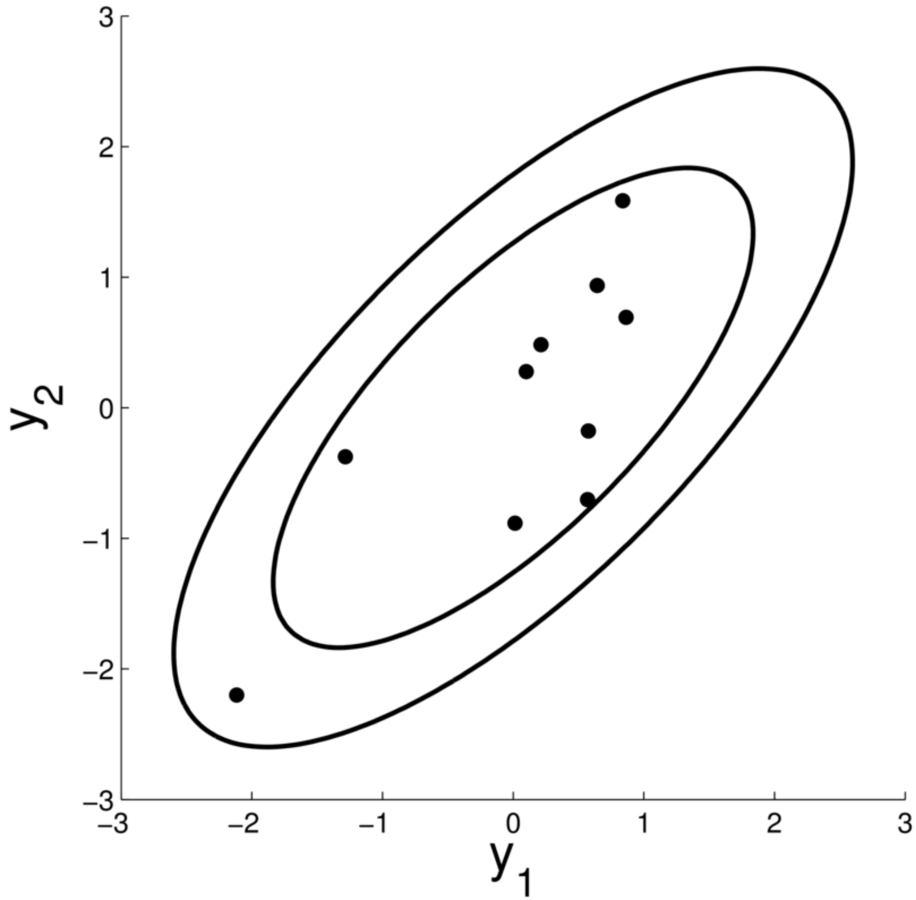

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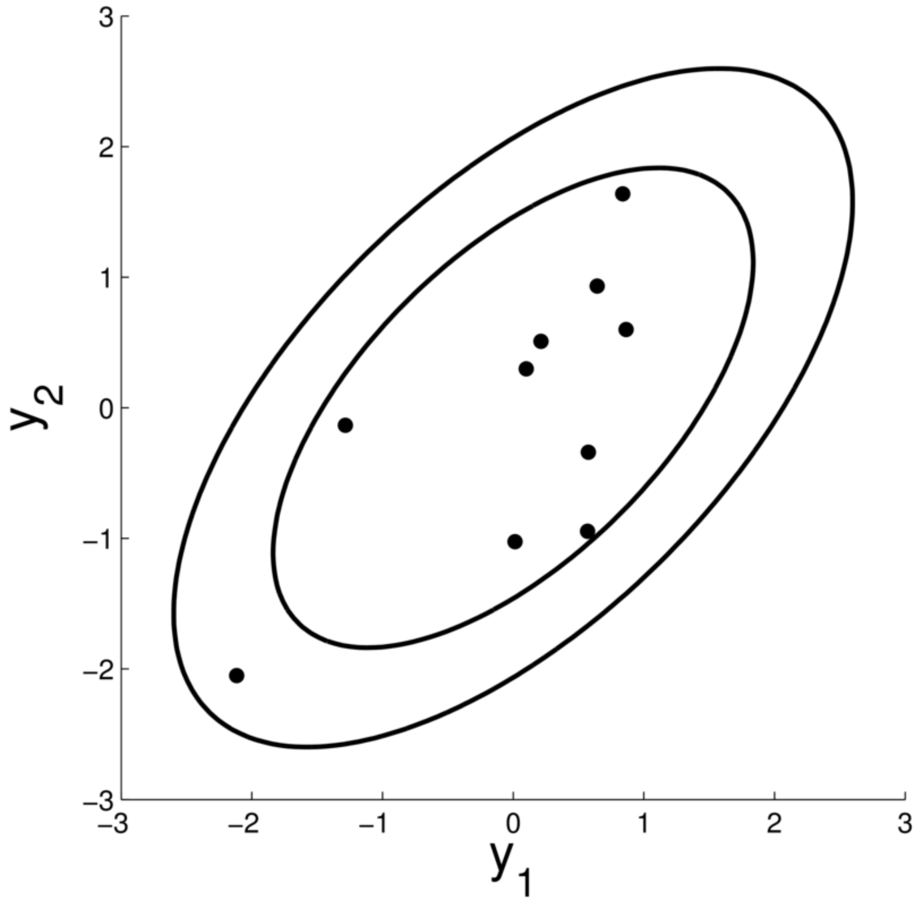
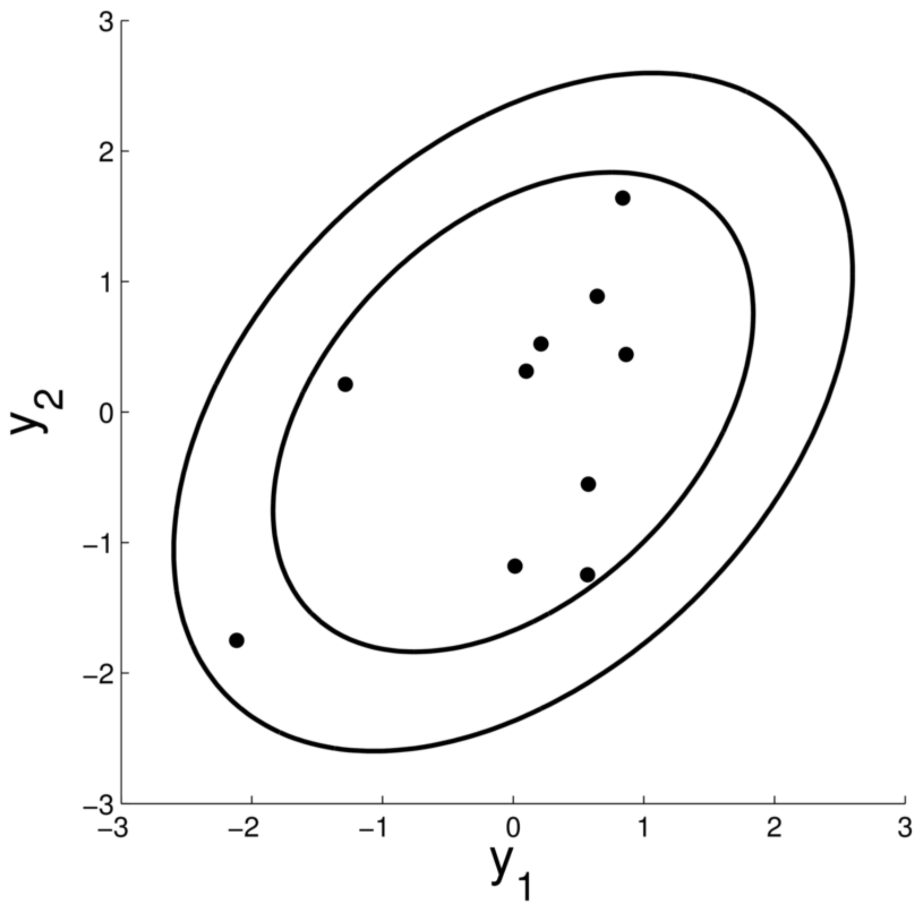
$$p(\mathbf{y}|\Sigma) \propto \exp\left(-\frac{1}{2}\mathbf{y}^{\top}\Sigma^{-1}\mathbf{y}\right) \qquad \Sigma = \begin{bmatrix} 1 & .6 \\ .6 & 1 \end{bmatrix}$$



Gaussian Distribution

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



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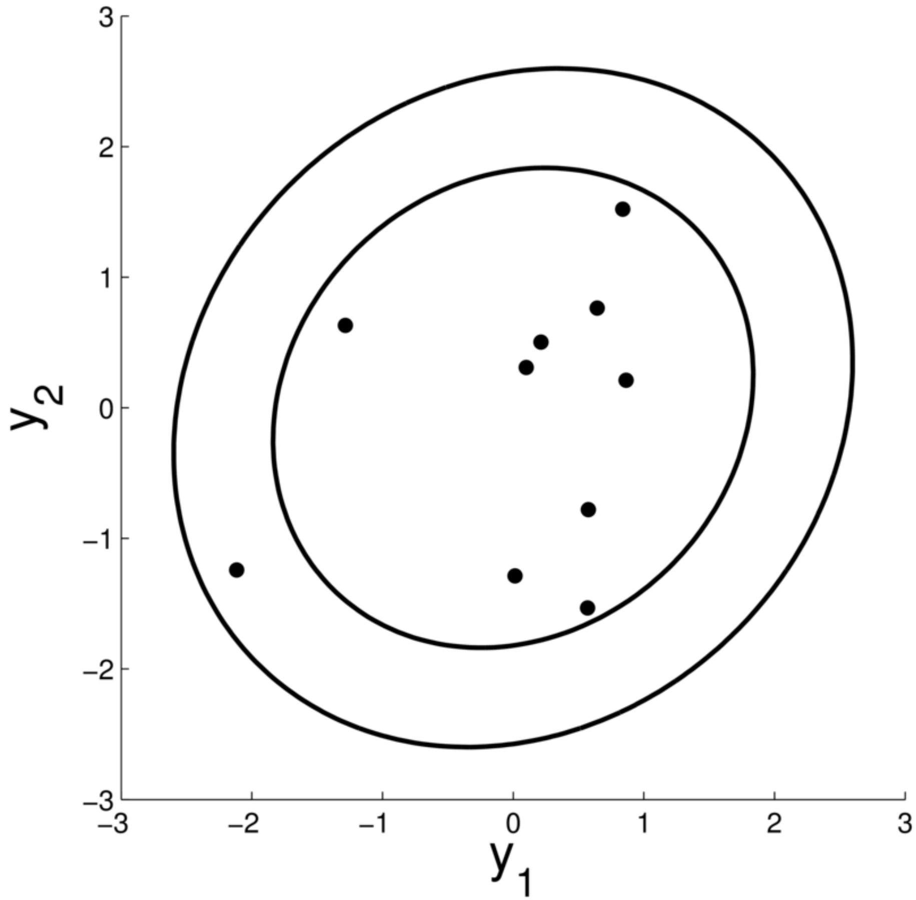

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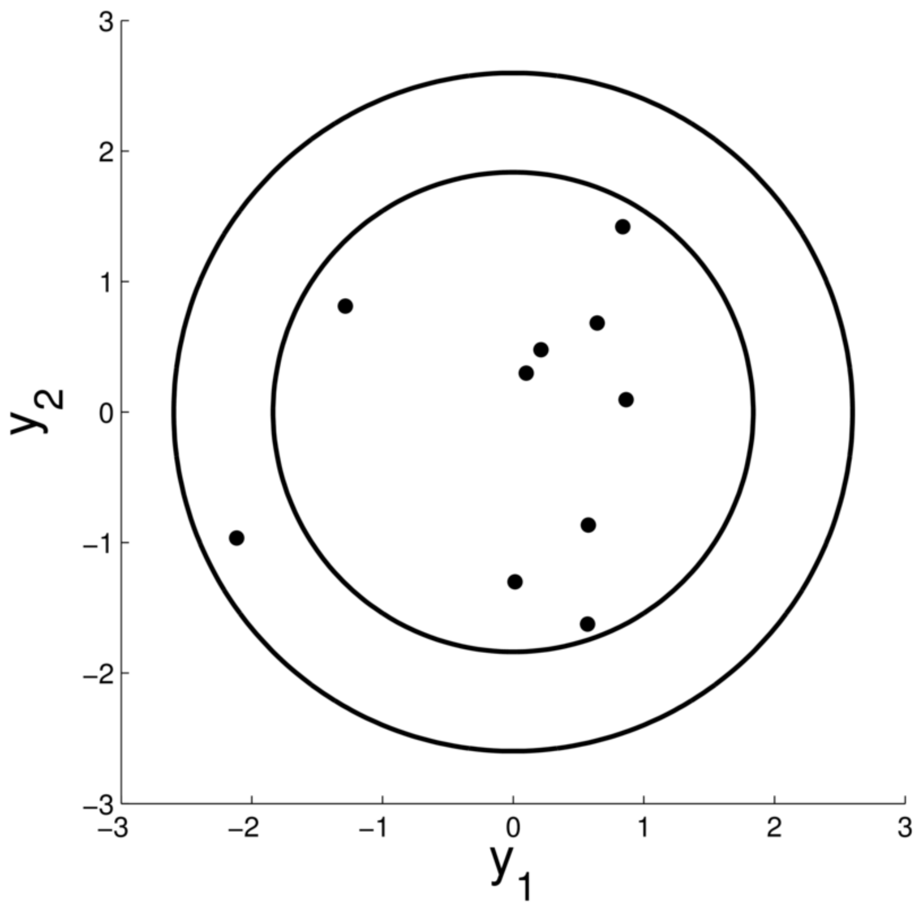

Gaussian Distribution: Conditional Distribution

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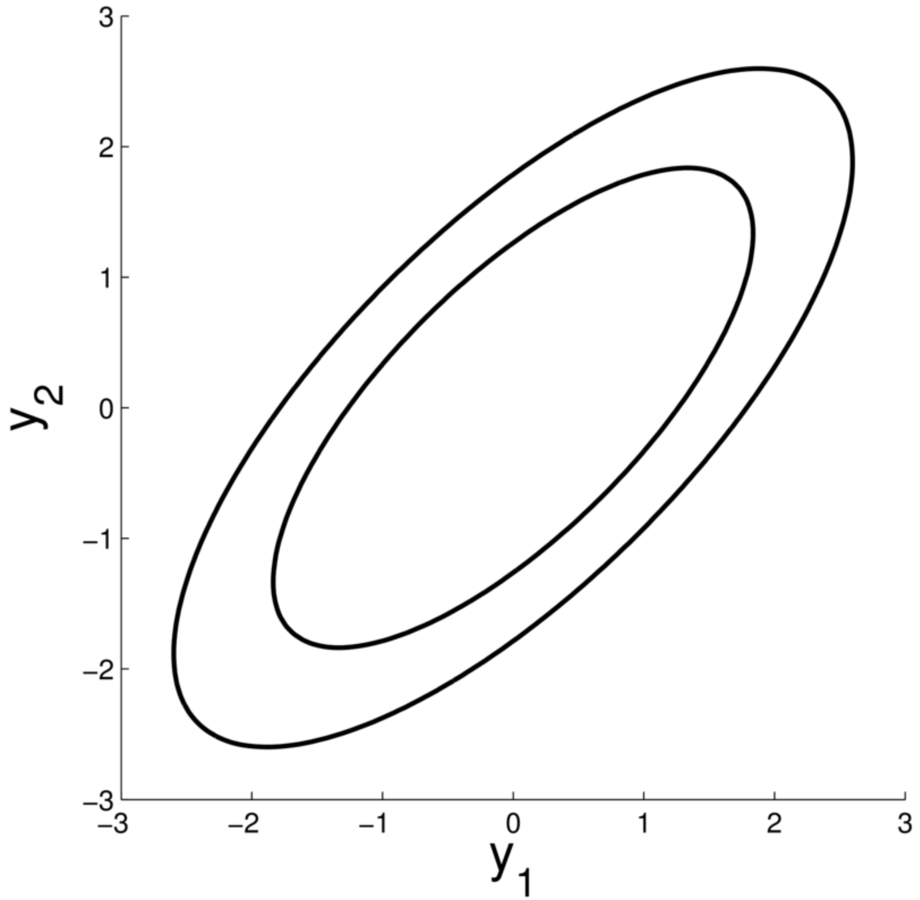

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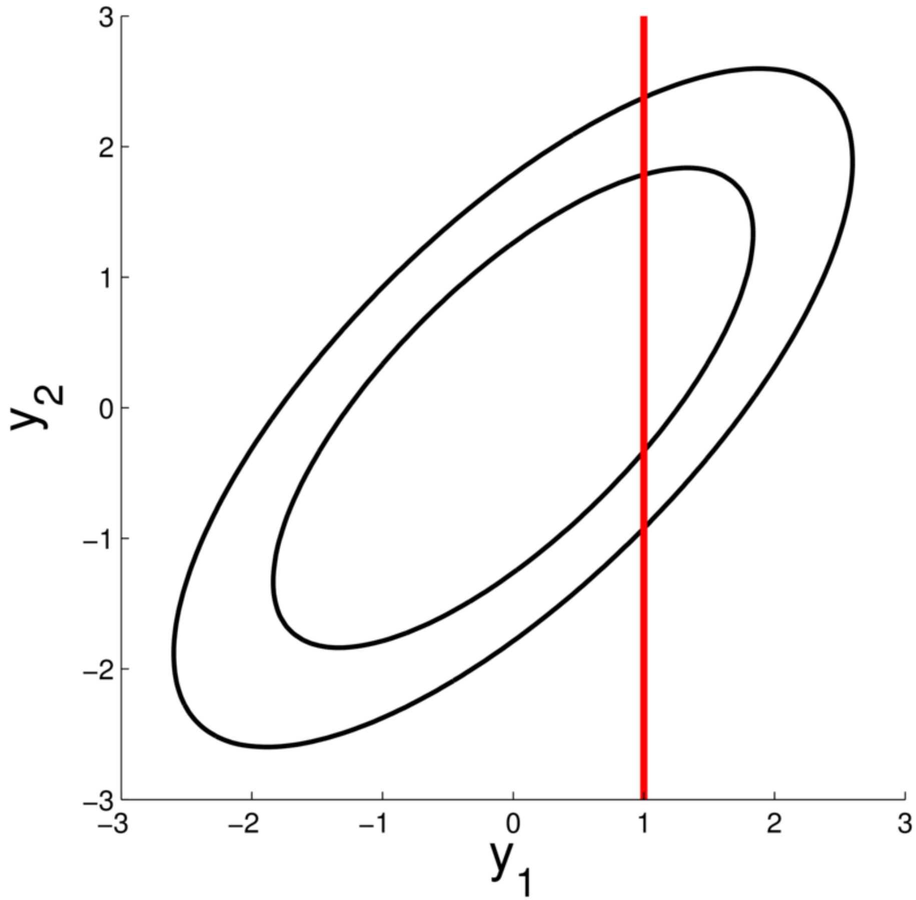
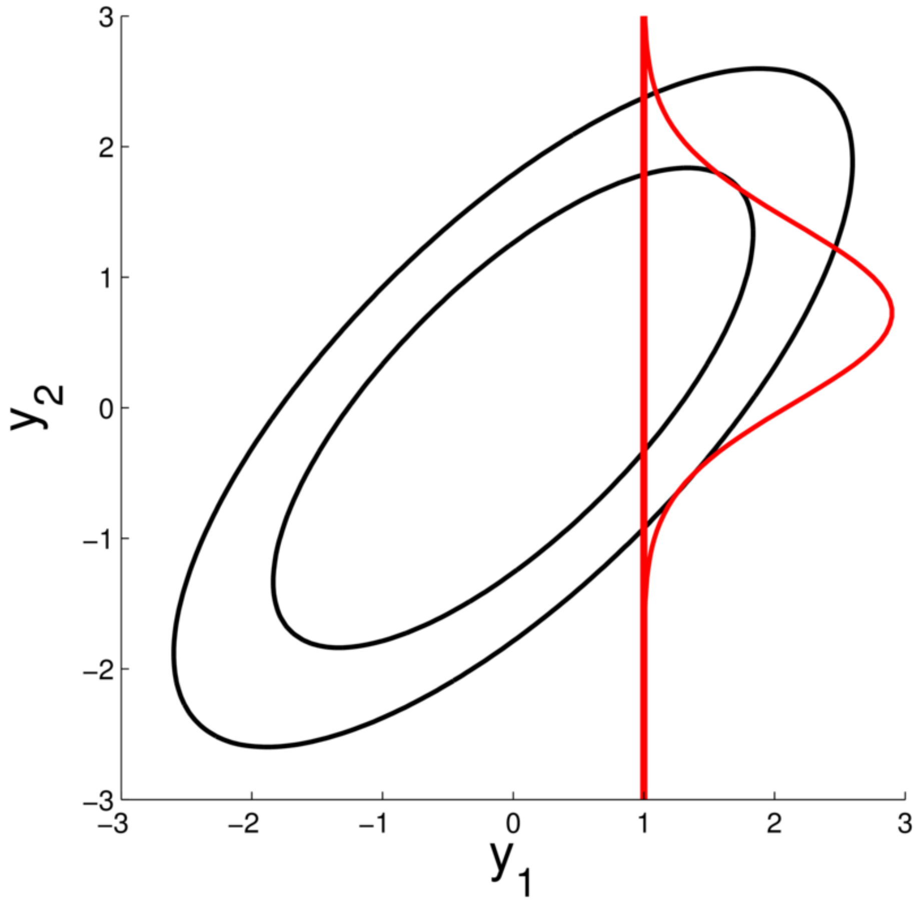


Gaussian Distribution: Conditional Distribution

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



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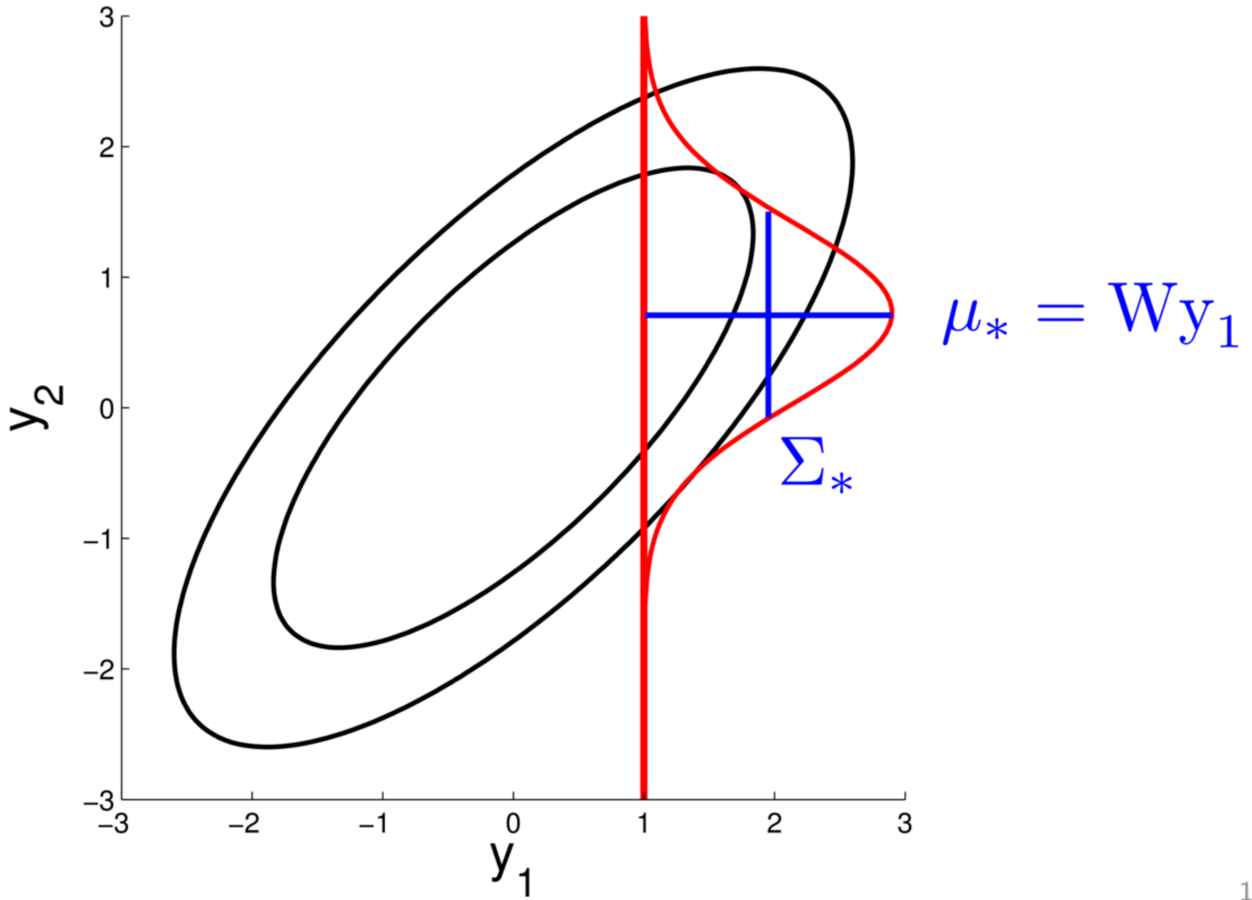

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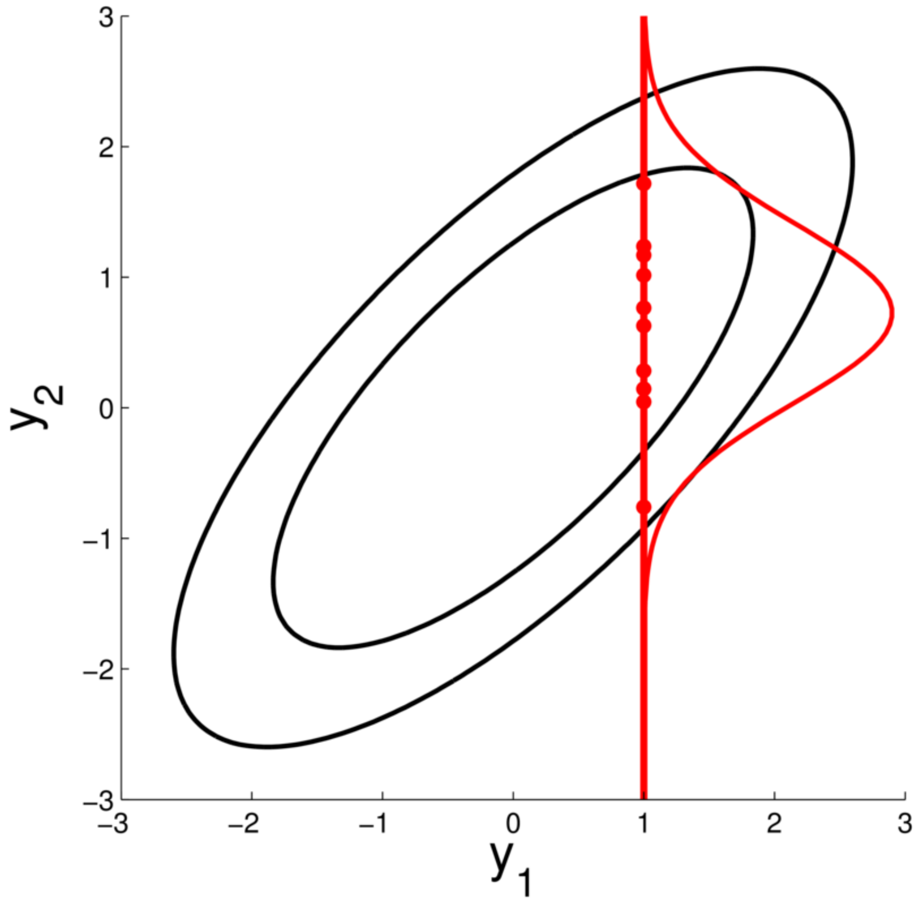

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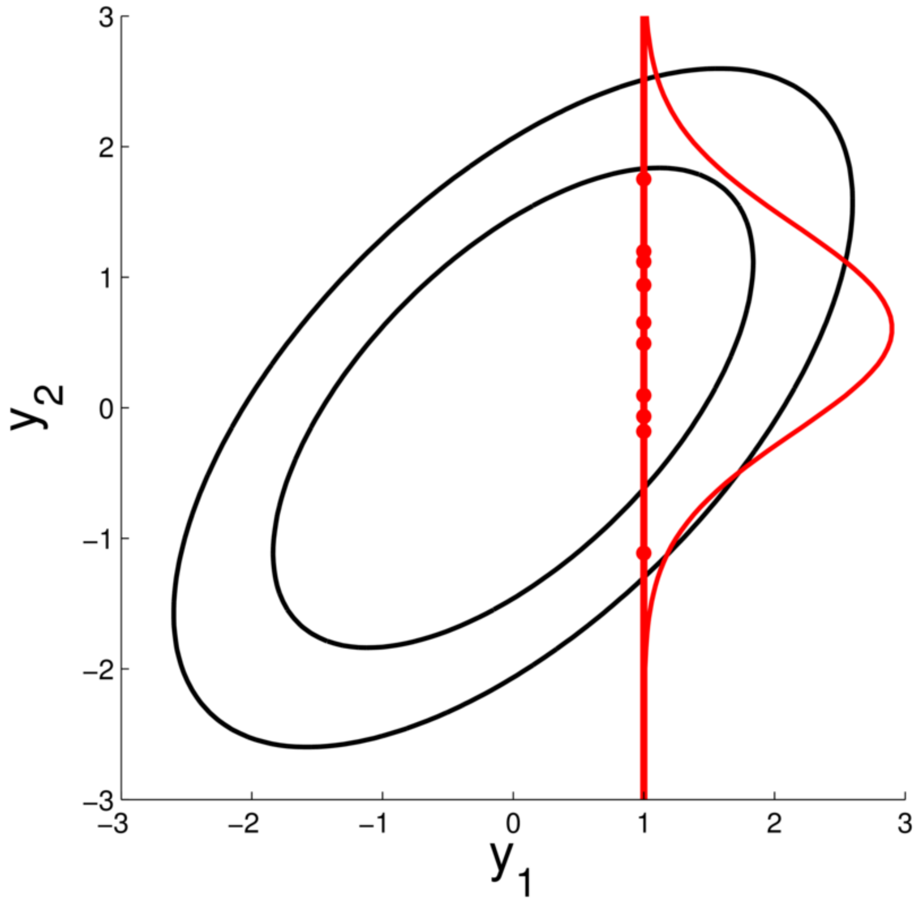

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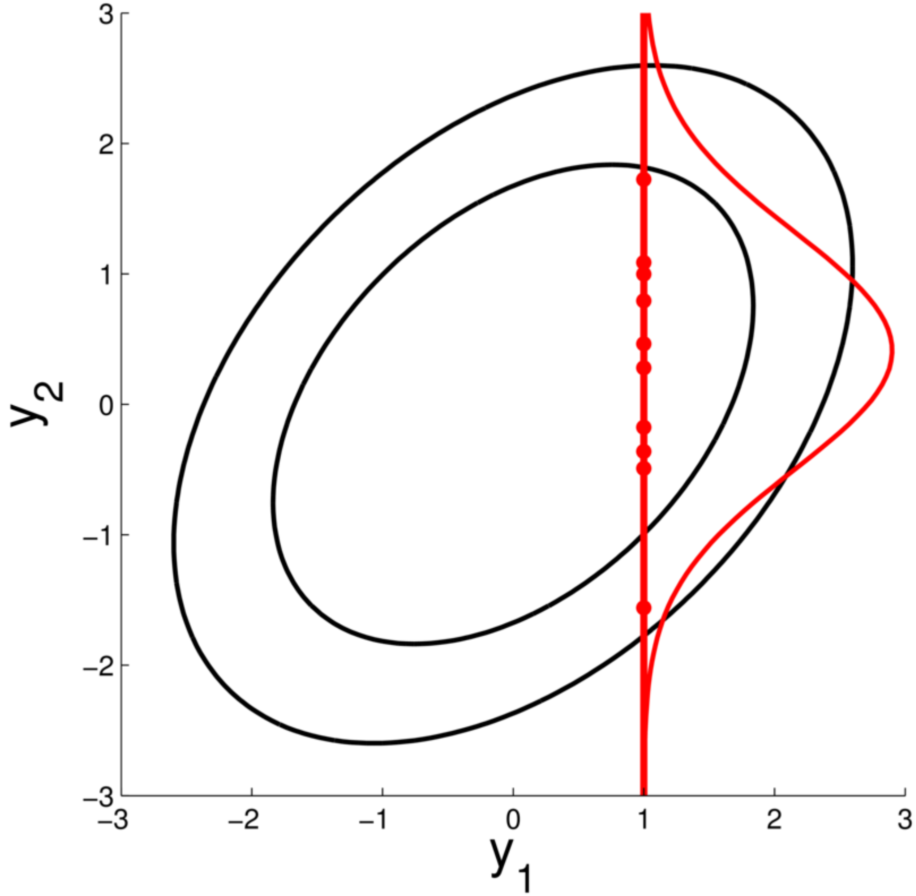

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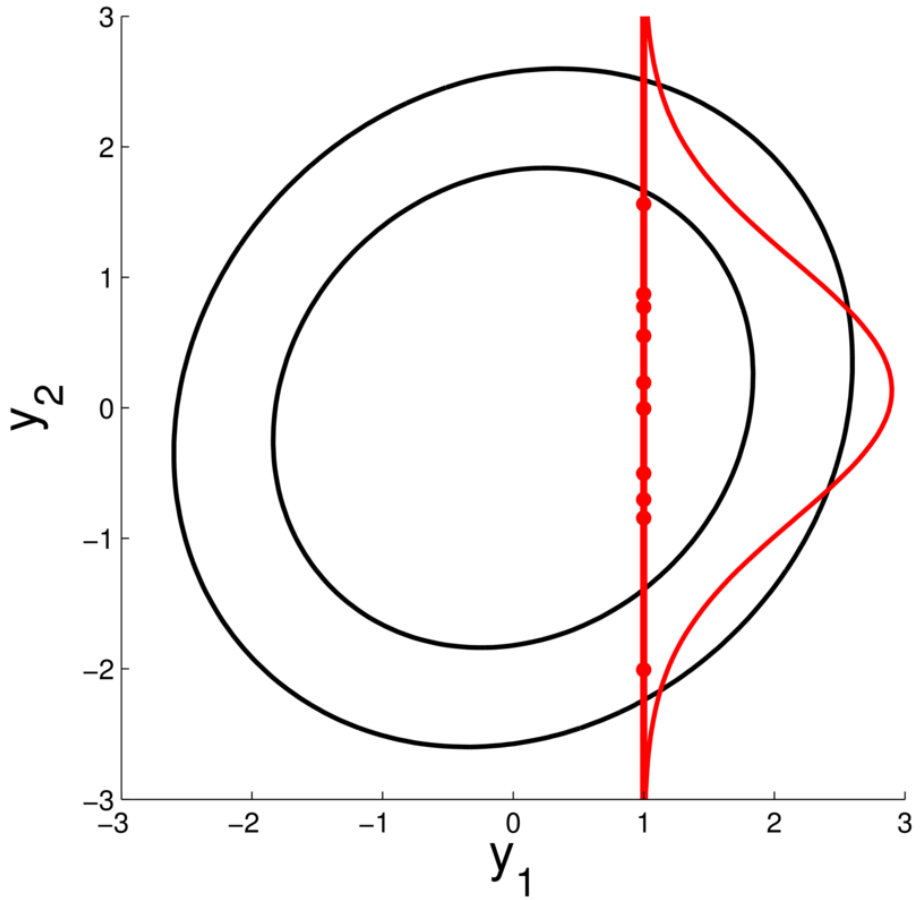

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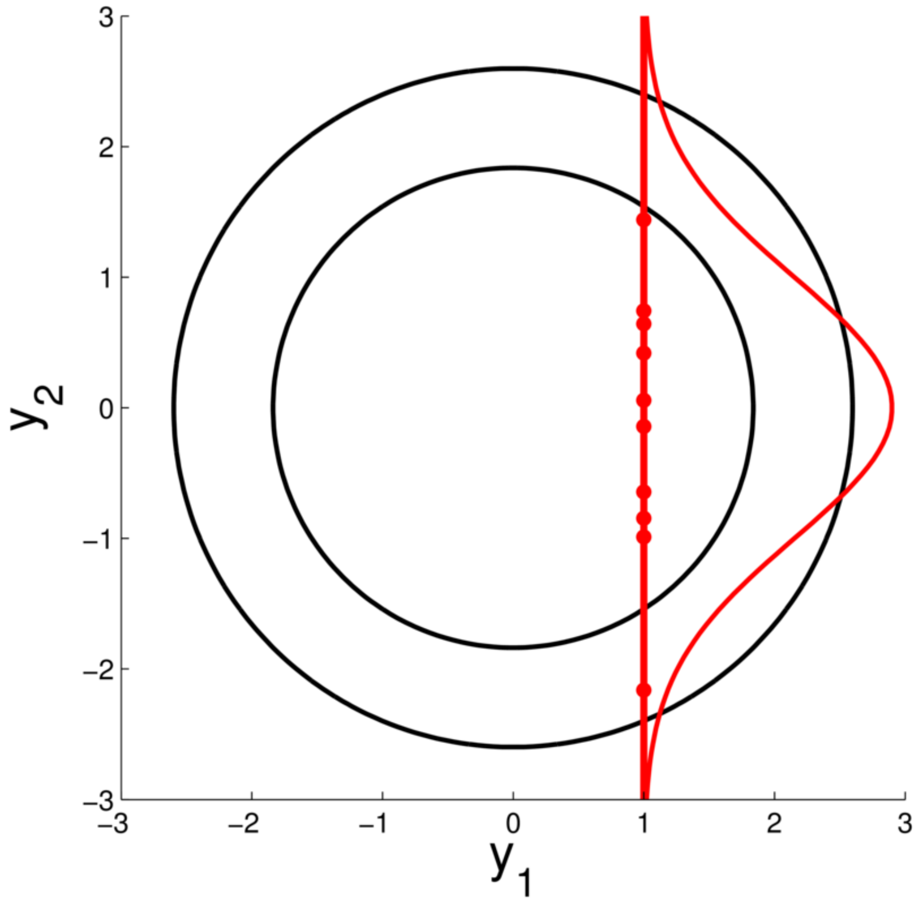
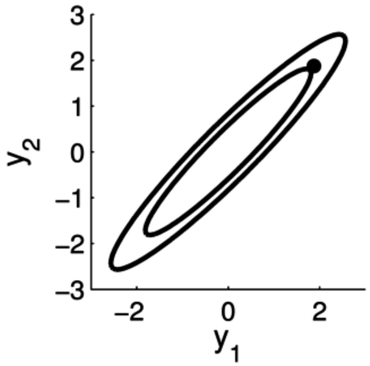


Visualizing Gaussian Processes



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

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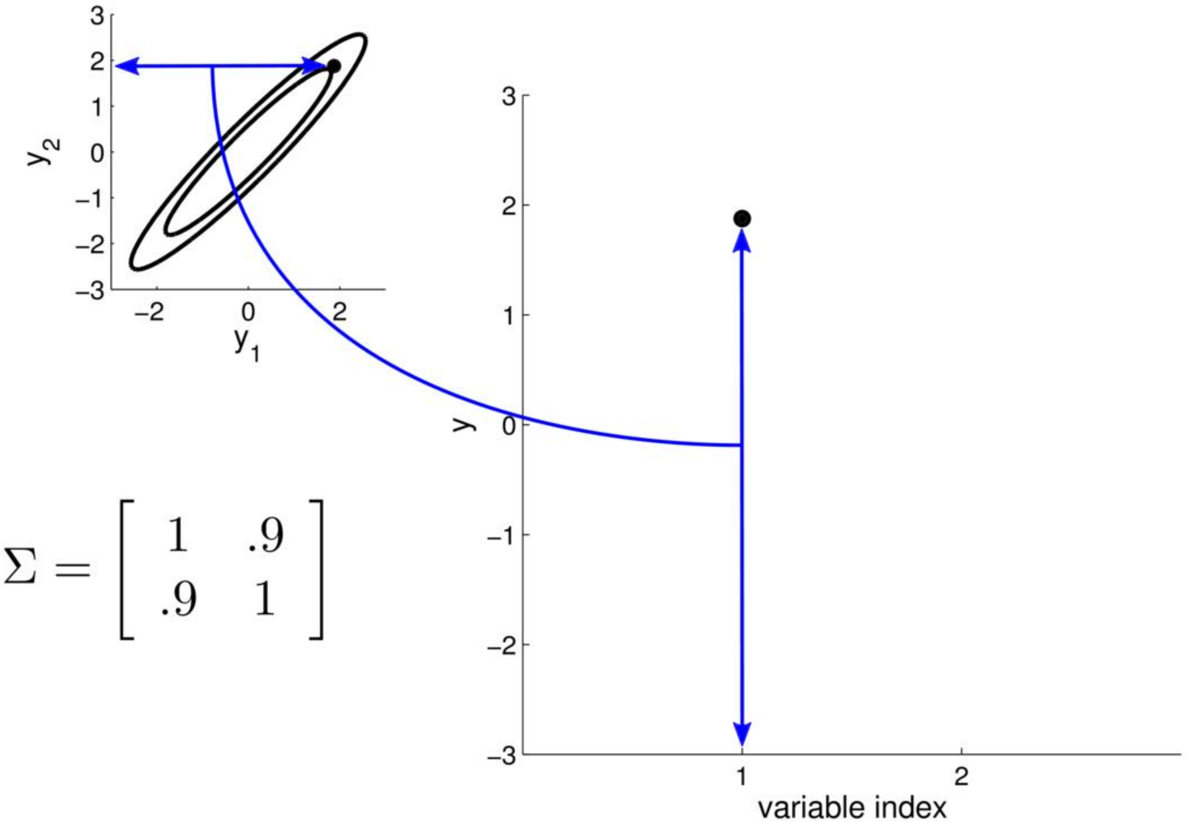

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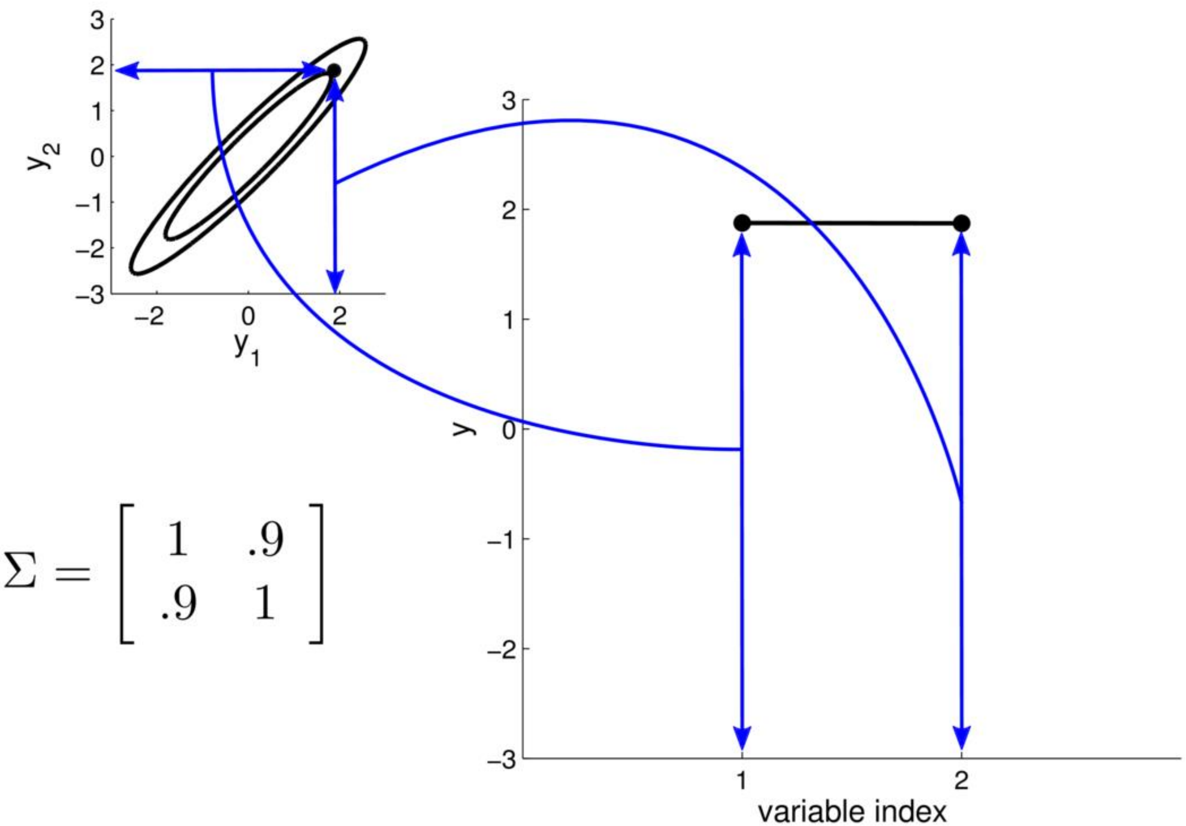

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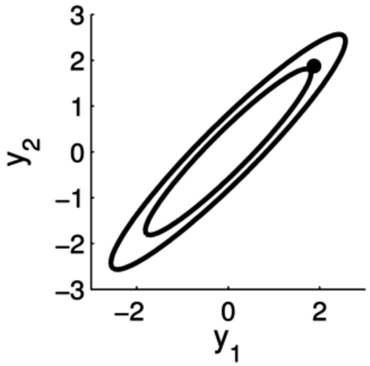

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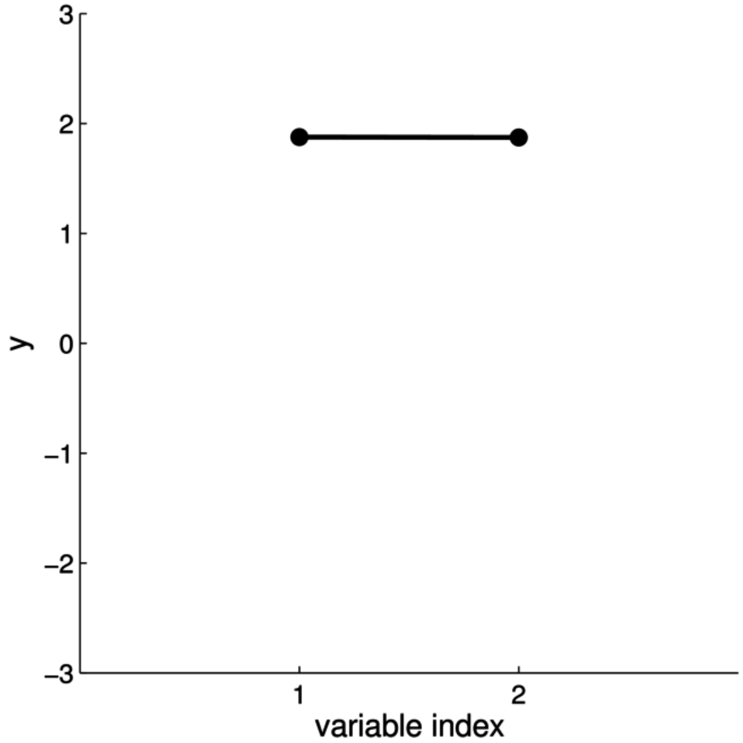

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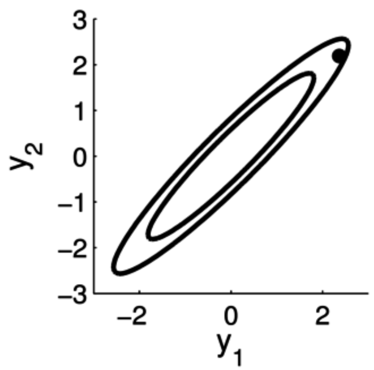

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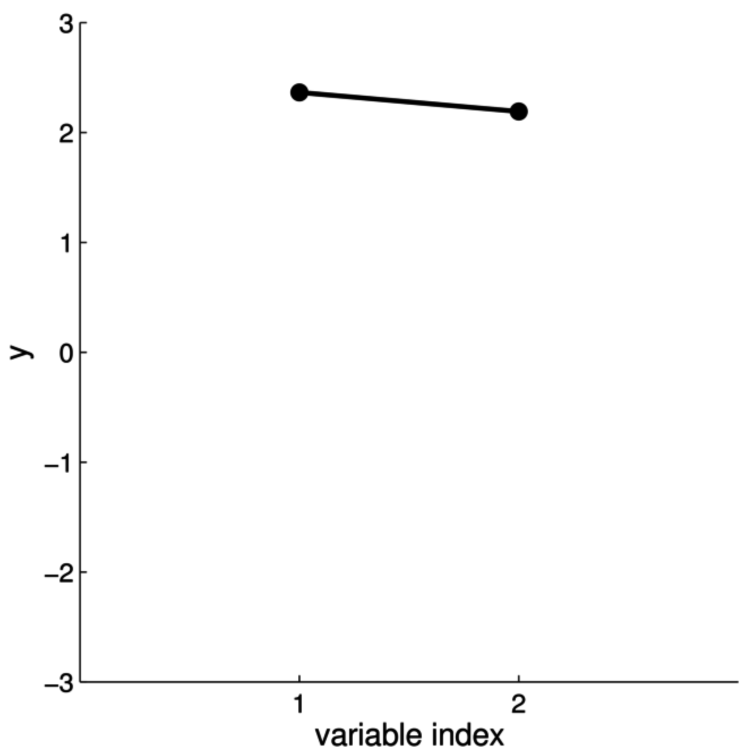

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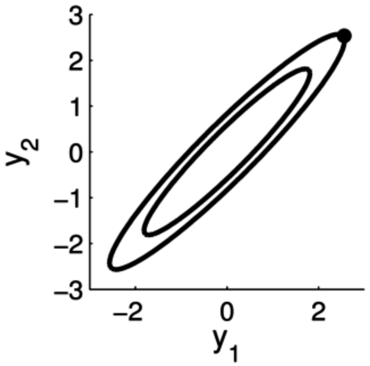

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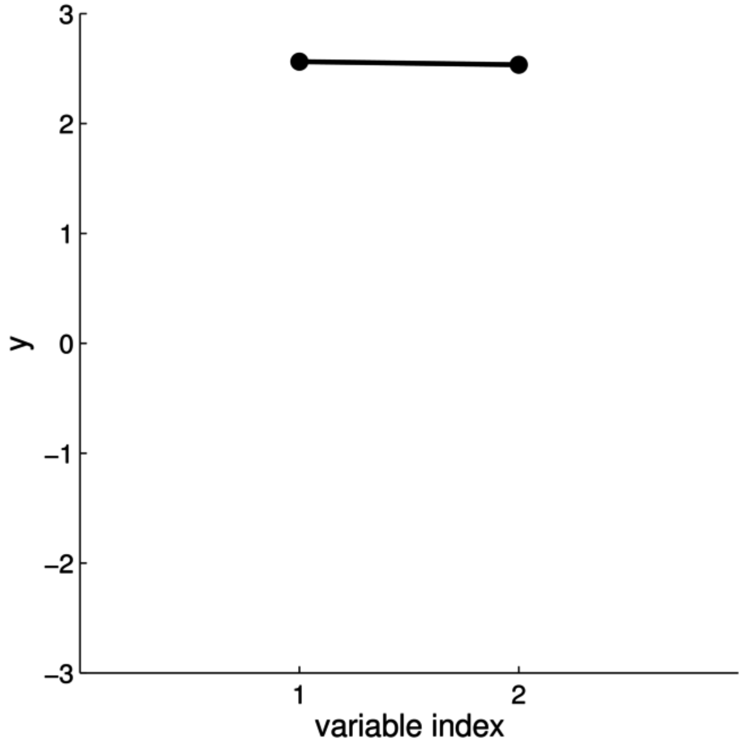

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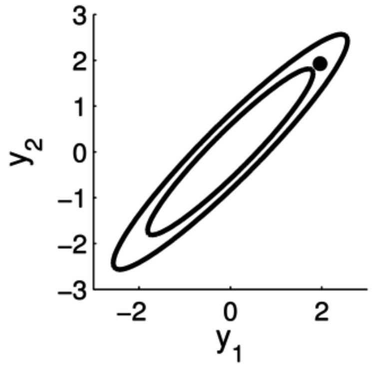

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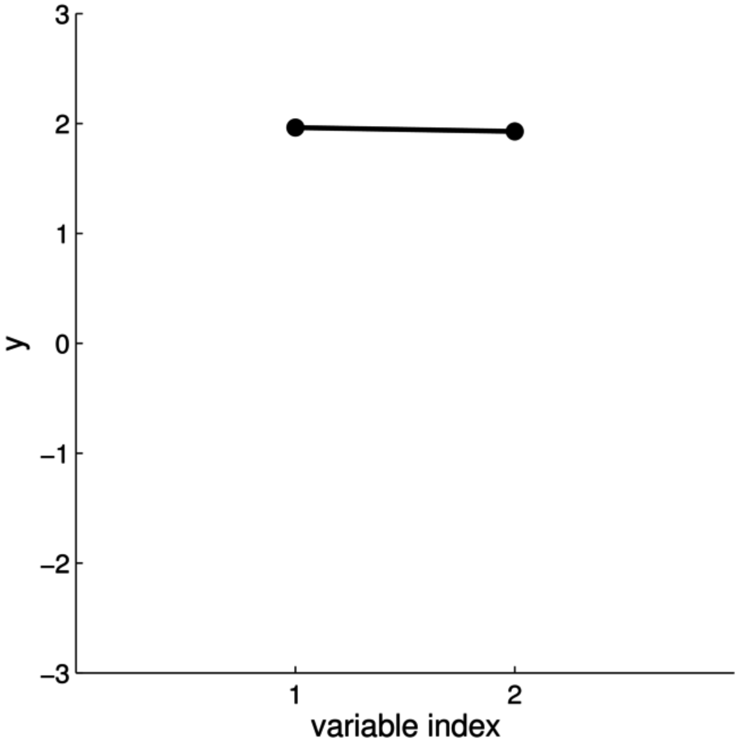

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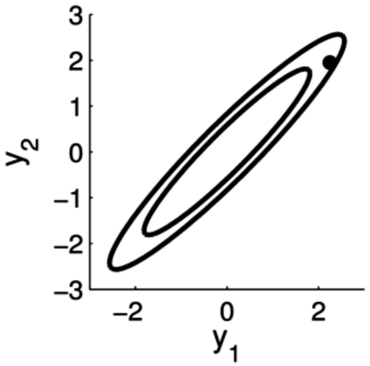

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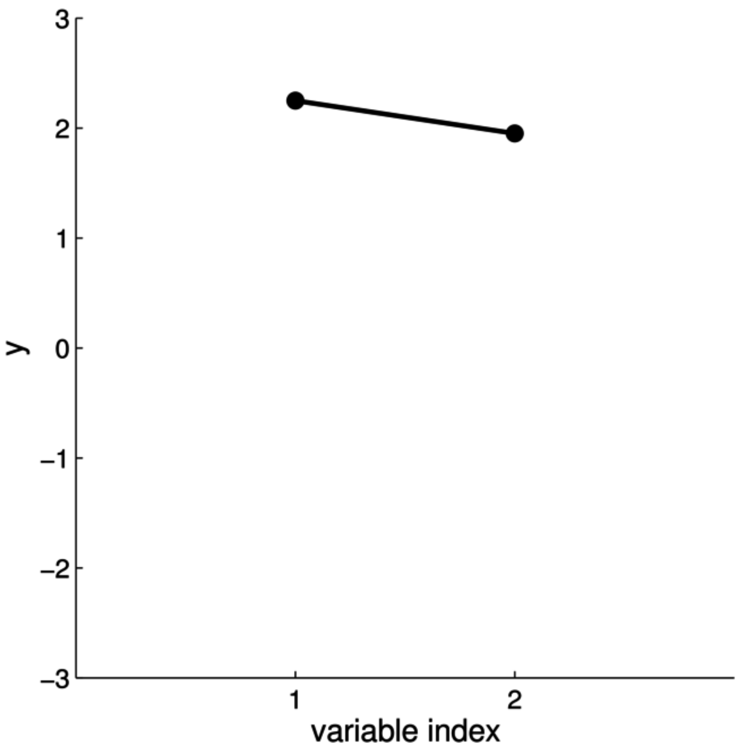

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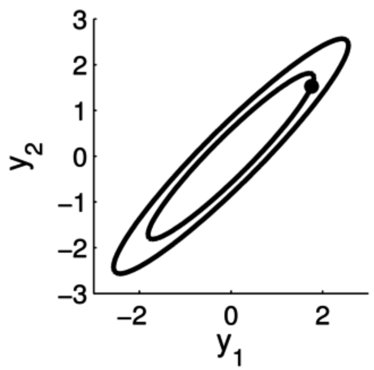

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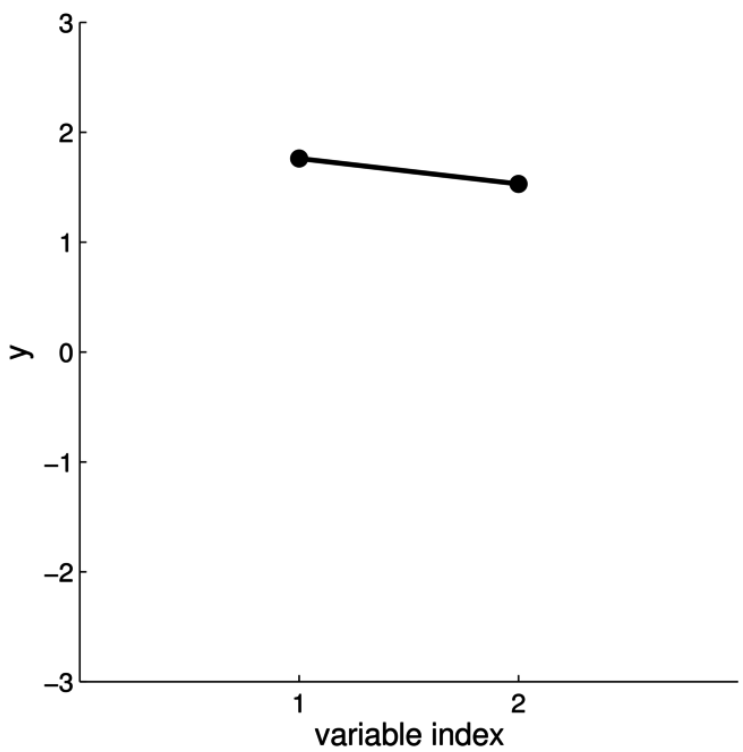

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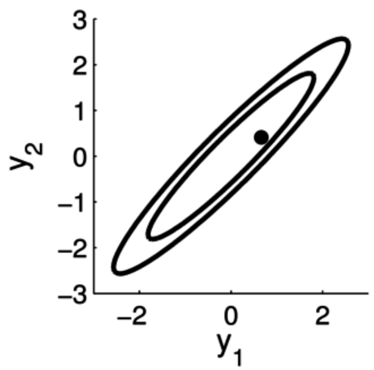

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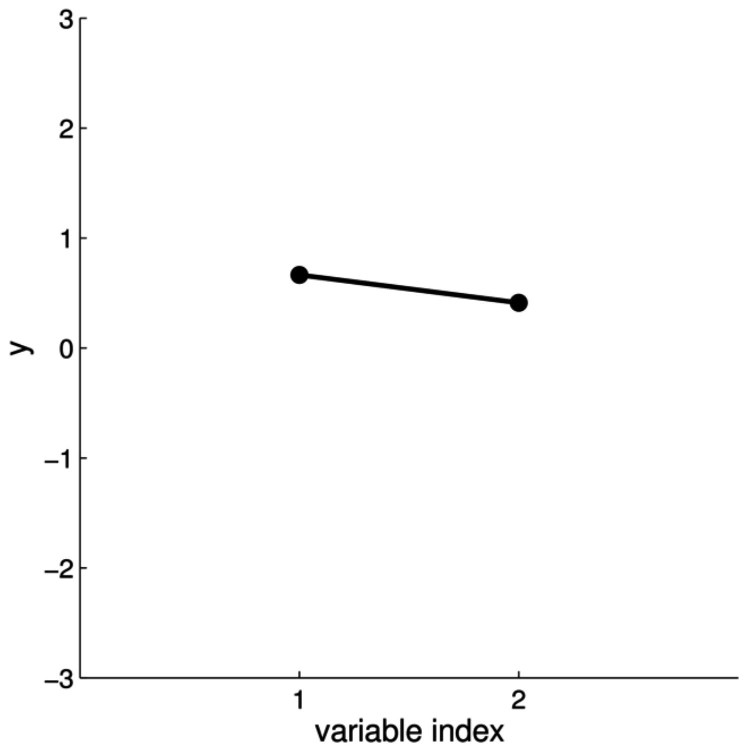

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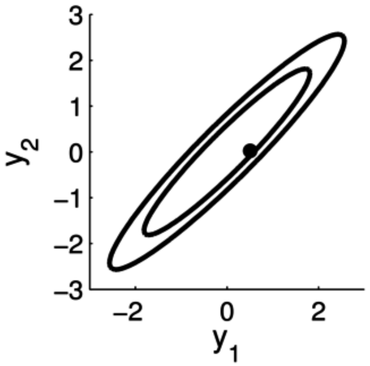

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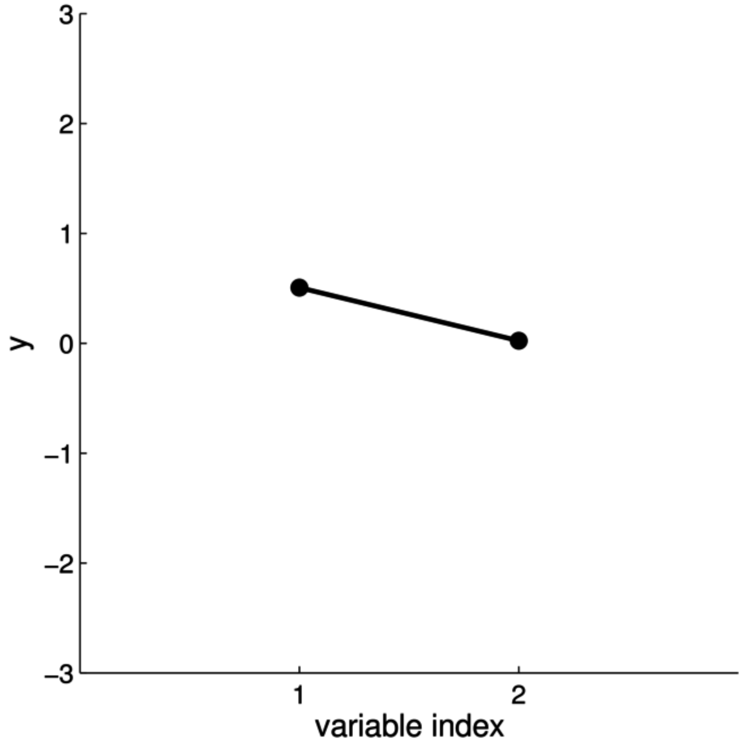

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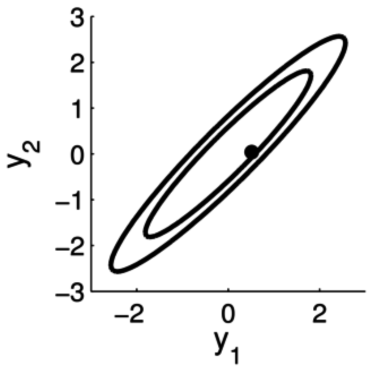

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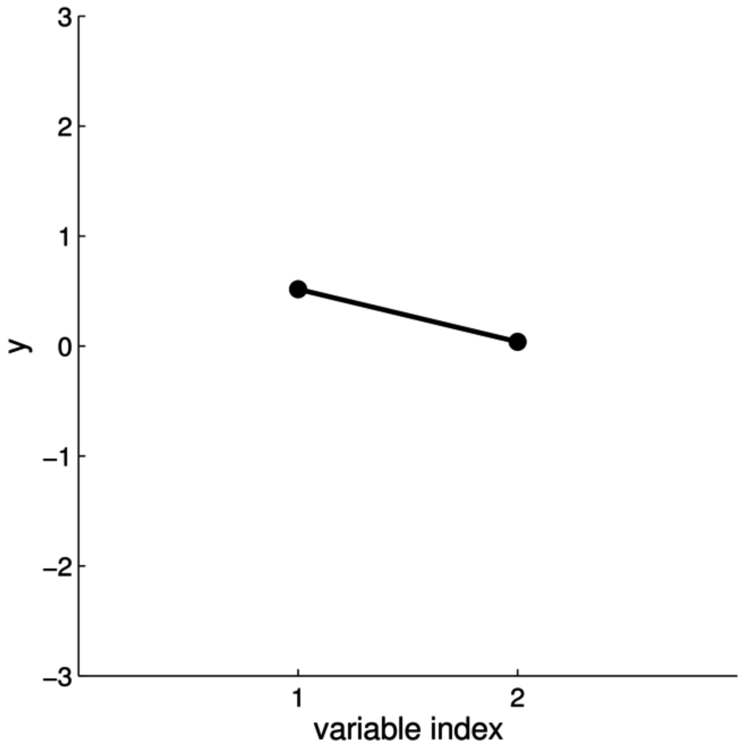

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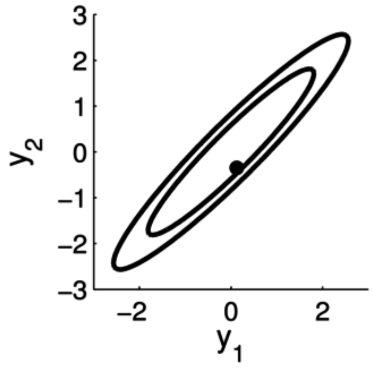

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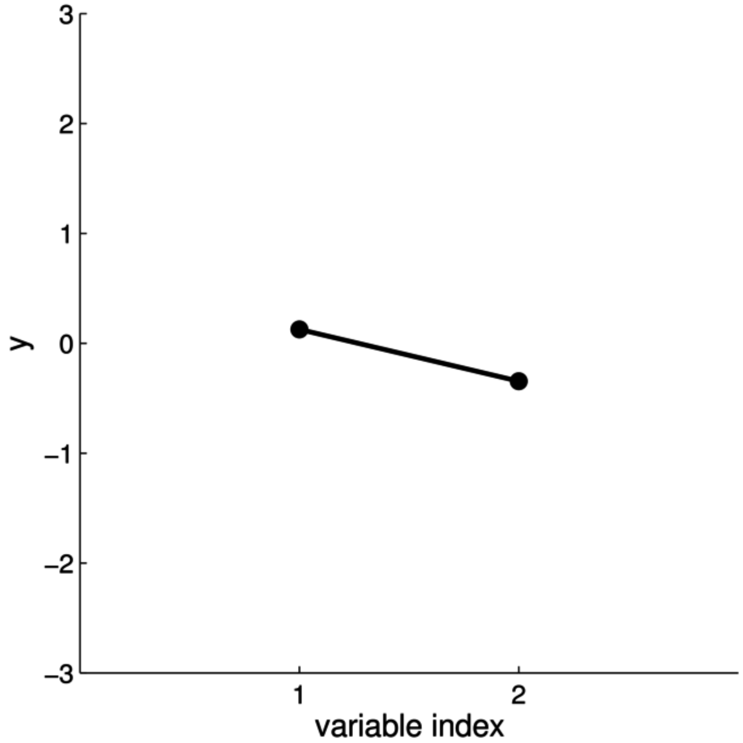

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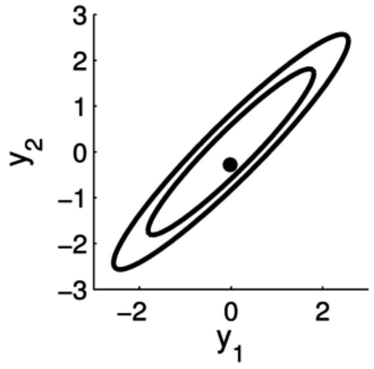

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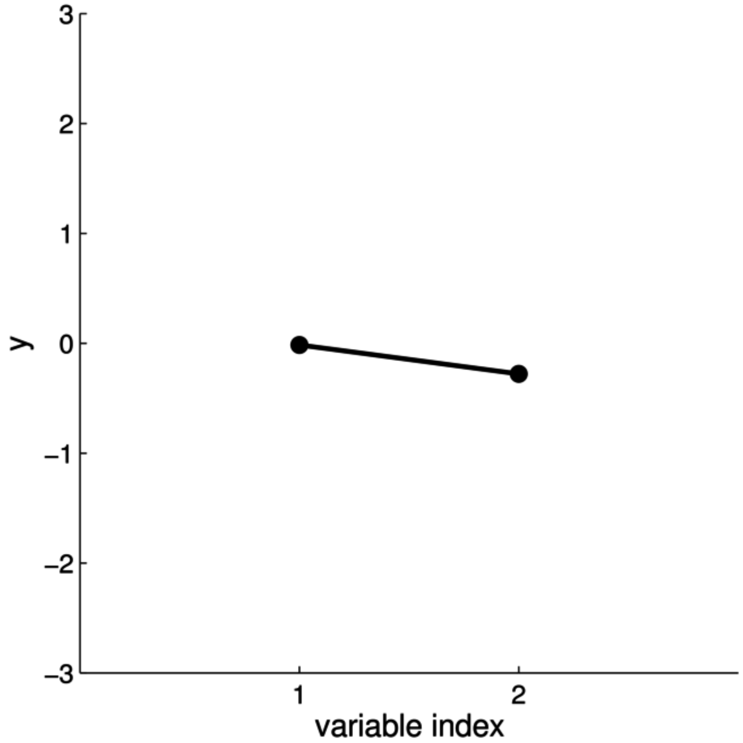

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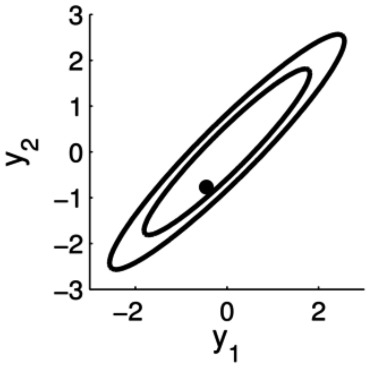

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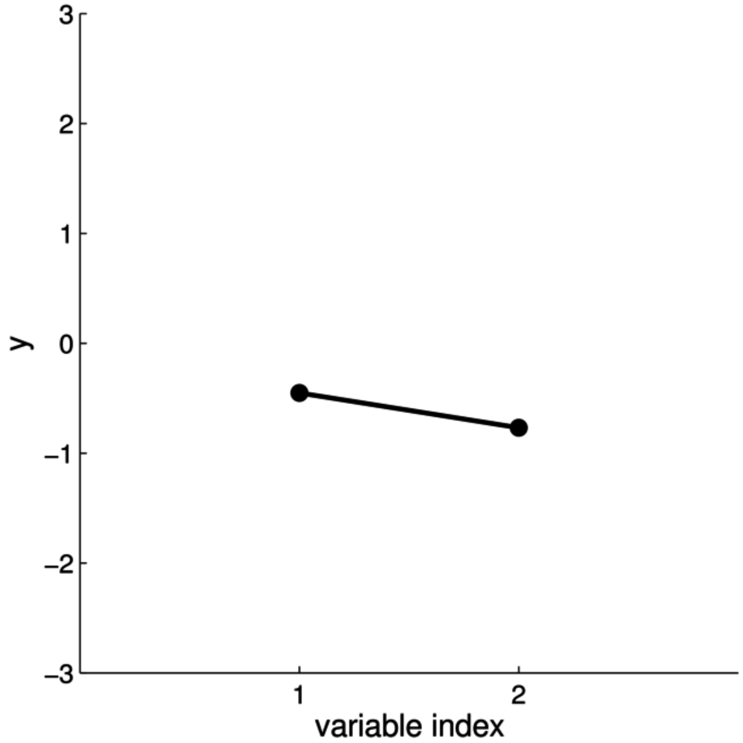

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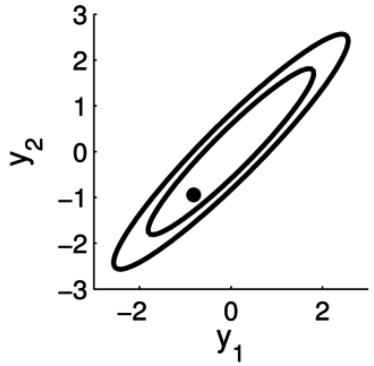

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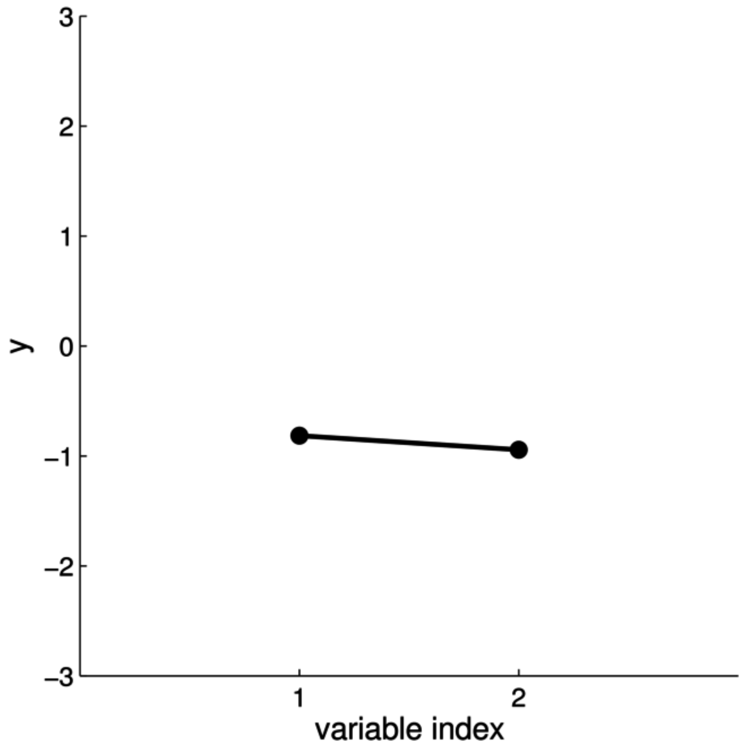

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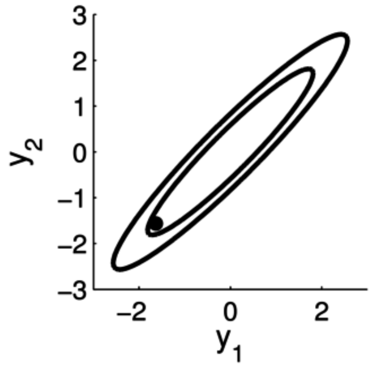

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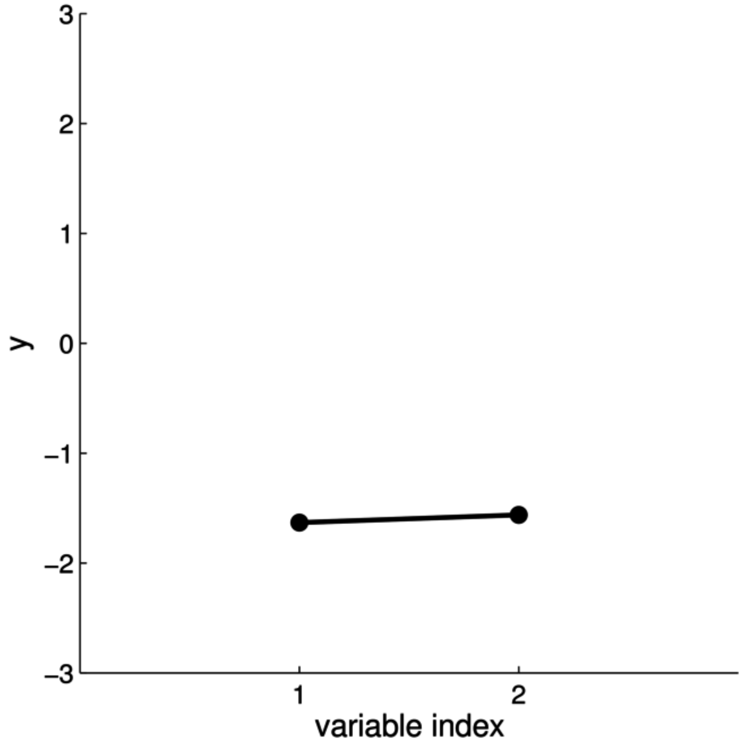

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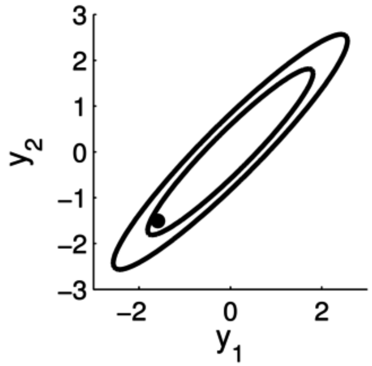

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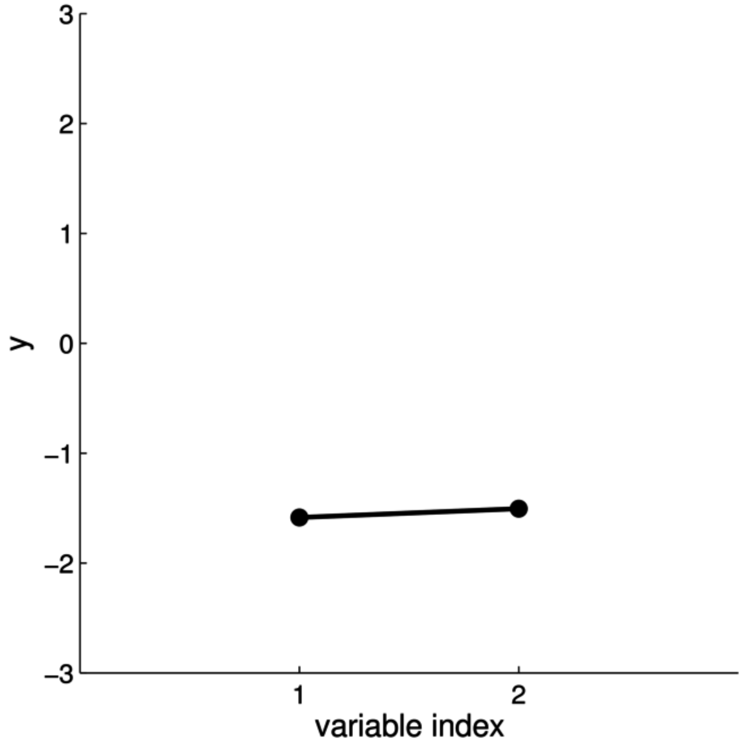

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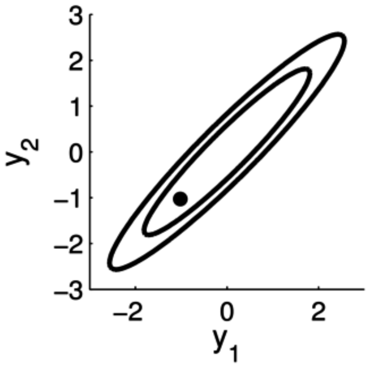

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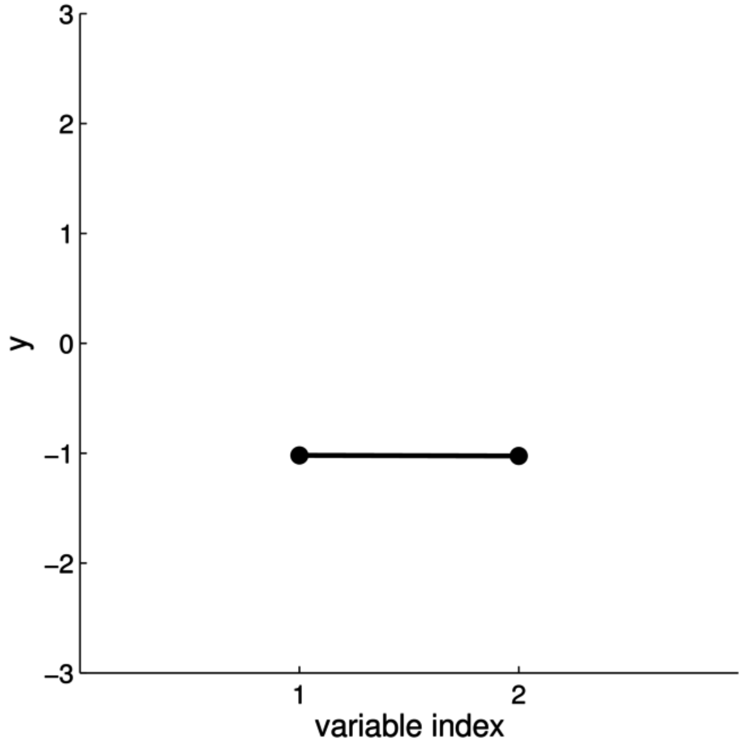

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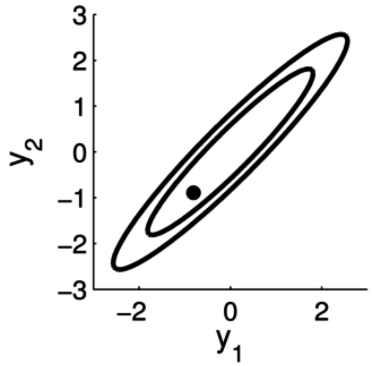

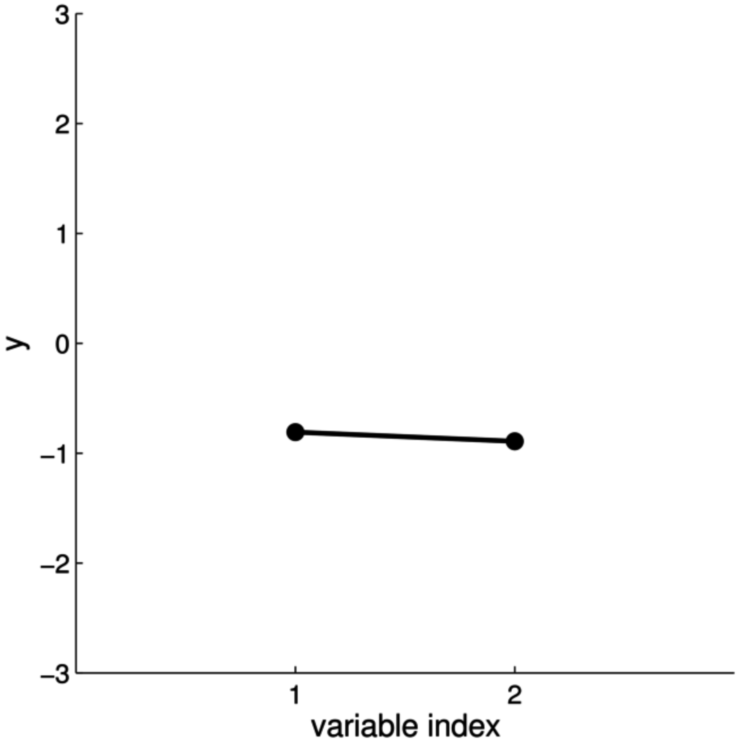

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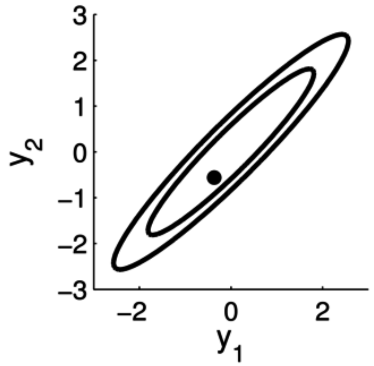

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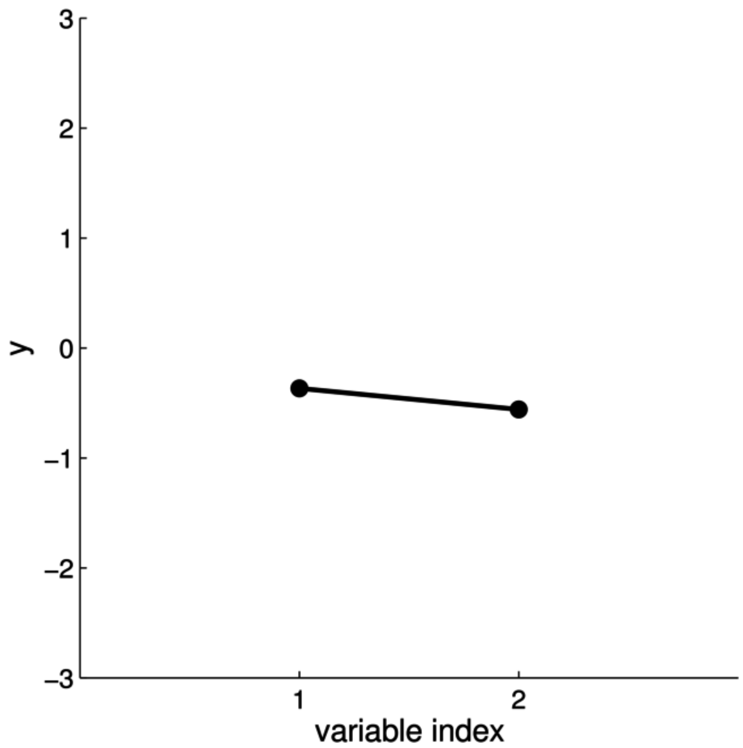
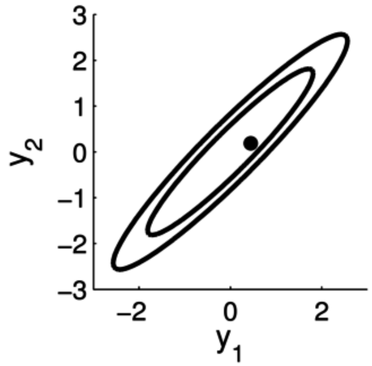
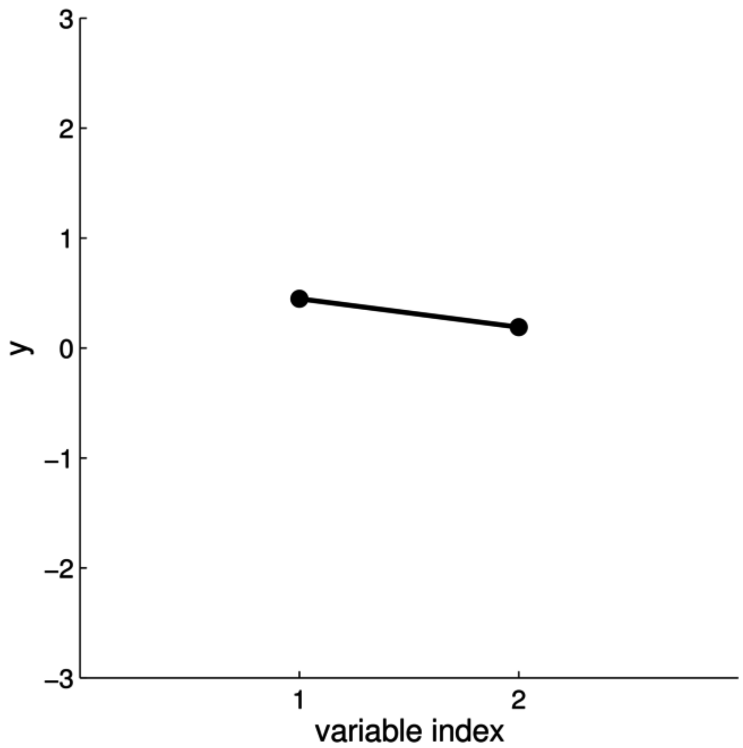


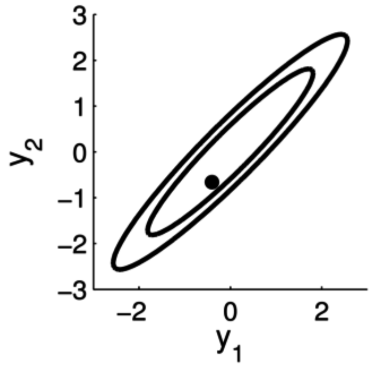
Visualizing Gaussian Processes



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



Visualizing Gaussian Processes



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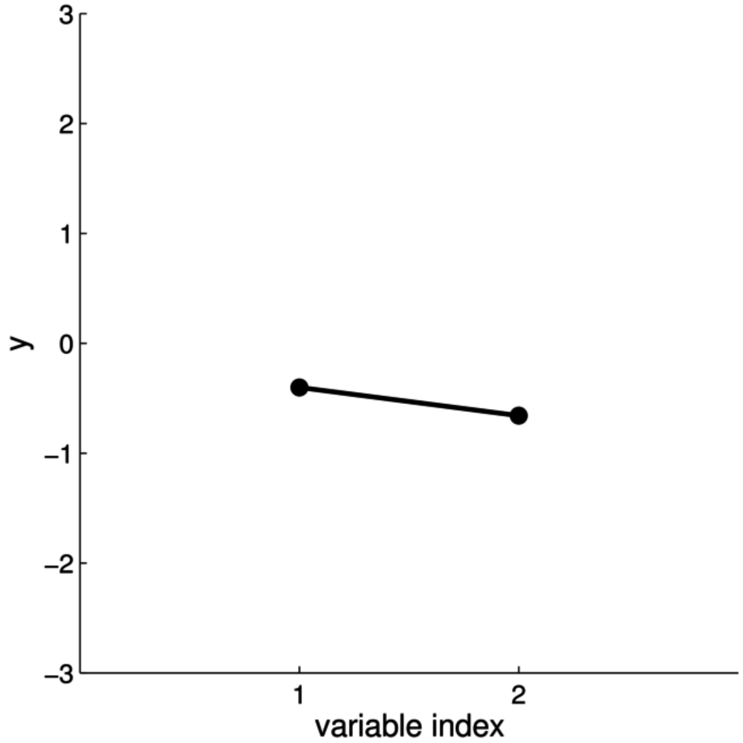
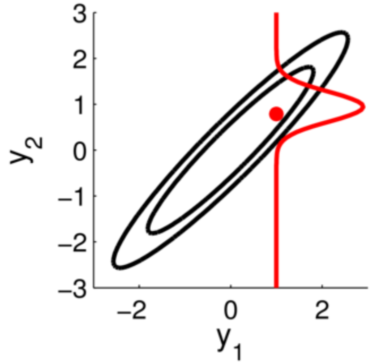


Visualizing Gaussian Processes



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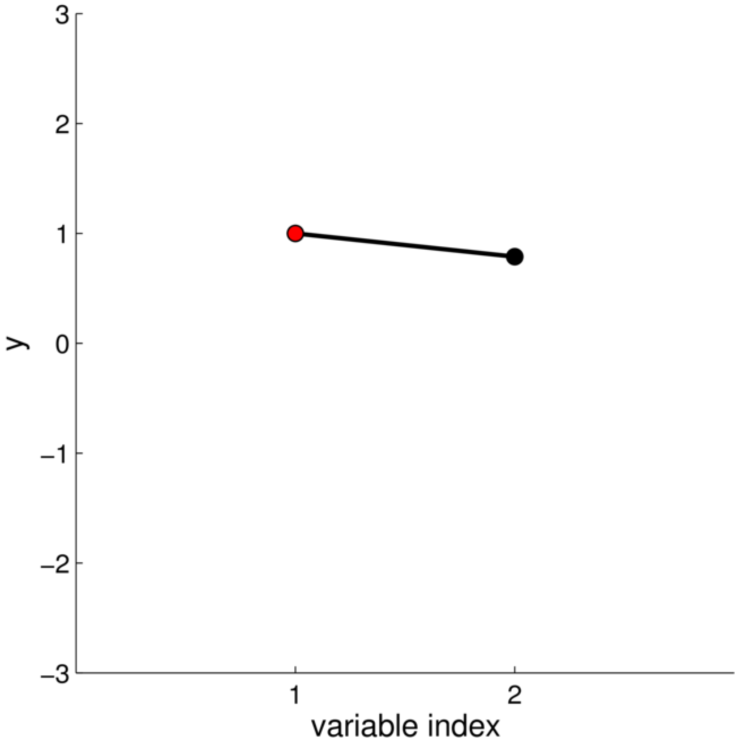
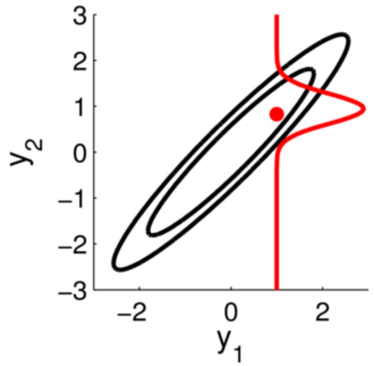


Visualizing Gaussian Processes



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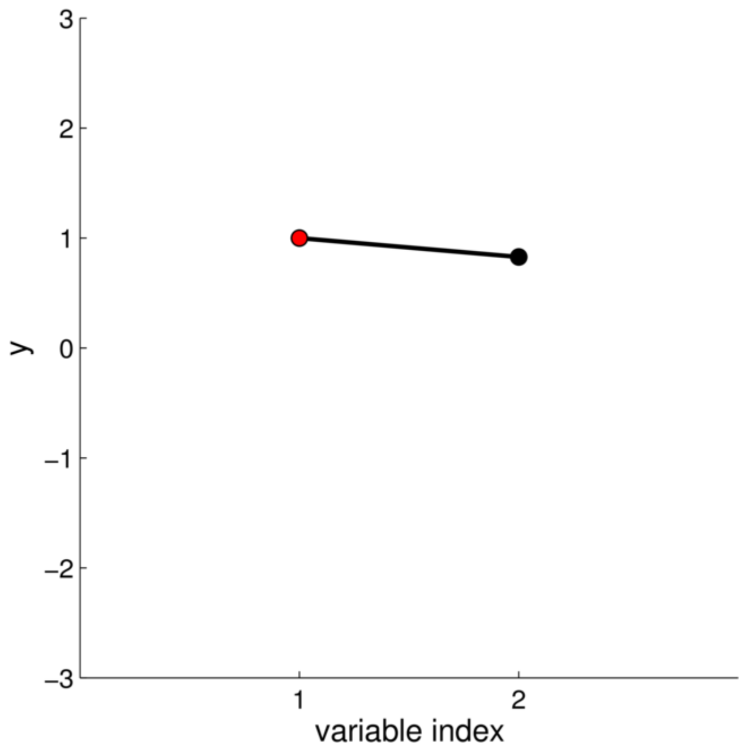
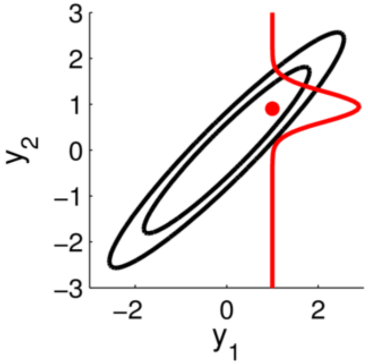


Visualizing Gaussian Processes



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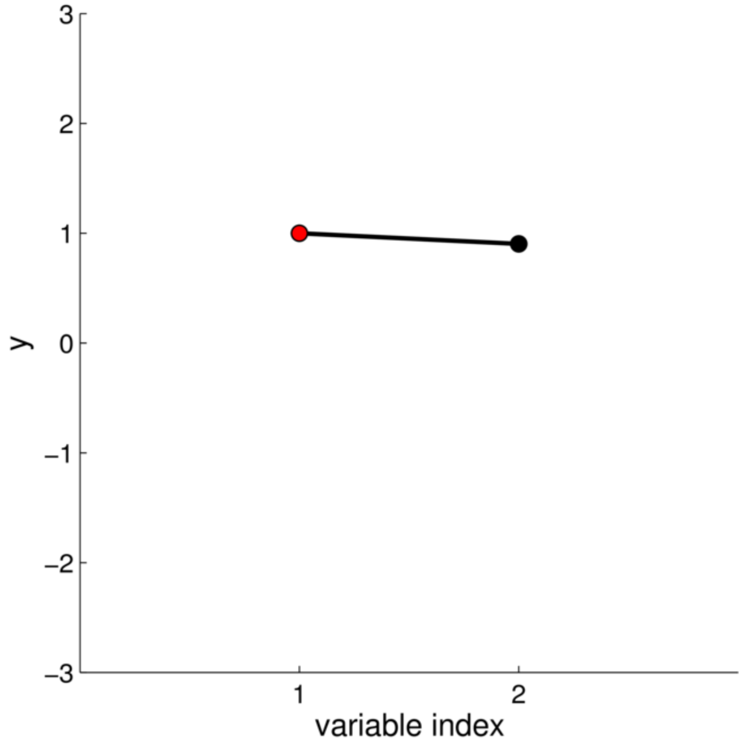
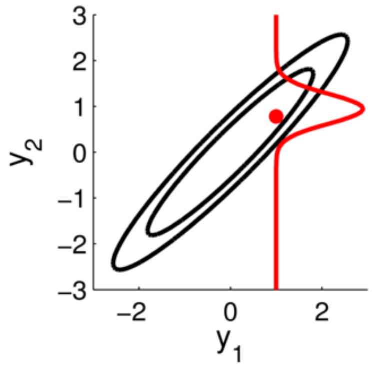
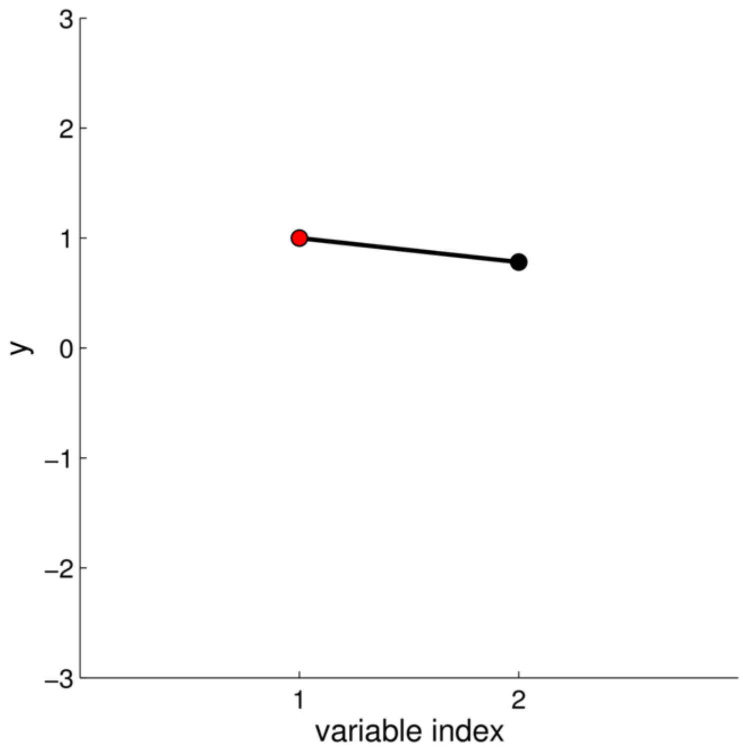


Visualizing Gaussian Processes





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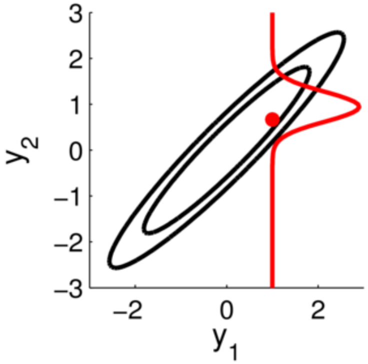
Visualizing Gaussian Processes



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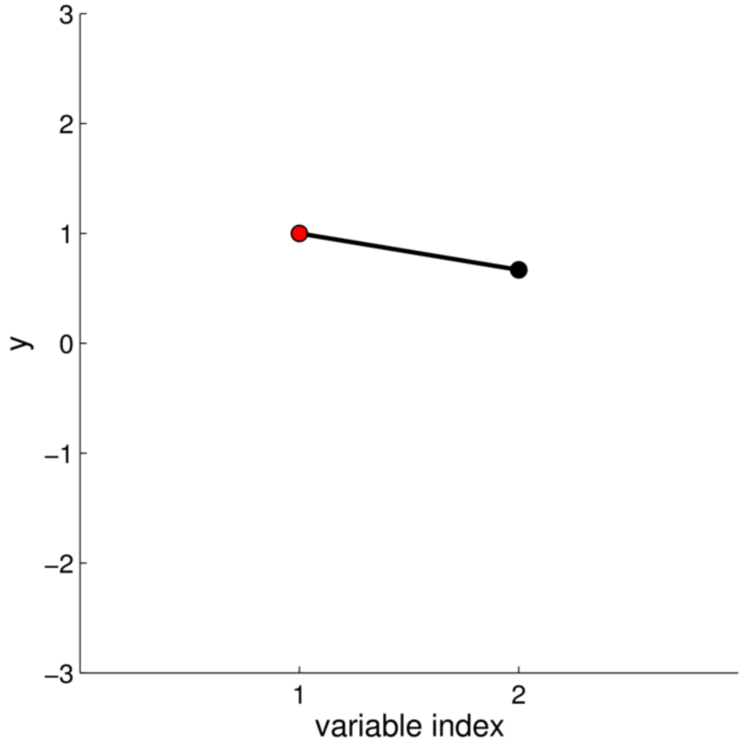
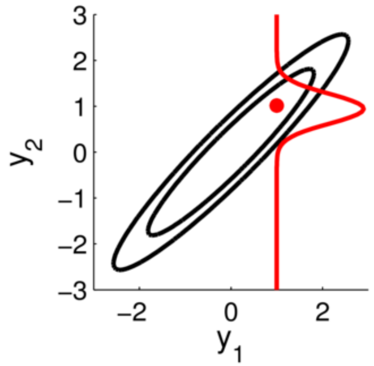


Visualizing Gaussian Processes



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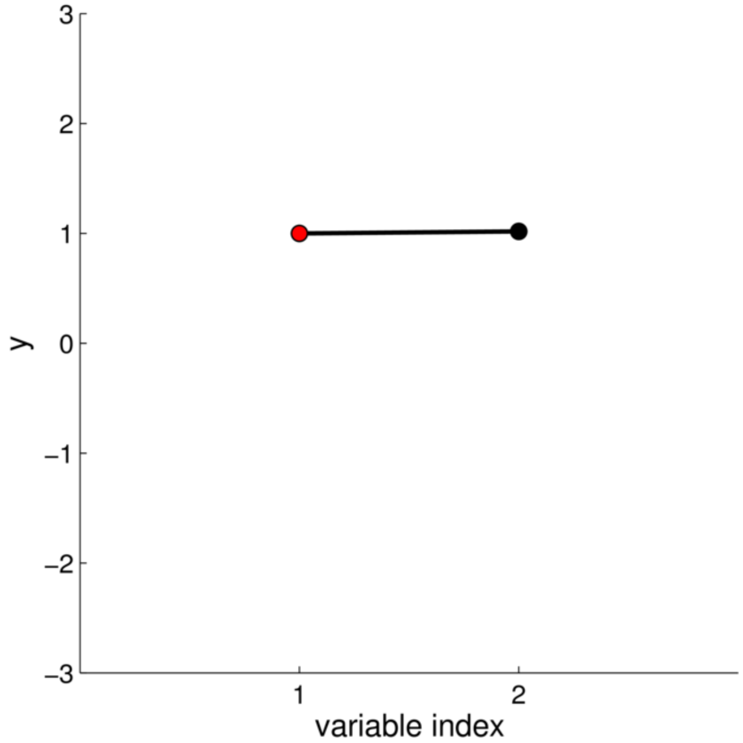
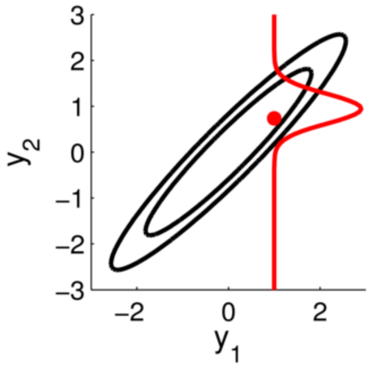
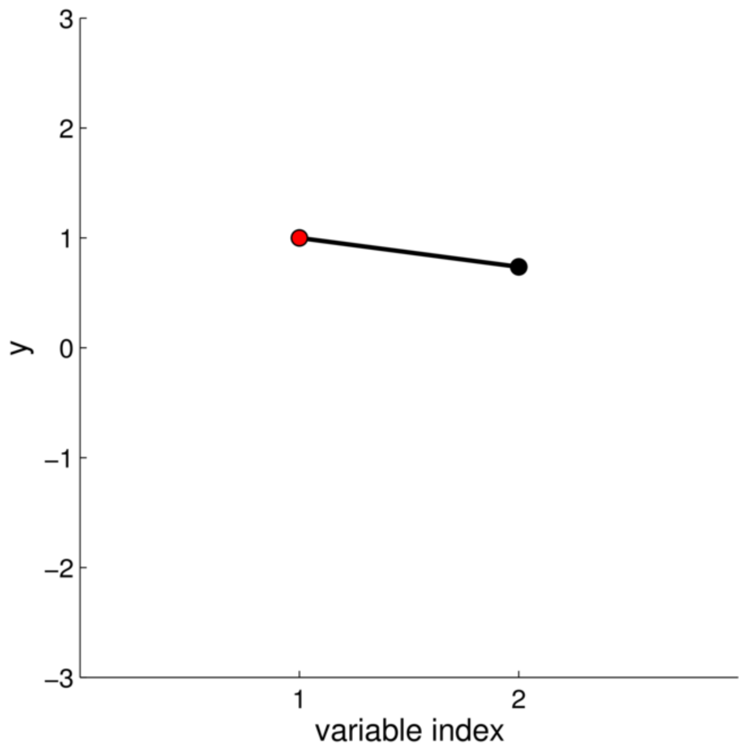


Visualizing Gaussian Processes





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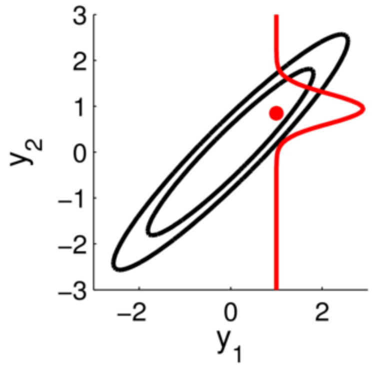
Visualizing Gaussian Processes



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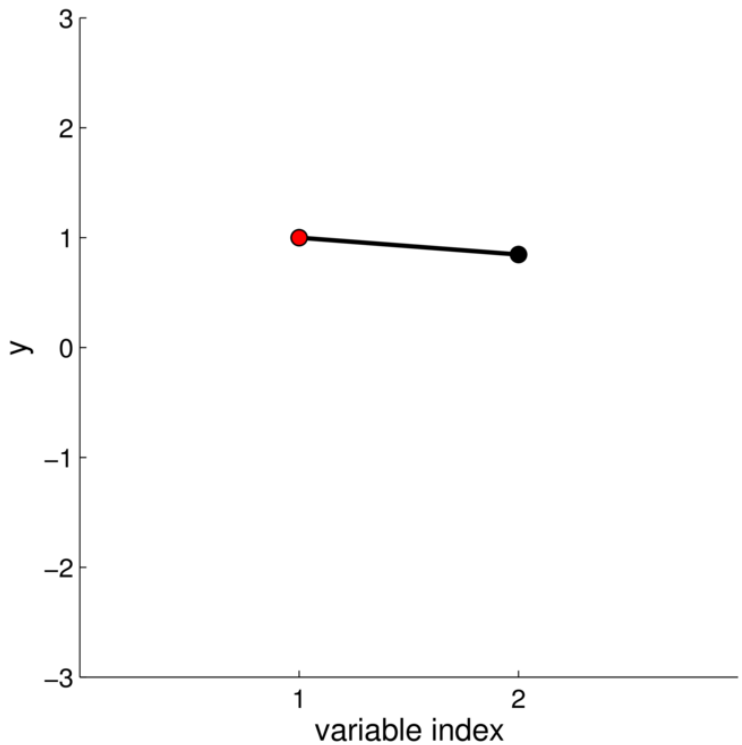

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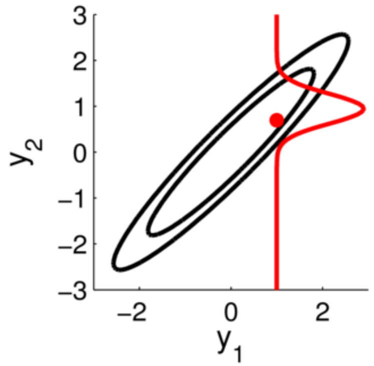

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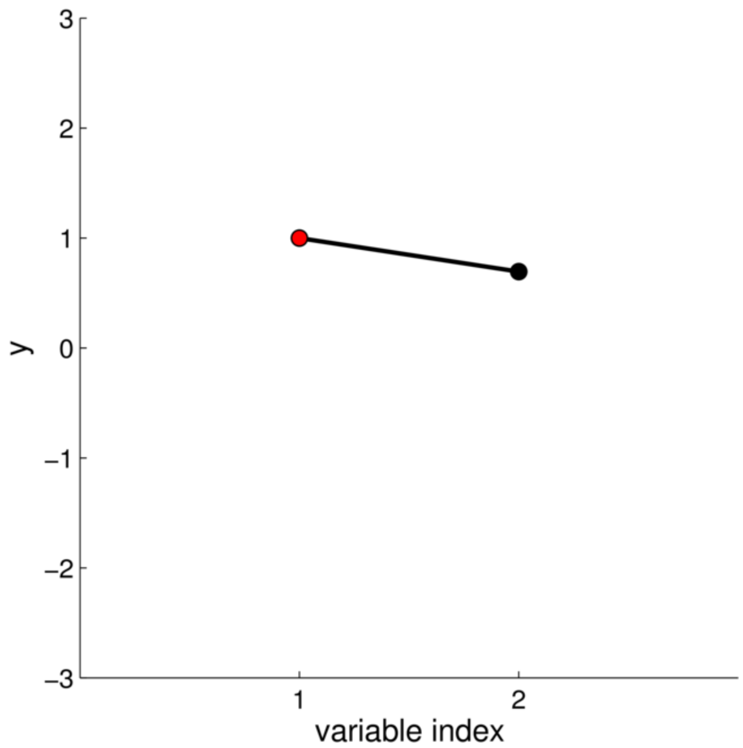
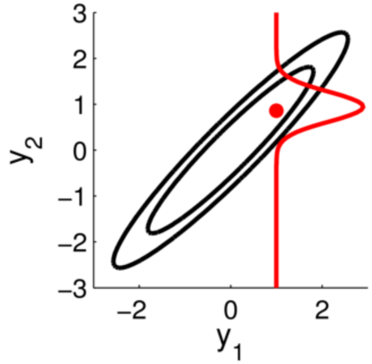


Visualizing Gaussian Processes



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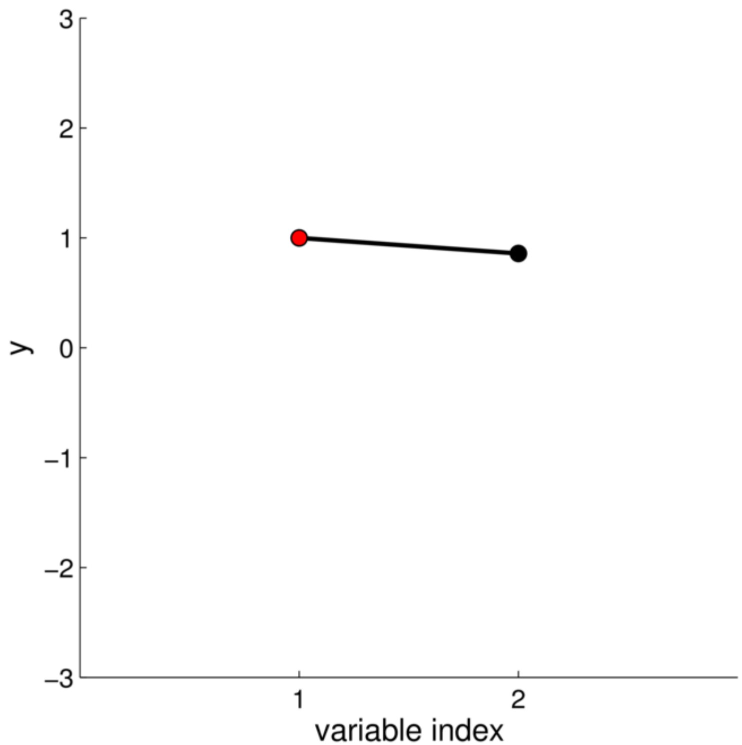
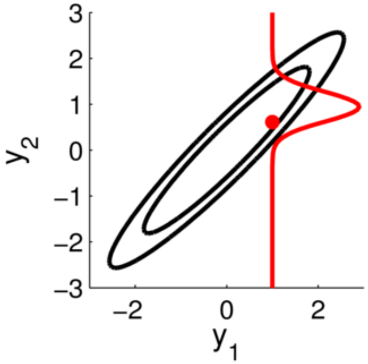


Visualizing Gaussian Processes



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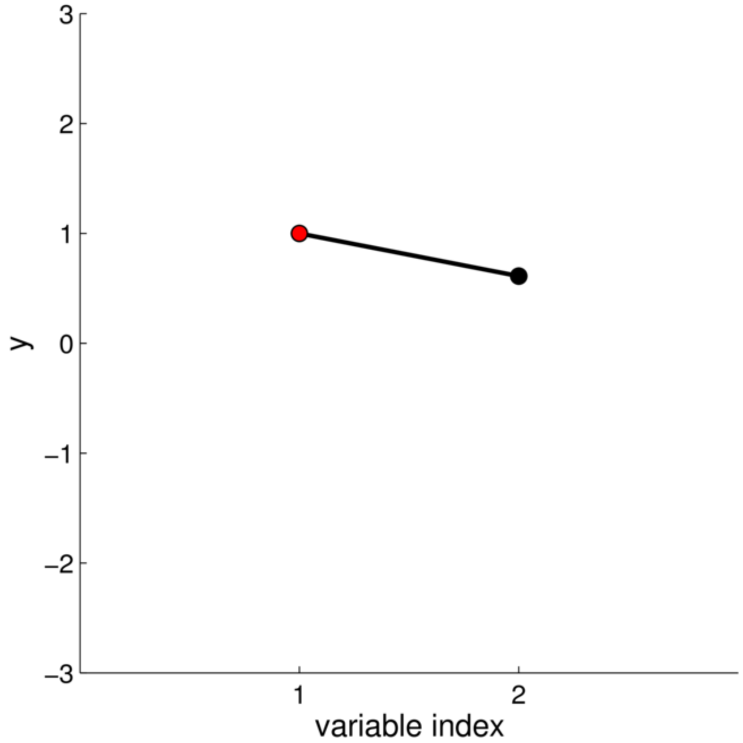
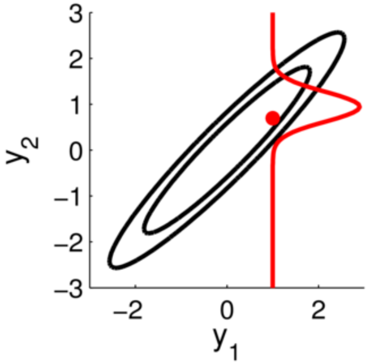
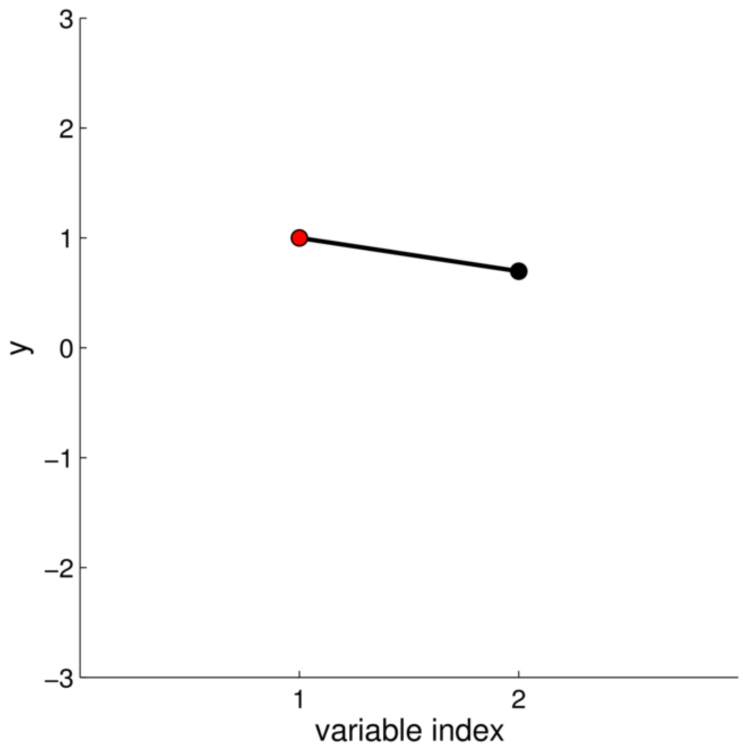


Visualizing Gaussian Processes





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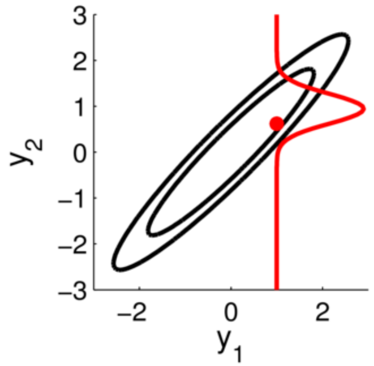
Visualizing Gaussian Processes



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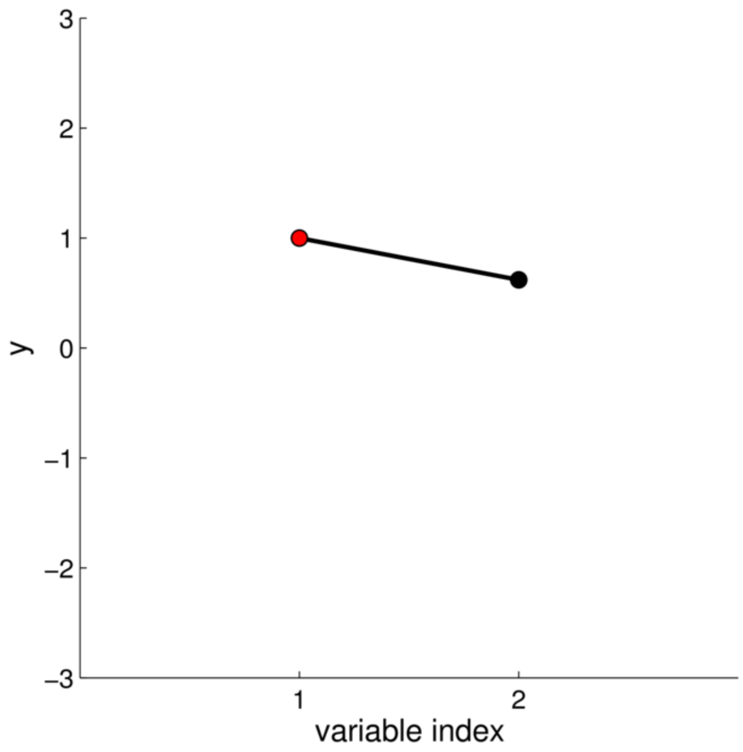
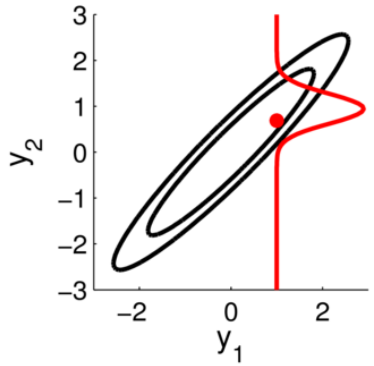


Visualizing Gaussian Processes



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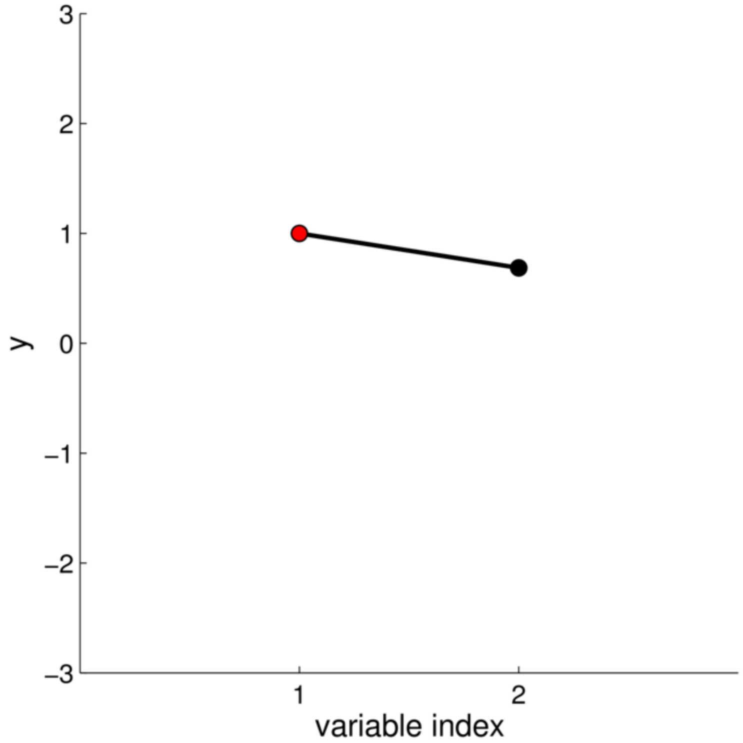
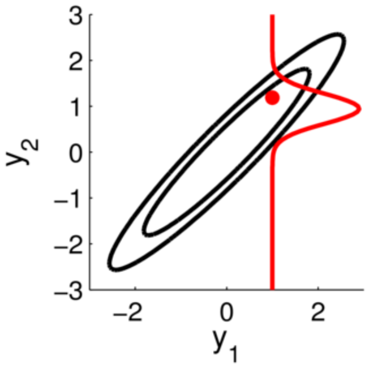


Visualizing Gaussian Processes



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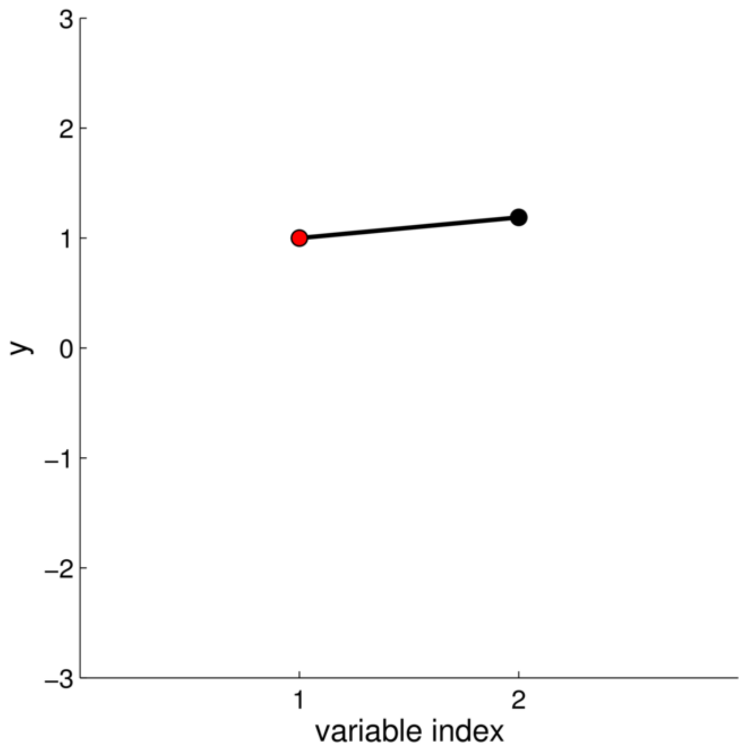

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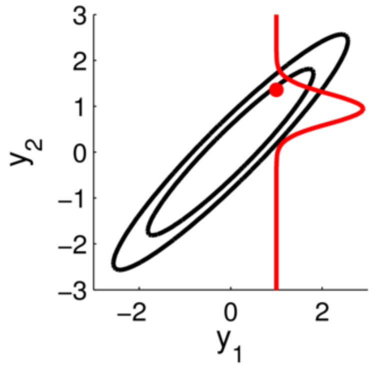

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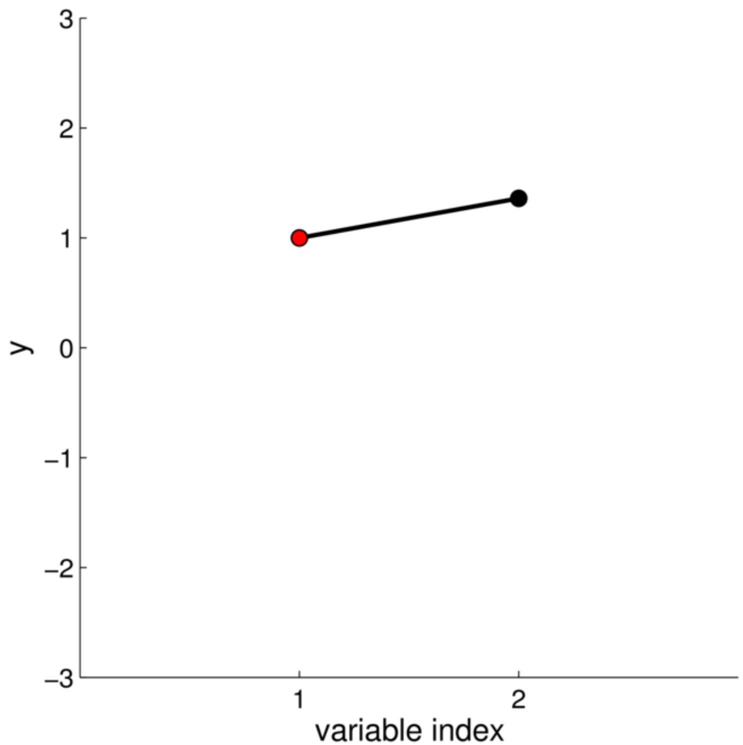
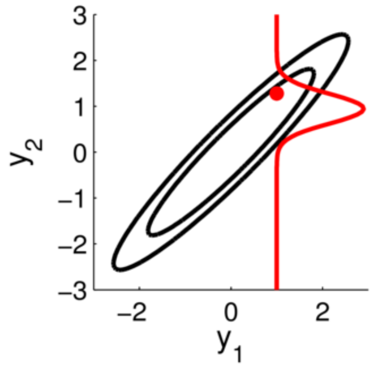


Visualizing Gaussian Processes



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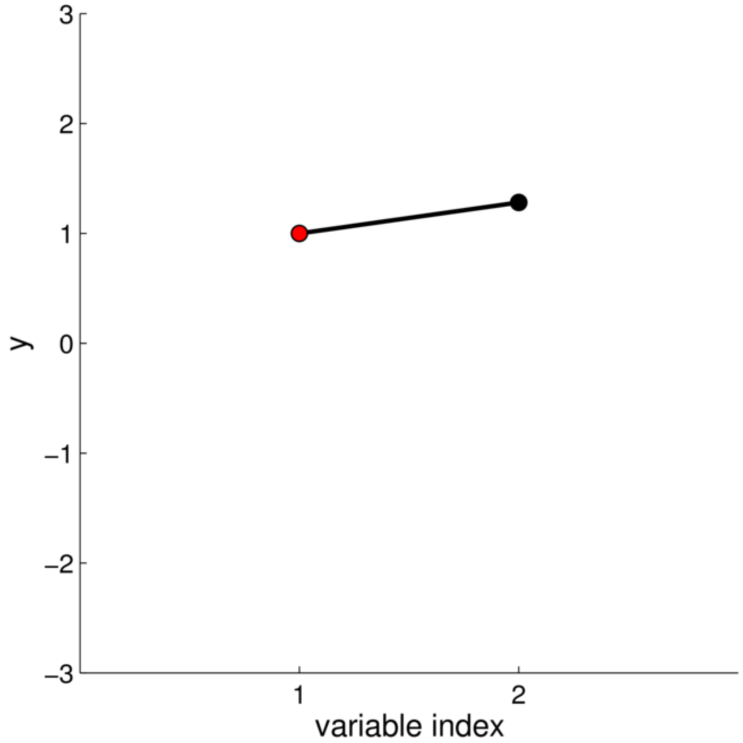
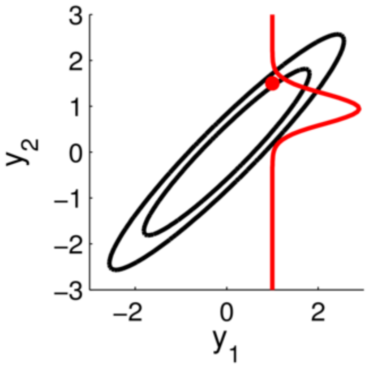


Visualizing Gaussian Processes



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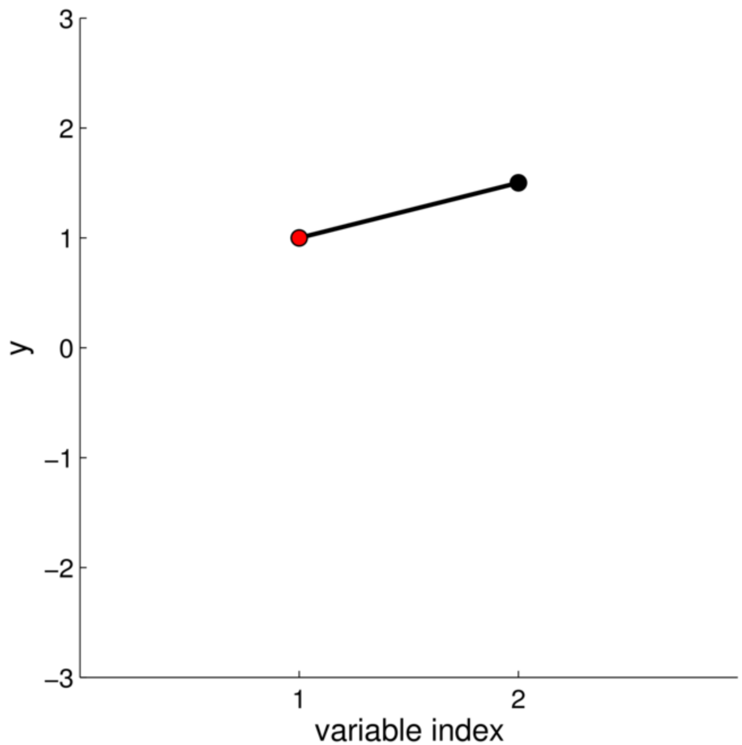

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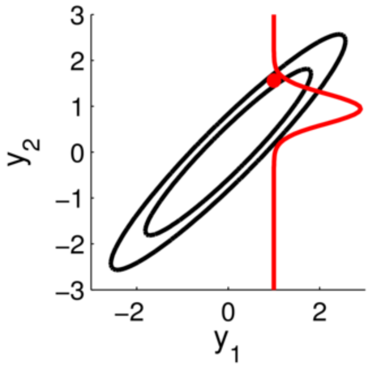

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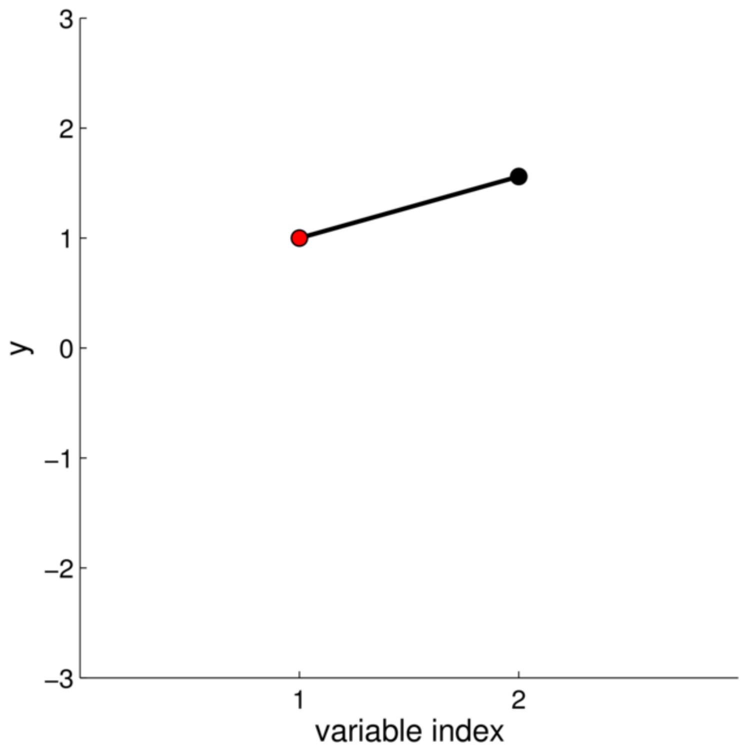

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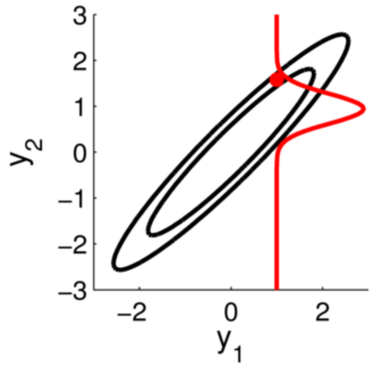

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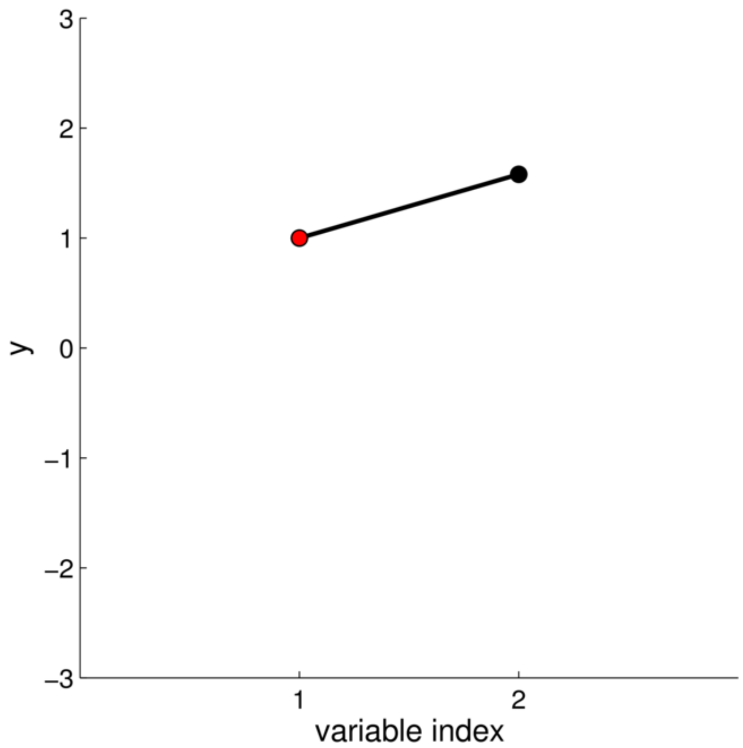
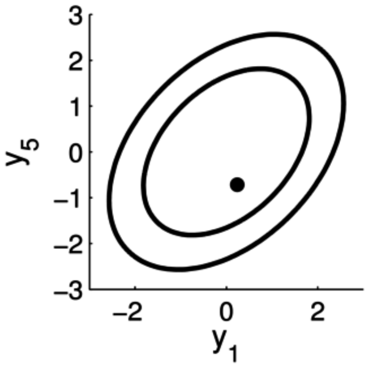


Visualizing Gaussian Processes



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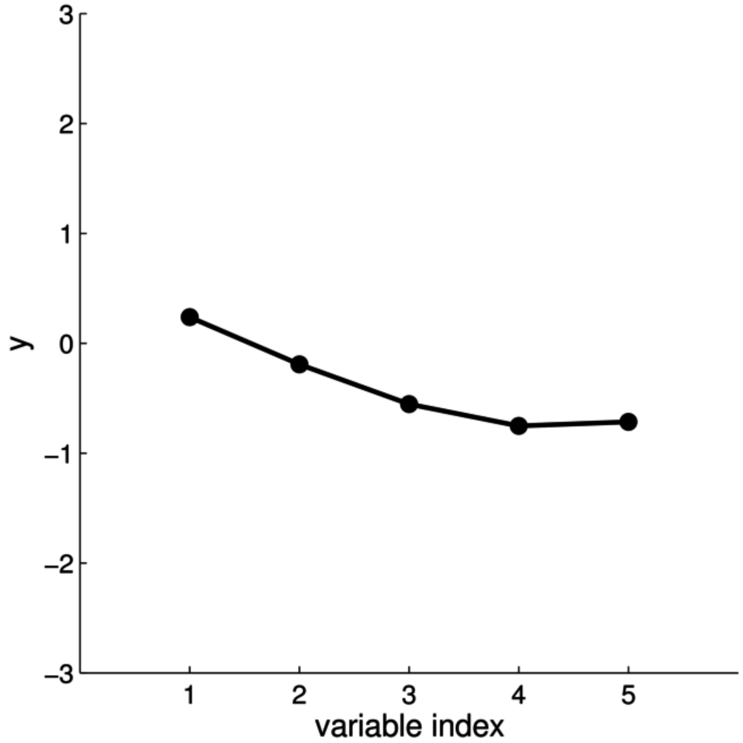

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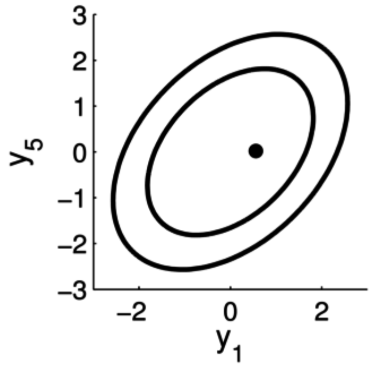

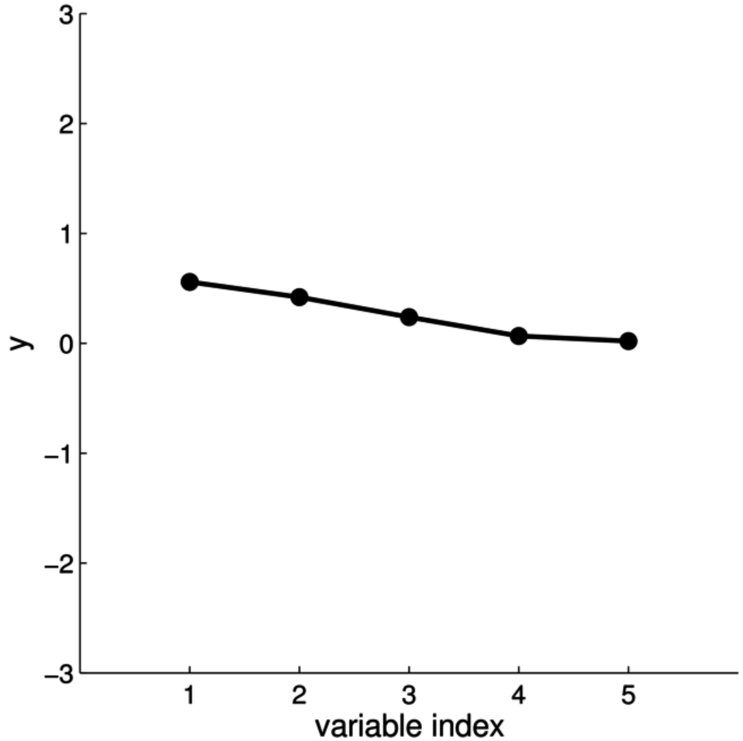

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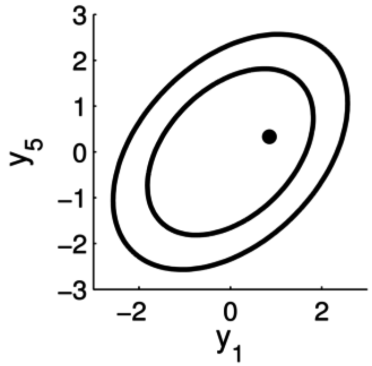
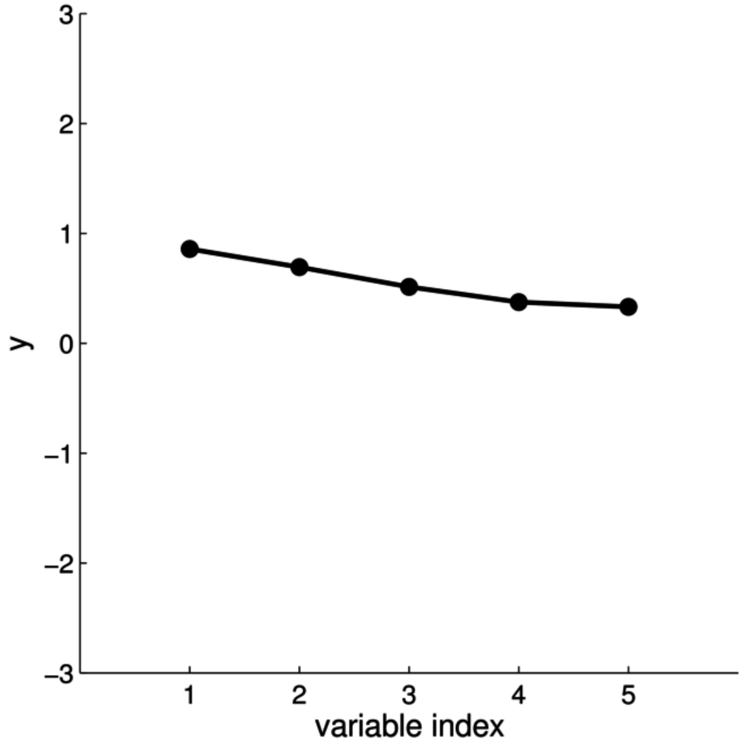
Visualizing Gaussian Processes





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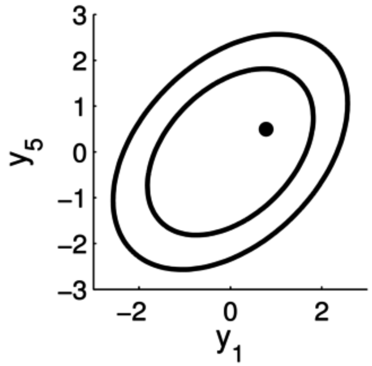
Visualizing Gaussian Processes



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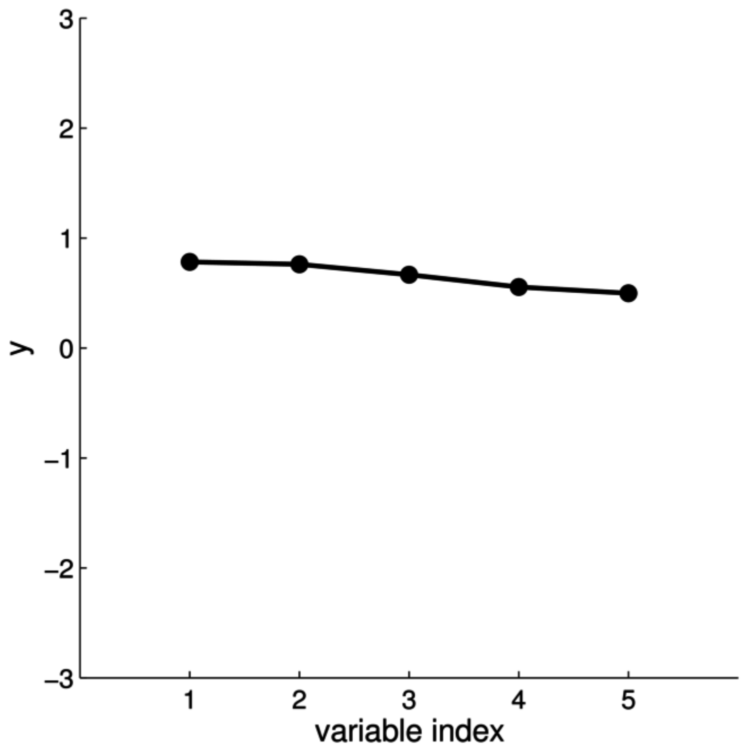

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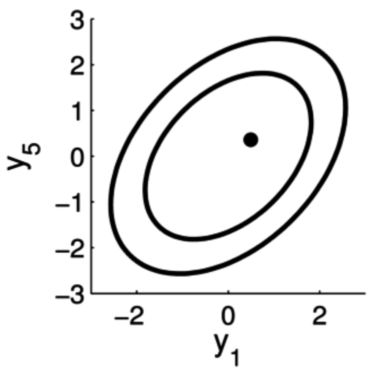

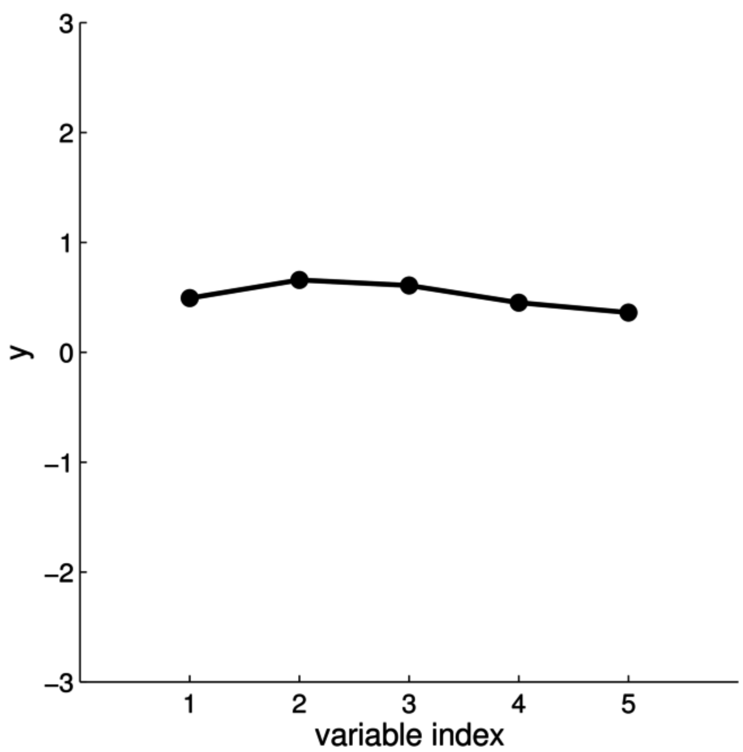

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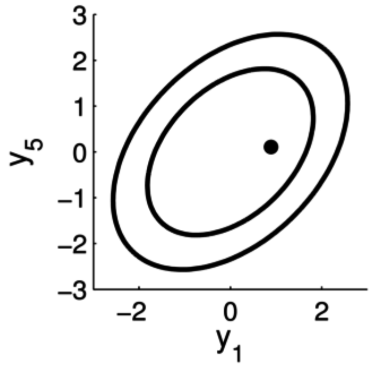

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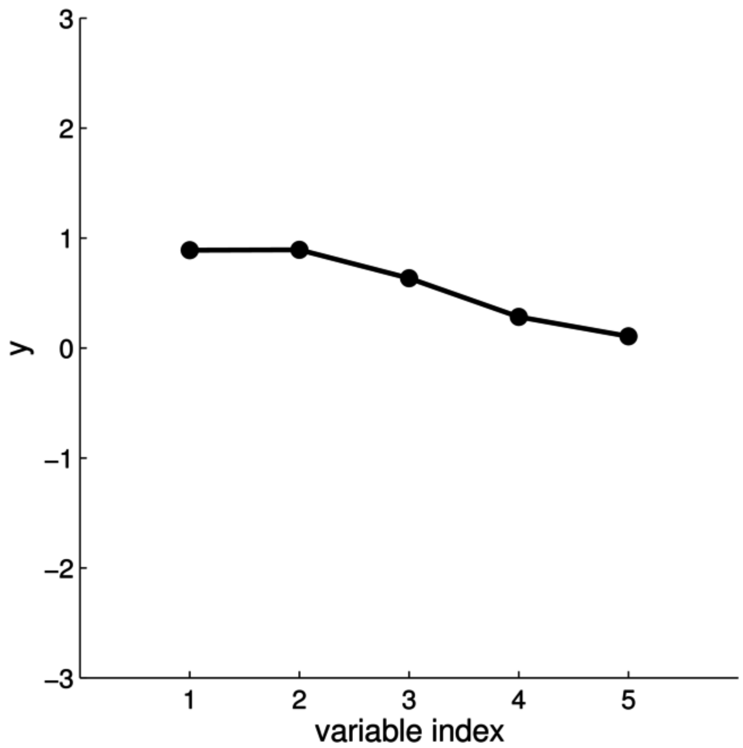

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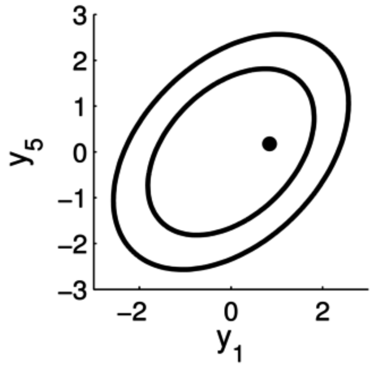

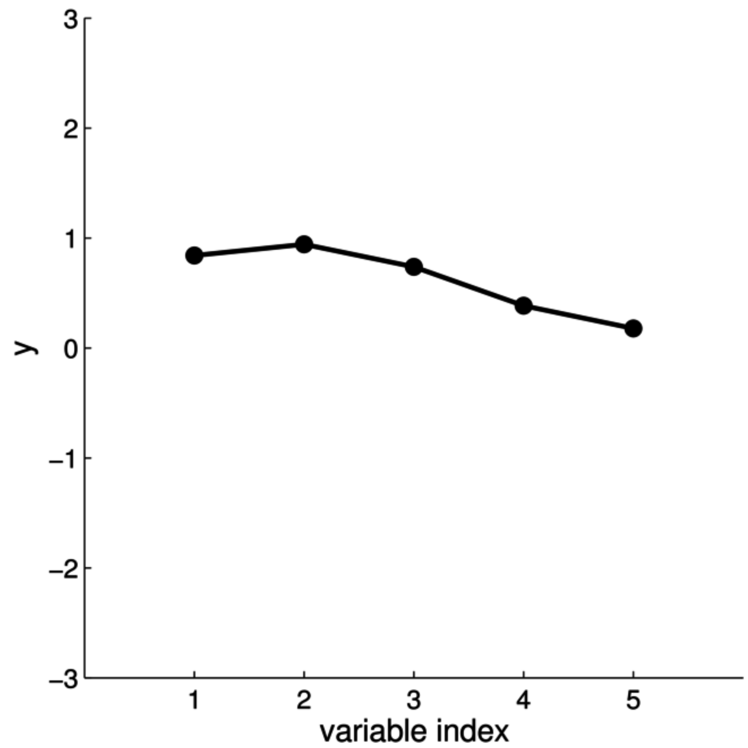

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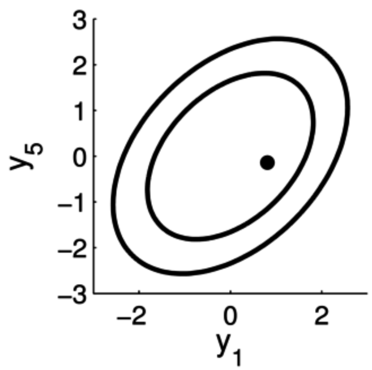
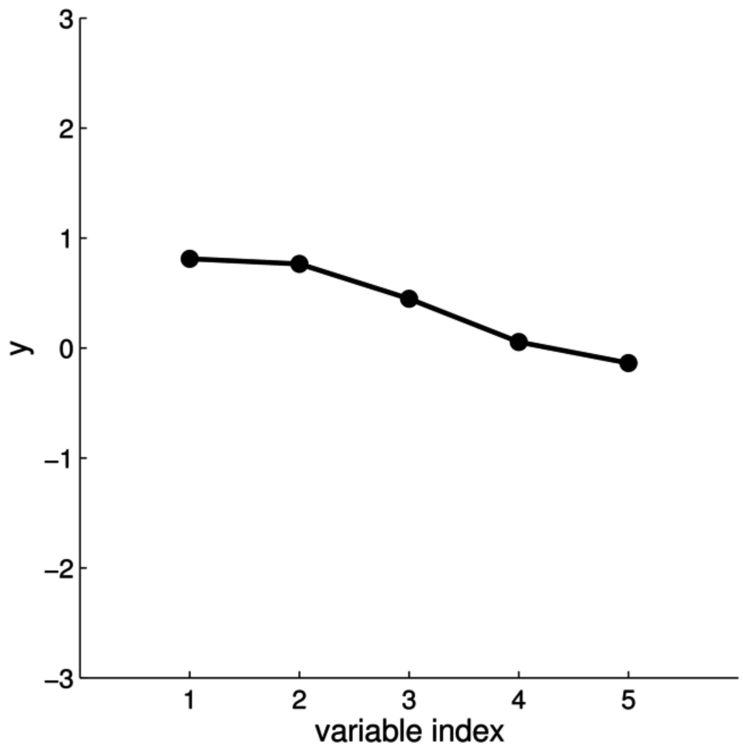
Visualizing Gaussian Processes





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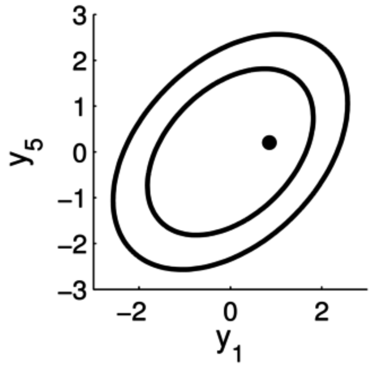
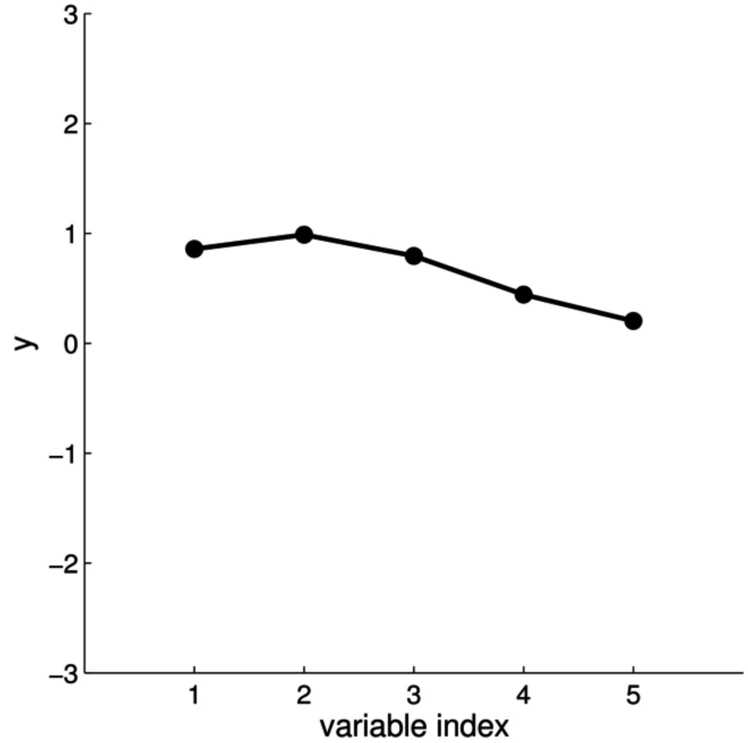
Visualizing Gaussian Processes





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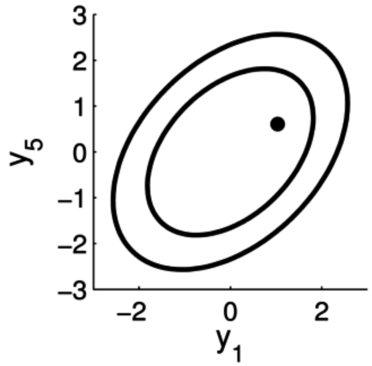
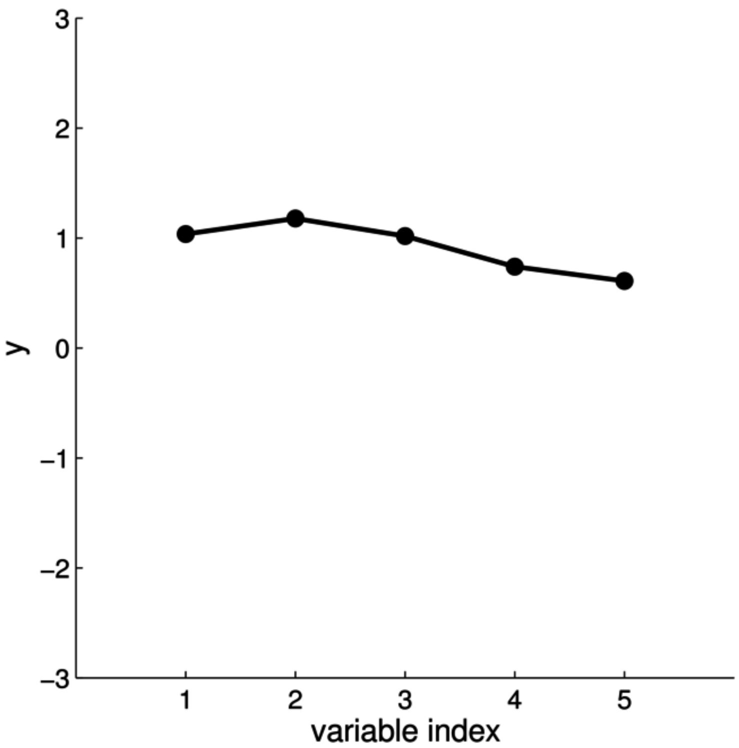
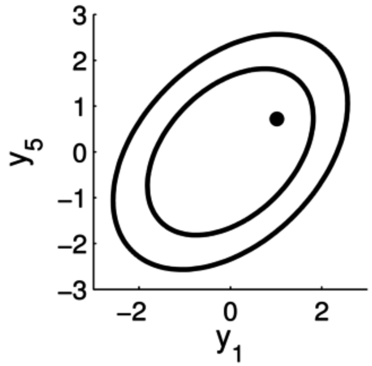
Visualizing Gaussian Processes

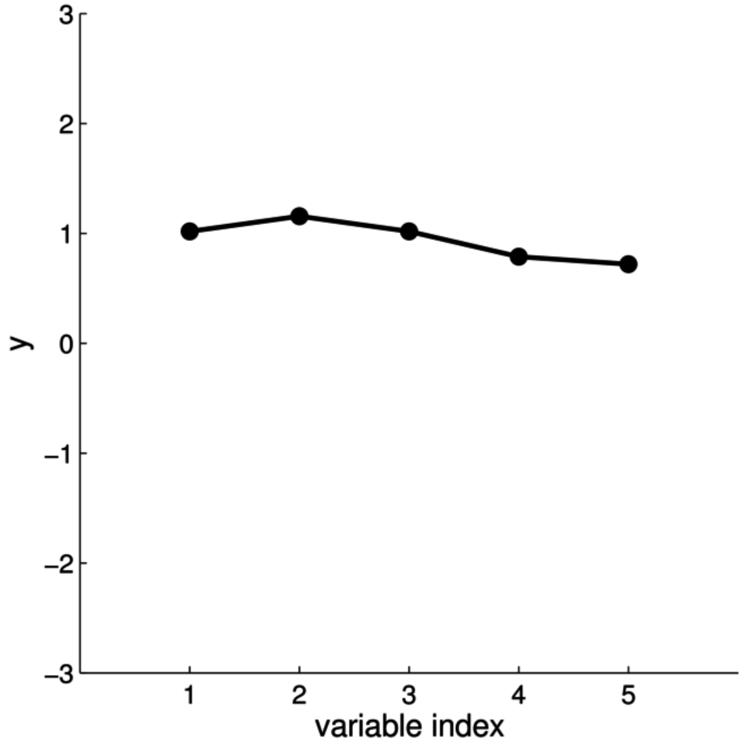




$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

Visualizing Gaussian Processes





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

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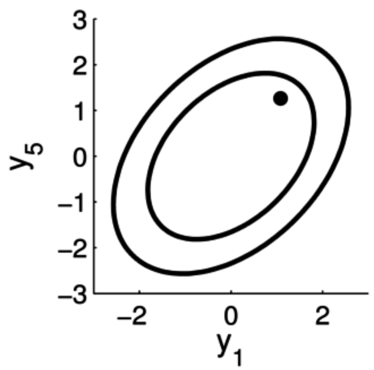

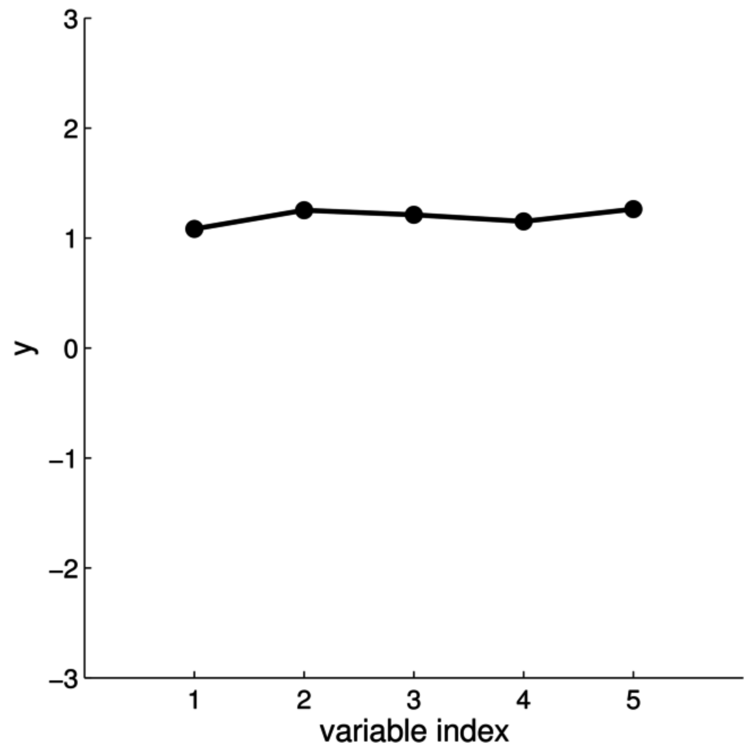

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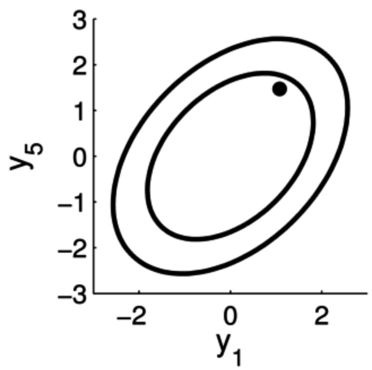
Visualizing Gaussian Processes



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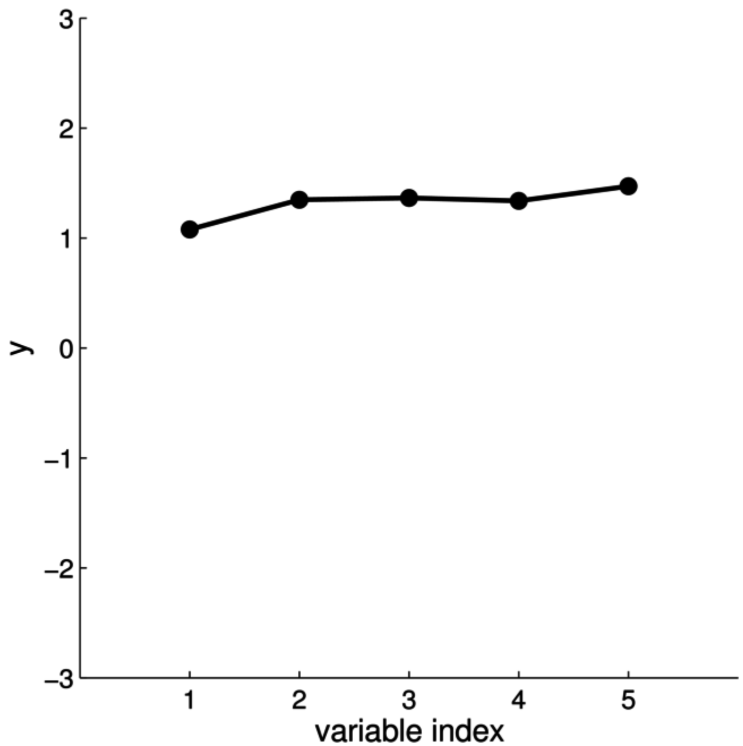
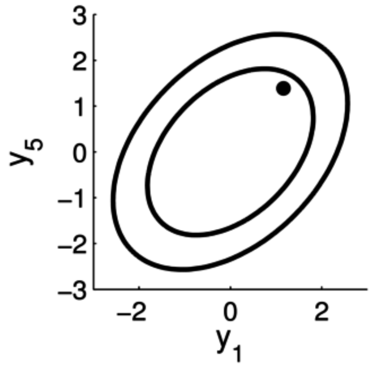
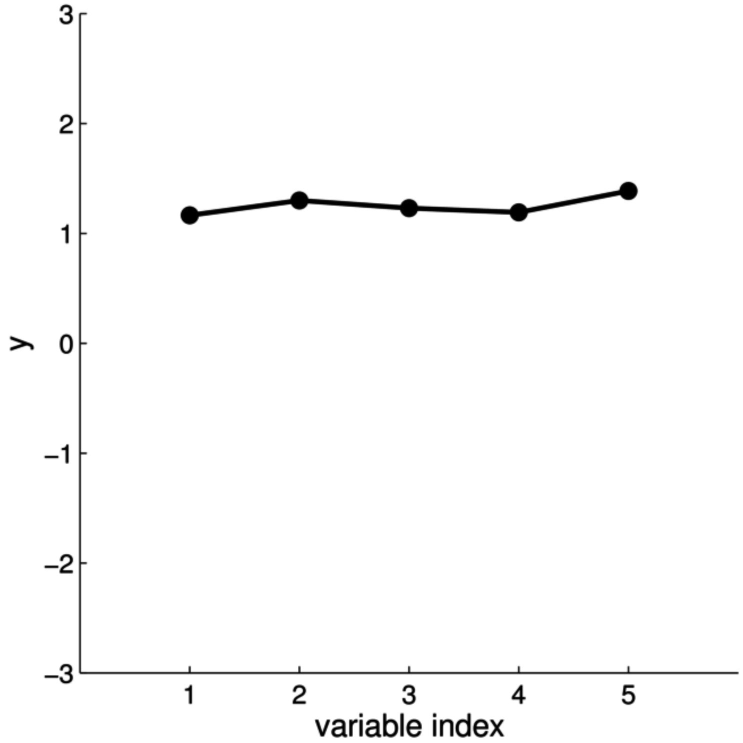


Visualizing Gaussian Processes





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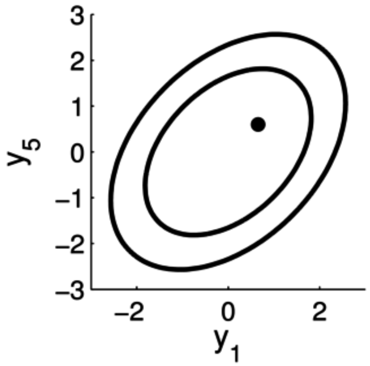
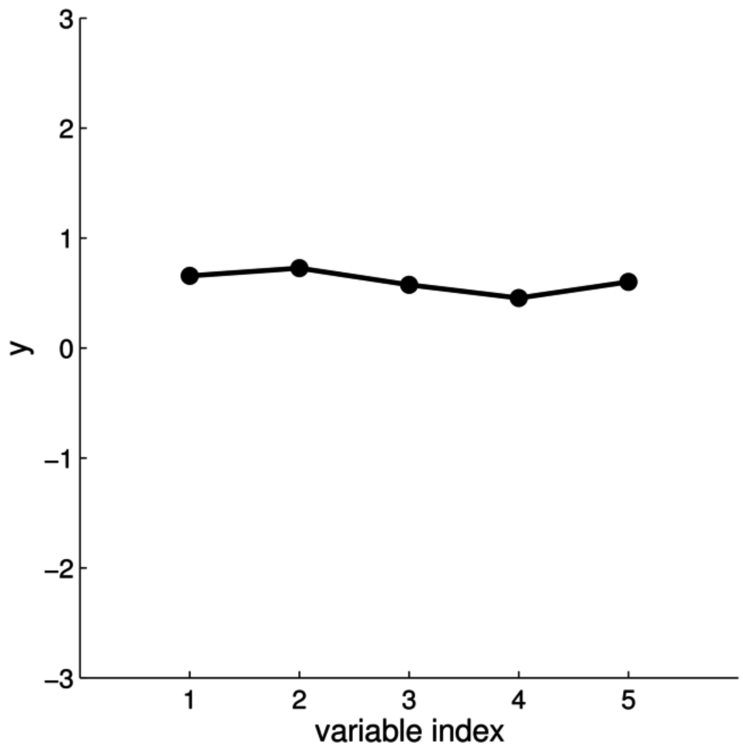
Visualizing Gaussian Processes





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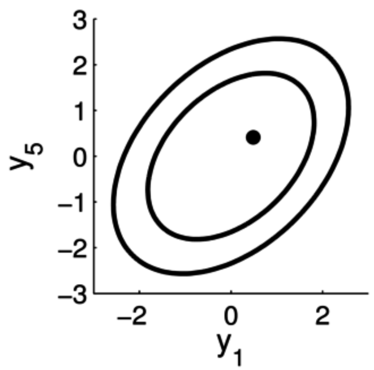
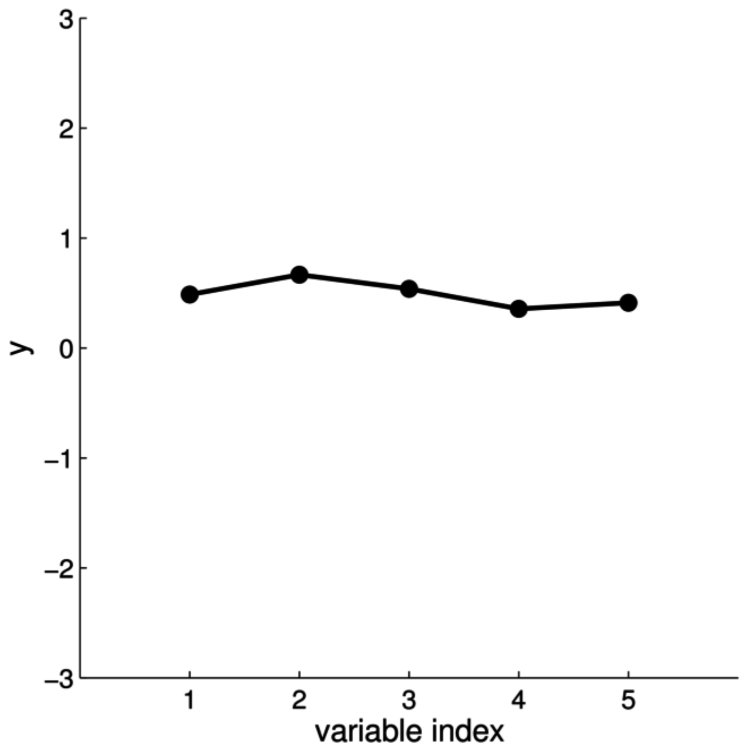
Visualizing Gaussian Processes





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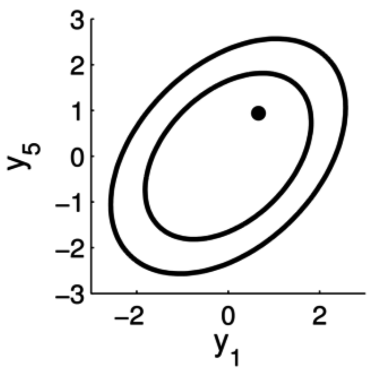
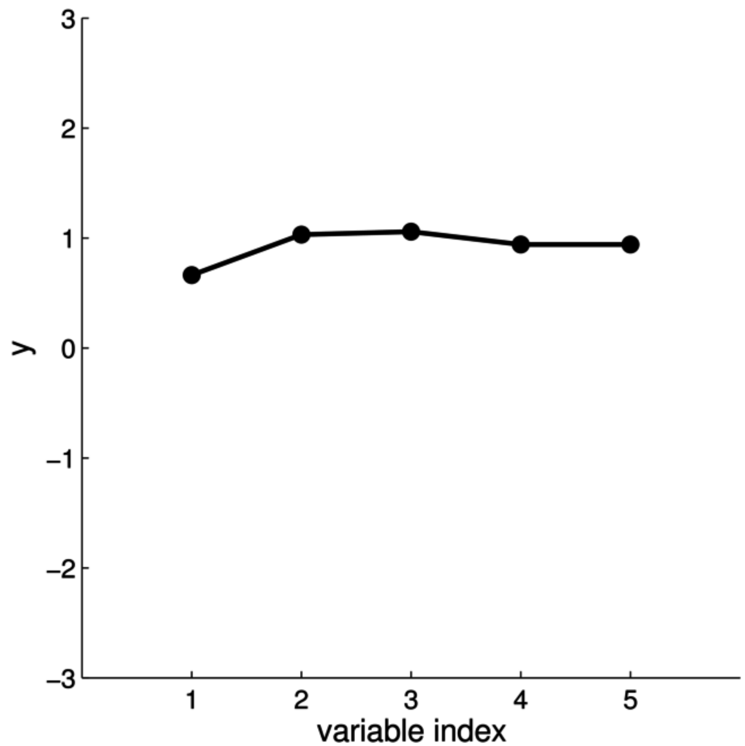
Visualizing Gaussian Processes





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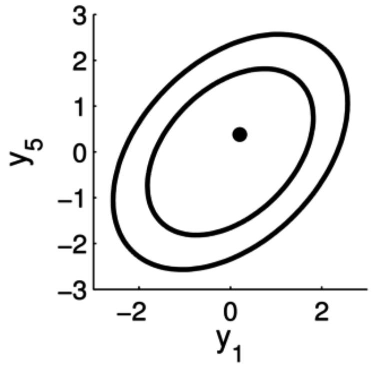
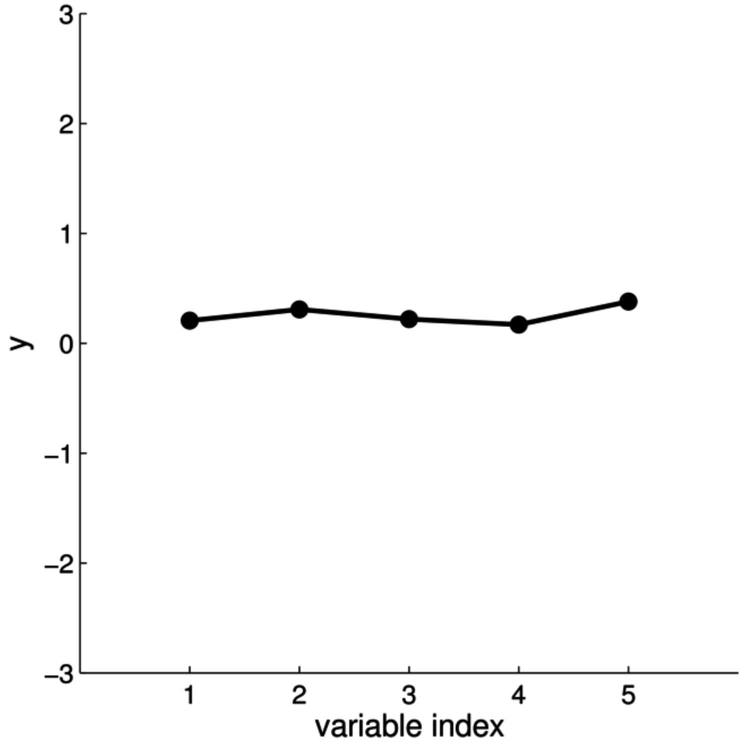
Visualizing Gaussian Processes





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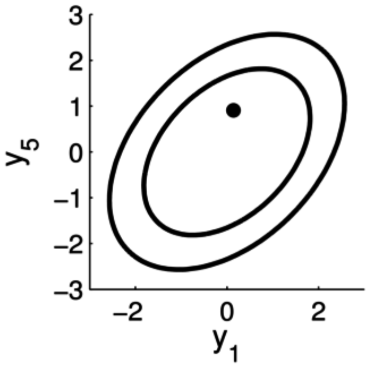
Visualizing Gaussian Processes



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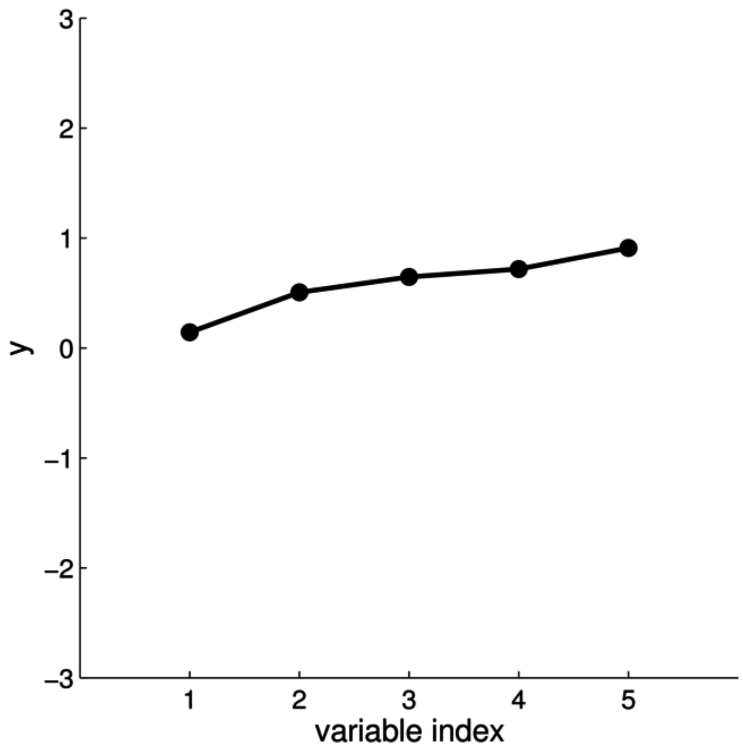
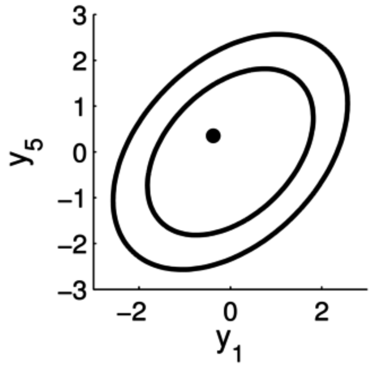
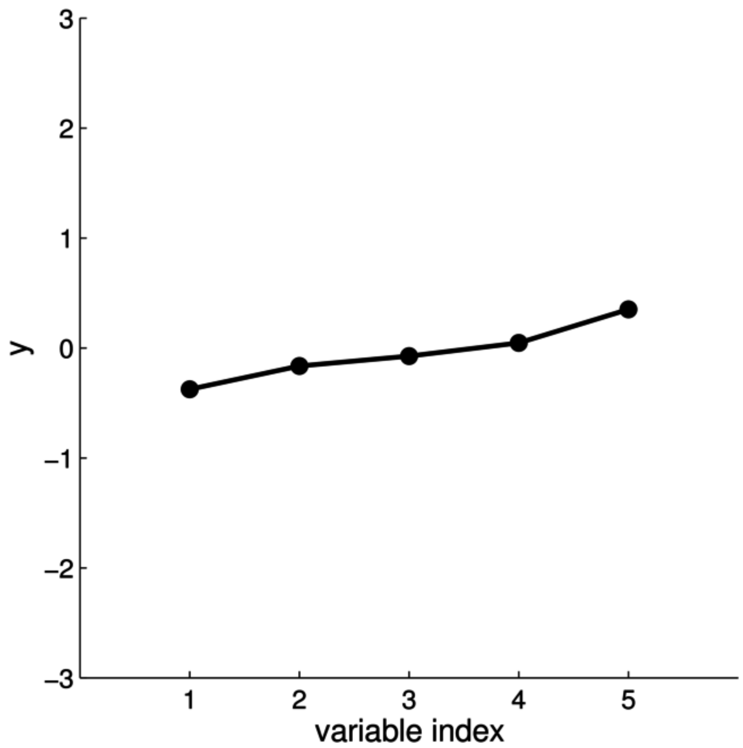


Visualizing Gaussian Processes





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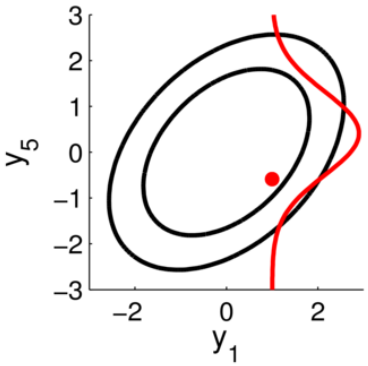
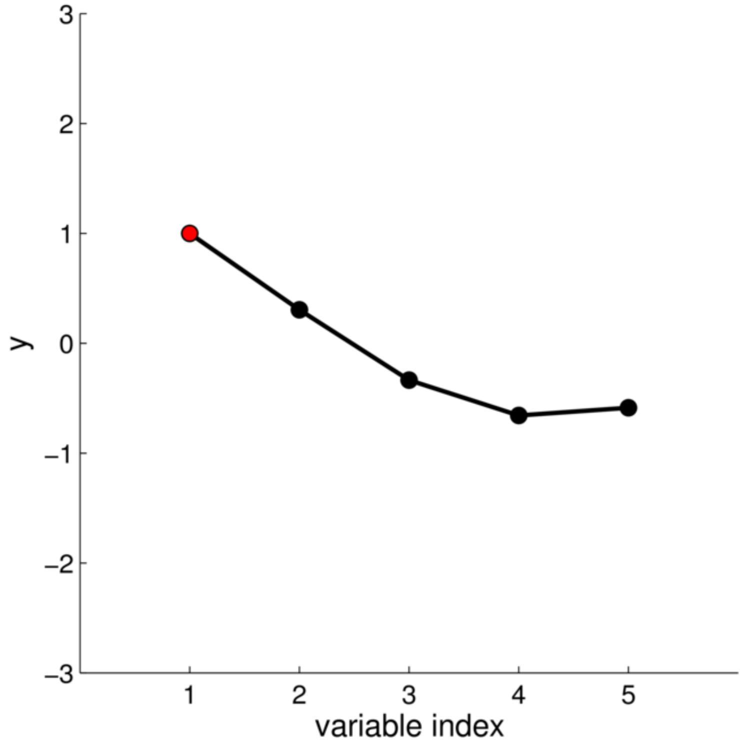
Visualizing Gaussian Processes





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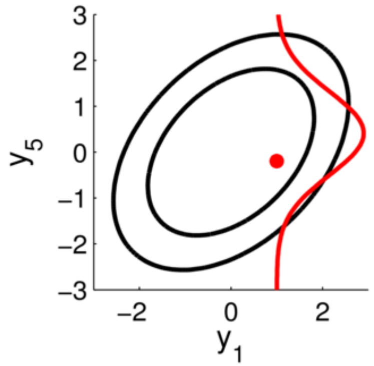

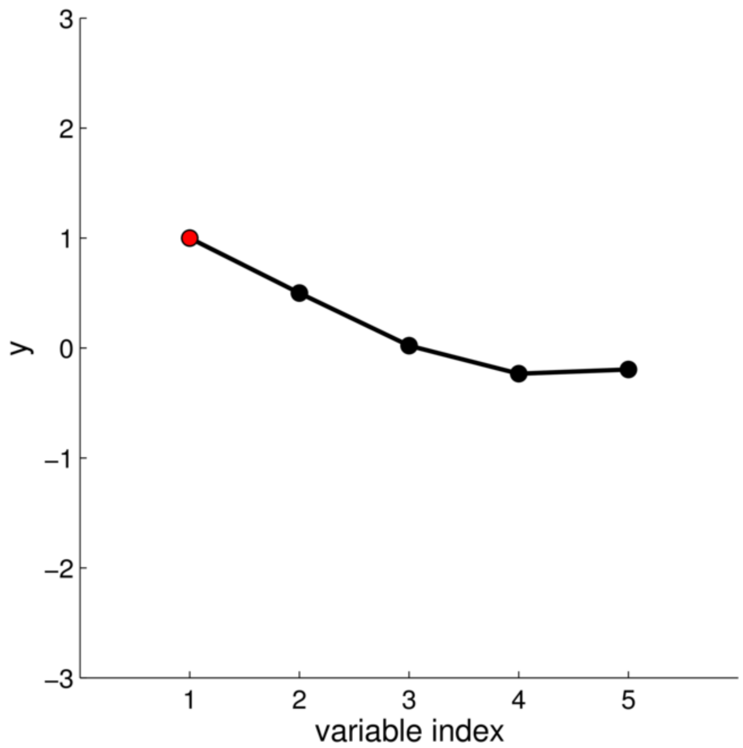

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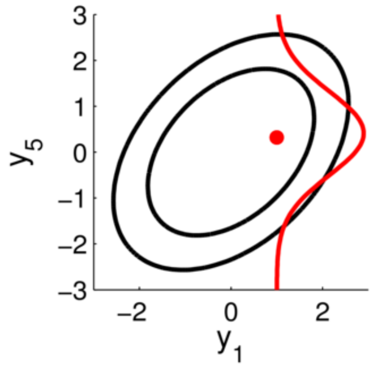

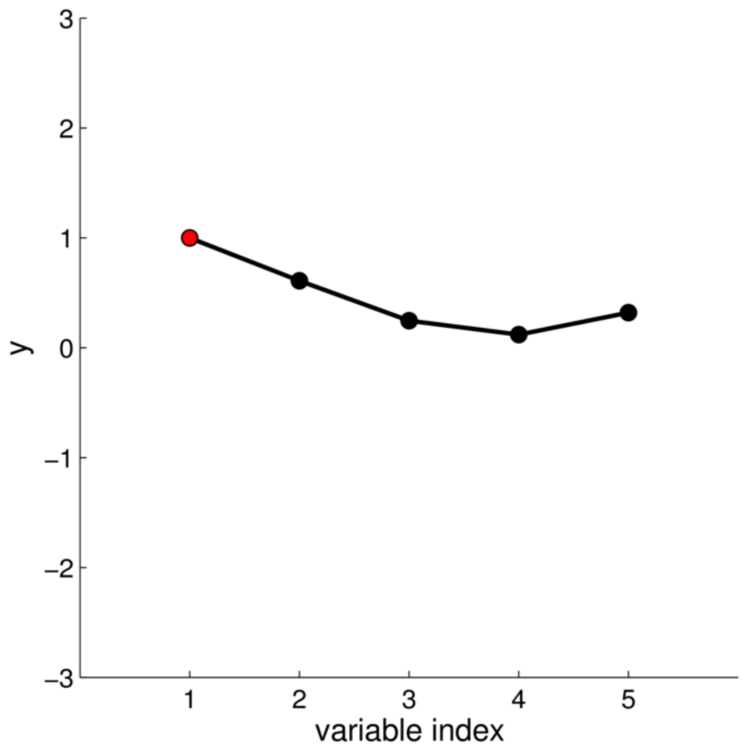

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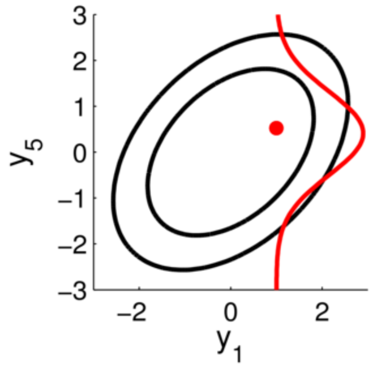

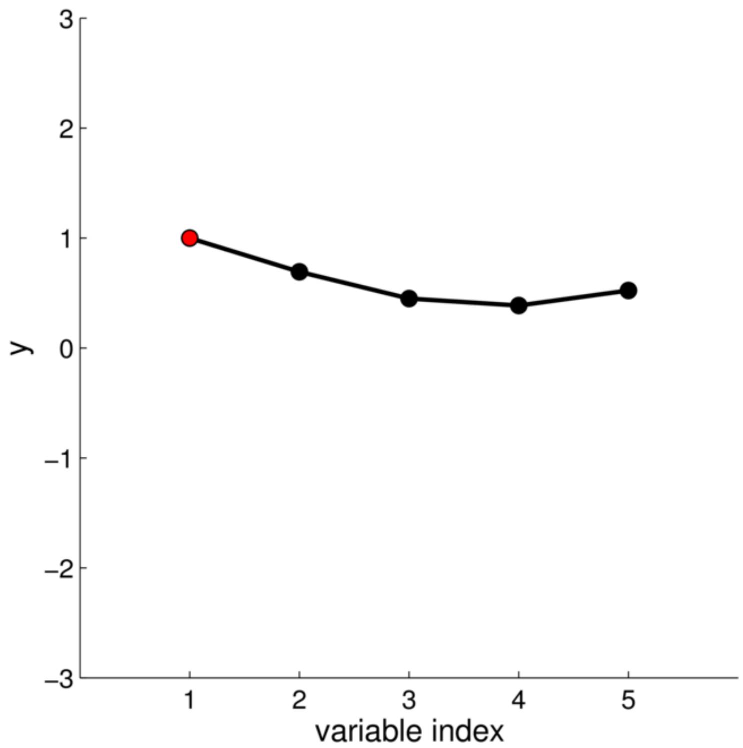

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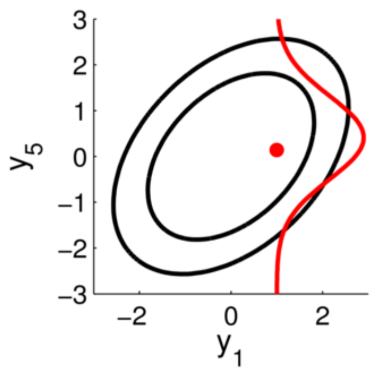

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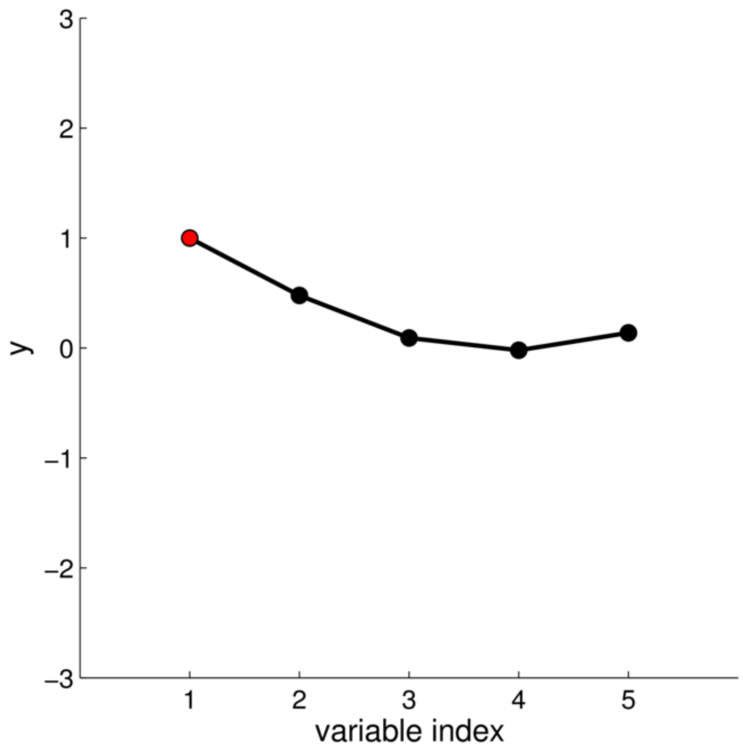
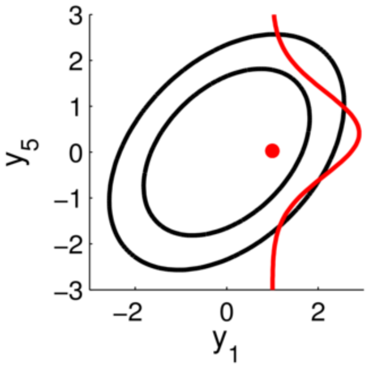
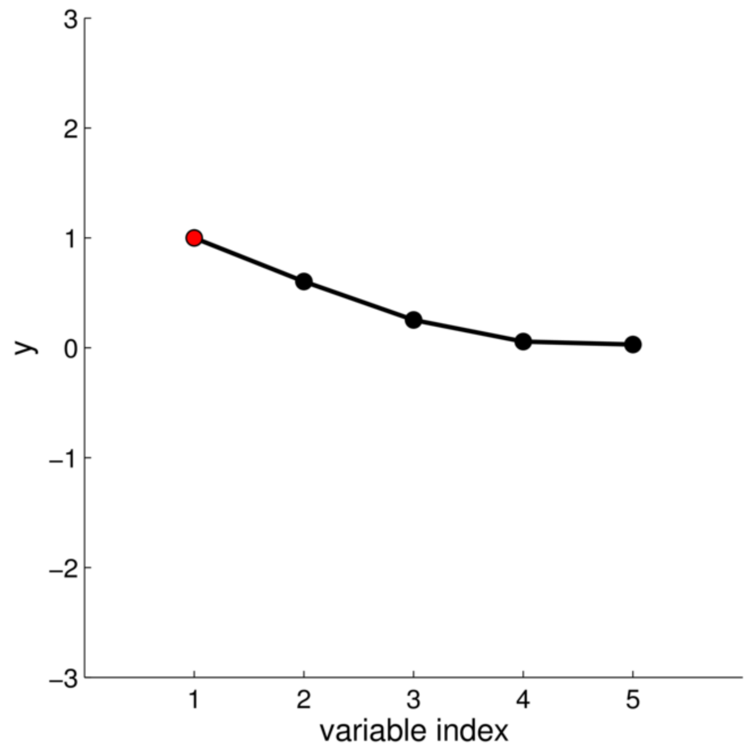


Visualizing Gaussian Processes





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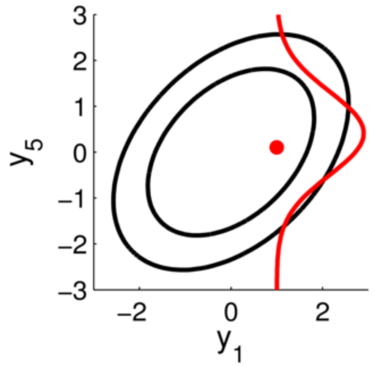

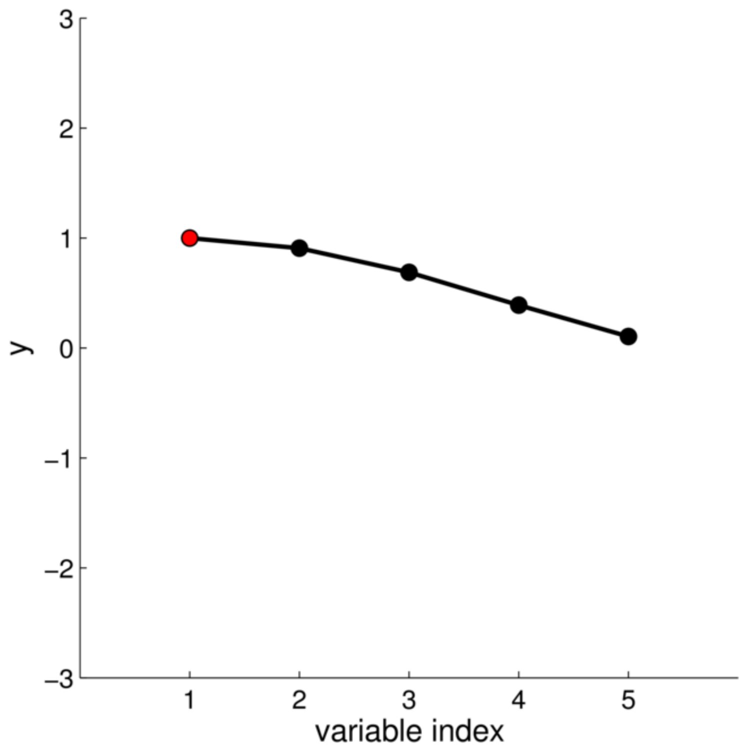

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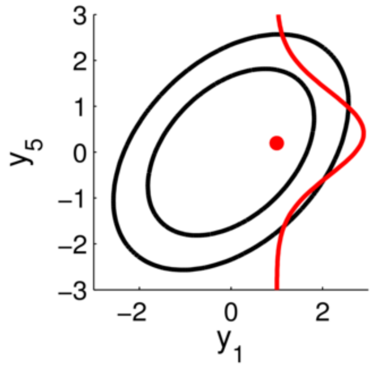

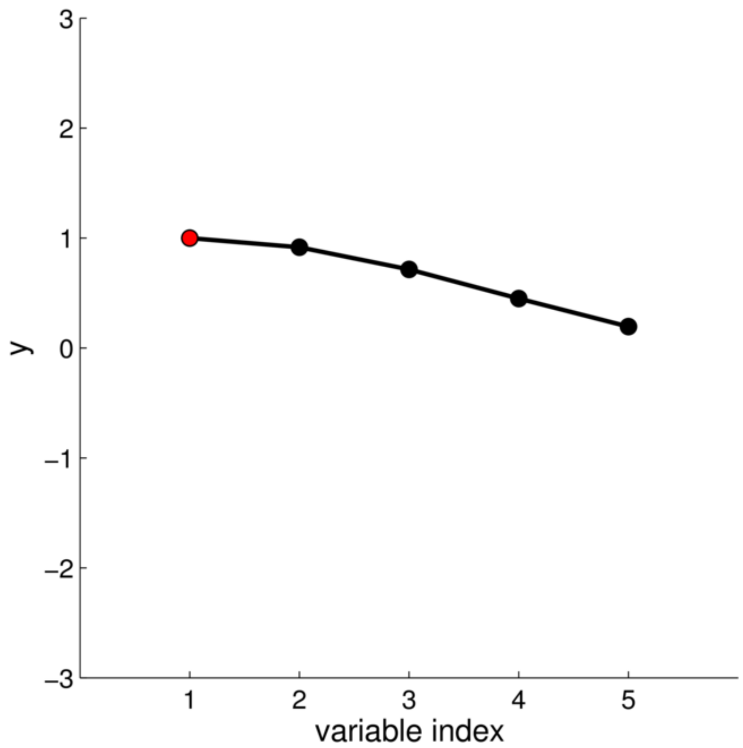

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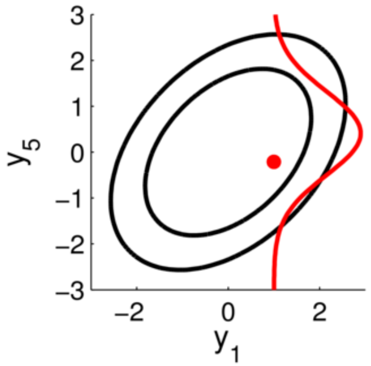

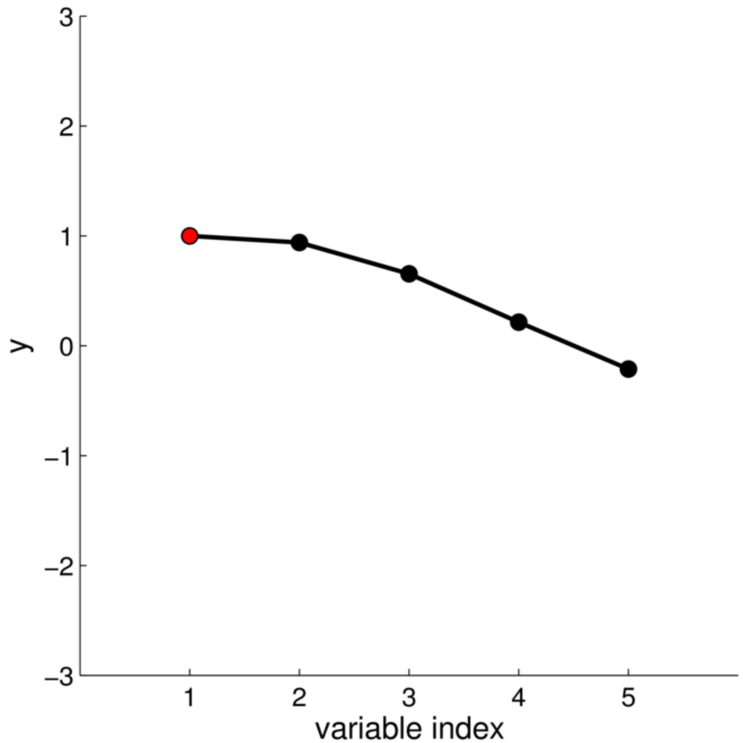

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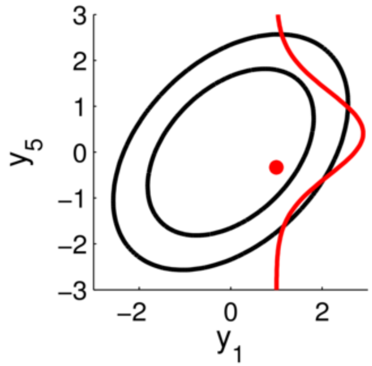
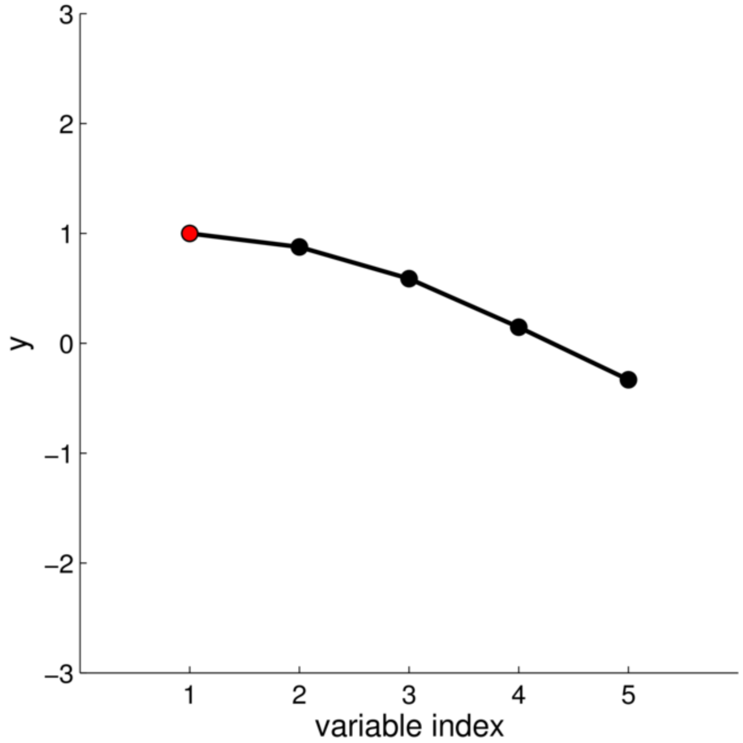
Visualizing Gaussian Processes





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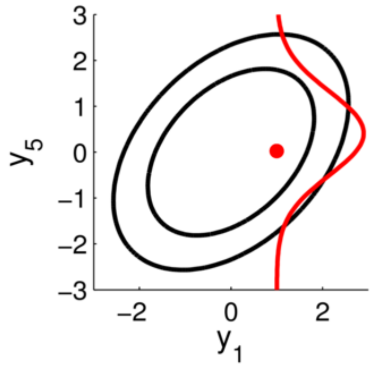
Visualizing Gaussian Processes



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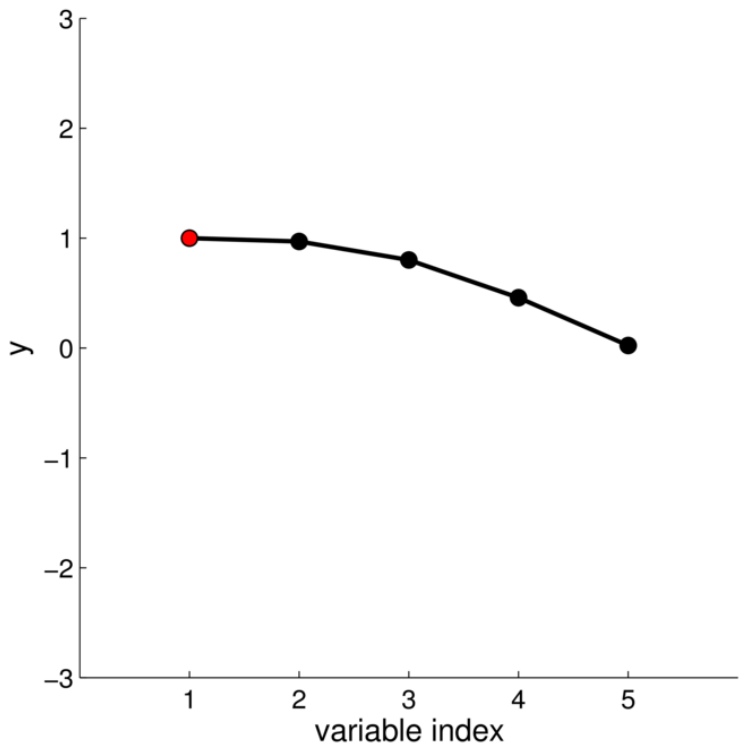

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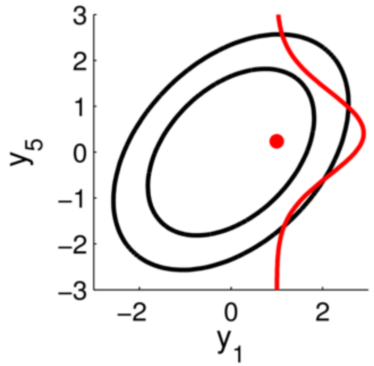

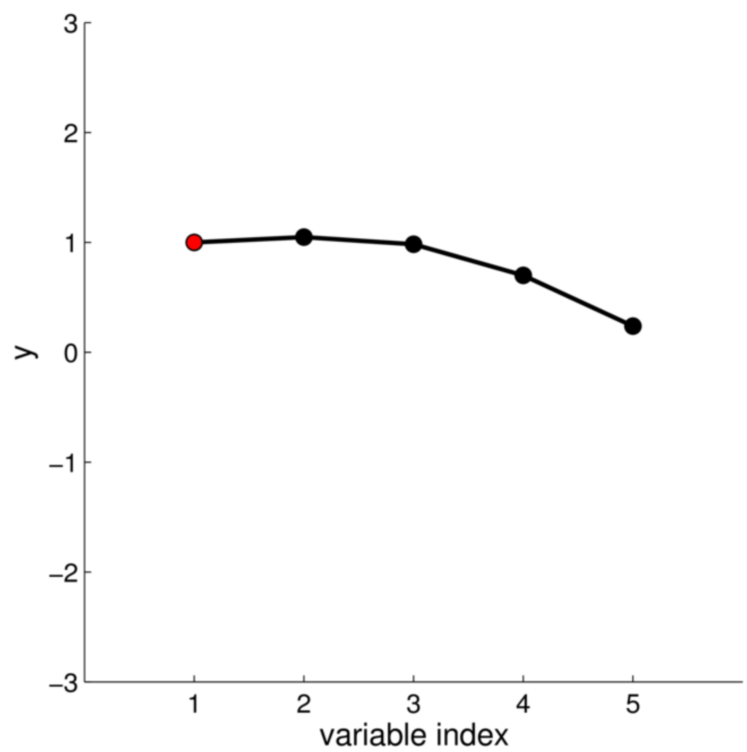

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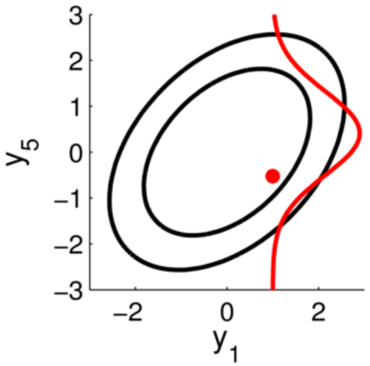

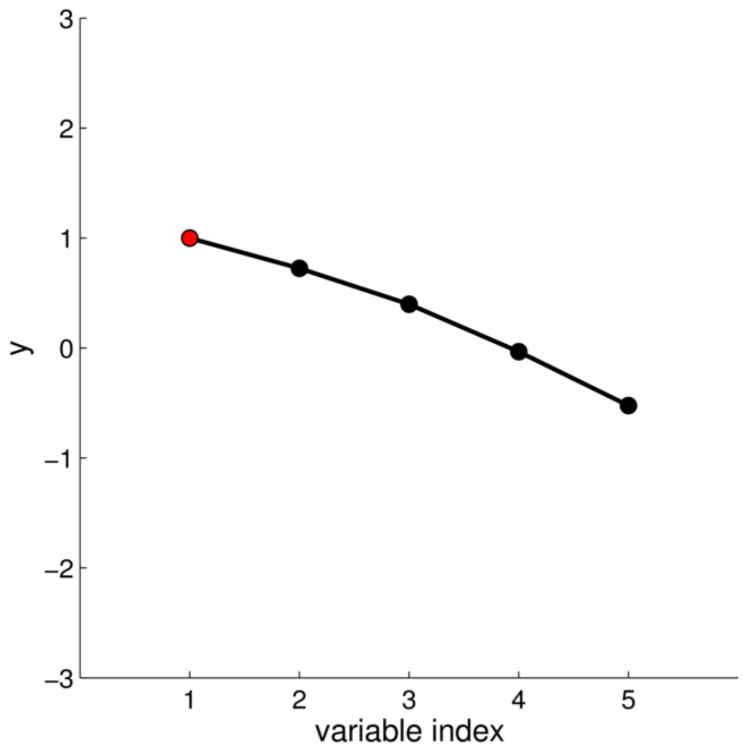

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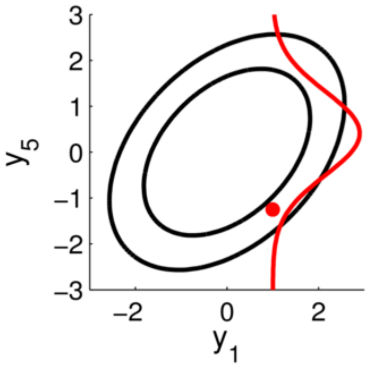

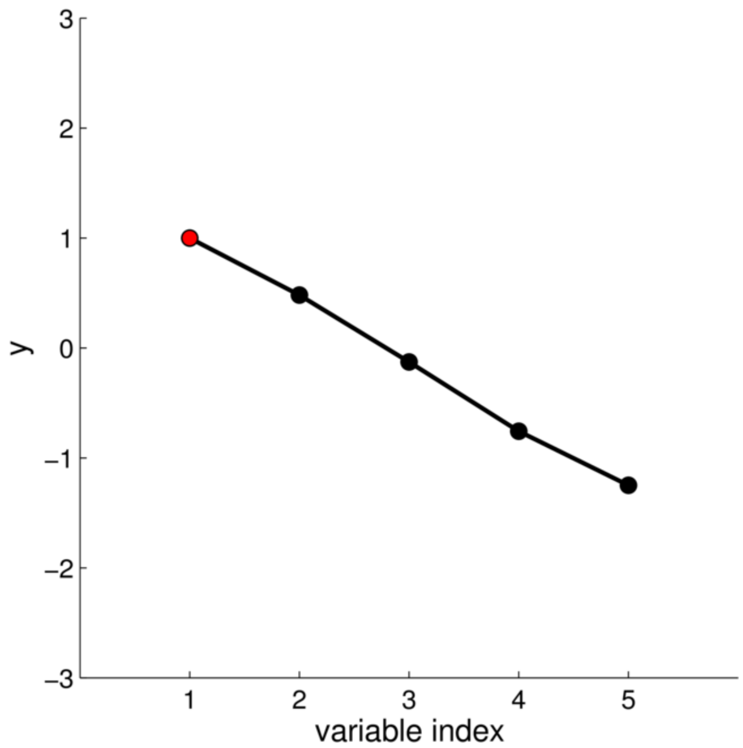

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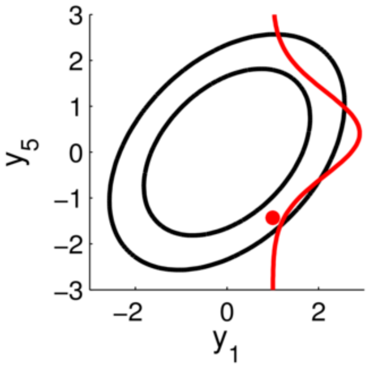

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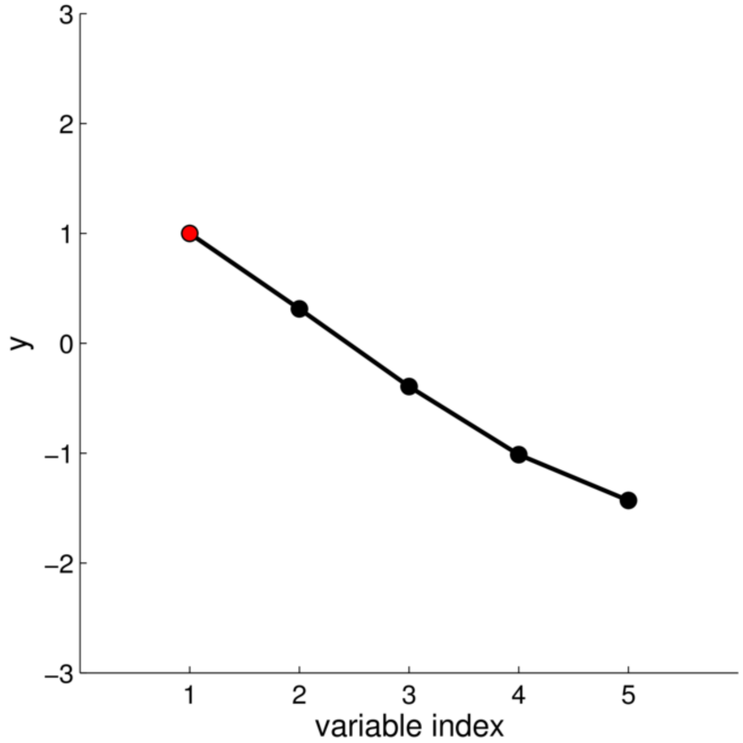

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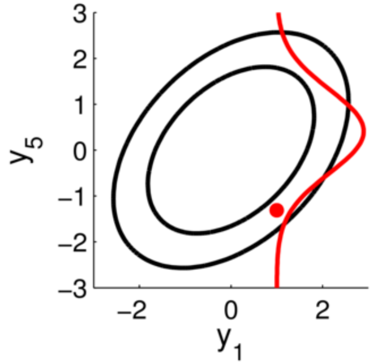

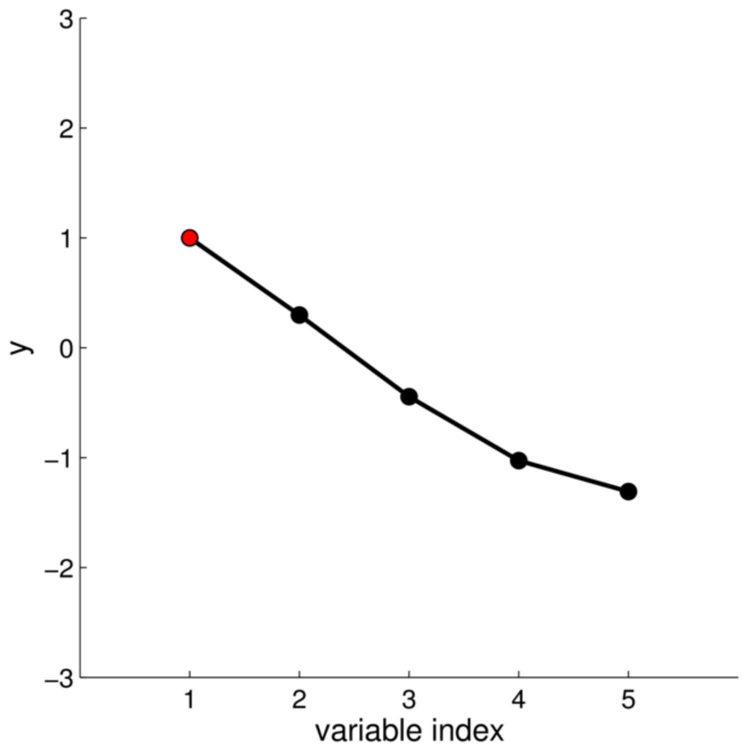

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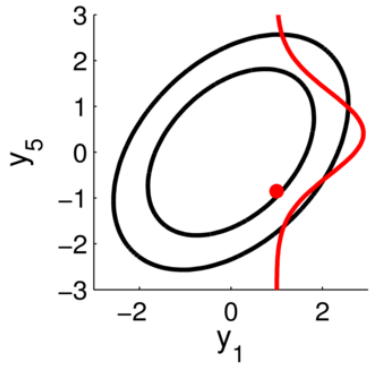
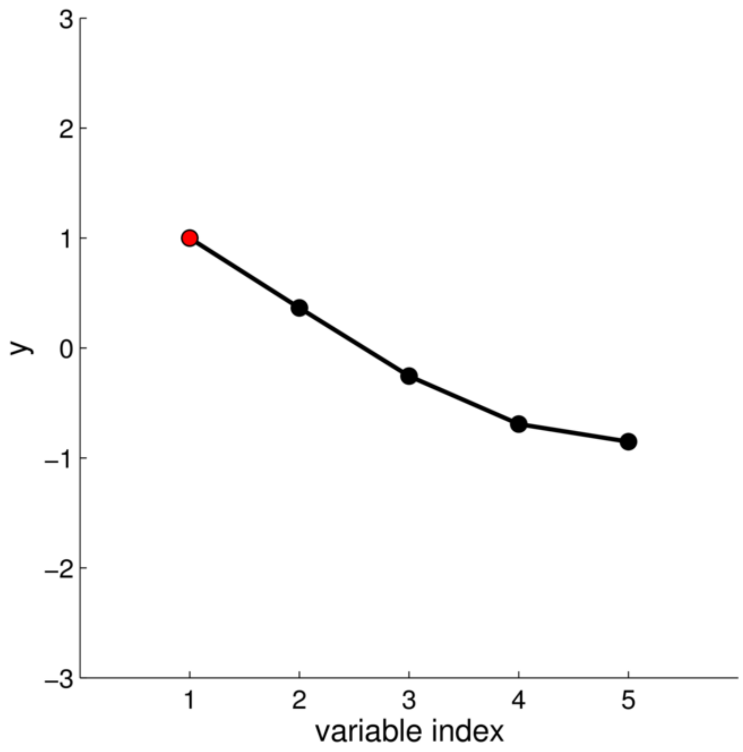
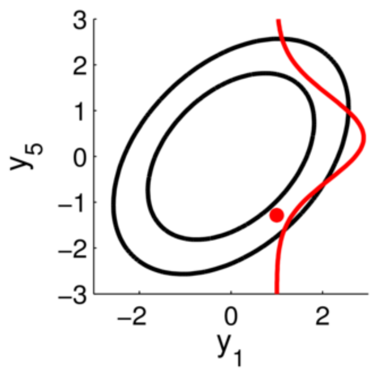
Visualizing Gaussian Processes

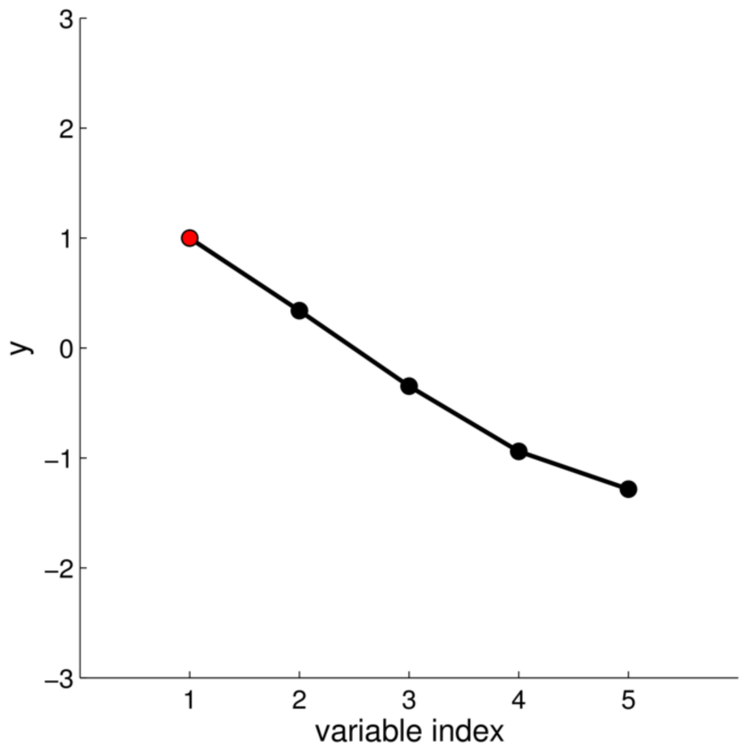




$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

Visualizing Gaussian Processes





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

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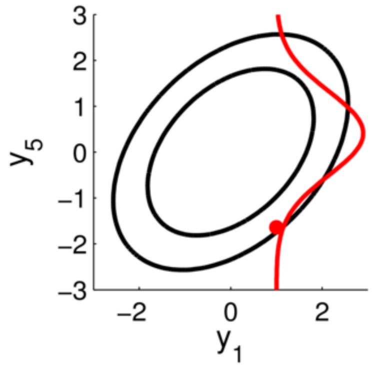

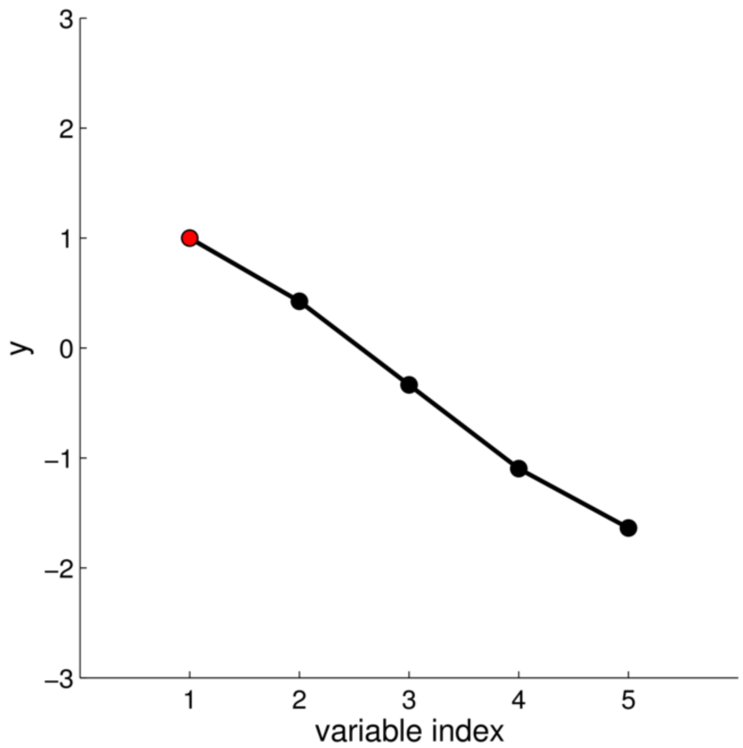

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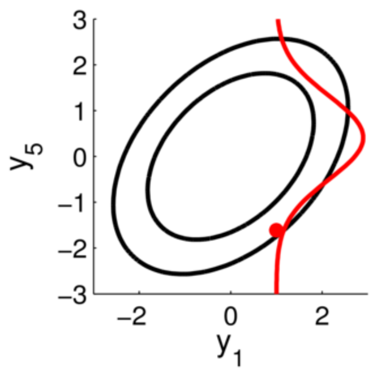
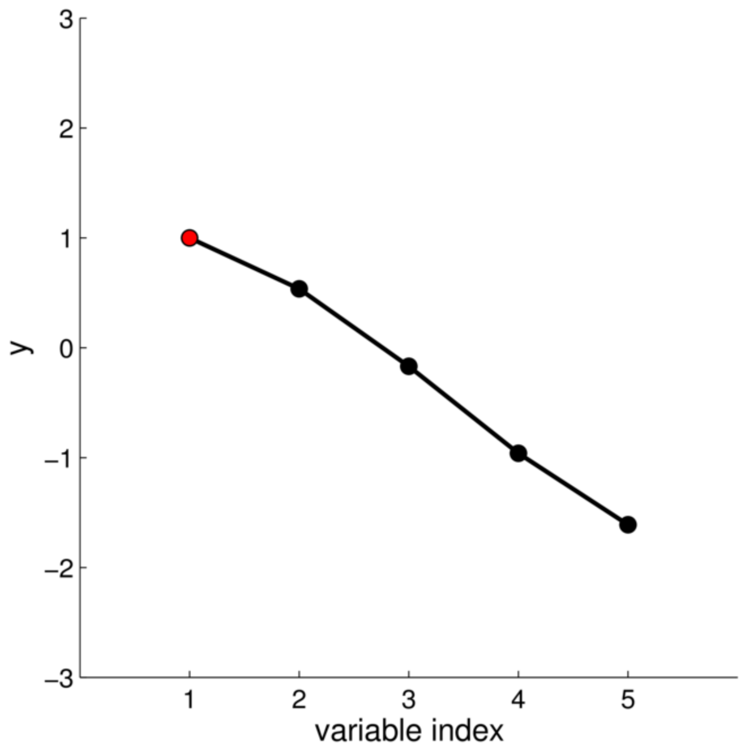
Visualizing Gaussian Processes





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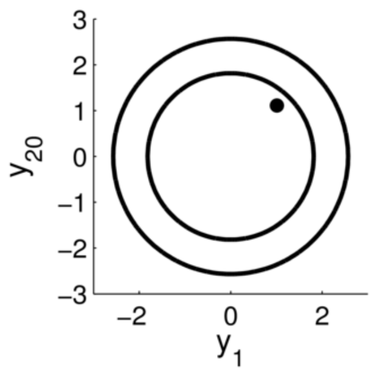
Visualizing Gaussian Processes



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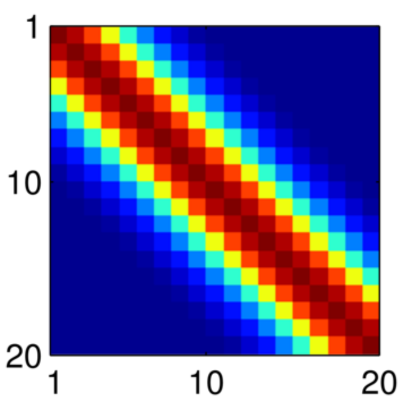

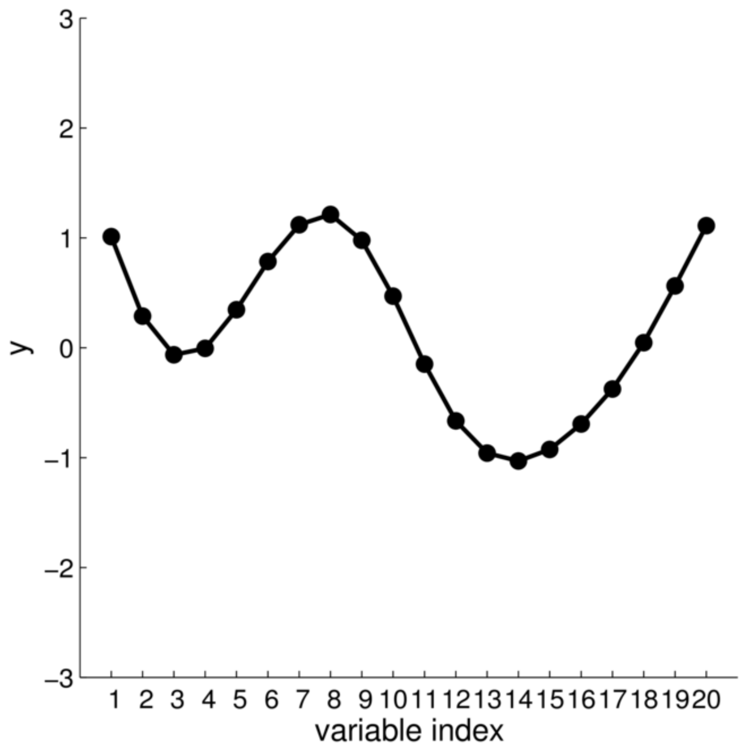

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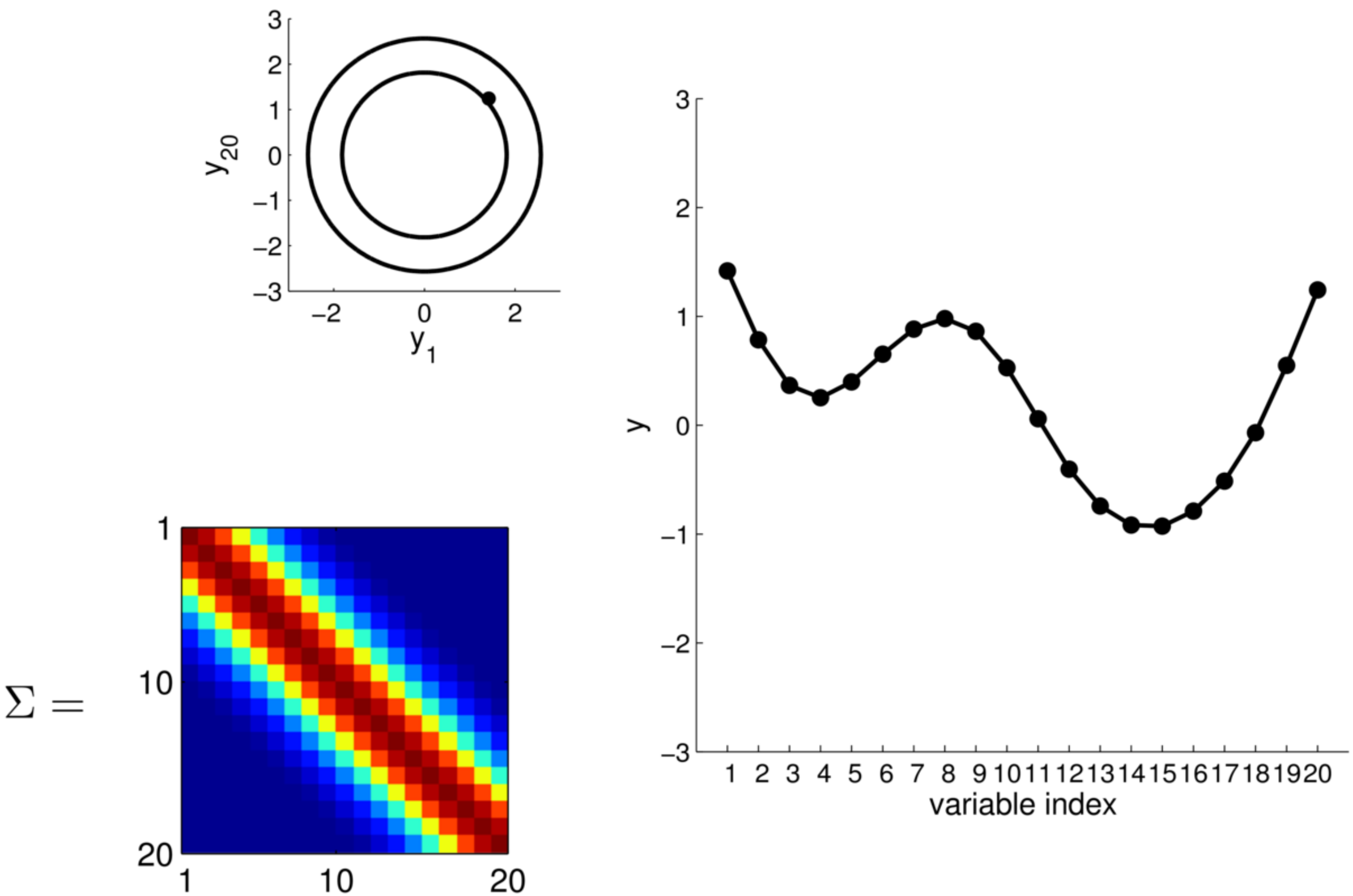

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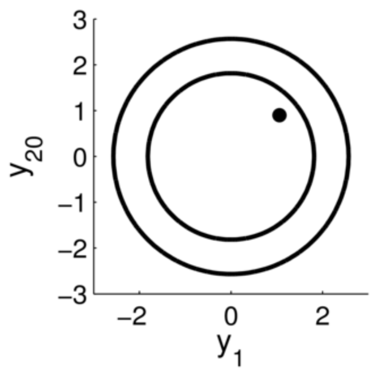

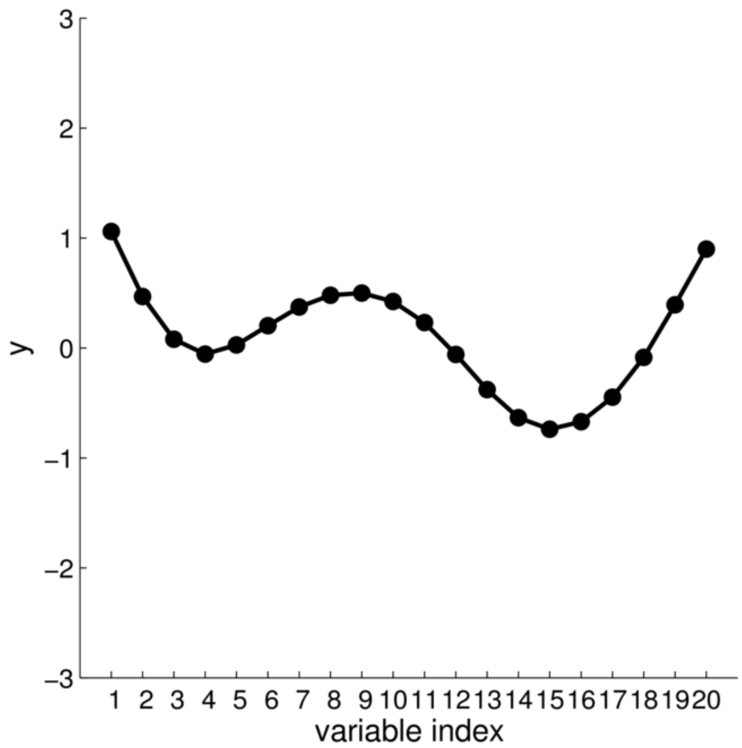

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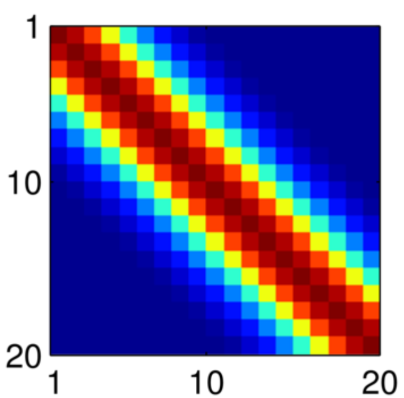

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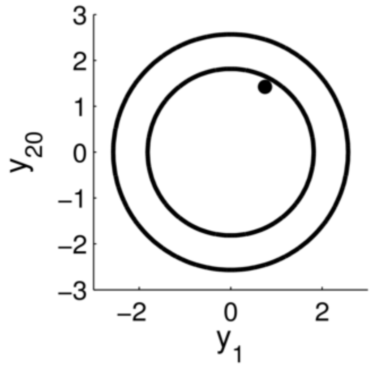
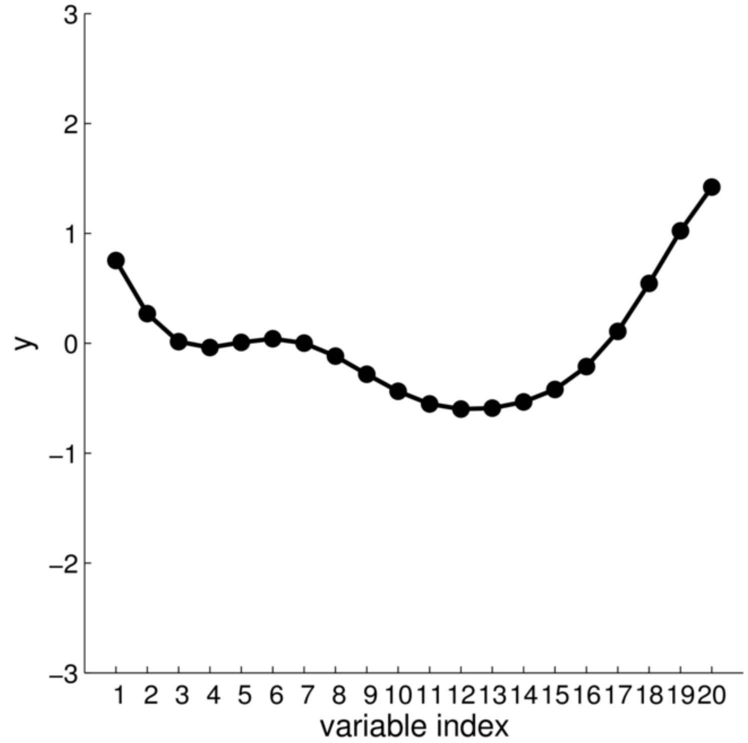
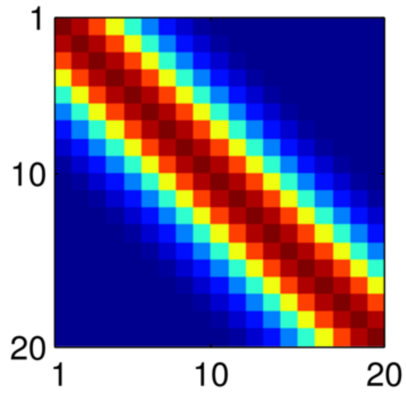




$\Sigma =$ 

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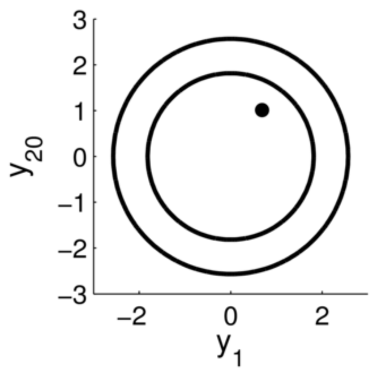

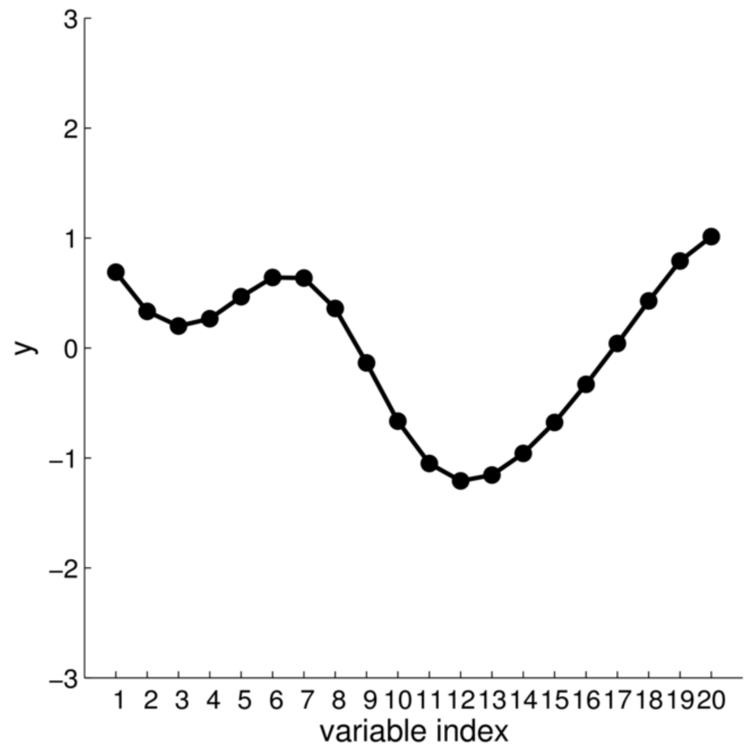

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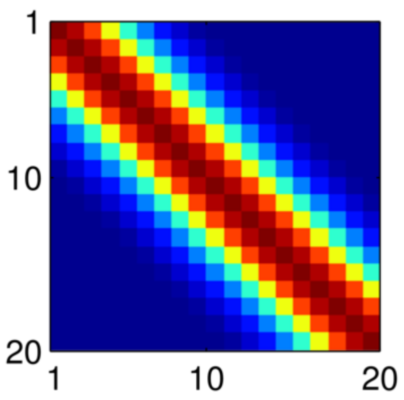

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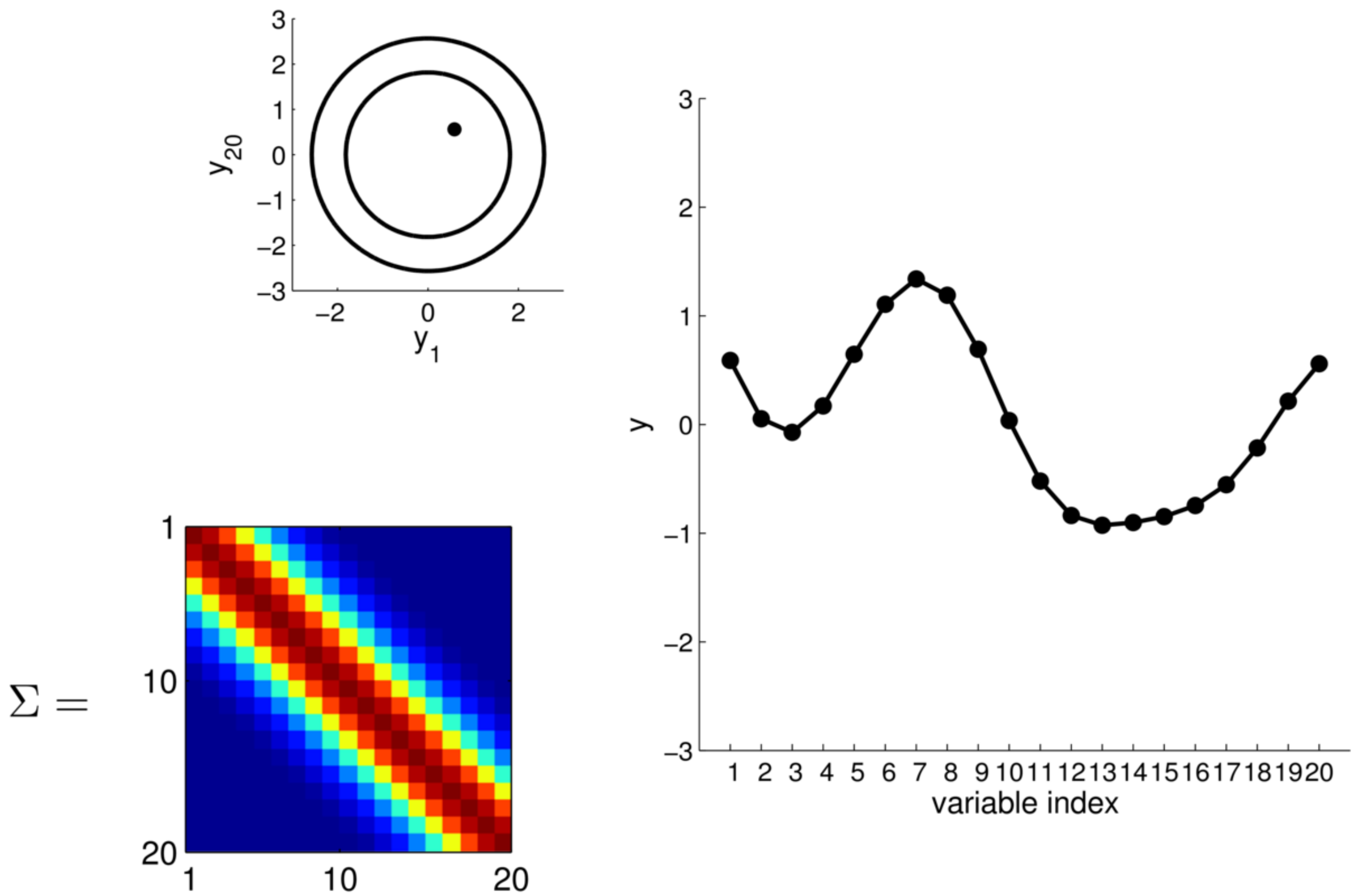

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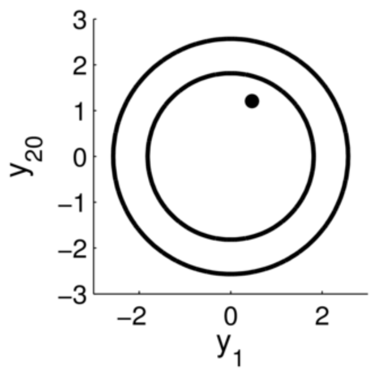

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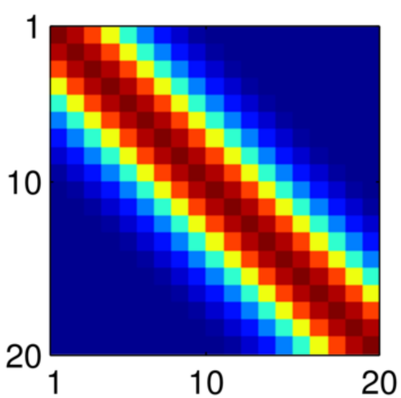

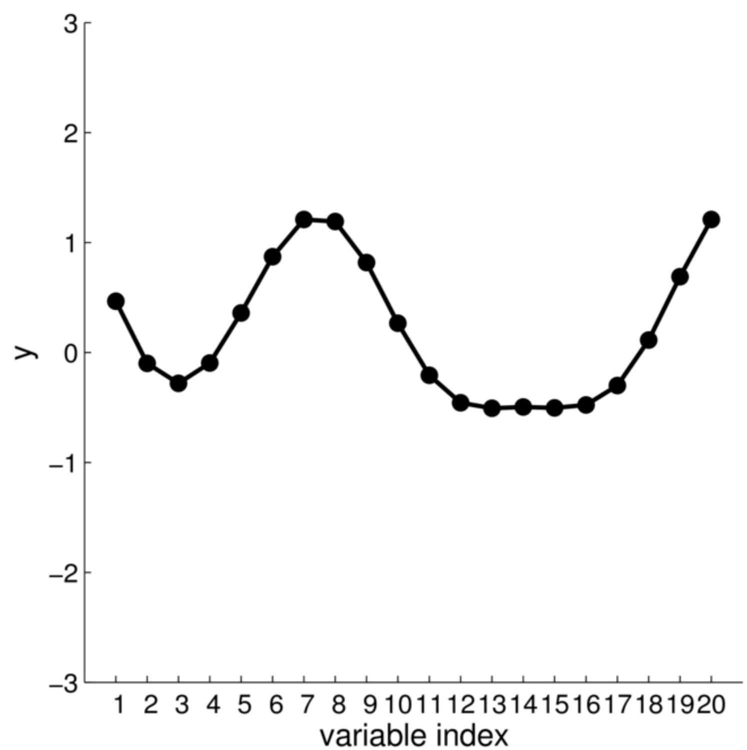

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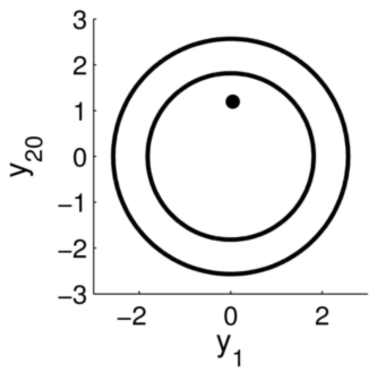

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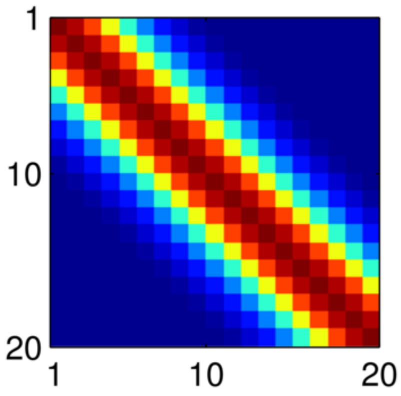

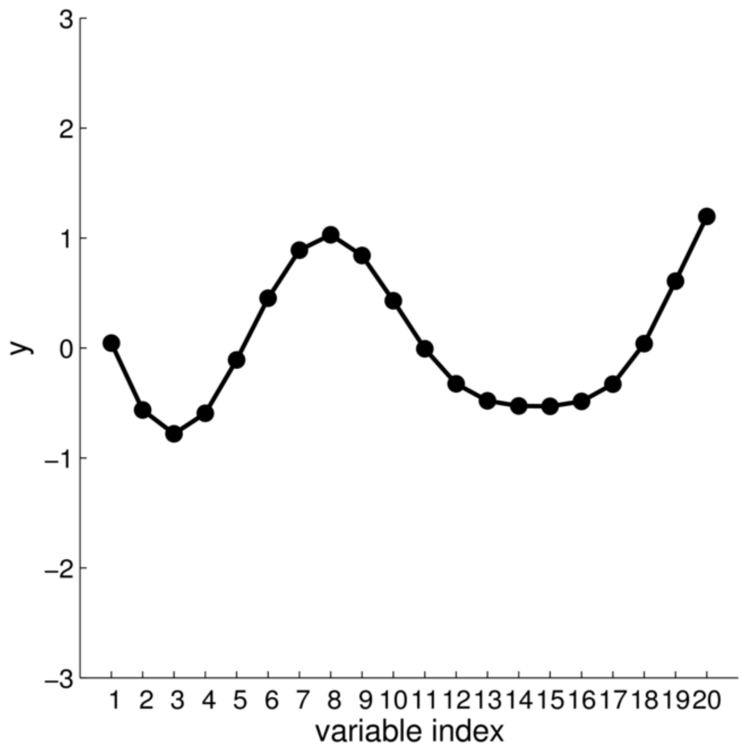

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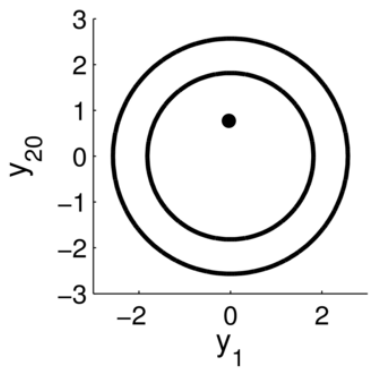

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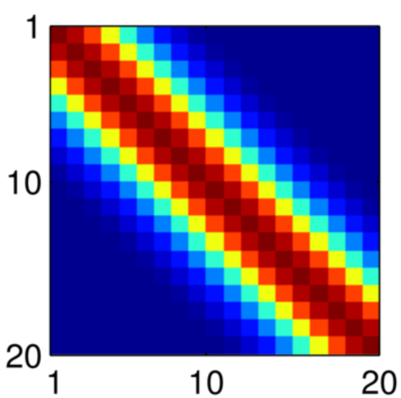

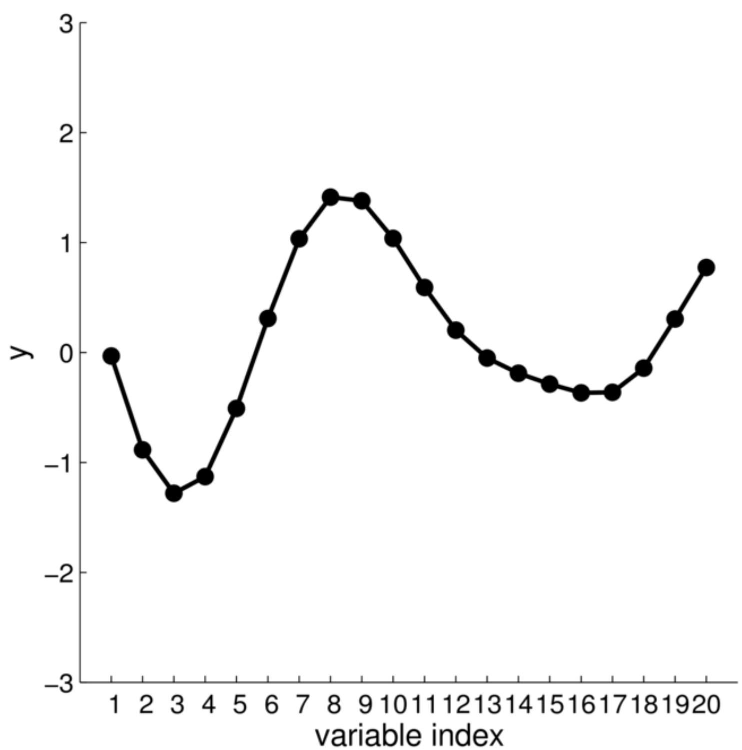

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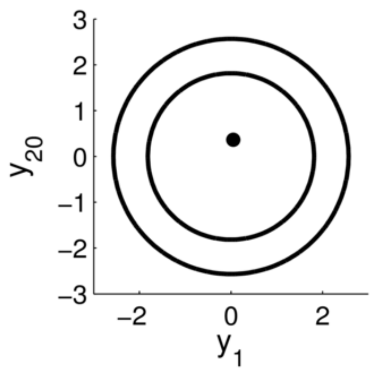

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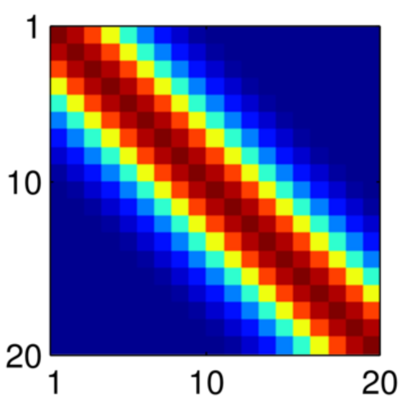

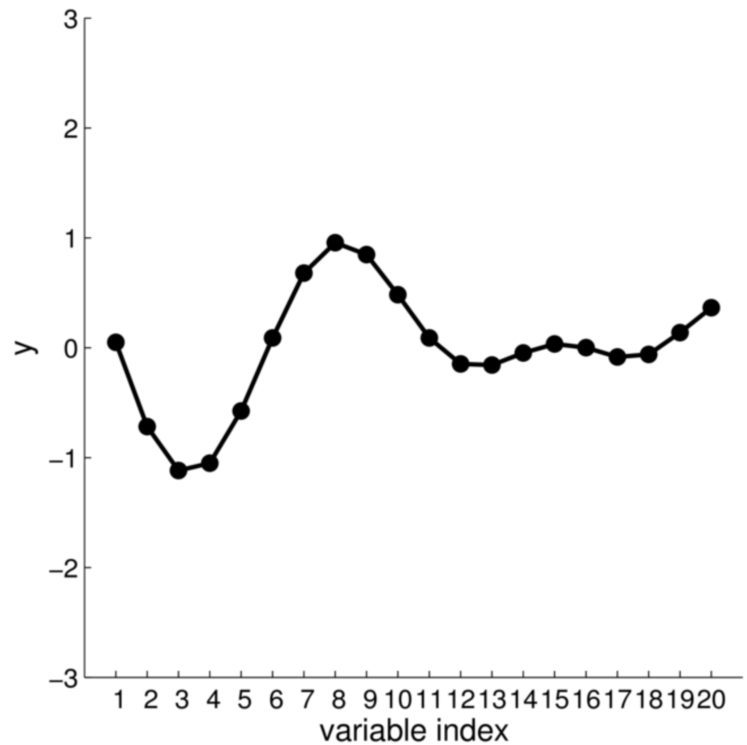

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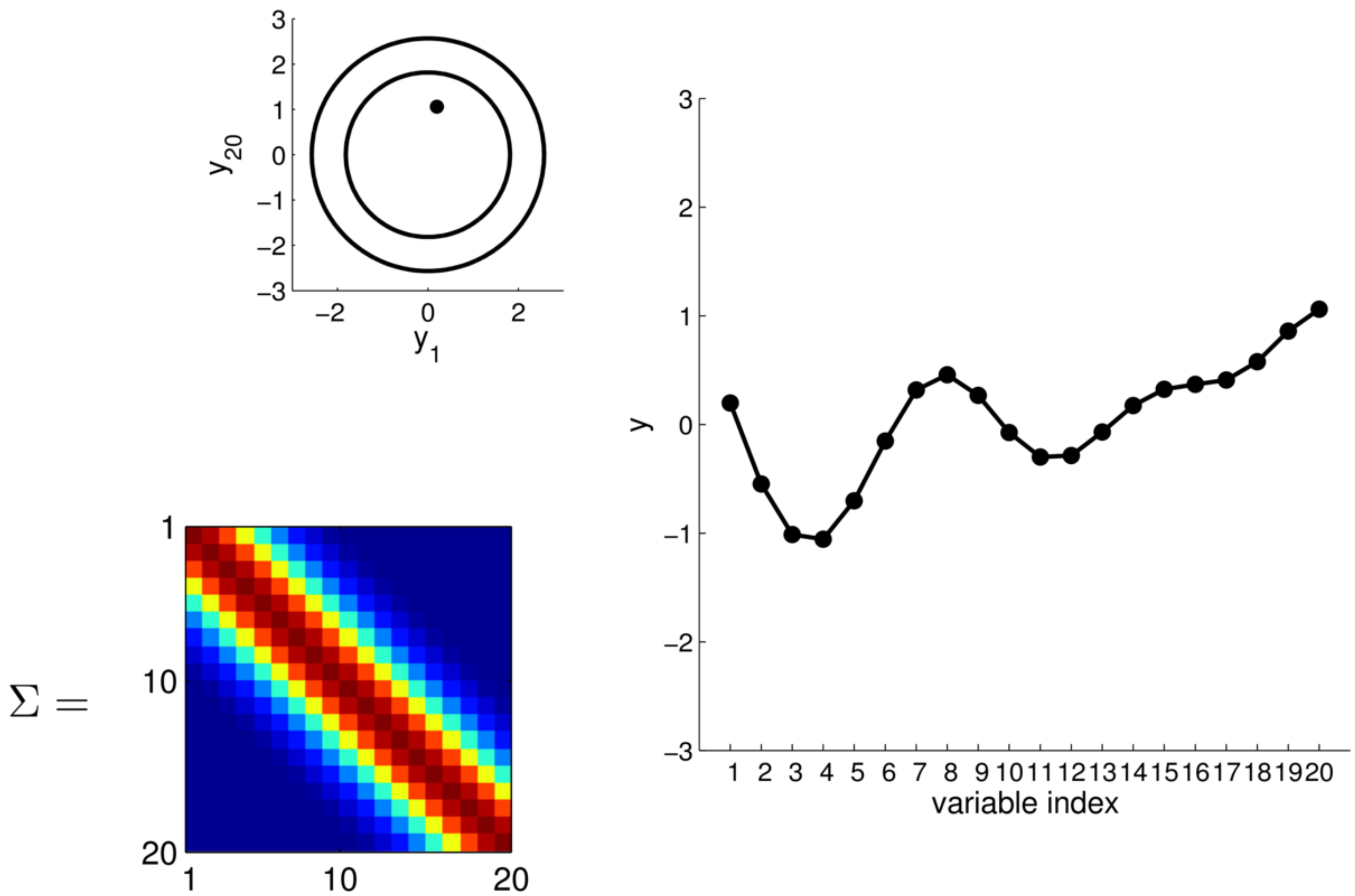

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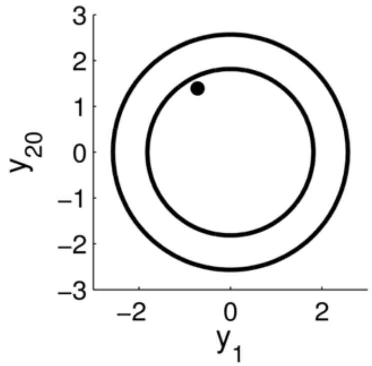

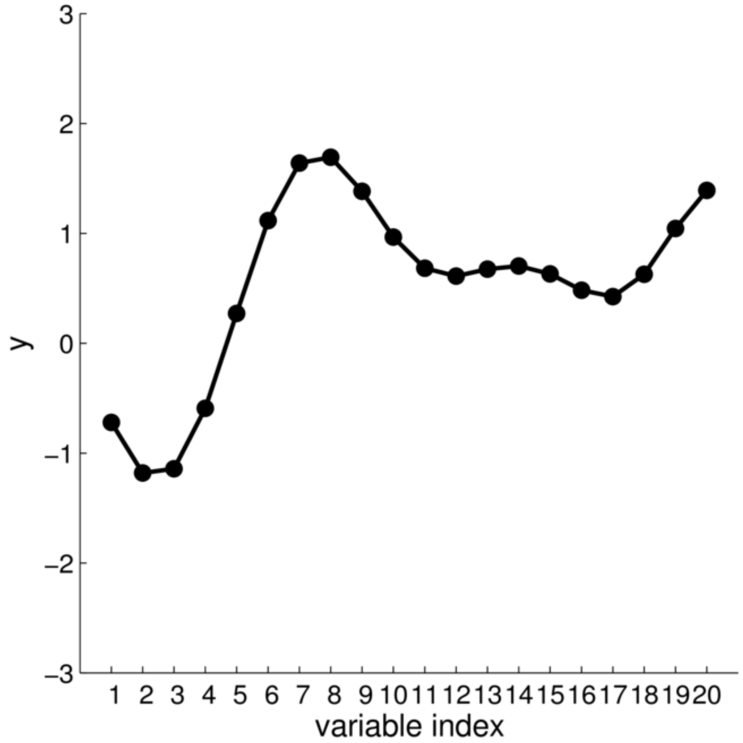

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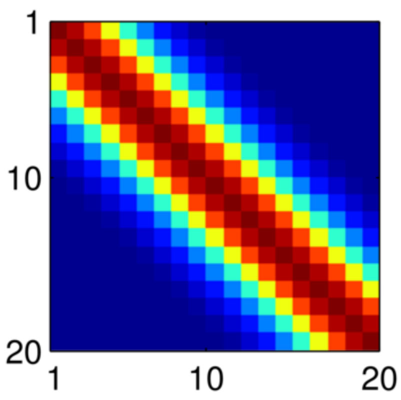

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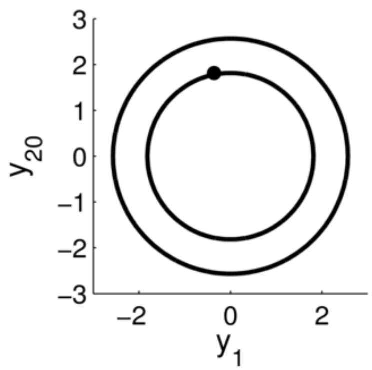

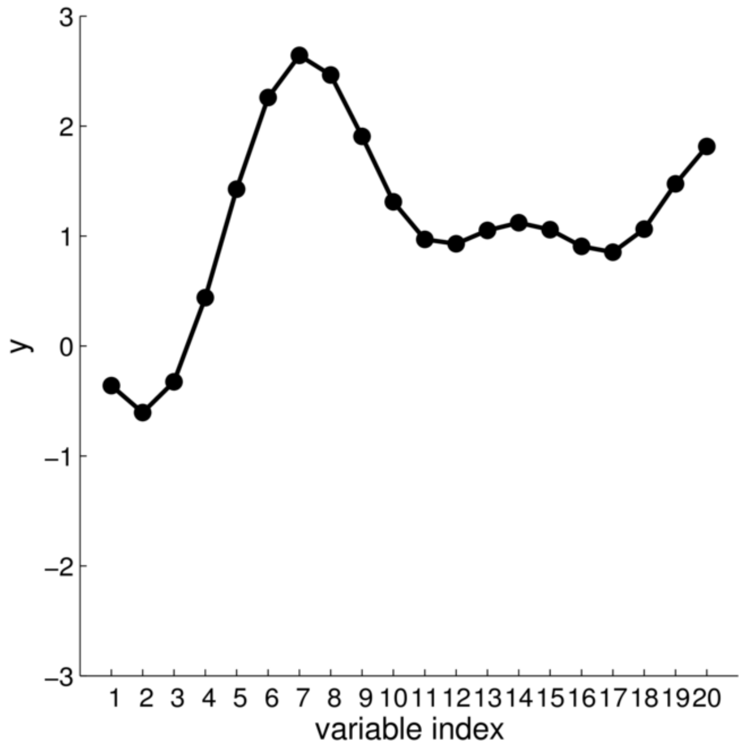

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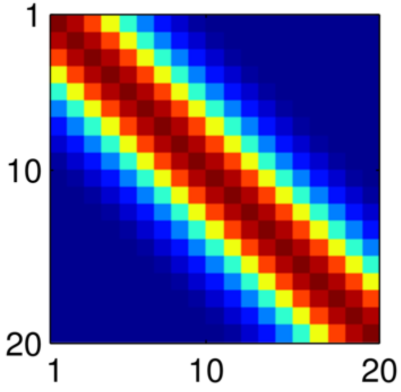

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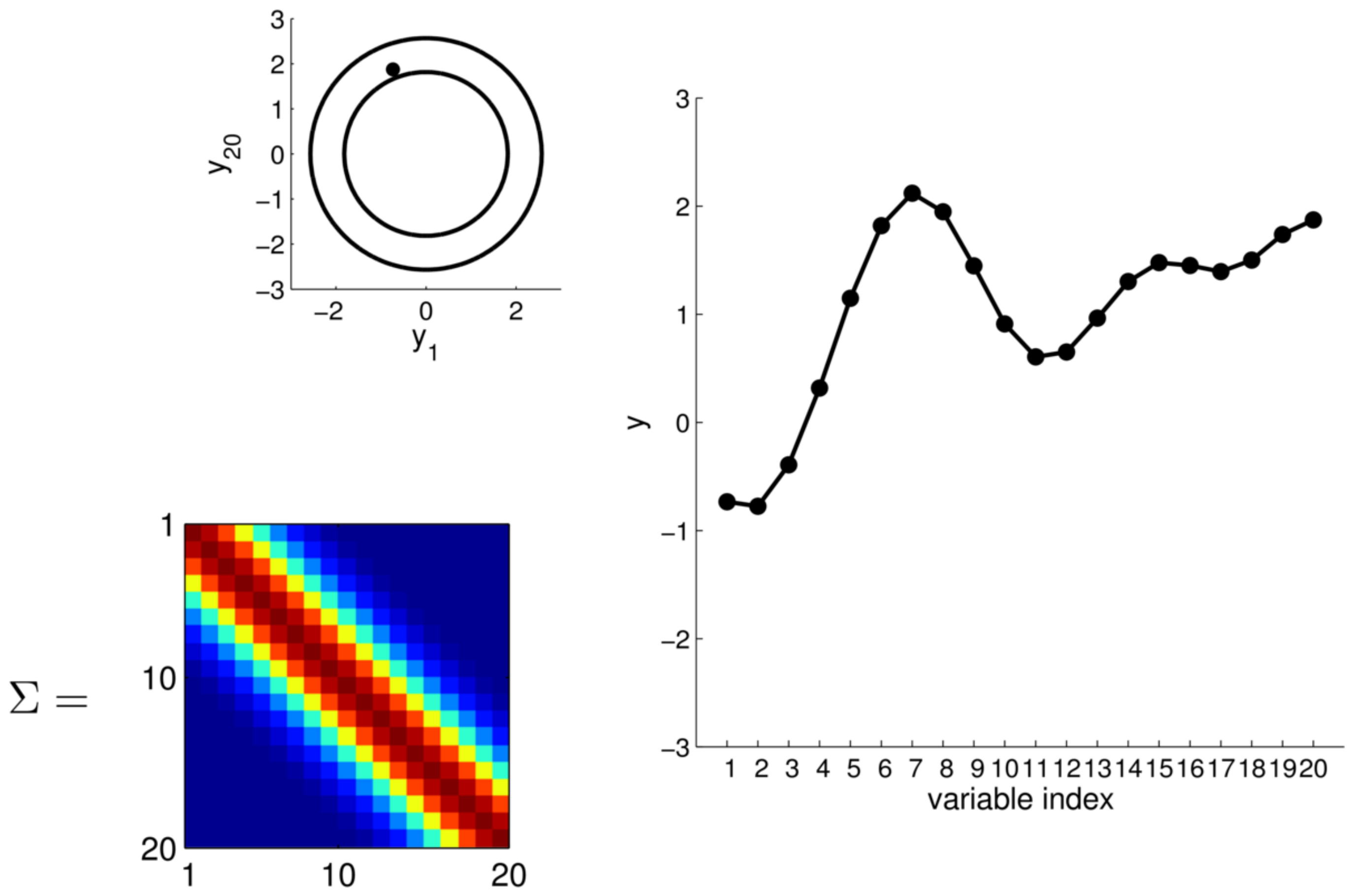

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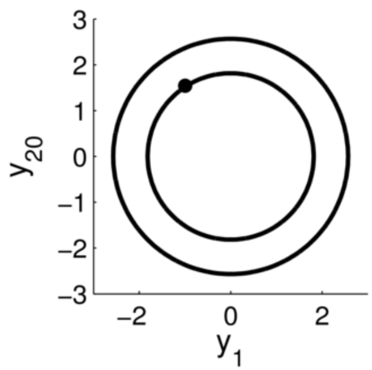

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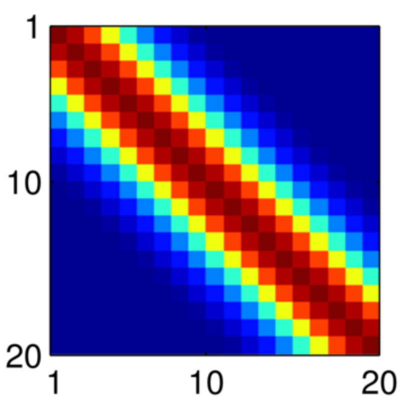

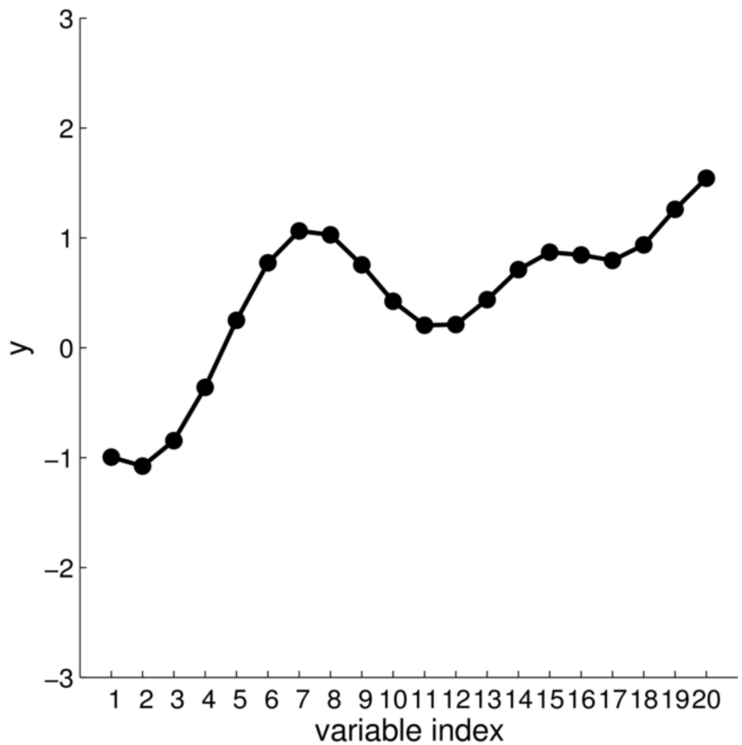

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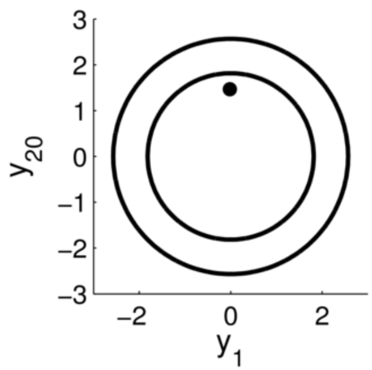

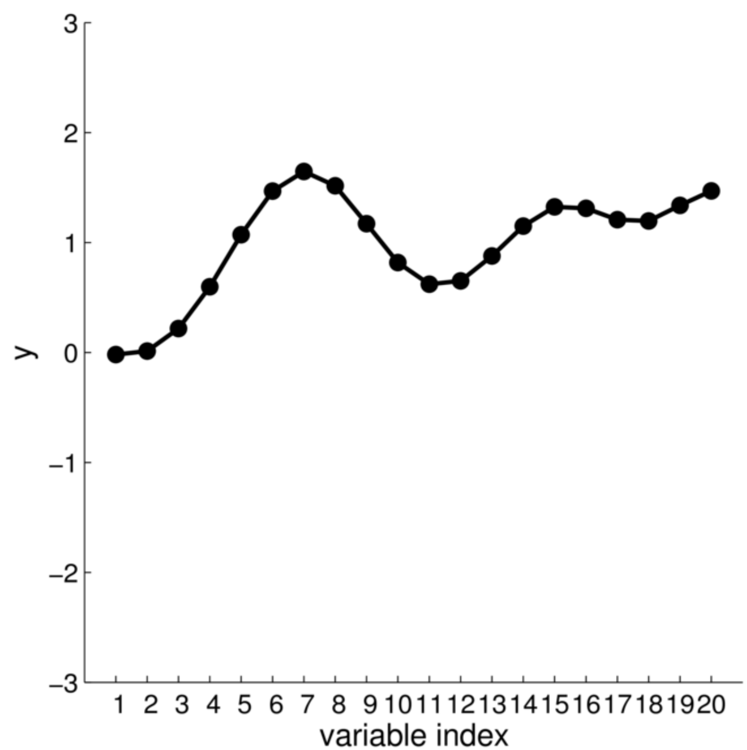

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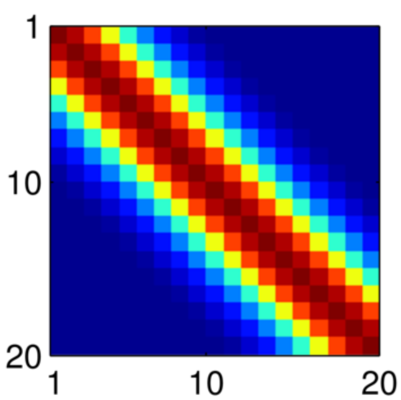

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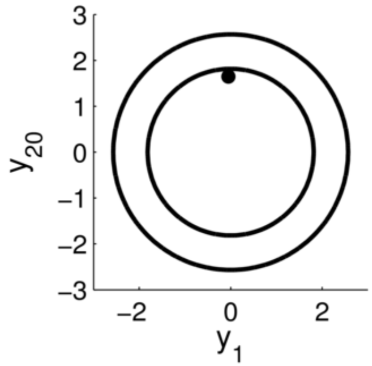
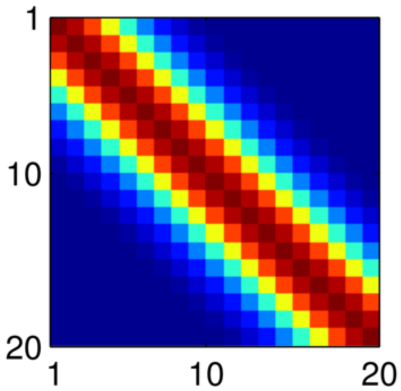
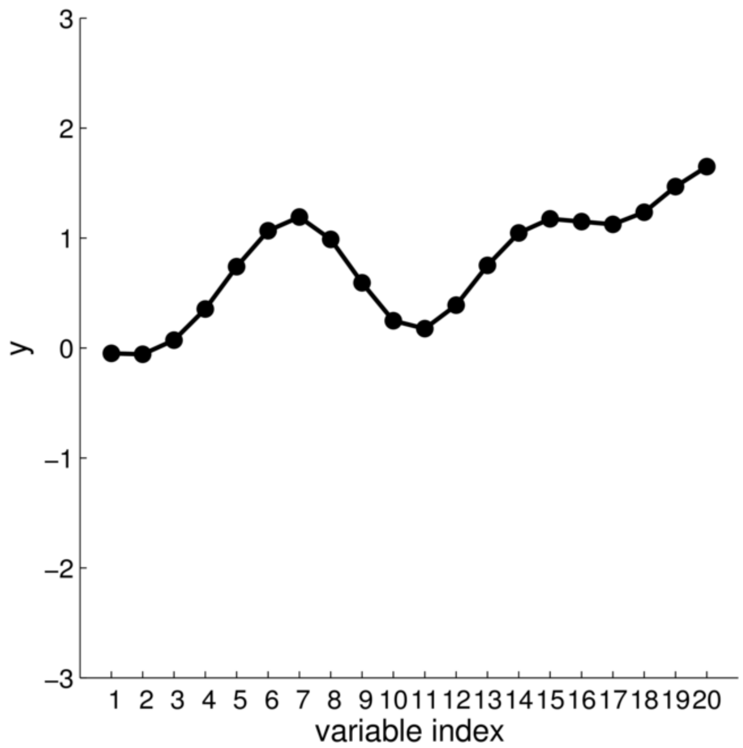


$\Sigma =$ 



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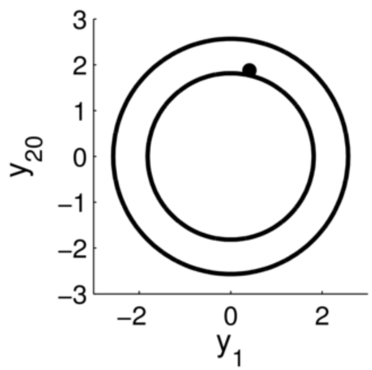

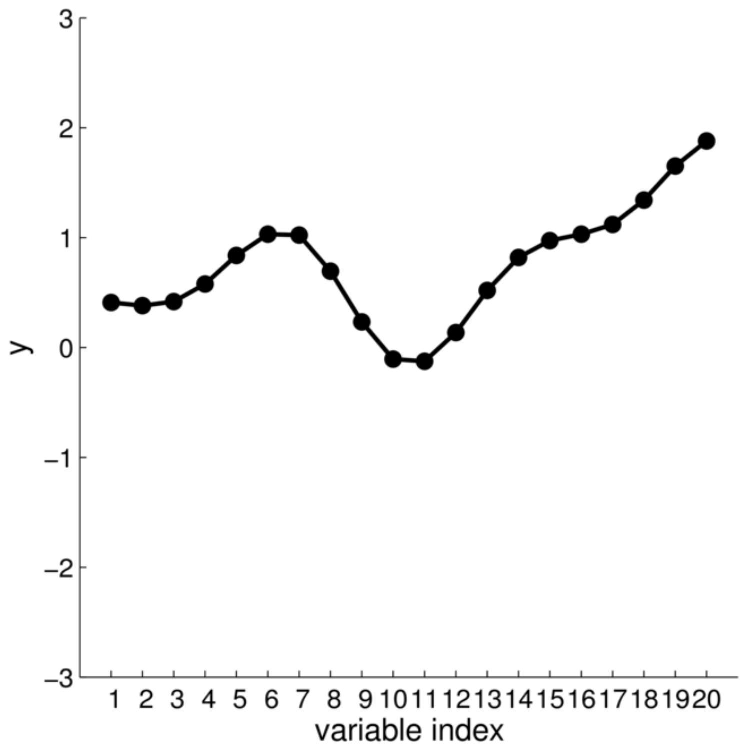

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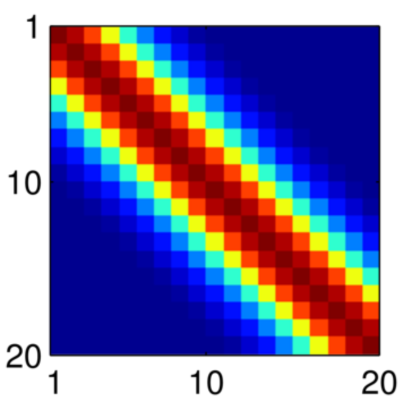

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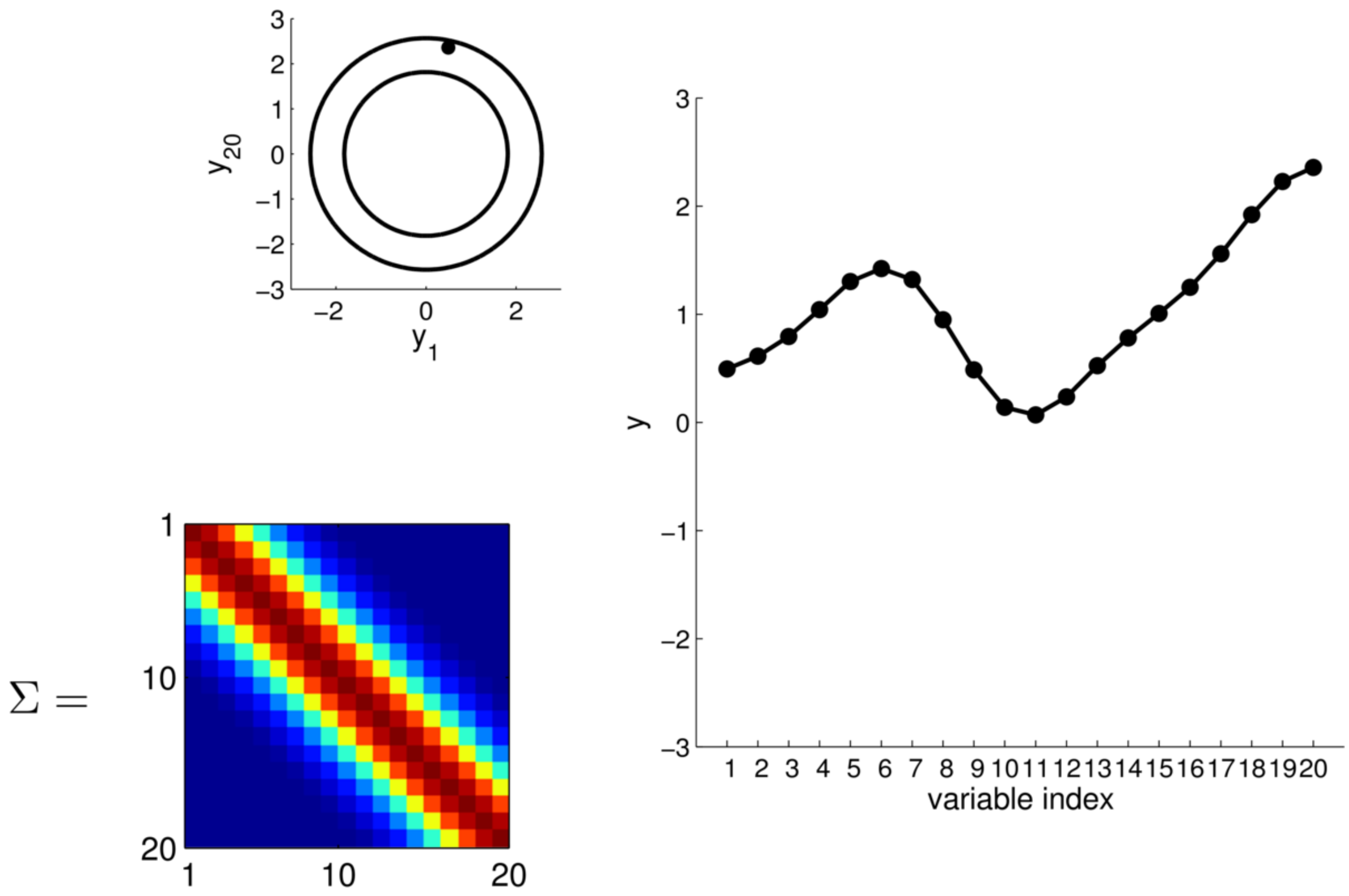

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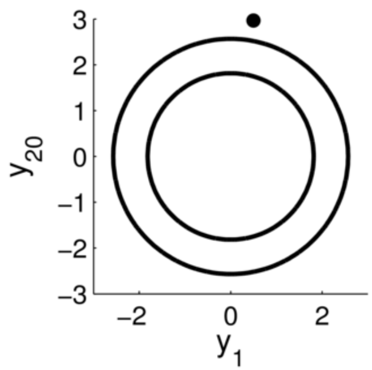

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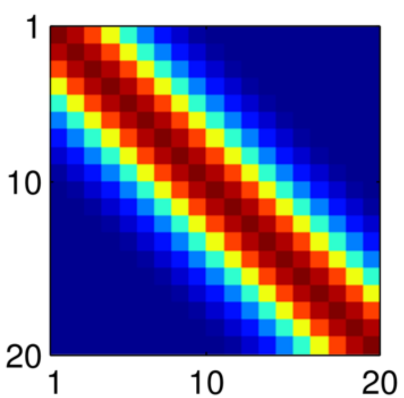

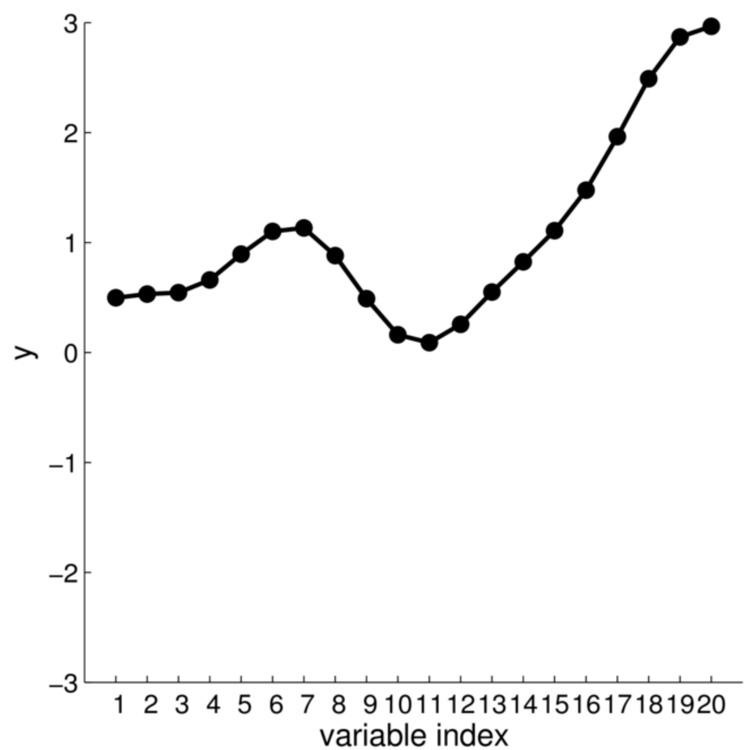

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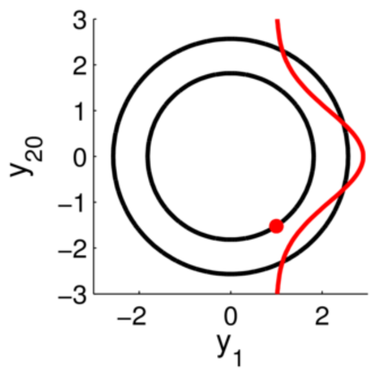

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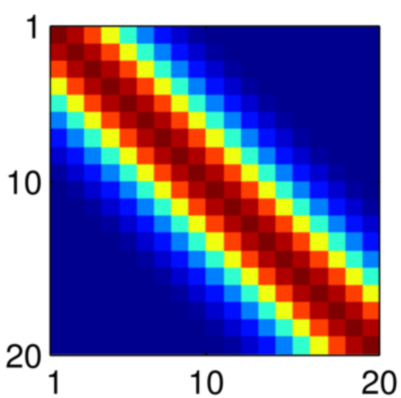

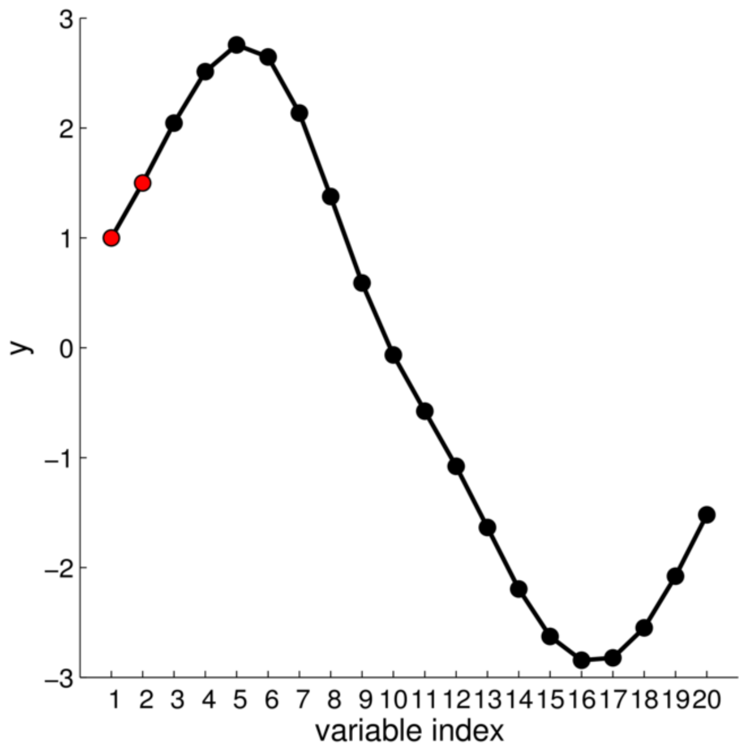

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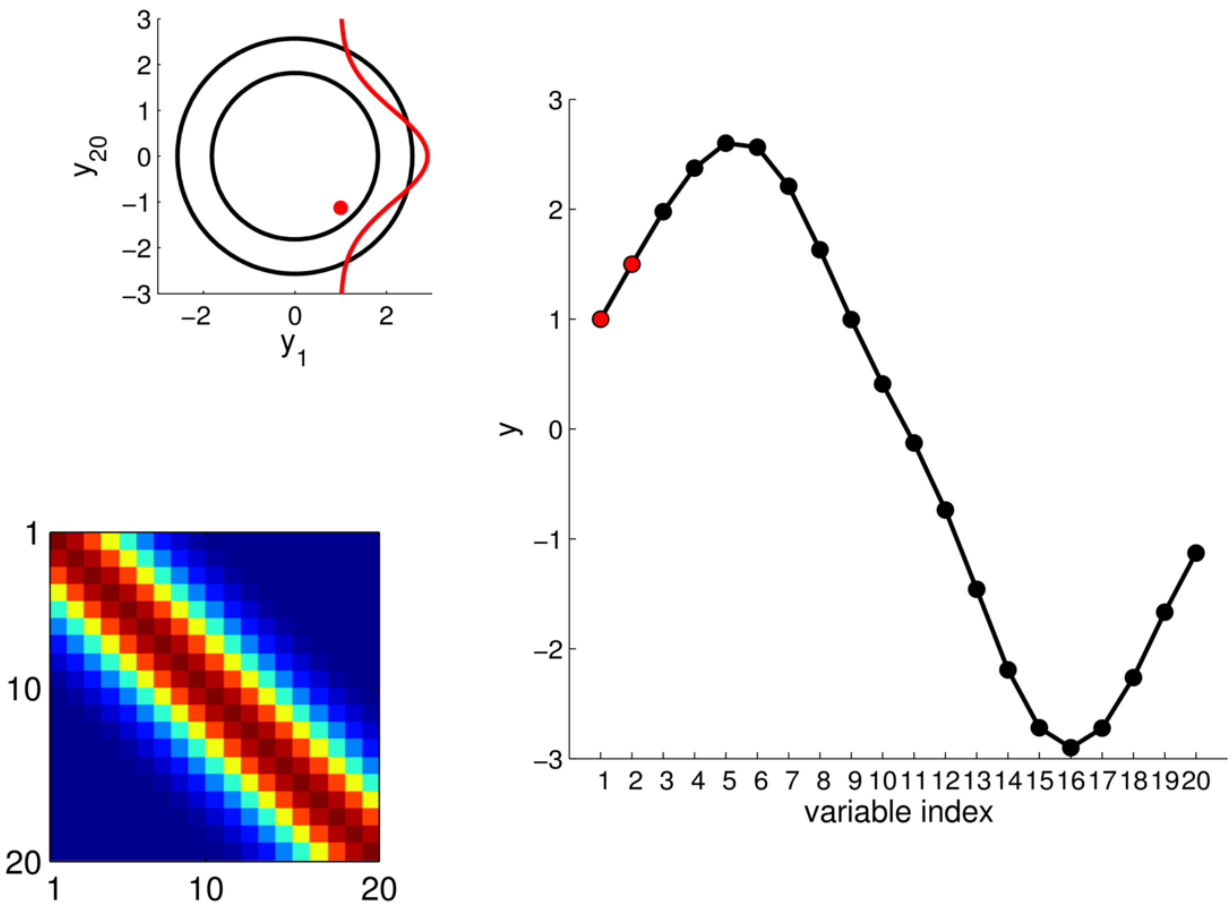

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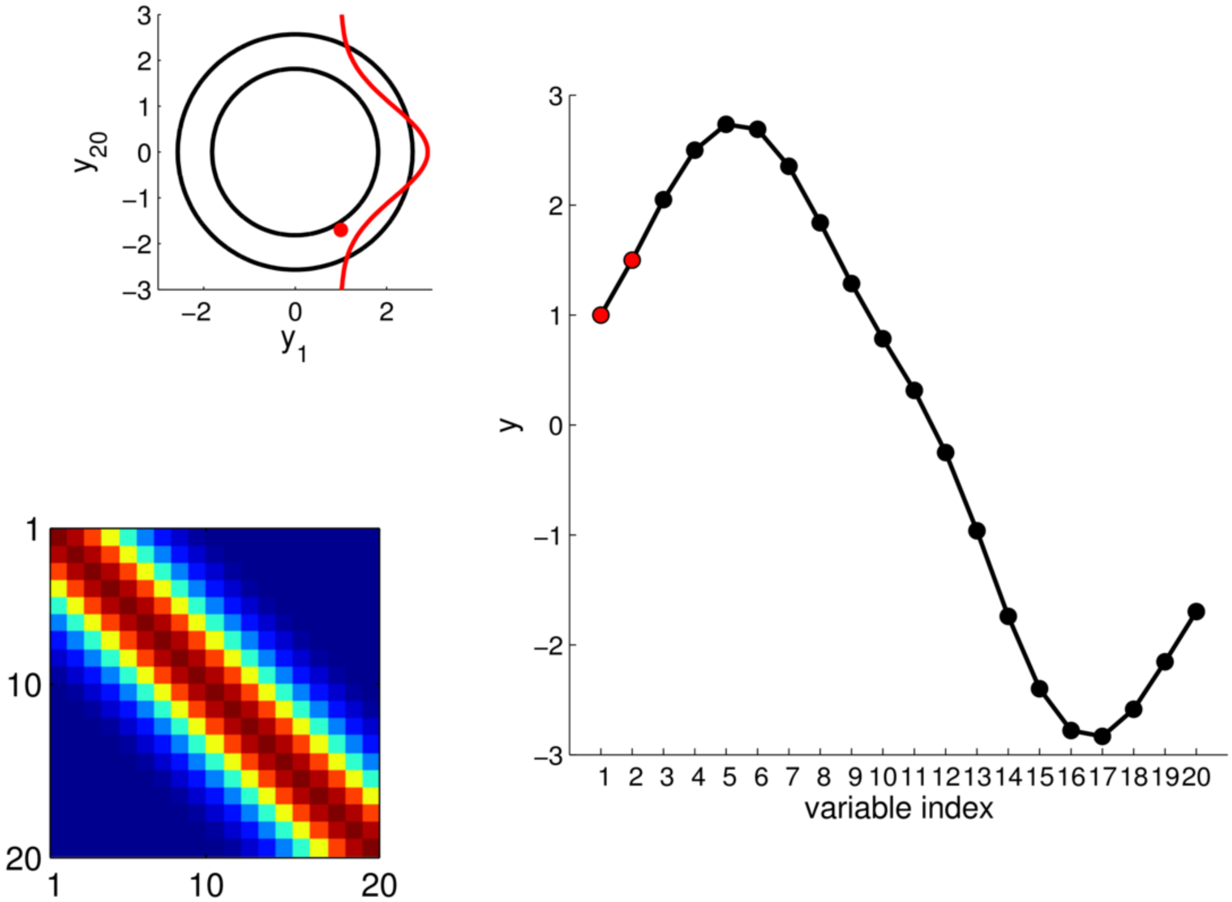

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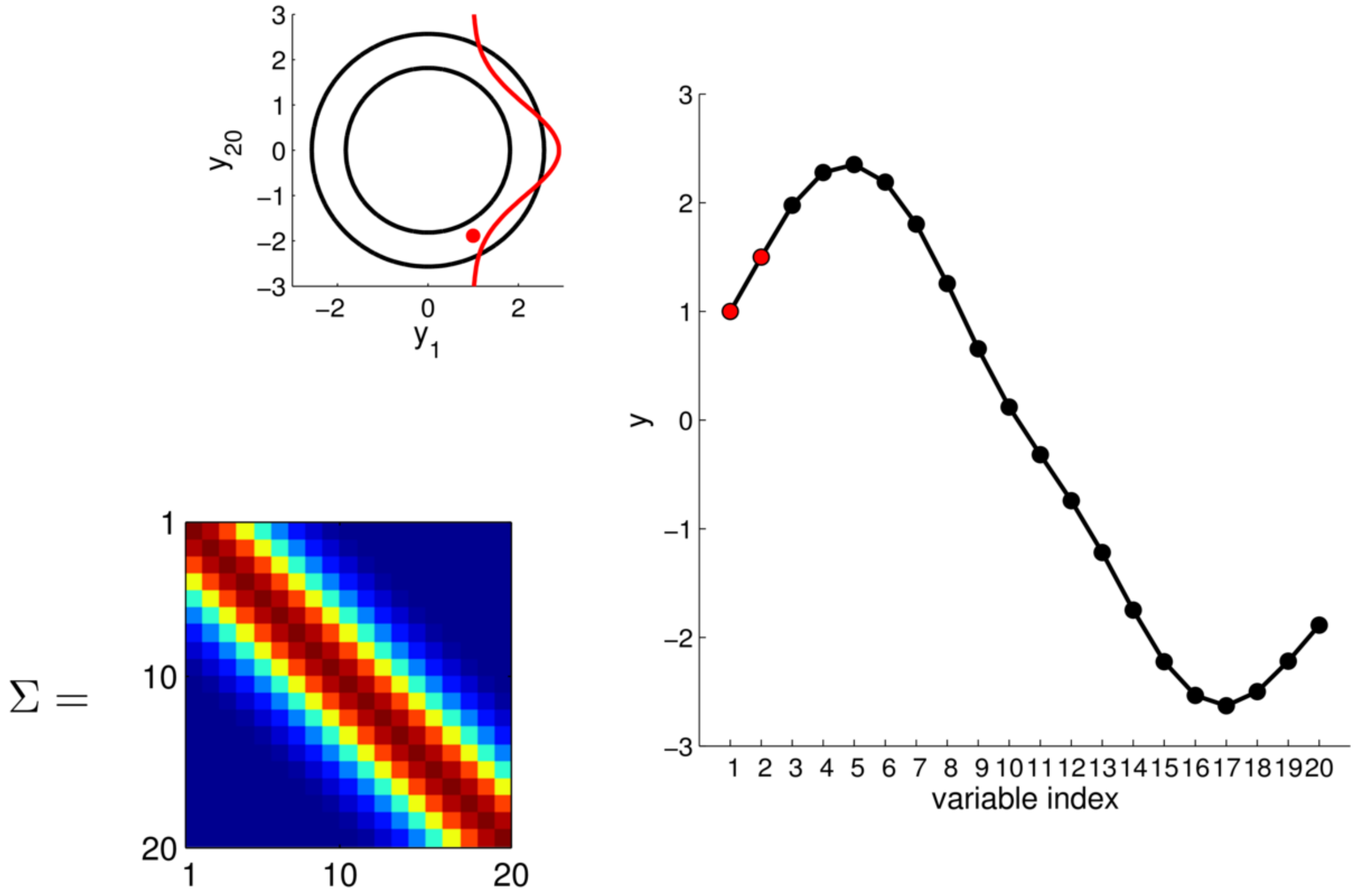

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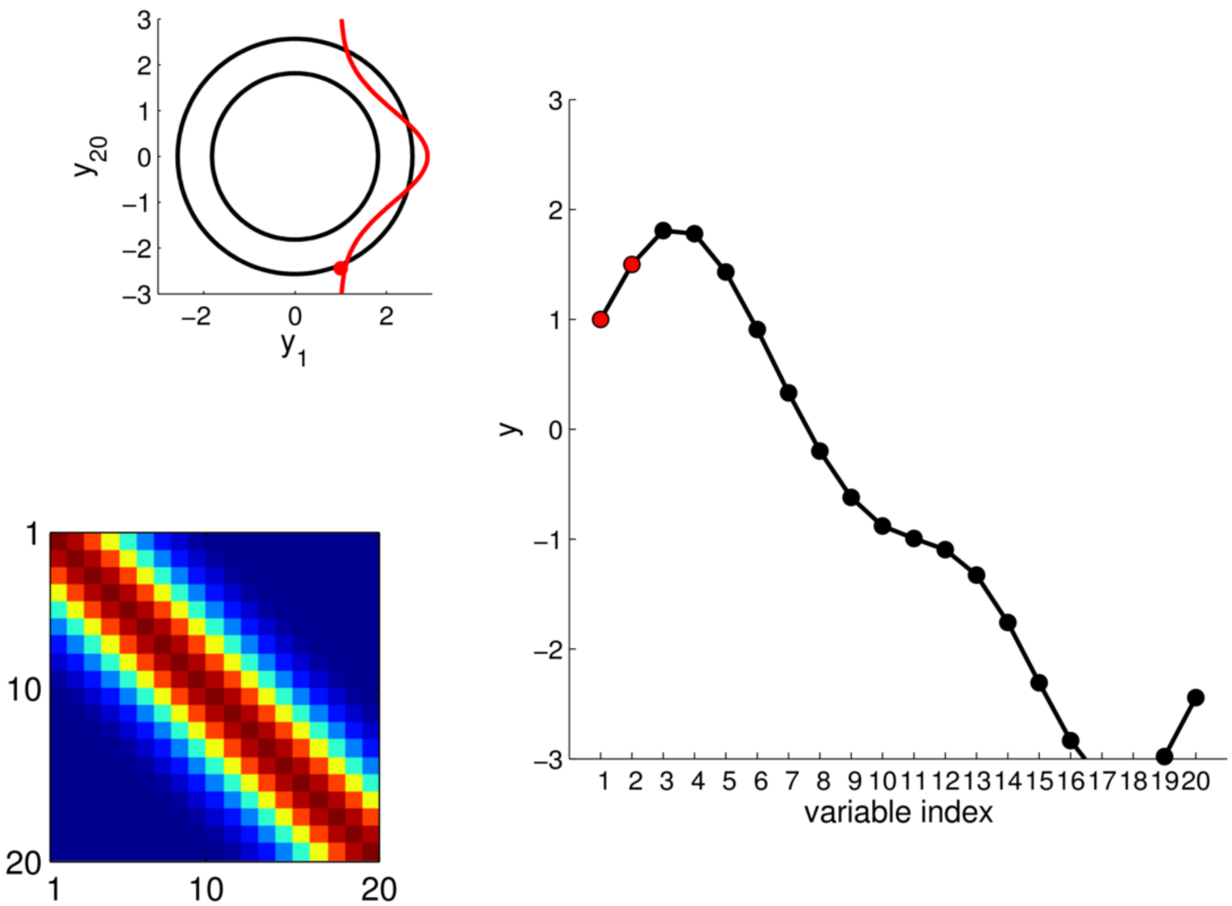

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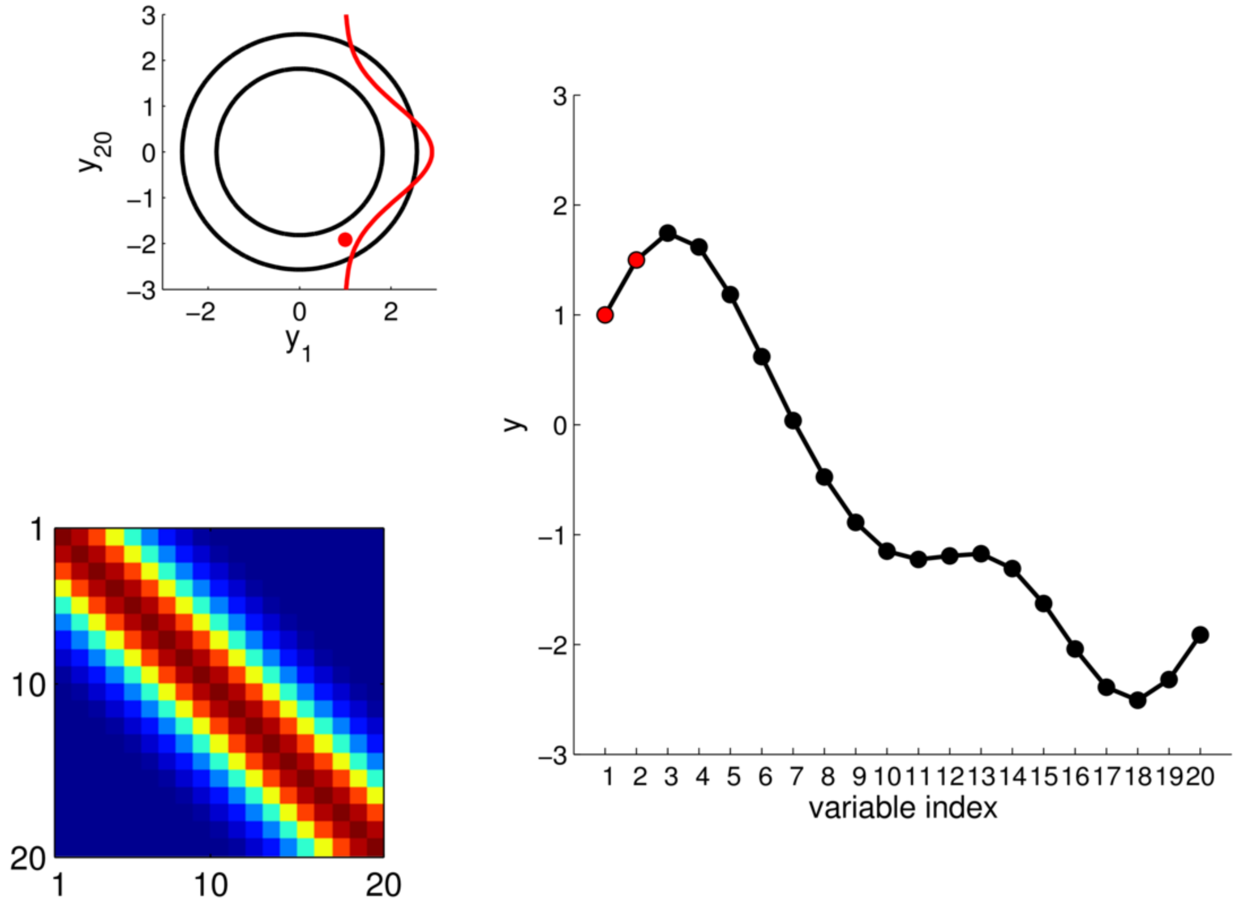

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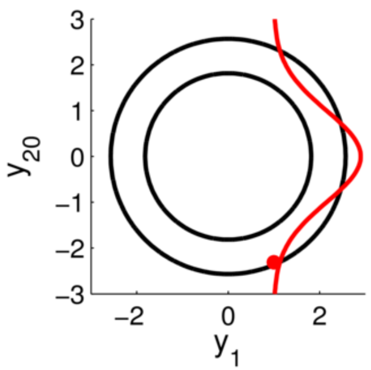

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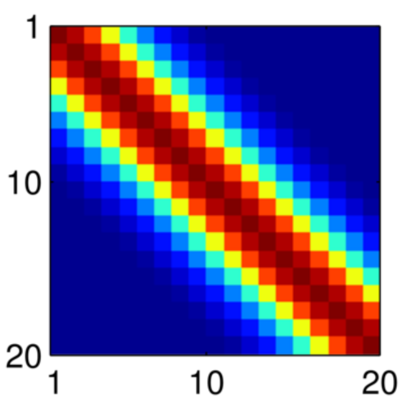

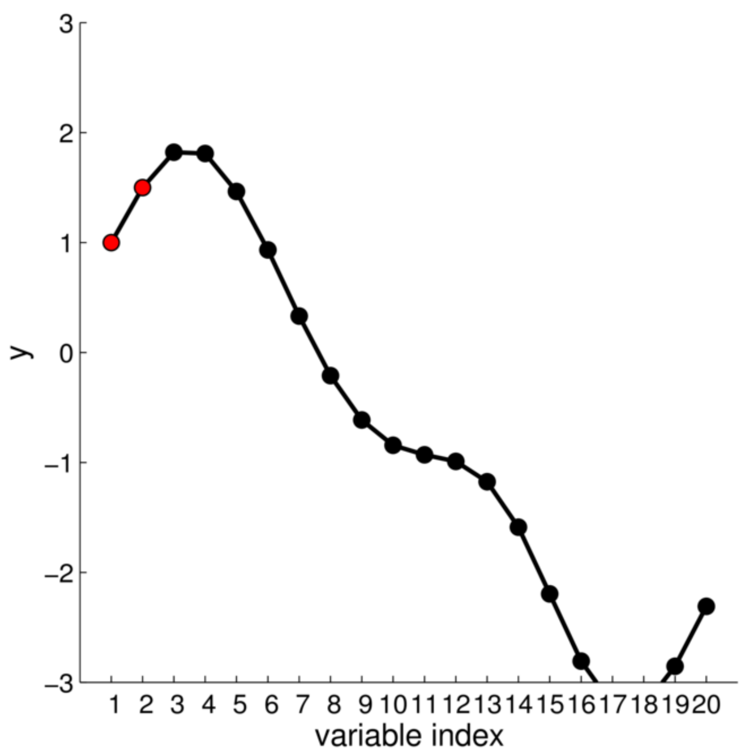

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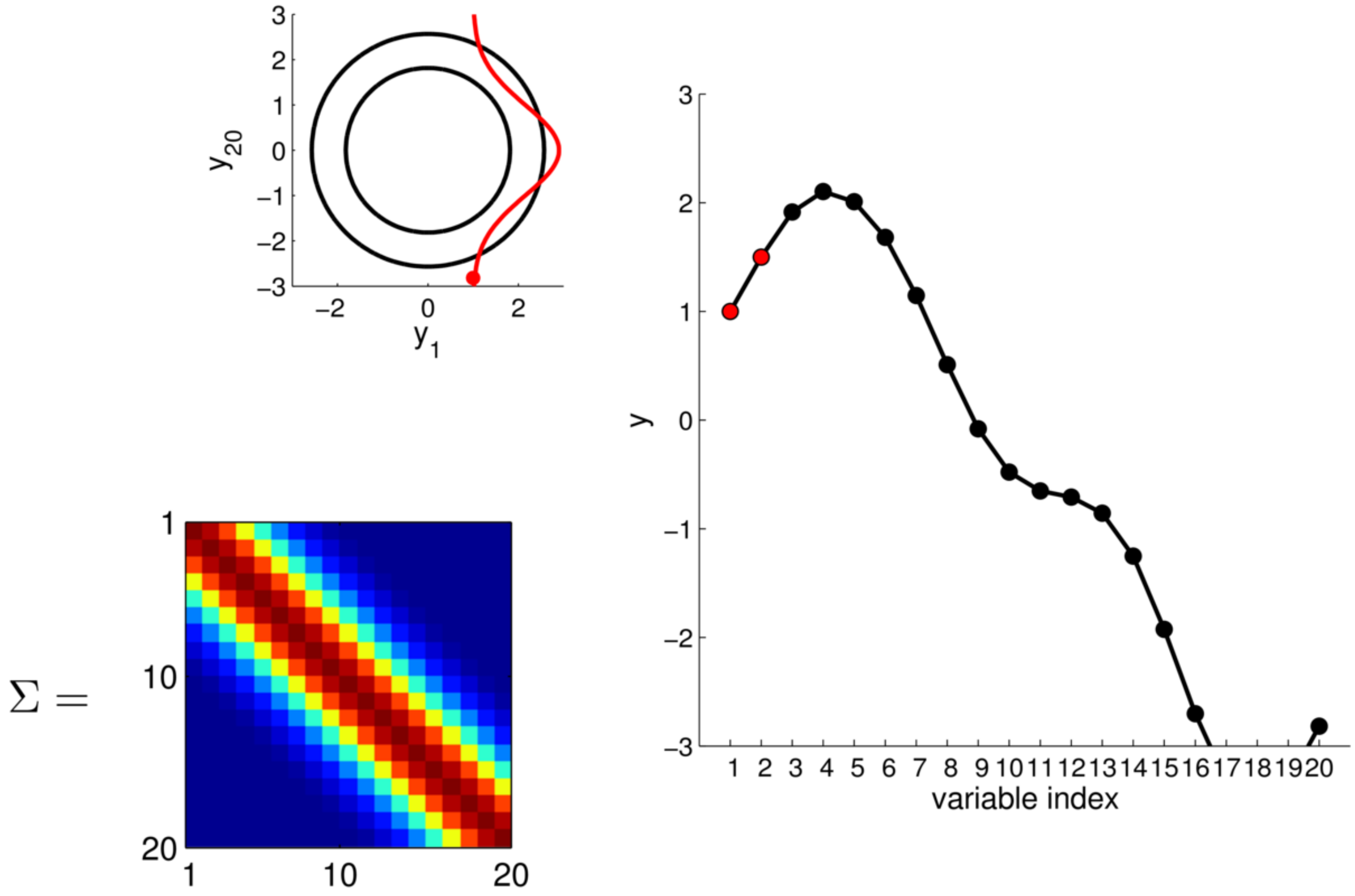

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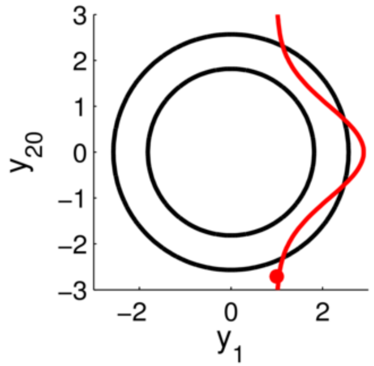
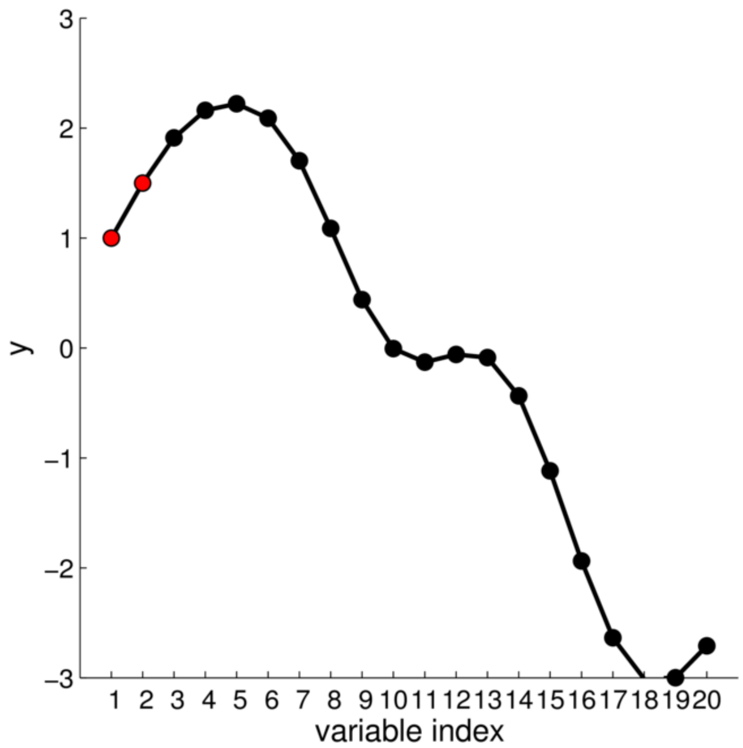
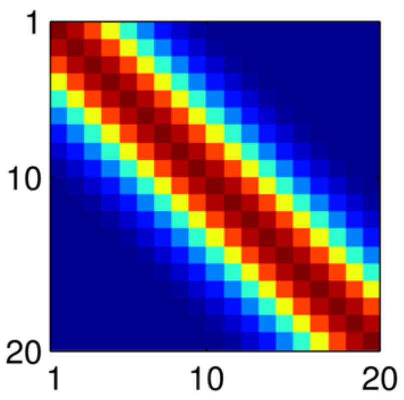
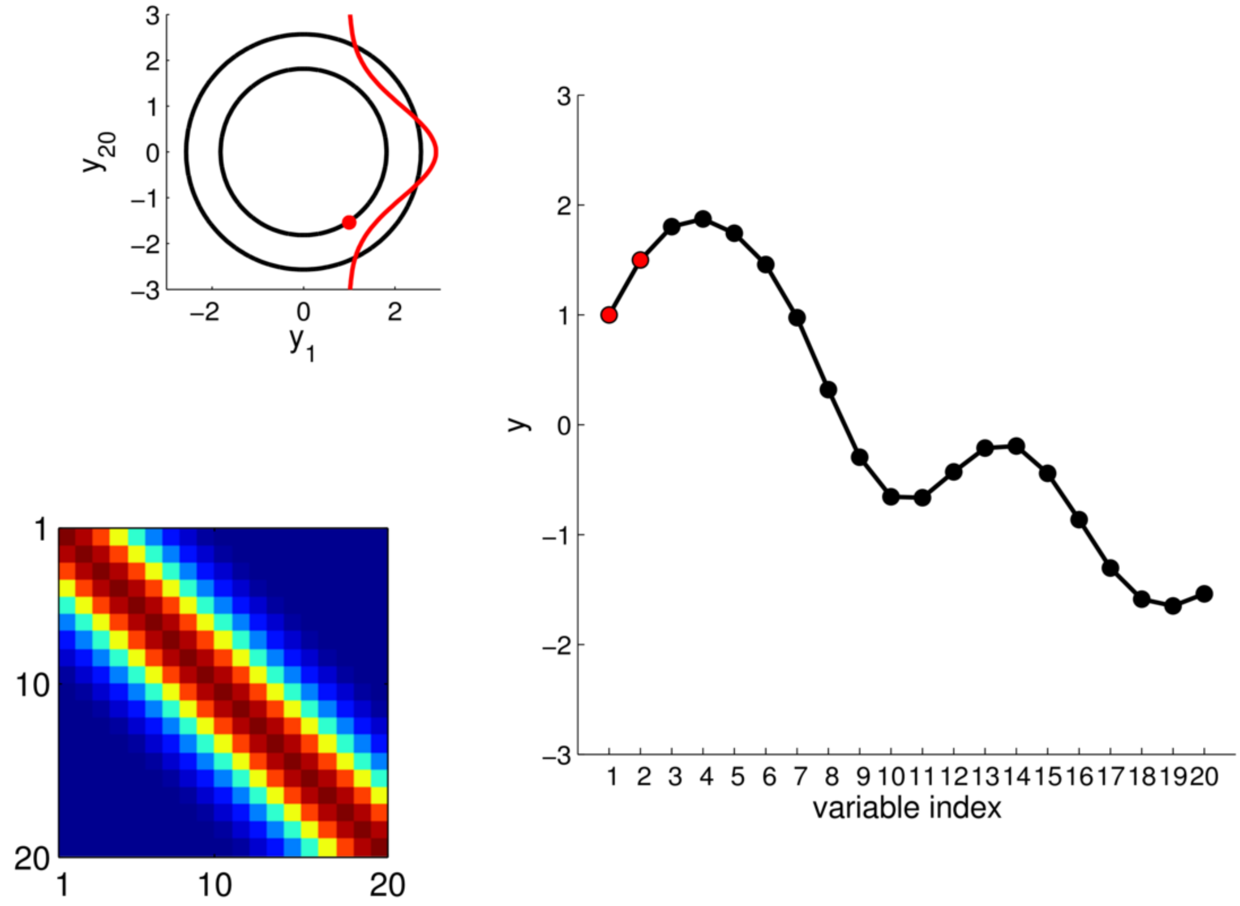




$\Sigma =$ 

Visualizing Gaussian Processes

$\Sigma =$



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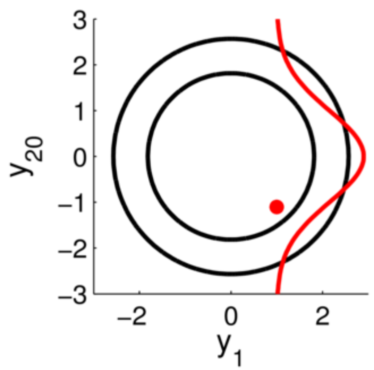

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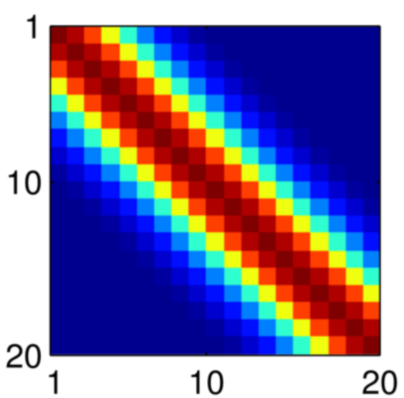

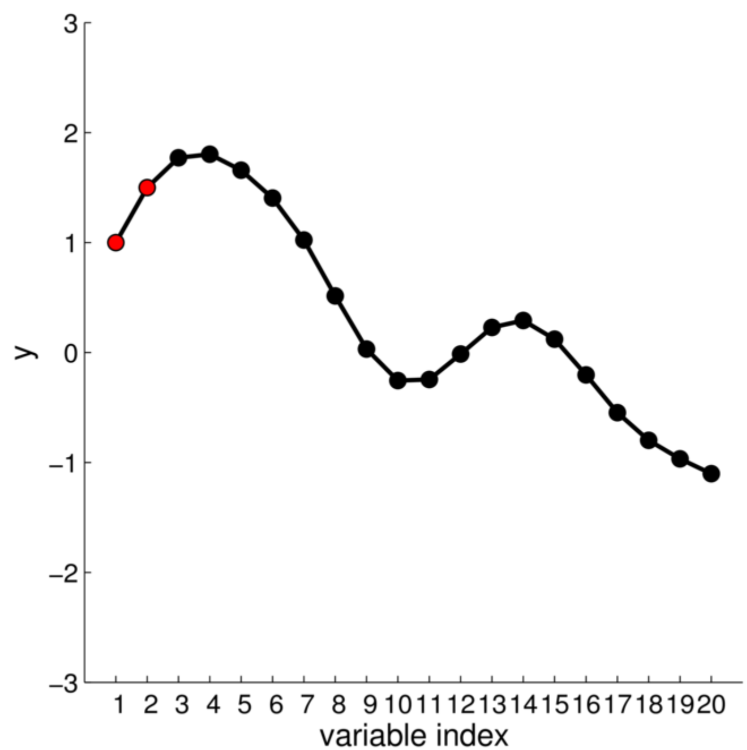

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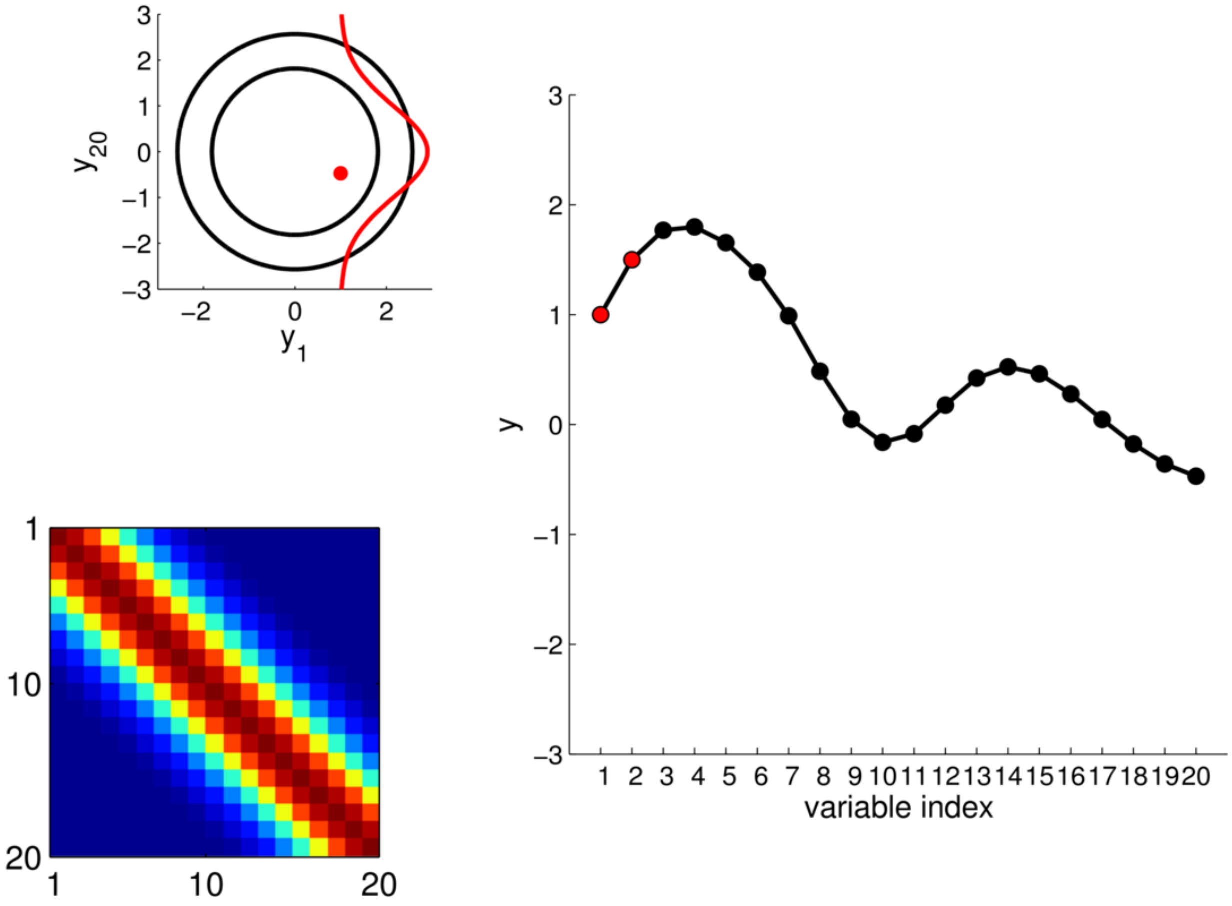

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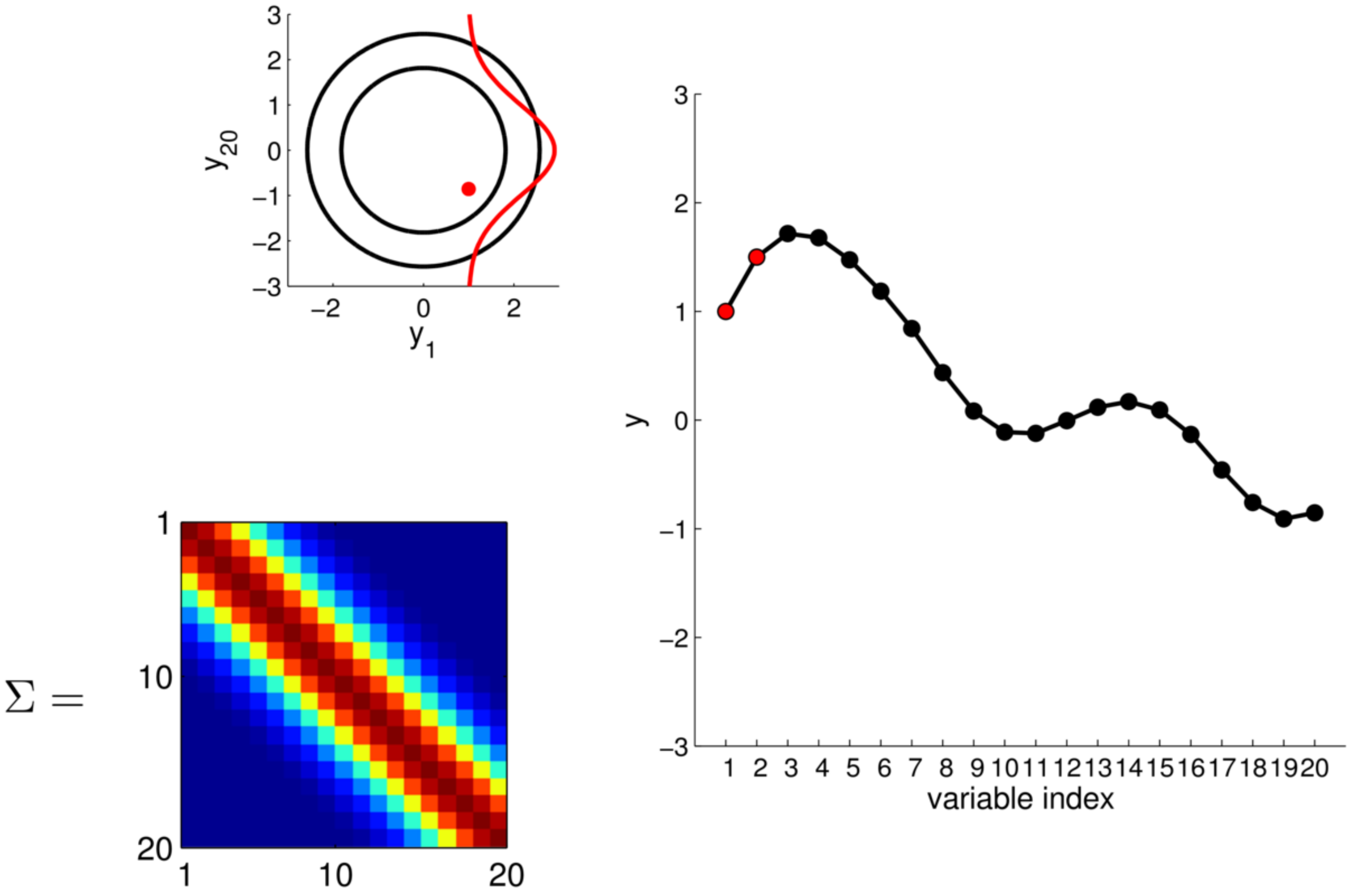

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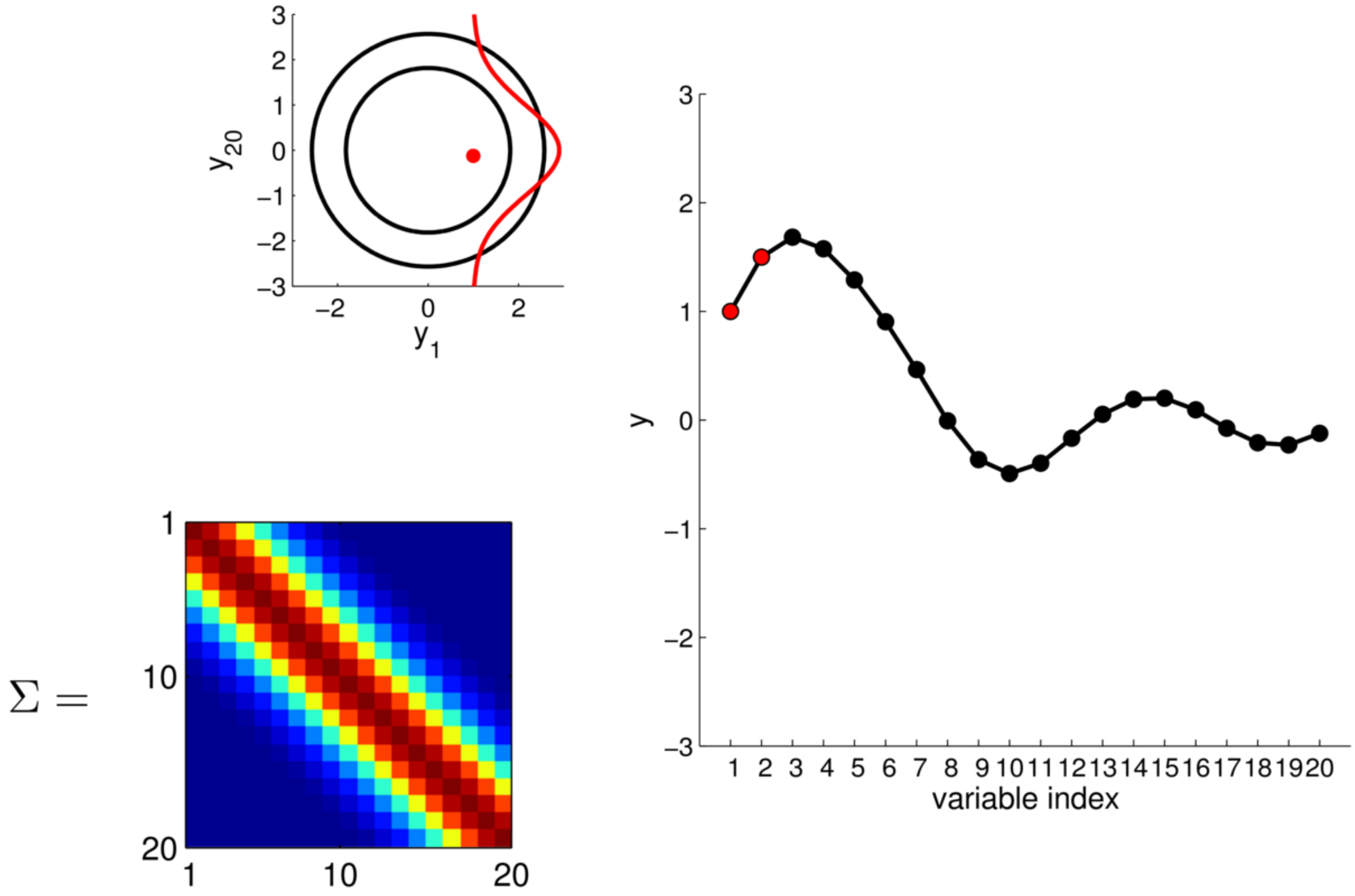

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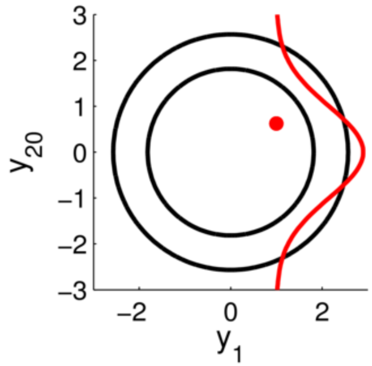

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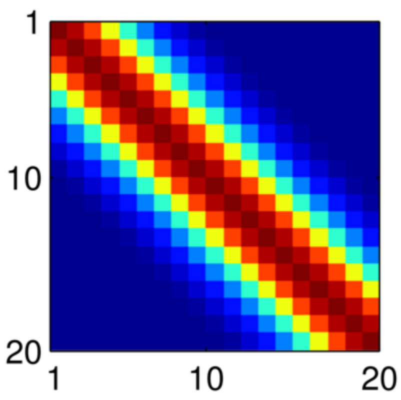

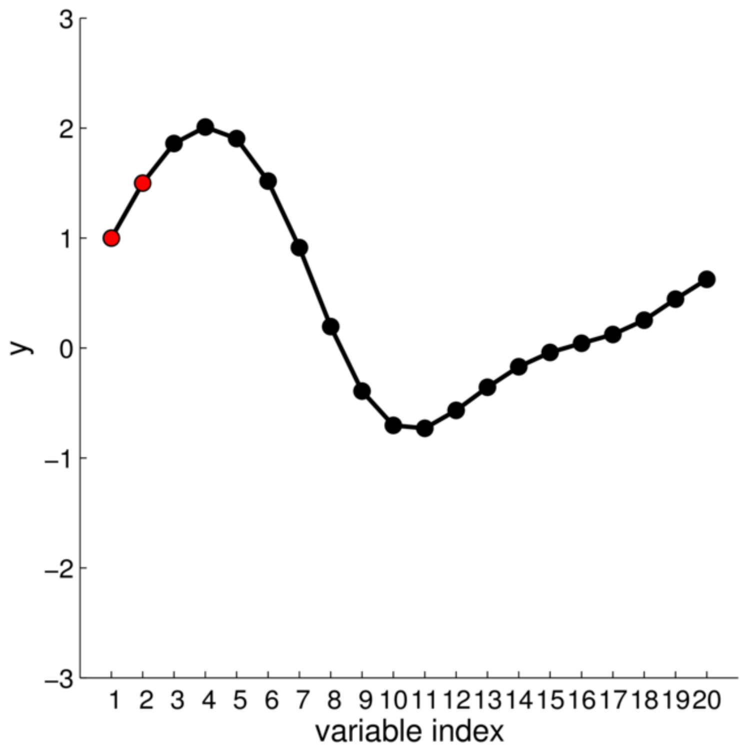

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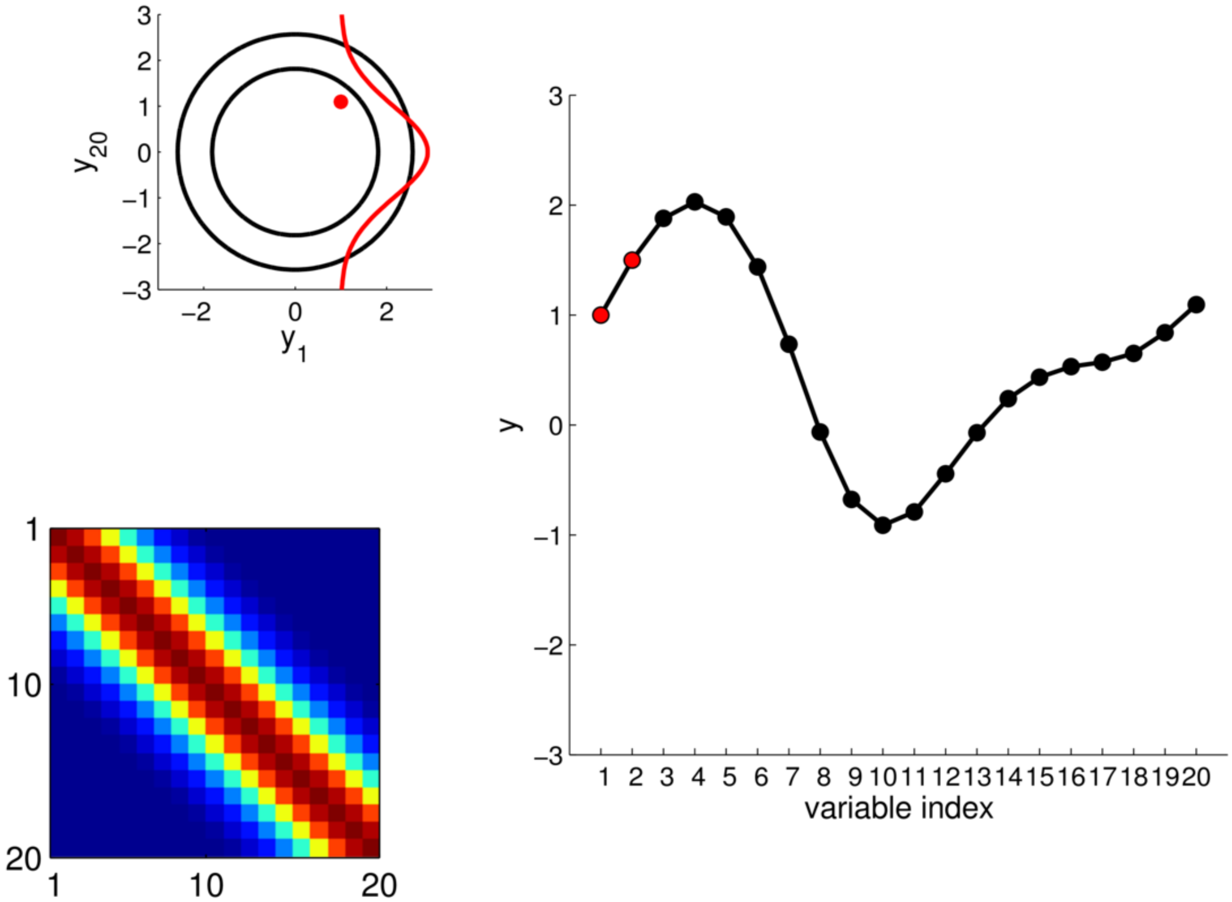

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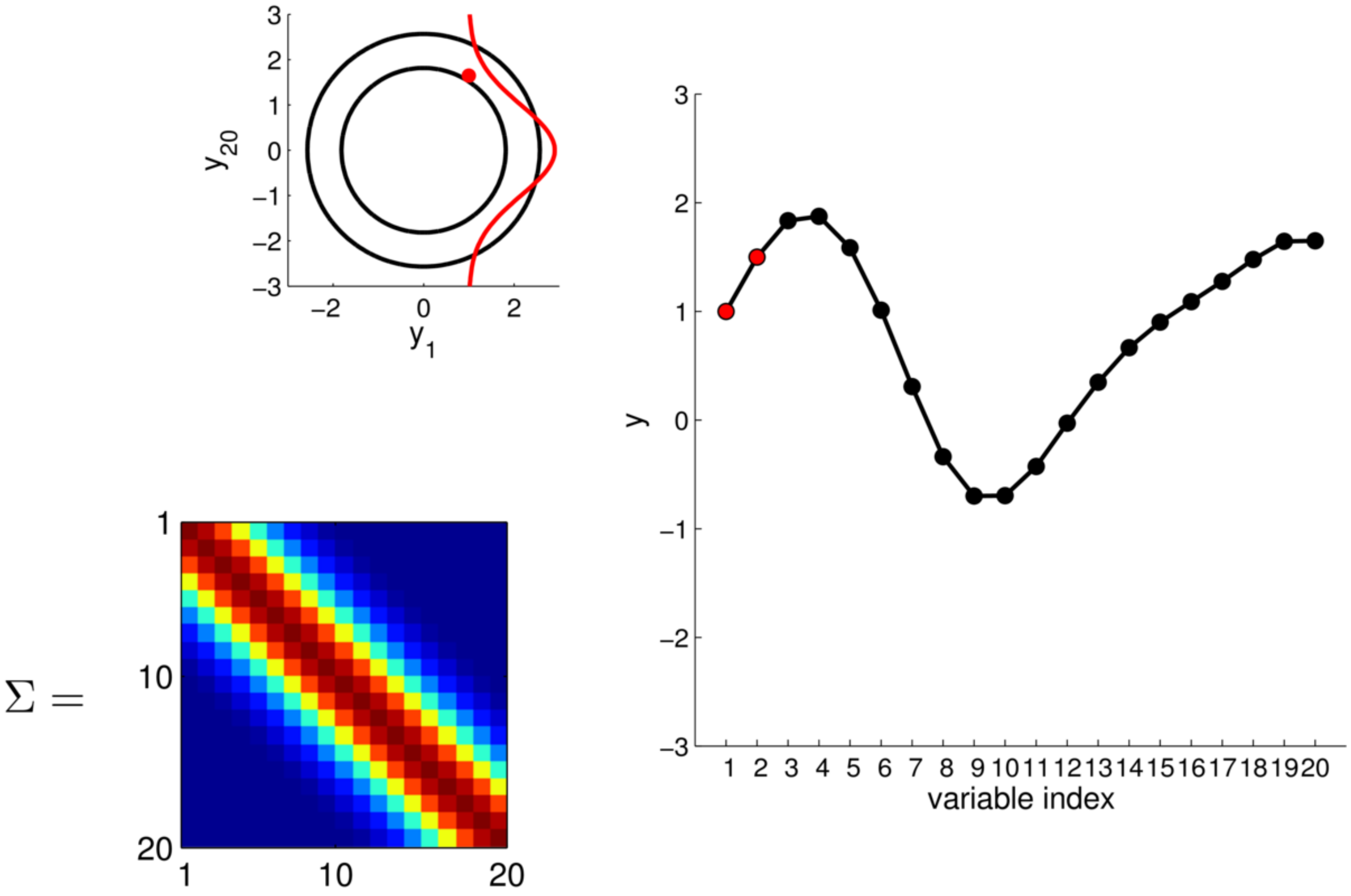

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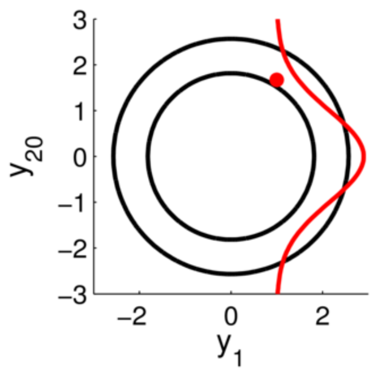

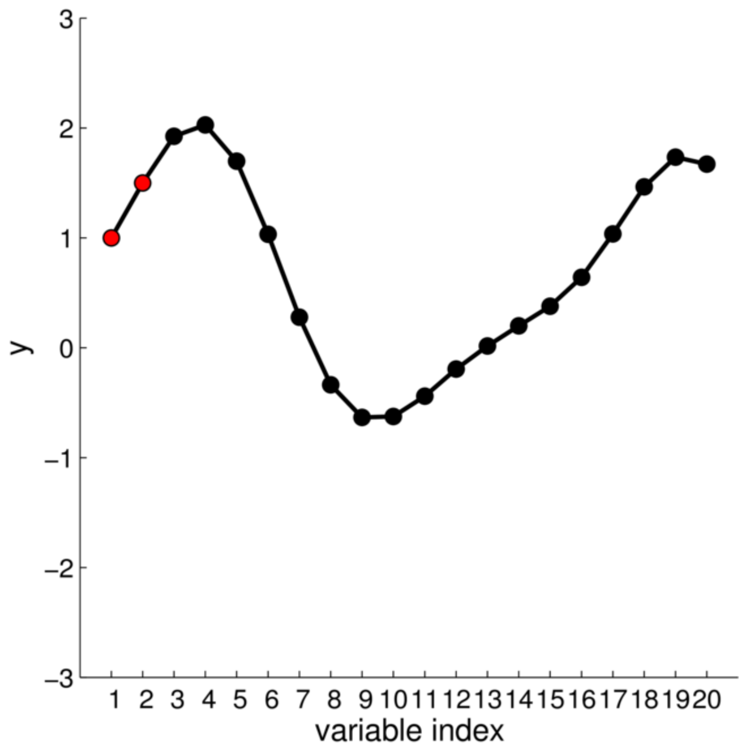

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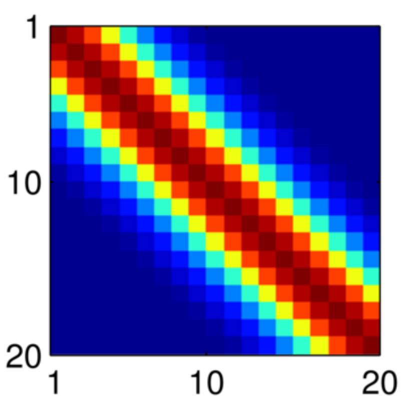

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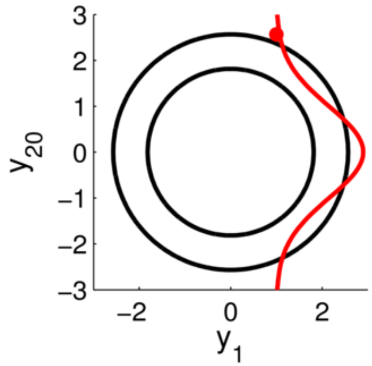
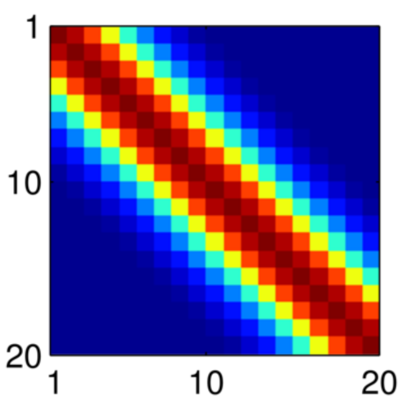
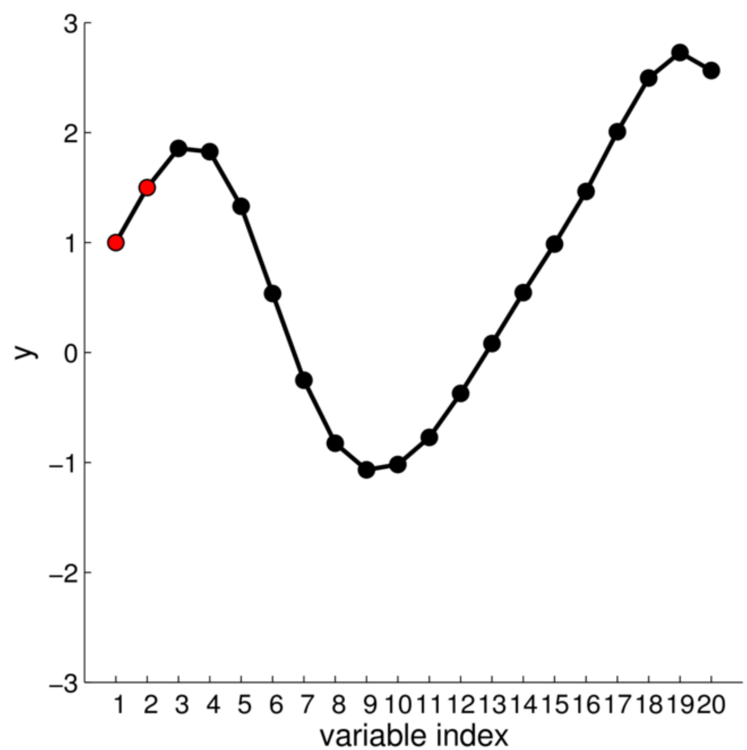
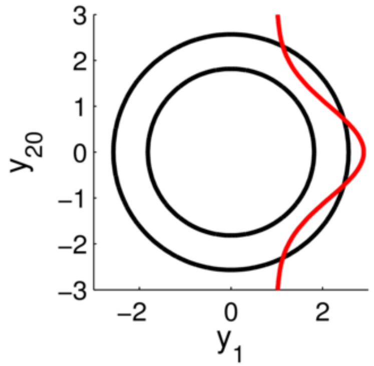


$\Sigma =$ 



Visualizing Gaussian Processes



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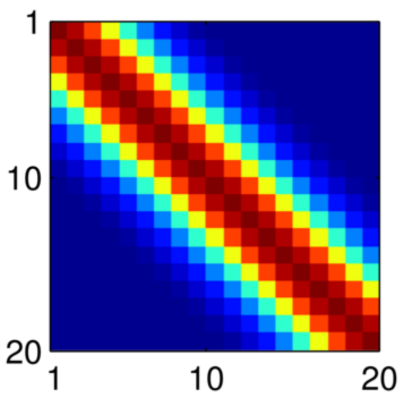
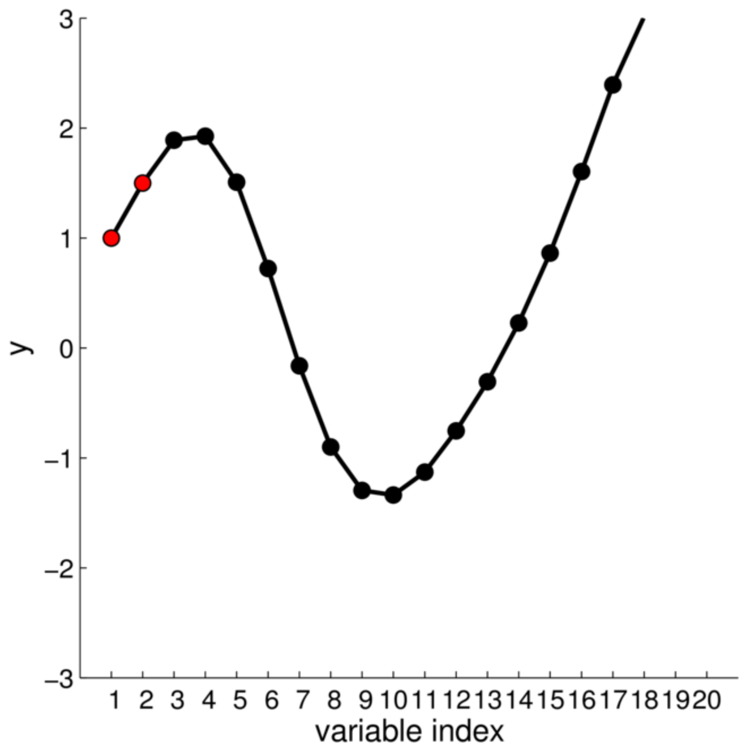
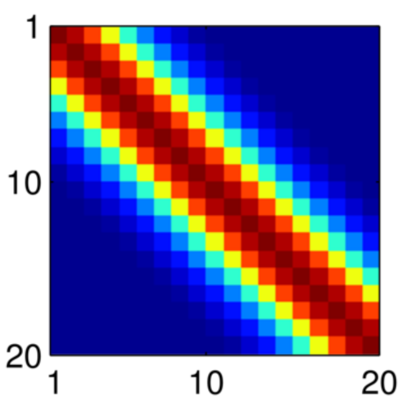
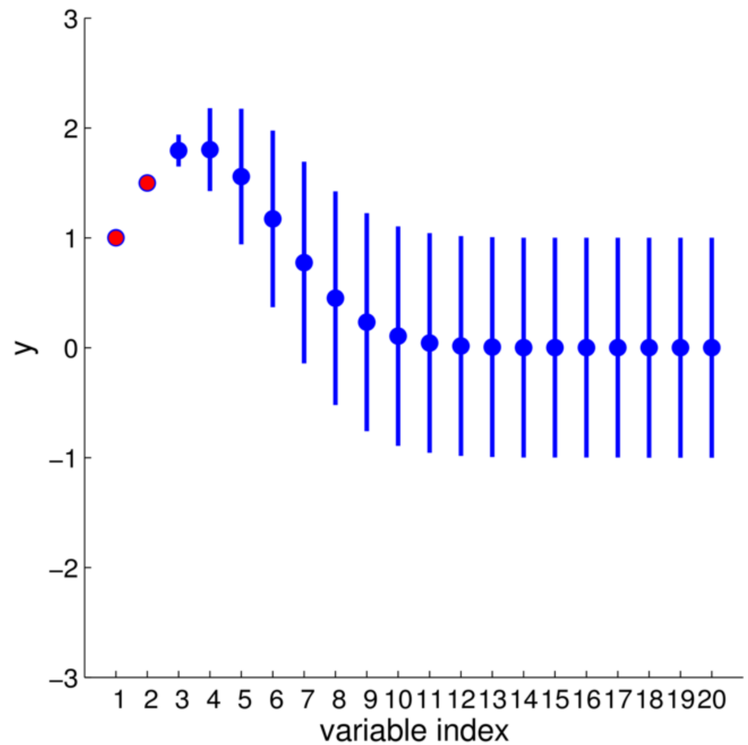




Regression via Gaussian Process

$\Sigma =$





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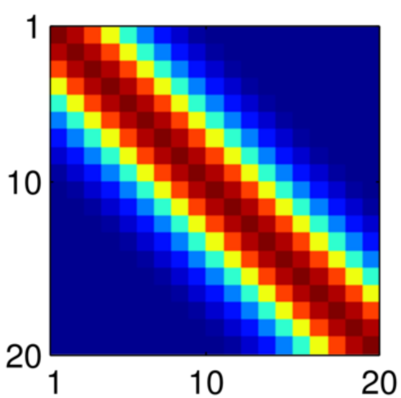

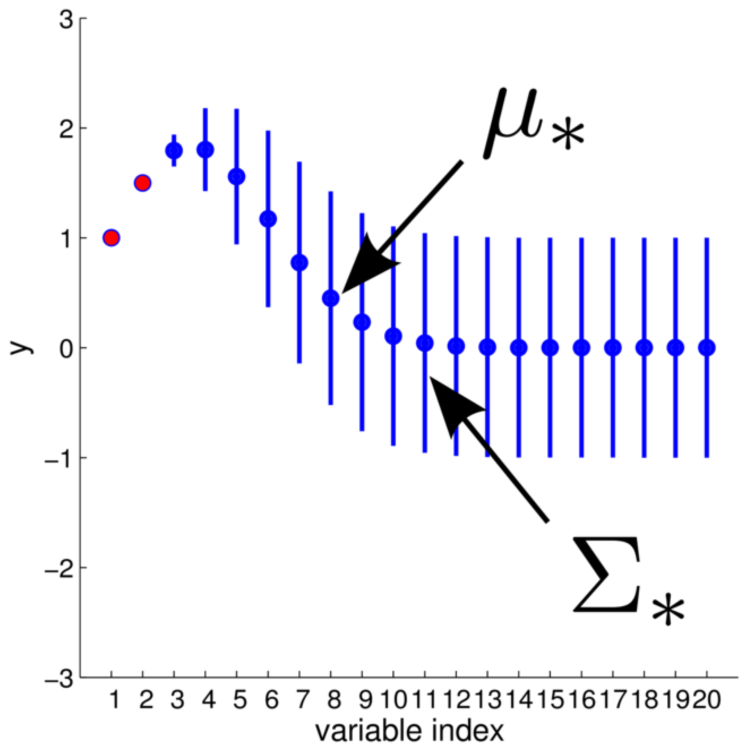

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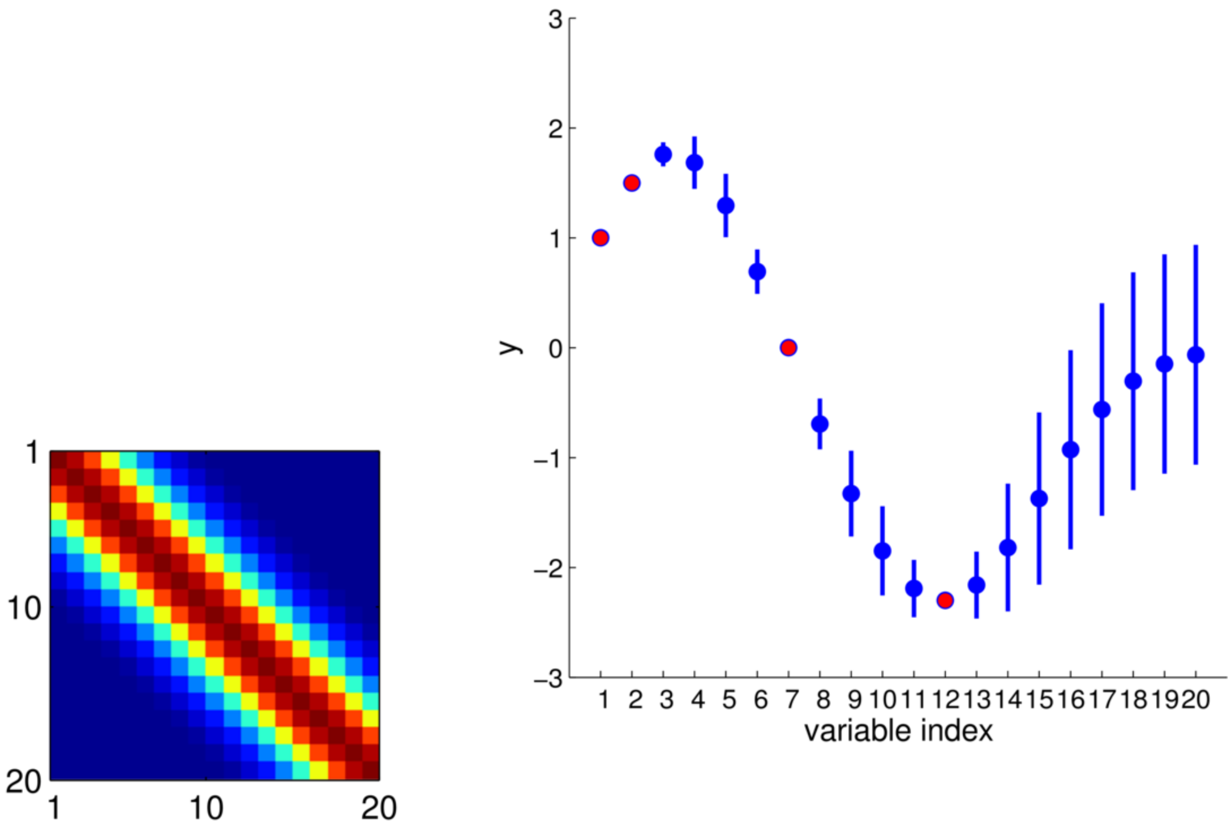


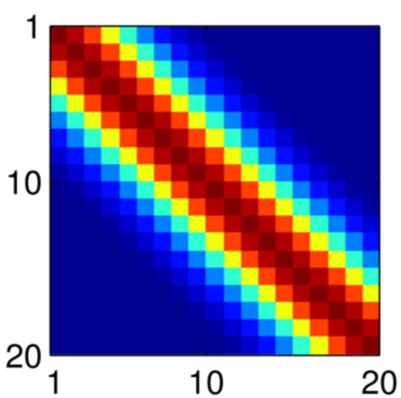
Regression via Gaussian Process

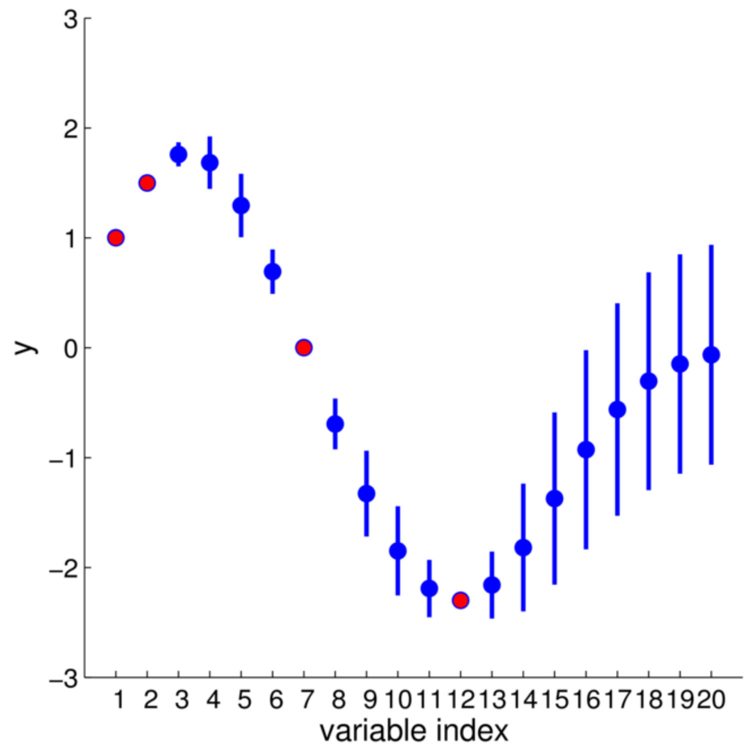
I: the Identity matrix

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

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

l: constant for horizontal scale

$\Sigma =$ 



Probabilistic Inference in Function Space

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

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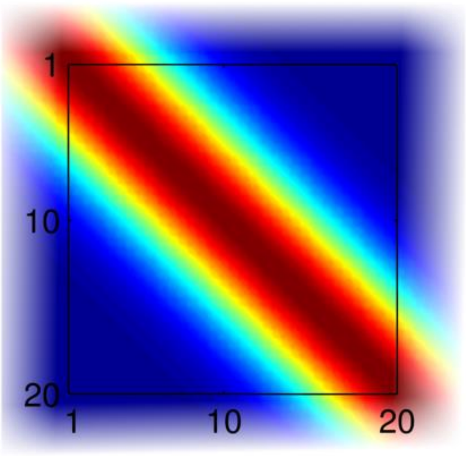

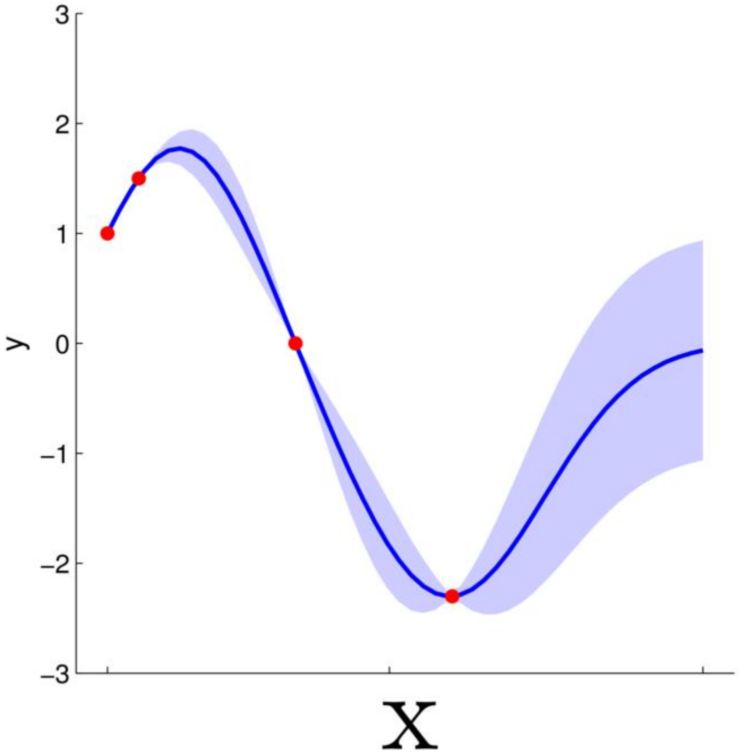

Probabilistic Inference in Function Space

Non-parametric (∞-parametric)

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

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

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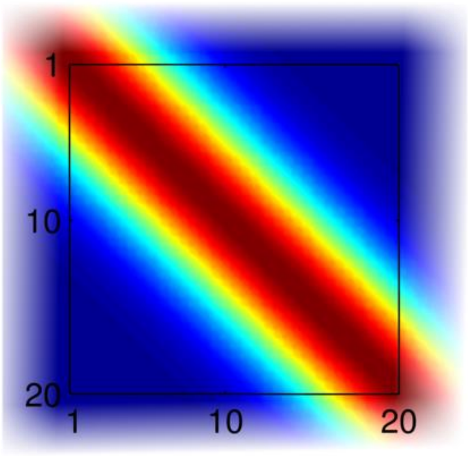
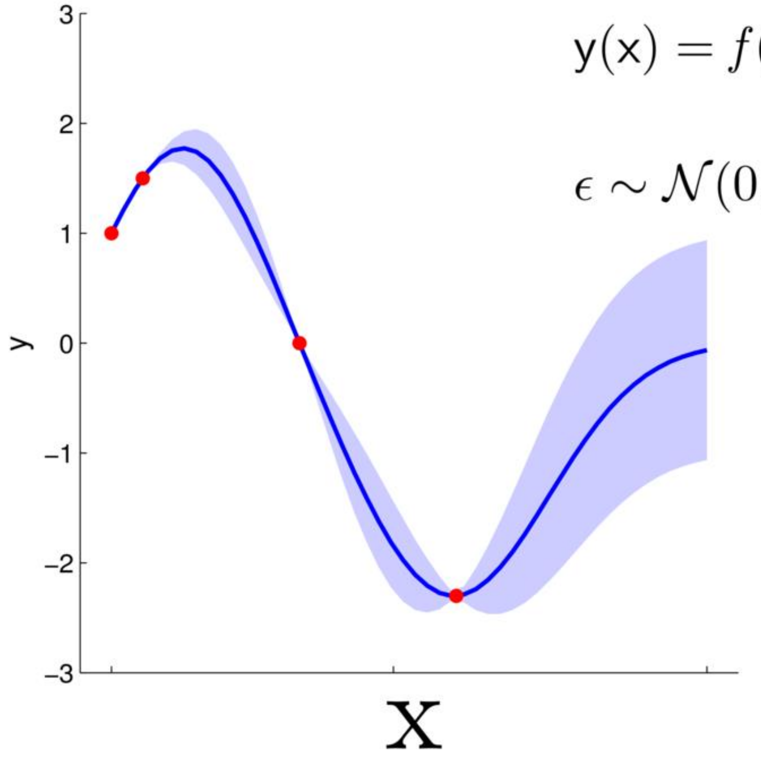
$\Sigma =$ 



Parametric model

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

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

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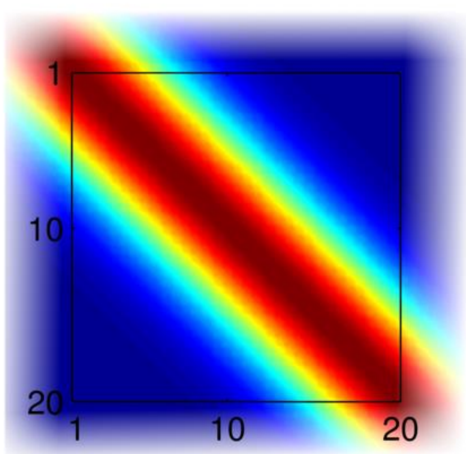
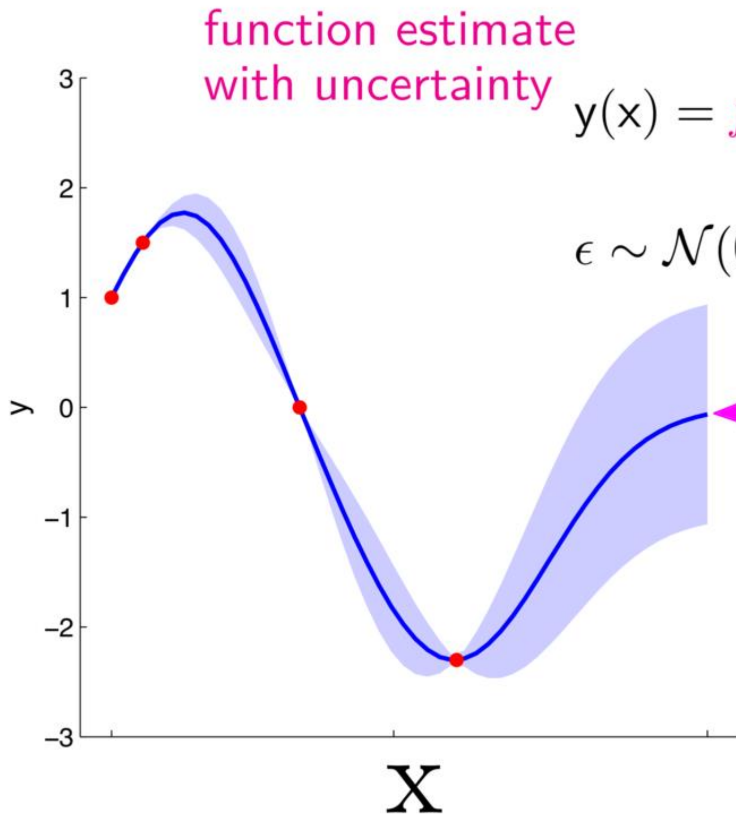
$\Sigma =$ 



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noise

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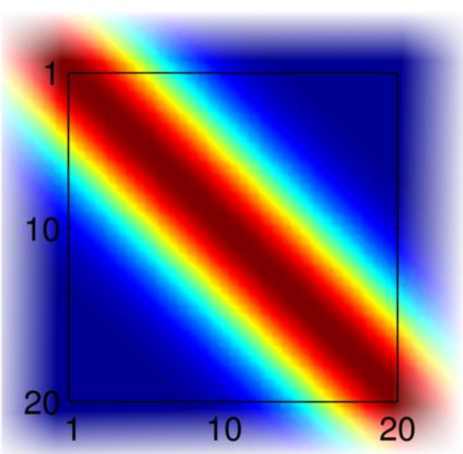
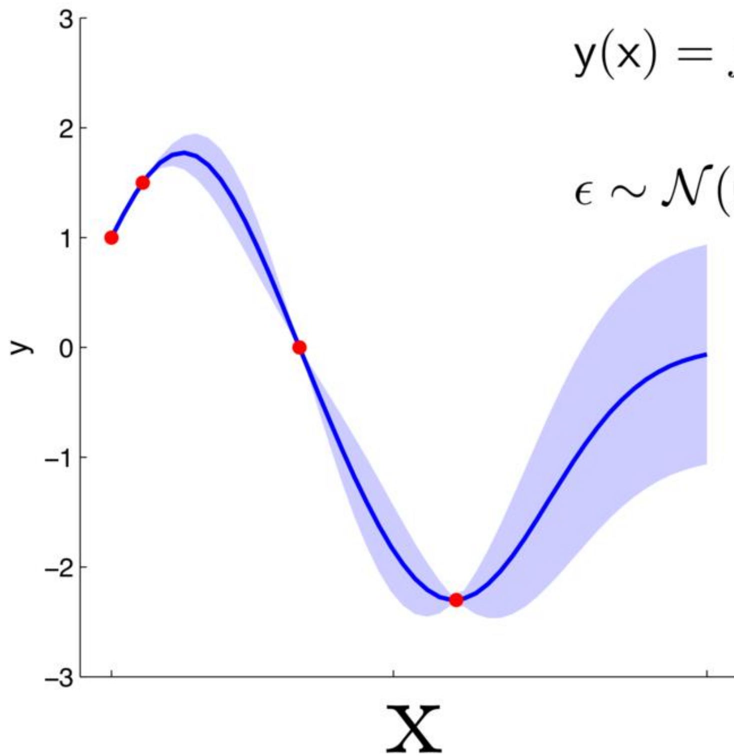
$\Sigma =$ 



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horizontal-scale

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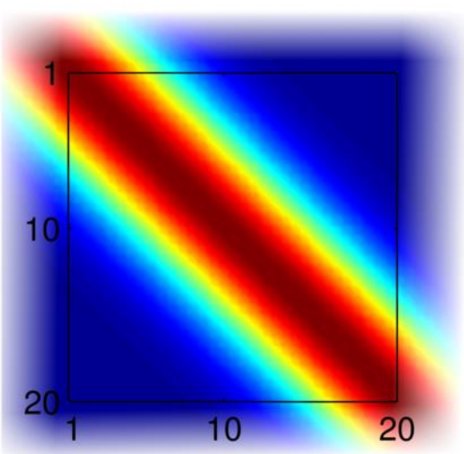

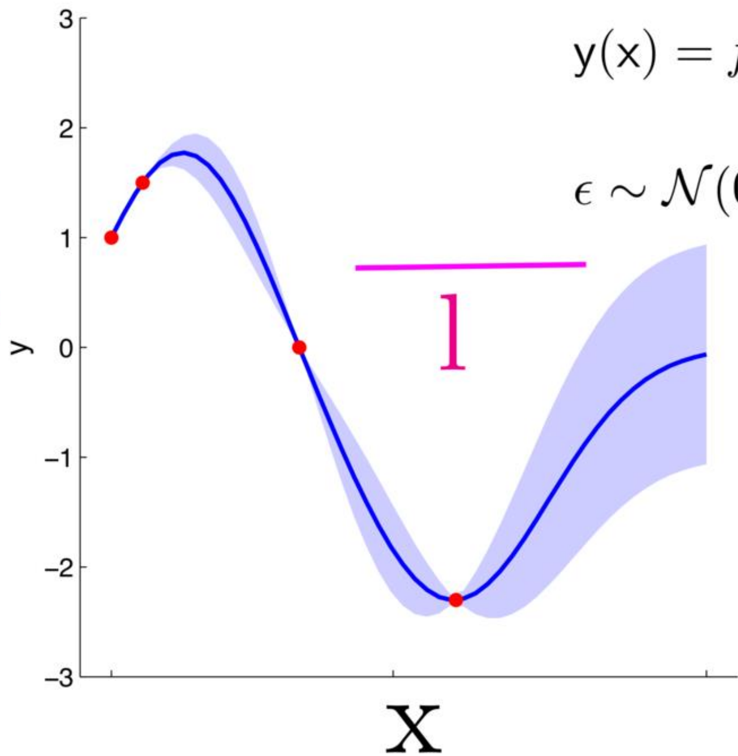

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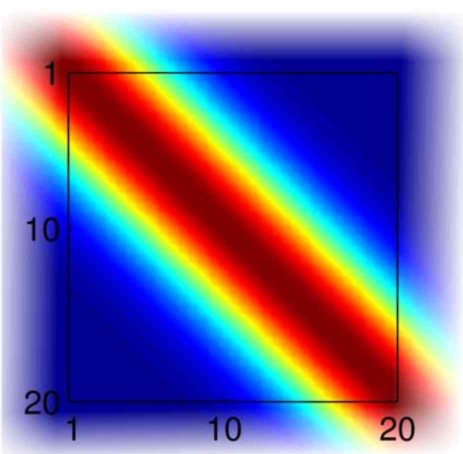
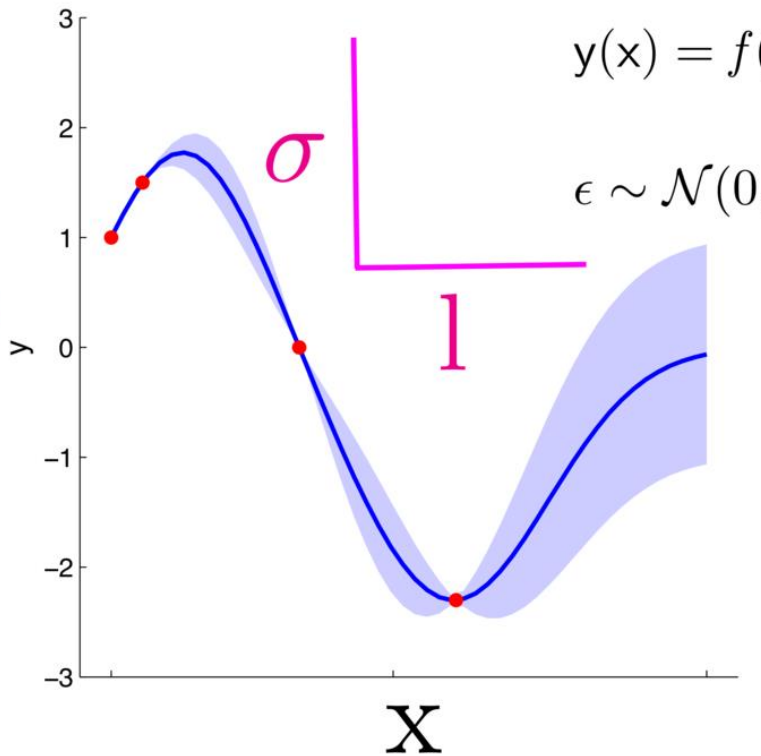
vertical-scale horizontal-scale

$\Sigma =$ 



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Mathematical Foundations: Definition

Gaussian process = generalisation 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:

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

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: Regression

Q1. What's the formal justification for how we were using GPs for regression?

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generative model (like non-linear regression)

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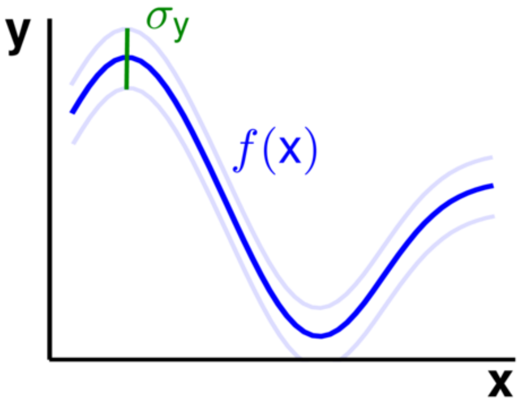

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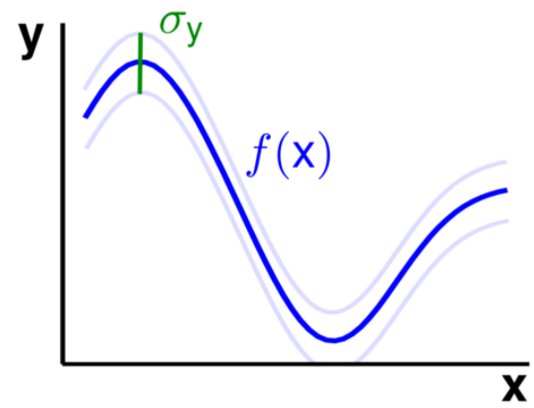

place GP prior over the non-linear function

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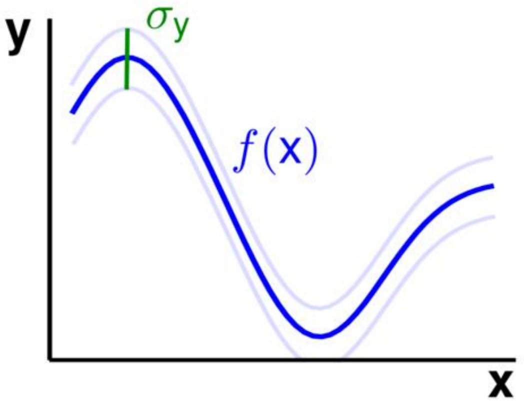

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sum of Gaussian variables = Gaussian: induces a GP over $\mathsf{y}(\mathsf{x})$

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

Mathematical Foundations: Marginalization

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

$$p(\mathbf{y}_1, \mathbf{y}_2) = \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \right)$$

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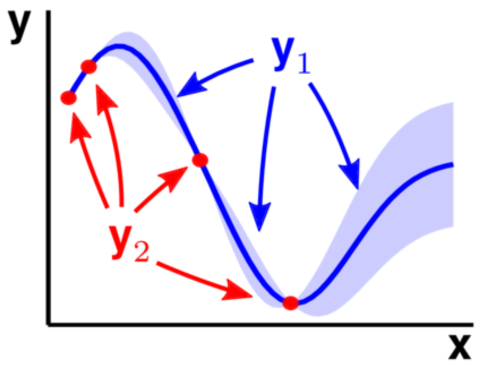
$\implies$ Only need to represent finite dimensional projections of GPs on computer.

Q3: How do we Make Predictions?



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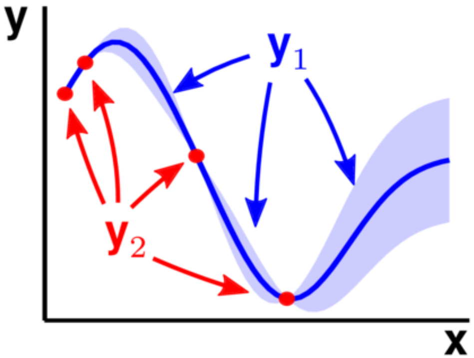

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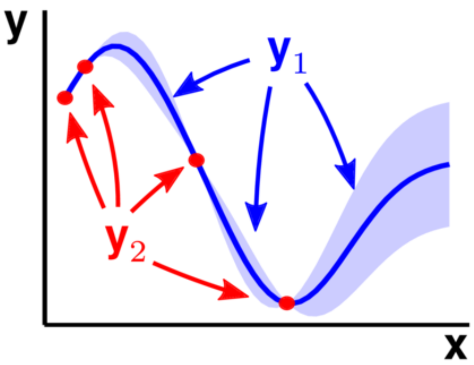
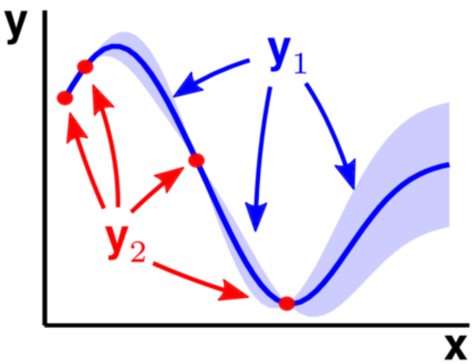
$$p(\mathbf{y}_1 | \mathbf{y}_2) = \frac{p(\mathbf{y}_1, \mathbf{y}_2)}{p(\mathbf{y}_2)}$$



Q3: How do we Make Predictions?

$$p(\mathbf{y}_1, \mathbf{y}_2) = \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{B}^\mathsf{T} & \mathsf{C} \end{bmatrix}\right)$$

$$p(\mathbf{y}_1 | \mathbf{y}_2) = \frac{p(\mathbf{y}_1, \mathbf{y}_2)}{p(\mathbf{y}_2)}$$



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

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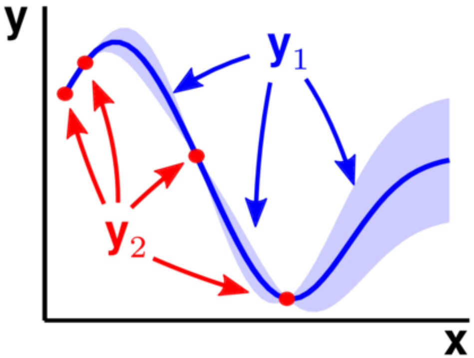
$$p(\mathbf{y}_1, \mathbf{y}_2) = \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{B}^\mathsf{T} & \mathsf{C} \end{bmatrix}\right)$$



$$p(\mathbf{y}_1 | \mathbf{y}_2) = \frac{p(\mathbf{y}_1, \mathbf{y}_2)}{p(\mathbf{y}_2)}$$

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

predictive mean

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

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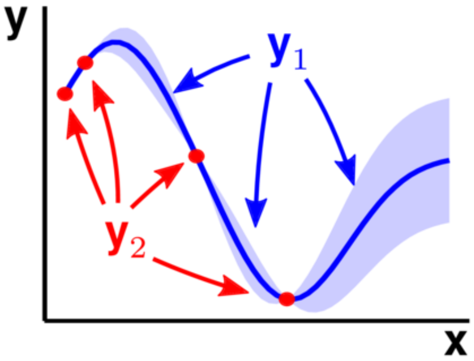

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predictive mean

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

linear in the data

Q3: How do we Make Predictions?

$$p(\mathbf{y}_1, \mathbf{y}_2) = \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{B}^\top & \mathsf{C} \end{bmatrix}\right)$$

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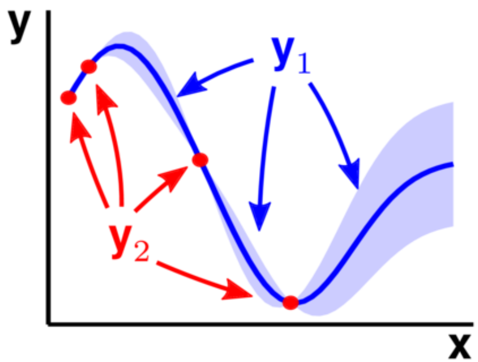


$$\Longrightarrow \quad p(\mathbf{y}_1|\mathbf{y}_2) = \mathcal{N}(\underline{\mathbf{a} + \mathsf{BC}^{-1}(\mathbf{y}_2 - \mathbf{b})}, \underline{\mathsf{A} - \mathsf{BC}^{-1}\mathsf{B}^\top})$$

predictive mean

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

linear in the data

predictive covariance

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

predictive uncertainty = prior uncertainty − reduction in uncertainty

predictions more confident than prior

Partitioned Gaussian Distributions

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

$$\mathbf{x} = \begin{pmatrix}\mathbf{x}_a \\ \mathbf{x}_b\end{pmatrix} \begin{array}{l}\text{Mx1} \\ \text{(D-M)x1}\end{array} \qquad \boldsymbol{\mu} = \begin{pmatrix}\boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b\end{pmatrix}$$

$$\underset{\text{DxD}}{\boldsymbol{\Sigma}} = \begin{array}{cc} \text{MxM} & \text{Mx(D-M)} \\ \end{array}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix}\boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb}\end{pmatrix}$$

$$\begin{array}{cc} \text{(D-M)xM} & \text{(D-M)x(D-M)} \end{array}$$

precision matrix $\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1}$

$$\boldsymbol{\Lambda} = \begin{pmatrix}\boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb}\end{pmatrix}$$

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} M & -MBD^{-1} \\ -D^{-1}CM & D^{-1} + D^{-1}CMBD^{-1} \end{bmatrix}$$

where $M = (A - BD^{-1}C)^{-1}$

Thus, $\Lambda_{aa} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$

Partitioned Conditional Distributions

- Conditional distribution $p(x_a|x_b)$ can be evaluated from the joint distribution $p(x) = p(x_a, x_b)$ by fixing x_b
- That is $p(x_a|x_b) \propto p(x_a, x_b)$ if we treat x_b as constant
- $\Delta^2 = -\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)$
- $= -\frac{1}{2}\left((x_a-\mu_a)^T \quad (x_b-\mu_b)^T\right)\begin{bmatrix}\Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb}\end{bmatrix}\begin{pmatrix}x_a-\mu_a \\ x_b-\mu_b\end{pmatrix}$
- $= -\frac{1}{2}(x_a-\mu_a)^T\Lambda_{aa}(x_a-\mu_a) - \frac{1}{2}(x_a-\mu_a)^T\Lambda_{ab}(x_b-\mu_b)$
  $- \frac{1}{2}(x_b-\mu_b)^T\Lambda_{ba}(x_a-\mu_a) - \frac{1}{2}(x_b-\mu_b)^T\Lambda_{bb}(x_b-\mu_b)$
- 2nd order of x_a: $-\frac{1}{2}(x_a)^T\Lambda_{aa}(x_a)$
- 1st order of x_a: $x_a^T\Lambda_{aa}\mu_a - \frac{1}{2}x_a^T\Lambda_{ab}(x_b-\mu_b) - \frac{1}{2}x_a^T\Lambda_{ba}^T(x_b-\mu_b)$

Completing the squares of the exponent

- General form $\Delta^2 = -\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)$
  $= -\frac{1}{2}\mathbf{x}^T\Sigma^{-1}\mathbf{x} + \mathbf{x}^T\Sigma^{-1}\boldsymbol{\mu} + const$
- Coefficient of the 2nd order term: covariance matrix $\sum^{-1}$
- Coefficient of the 1st order term: $\sum^{-1}\mu$

2nd order of x_a $\quad -\frac{1}{2}\mathbf{x}_a^T\Lambda_{aa}\mathbf{x}_a$ $\quad \Rightarrow \Sigma_{a|b} = \Lambda_{aa}^{-1}$

1st order of x_a $\quad \mathbf{x}_a^T\Lambda_{aa}\boldsymbol{\mu}_a - \frac{1}{2}\mathbf{x}_a^T\Lambda_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b) - \frac{1}{2}\mathbf{x}_a^T\Lambda_{ba}^T(\mathbf{x}_b - \boldsymbol{\mu}_b)$

$$= x_a^T\{\Lambda_{aa}\mu_a - \Lambda_{ab}(x_b - \mu_b)\}$$
$$= x_a^T\Sigma_{a|b}^{-1}\mu_{a|b}$$

$$\Rightarrow \mu_{a|b} = \Sigma_{a|b}\{\Lambda_{aa}\mu_a - \Lambda_{ab}(x_b - \mu_b)\} = \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(x_b - \mu_b)$$

Conditional Distribution of Multivariate Gaussian

- $\Sigma_{a|b} = \Lambda_{\mathrm{aa}}^{-1} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$
- $\mu_{a|b} = \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(x_b - \mu_b)$
- Moreover, $\begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}^{-1} = \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix}$
- and, $\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} M & -MBD^{-1} \\ -D^{-1}CM & D^{-1} + D^{-1}CMBD^{-1} \end{bmatrix}$,
- $M = (A - BD^{-1}C)^{-1}$
- Thus, $\Lambda_{aa} = \left(\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}\right)^{-1}$,
- $\Lambda_{ab} = -\left(\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}\right)^{-1}\Sigma_{ab}\Sigma_{bb}^{-1}$
- As a result, $\mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b)$

Conditional Distribution of Multivariate Gaussian

- Let $x = [x_1\ x_2 \cdots x_D]$ be jointly Gaussian
- $x \sim MN(\mu, \Sigma)$
- Partitioned x into two groups $x = \begin{bmatrix} x_a \\ x_b \end{bmatrix}$; $x_a = [x_1\ x_2\ \ldots x_M]^T$, and $x_b = [x_{M+1}\ \ldots x_D]^T$
- Think of x_a as the target variables and x_b as the features.
- $p(x_a|x_b) = MN(\mu_{a|b}, \Sigma_{a|b})$
- $\Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$
- $\mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b)$

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \begin{array}{l} \text{Mx1} \\ \text{(D-M)x1} \end{array} \qquad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix}$$

$$\underset{\text{DxD}}{\boldsymbol{\Sigma}} = \begin{array}{cc} \text{MxM} & \text{Mx(D-M)} \end{array} \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix} \begin{array}{cc} \text{(D-M)xM} & \text{(D-M)x(D-M)} \end{array}$$

Kernel Hyper-parameters

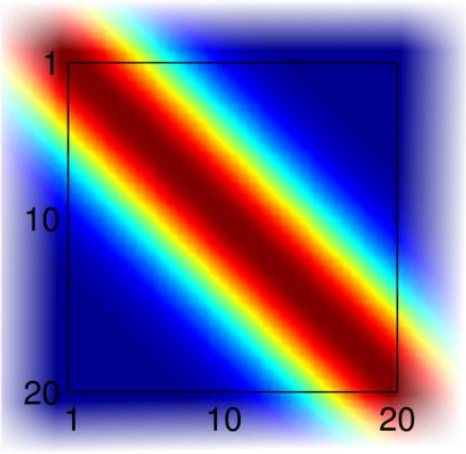
Non-parametric (∞-parametric)

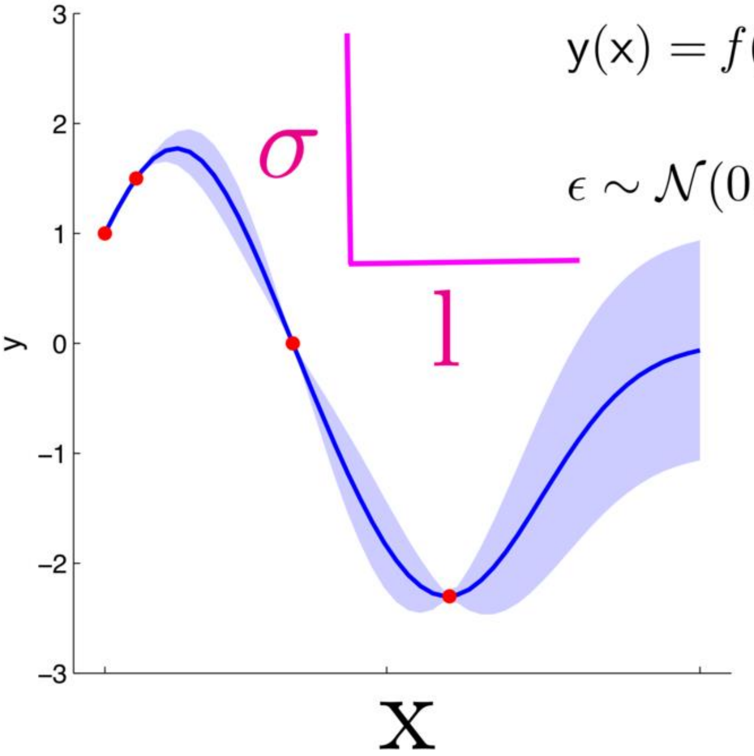
$$p(\mathrm{y}|\theta) = \mathcal{N}(0, \Sigma)$$

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

$$\mathrm{K}(\mathrm{x}_1, \mathrm{x}_2) = \sigma^2 e^{-\frac{1}{2l^2}(\mathrm{x}_1 - \mathrm{x}_2)^2}$$

vertical-scale horizontal-scale

$\Sigma =$ 



Parametric model

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

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

Comparing Three Kernel Parameter Settings

- Changing l will affect the horizontal length scale
- l larger→ correlation decays faster

Non-parametric (∞-parametric)

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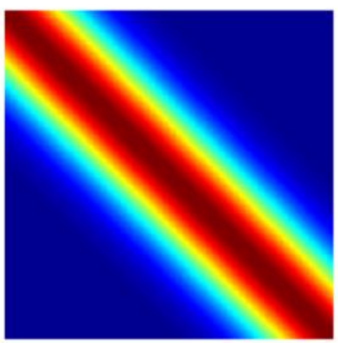
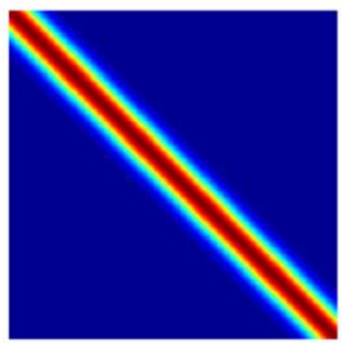
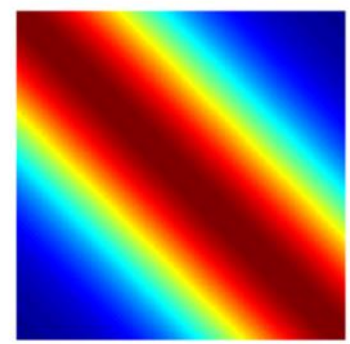
$$\Sigma(\mathrm{x}_1, \mathrm{x}_2) = \mathrm{K}(\mathrm{x}_1, \mathrm{x}_2) + \mathrm{I}\sigma_{\mathrm{y}}^2$$

$$\mathrm{K}(\mathrm{x}_1, \mathrm{x}_2) = \sigma^2 e^{-\frac{1}{2l^2}(\mathrm{x}_1 - \mathrm{x}_2)^2}$$

- l median | l large | l small
- median scale | short scale | long scale

$\Sigma =$ 

$\Sigma =$ 

$\Sigma =$ 

What effect do the Hyper-parameters Have?

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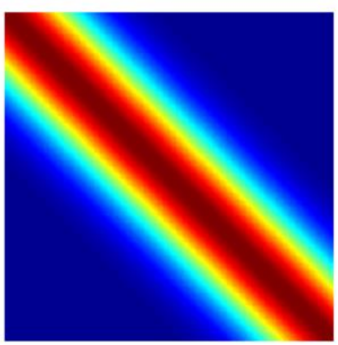
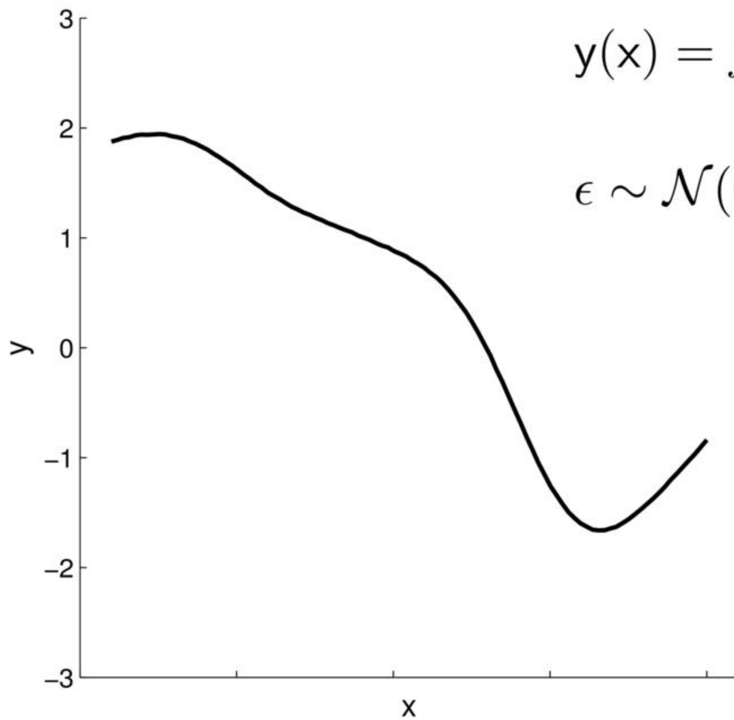
$$\Sigma =$$





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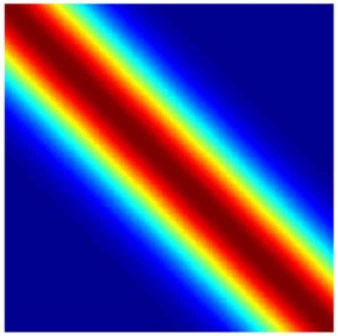
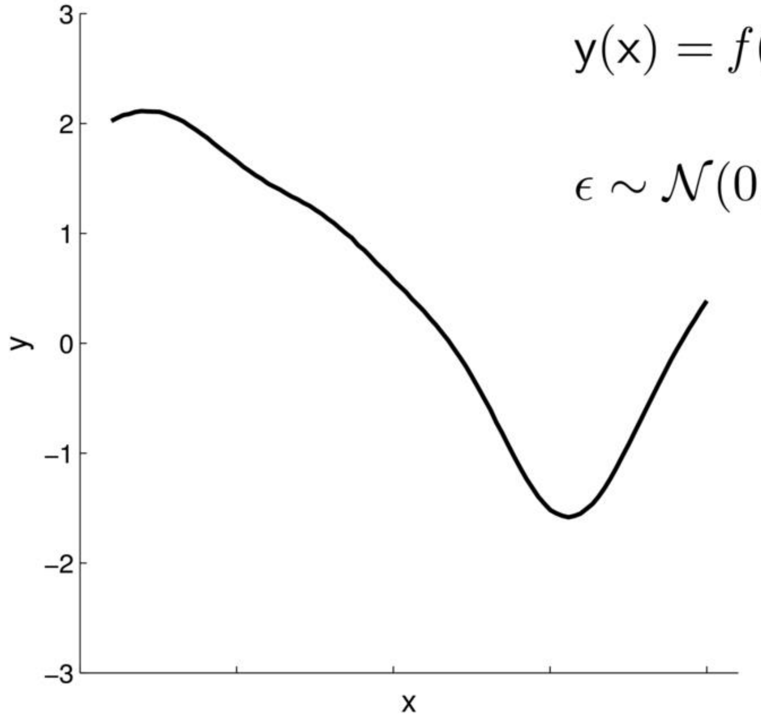
$\Sigma =$ 



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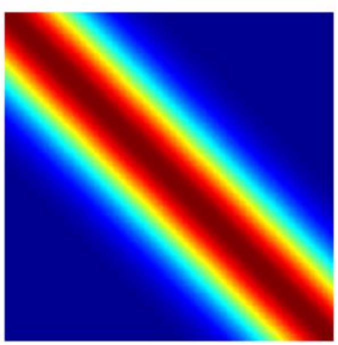
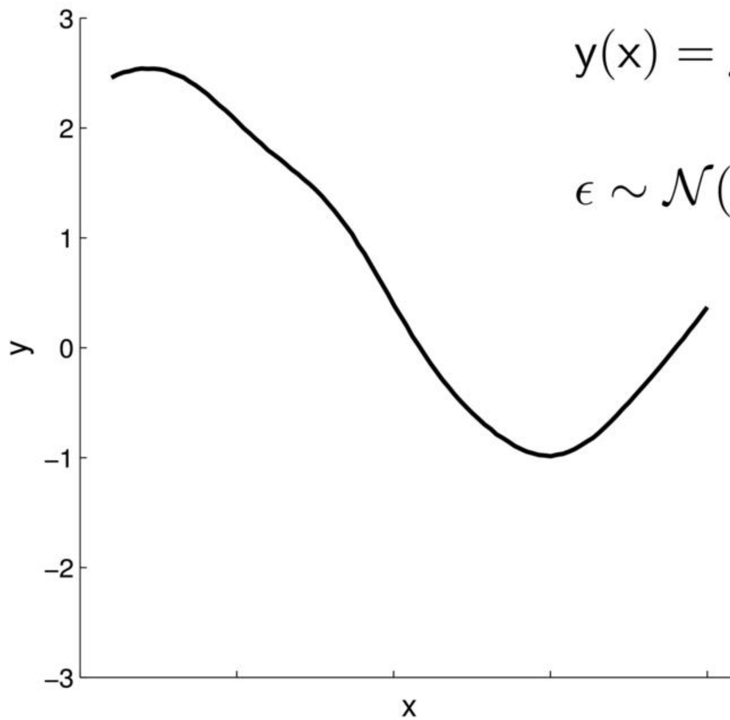
$\Sigma =$ 



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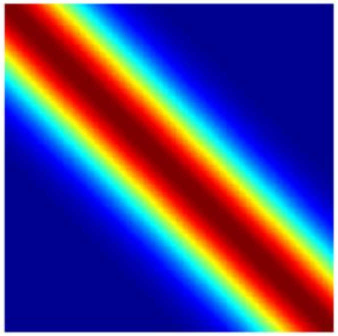
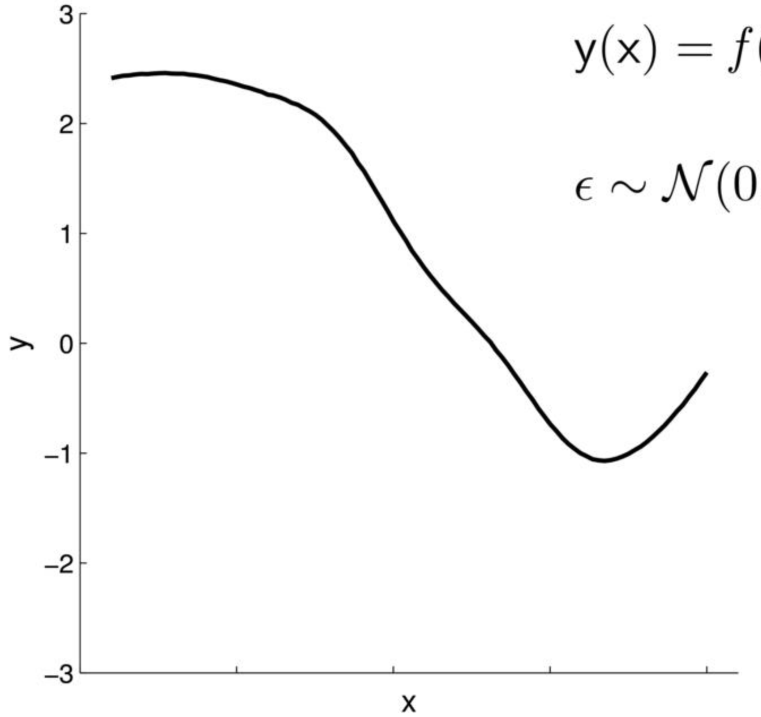
$\Sigma =$ 



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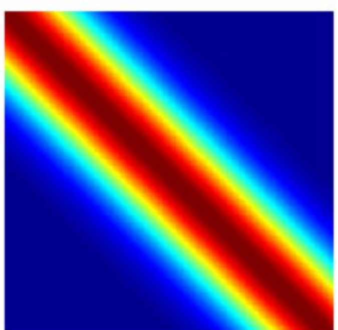
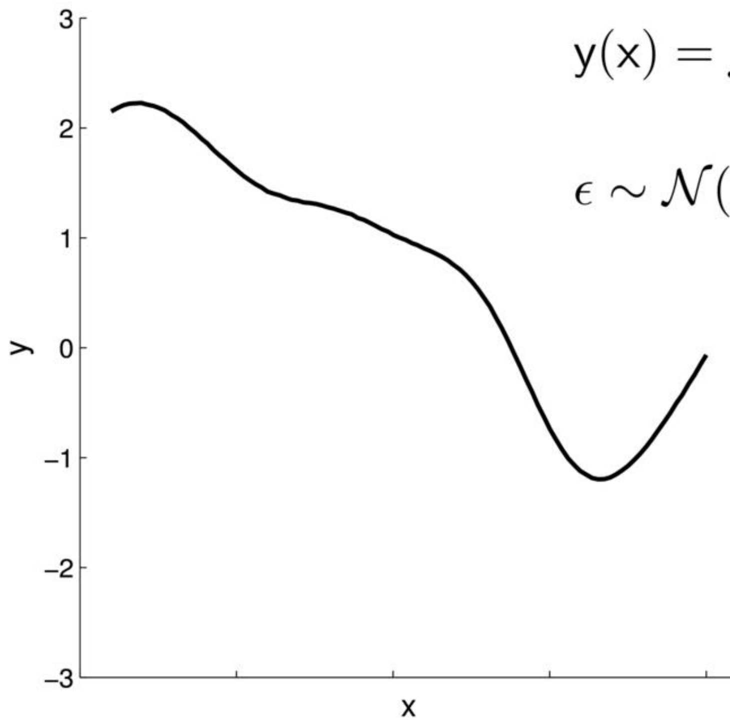
$\Sigma =$ 



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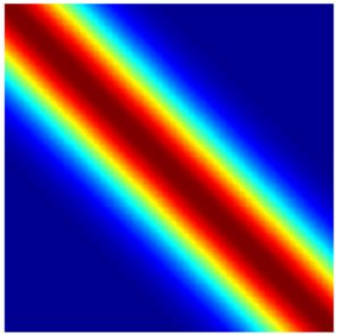
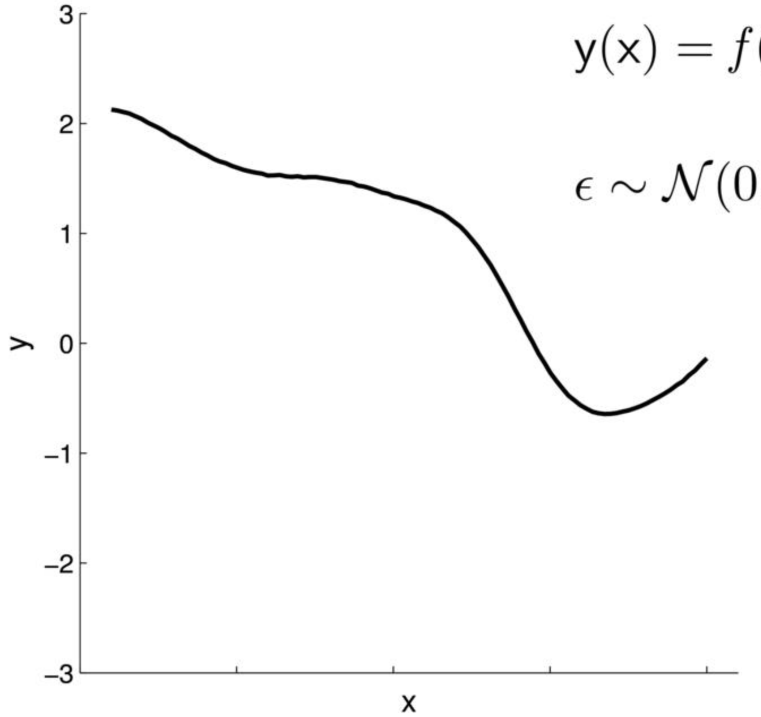
$\Sigma =$ 



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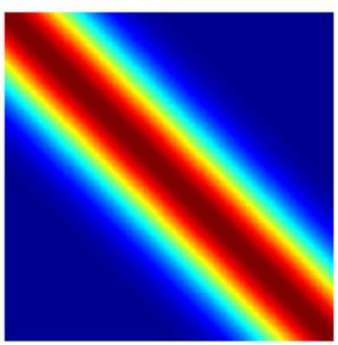
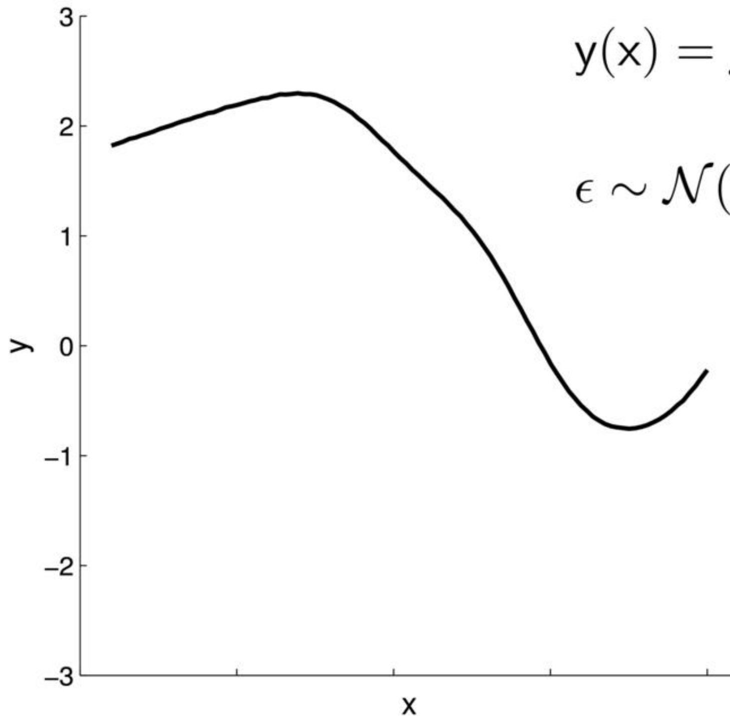
$\Sigma =$ 



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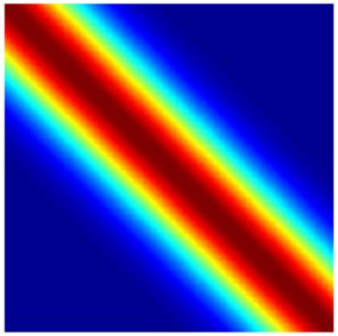
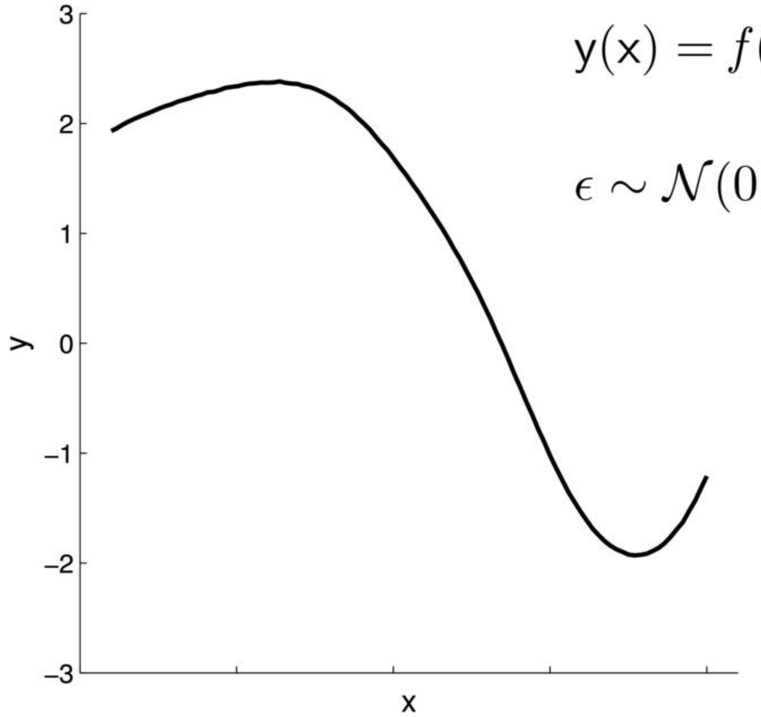
$\Sigma =$ 



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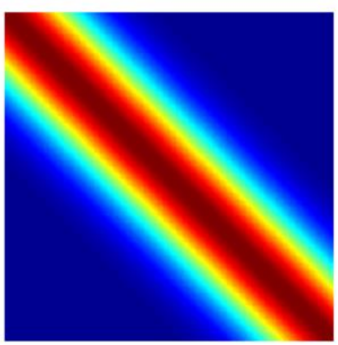
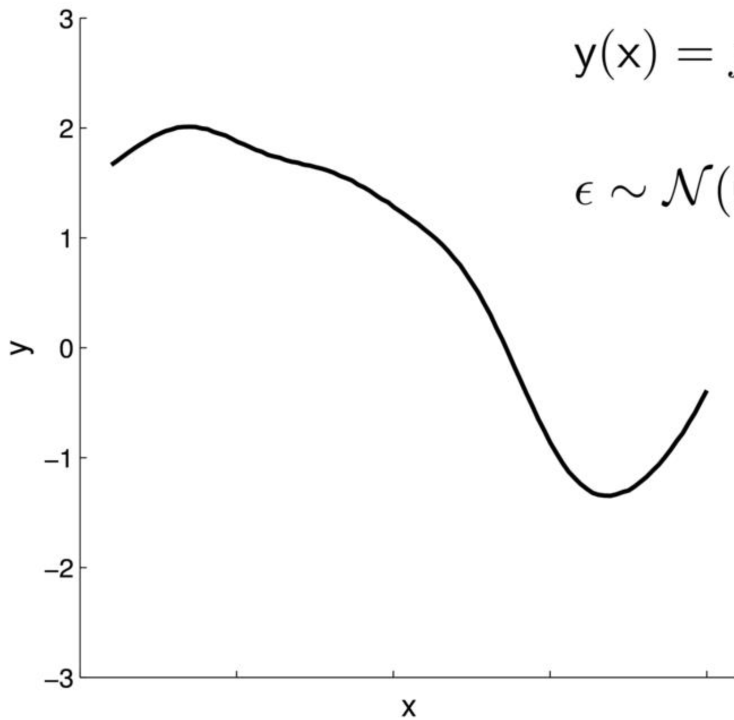
$\Sigma =$ 



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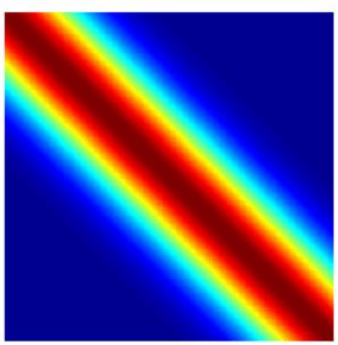
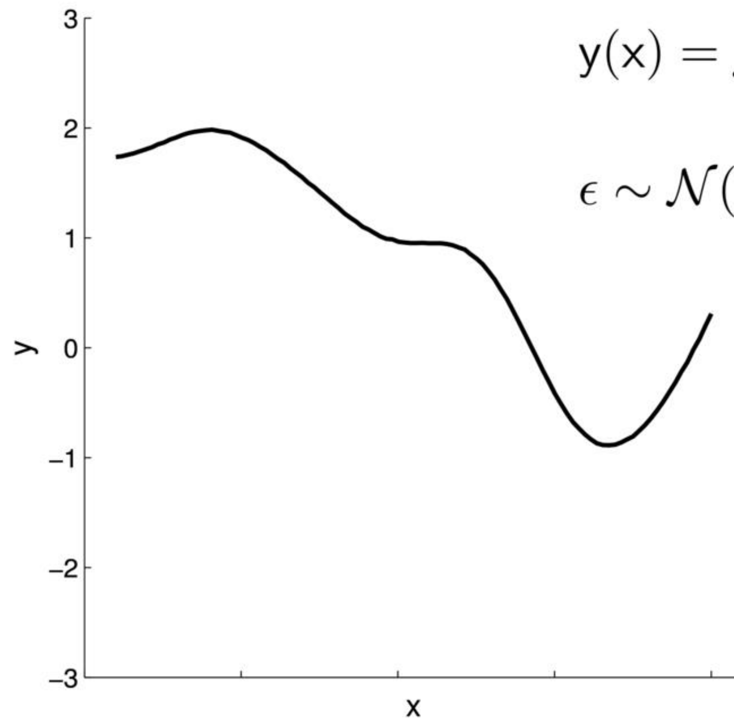
$\Sigma =$ 



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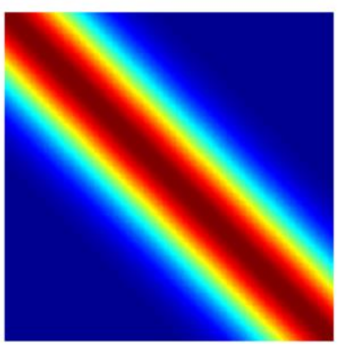
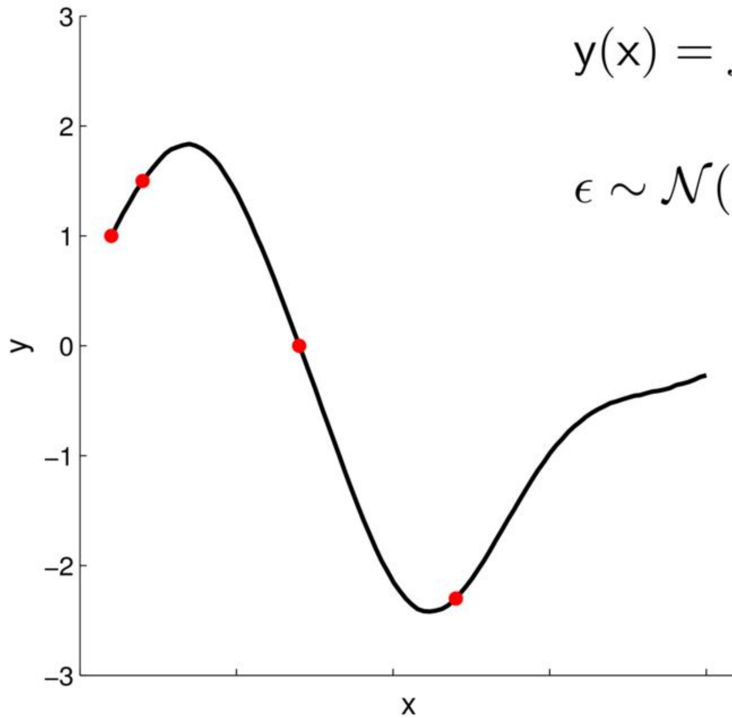
$\Sigma =$ 



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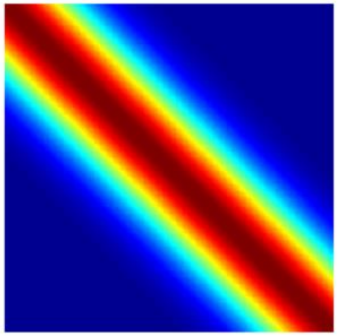
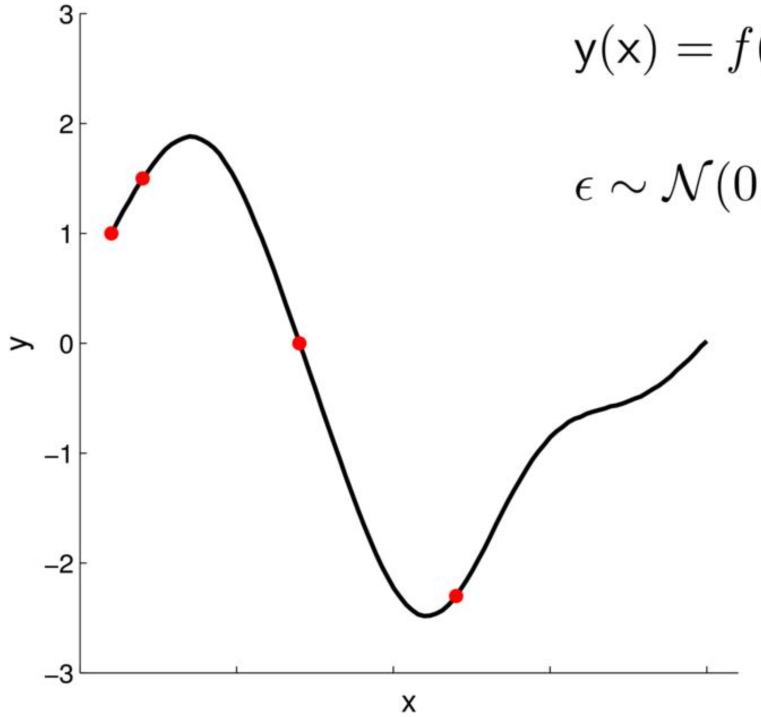
$\Sigma =$ 



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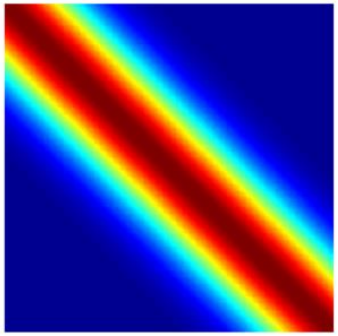
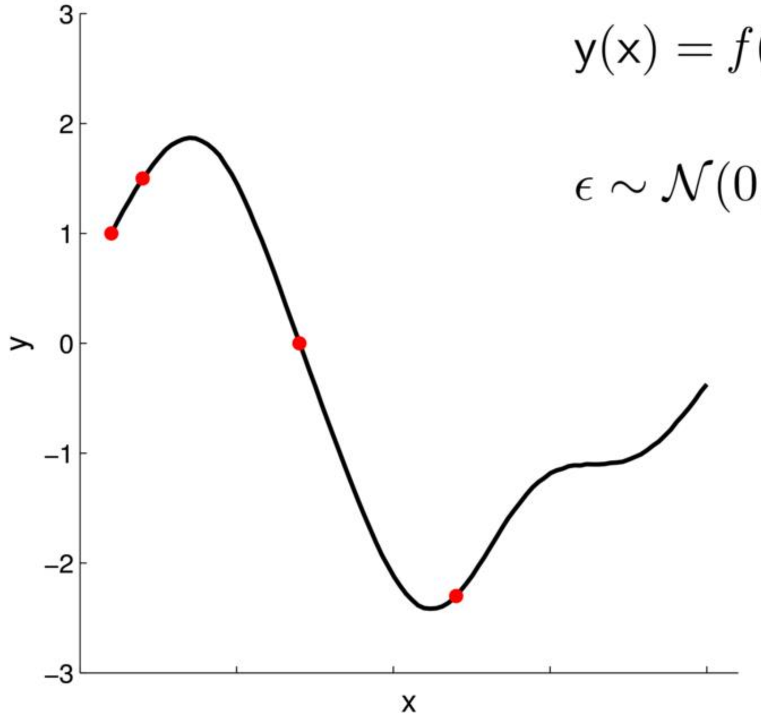
$\Sigma =$ 



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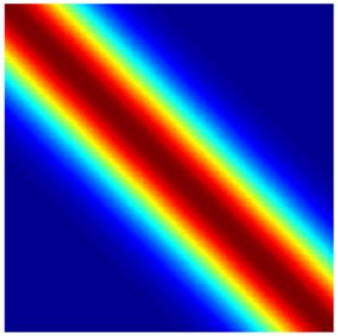
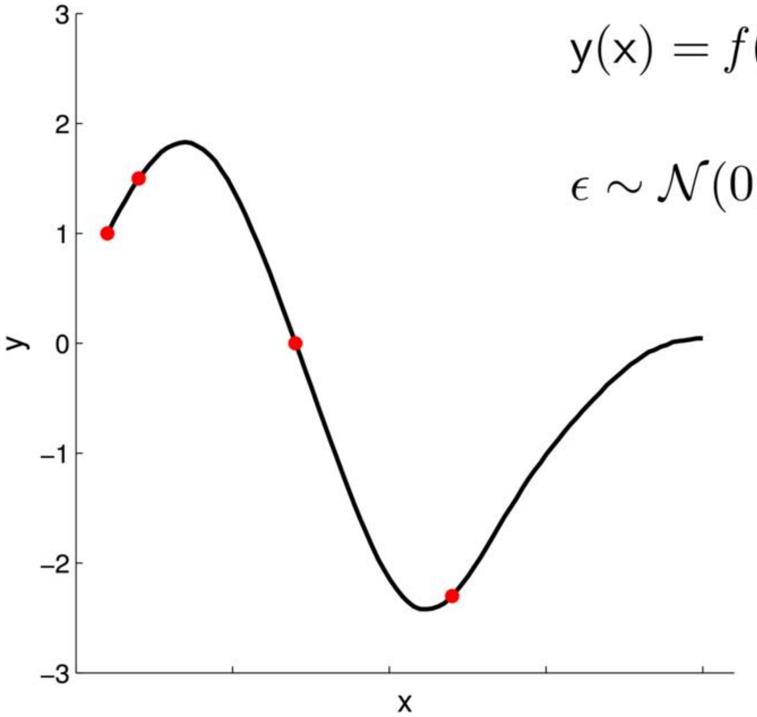
$\Sigma =$ 



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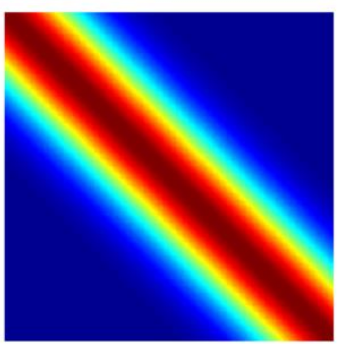
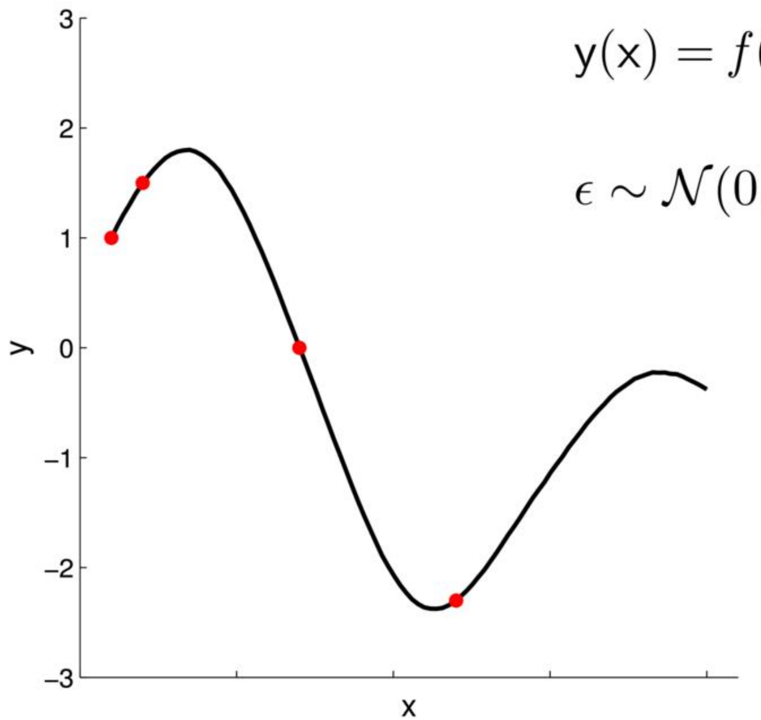
$\Sigma =$ 



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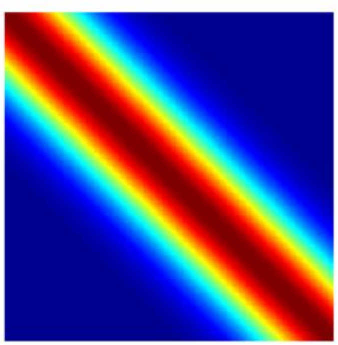
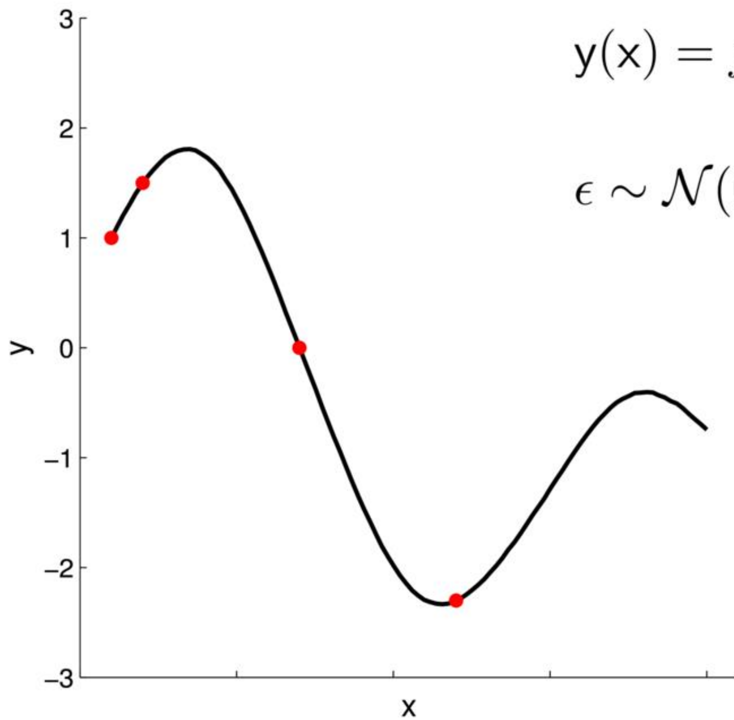
$\Sigma =$ 



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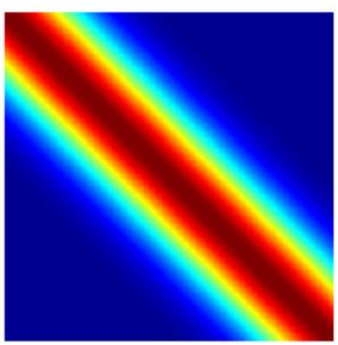
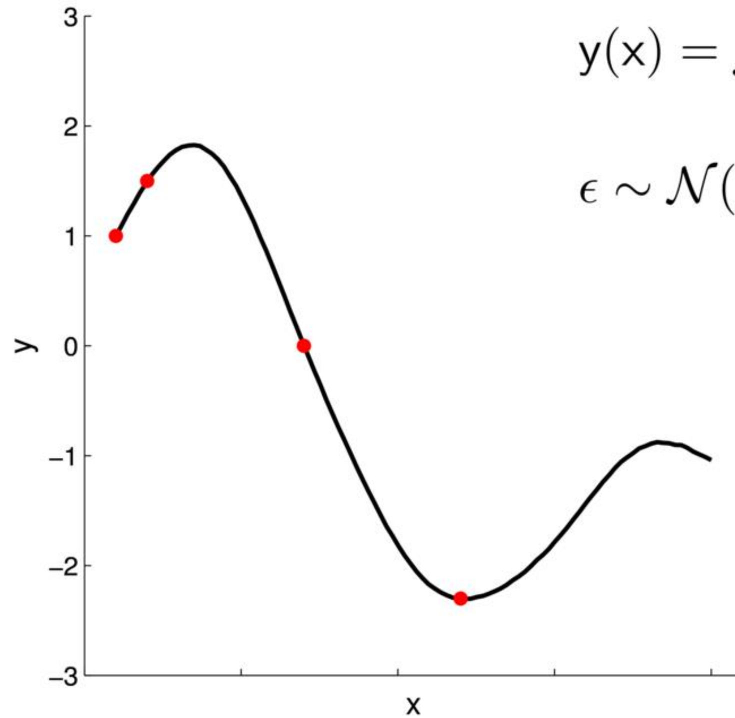
$\Sigma =$ 



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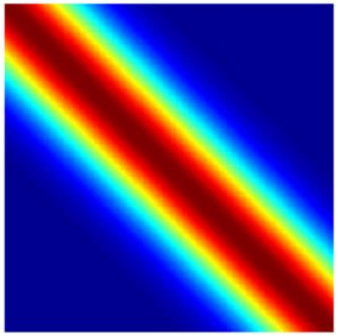
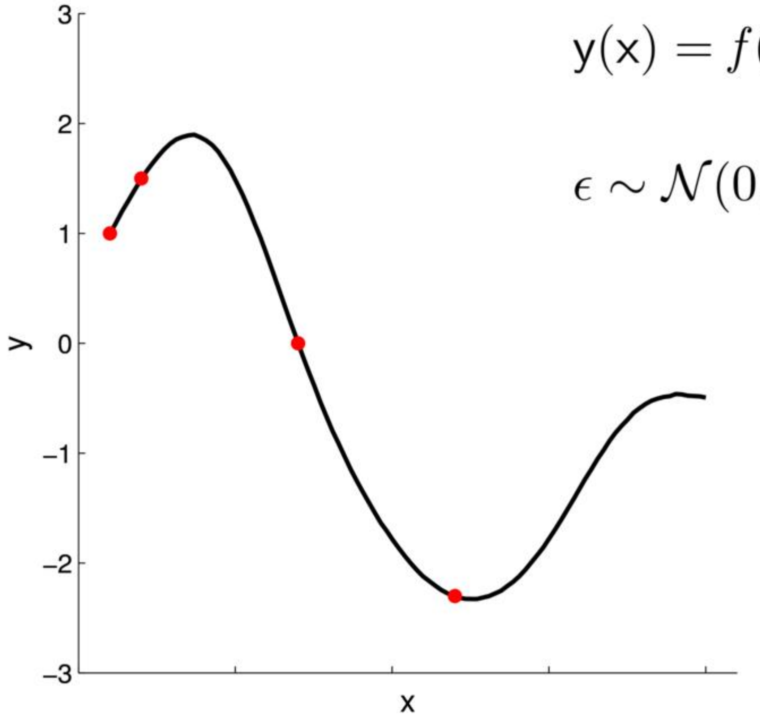
$\Sigma =$ 



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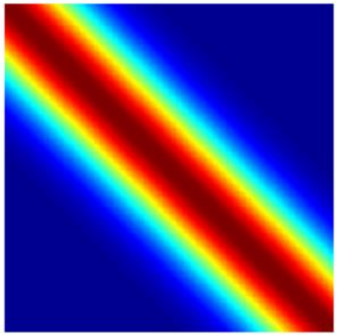
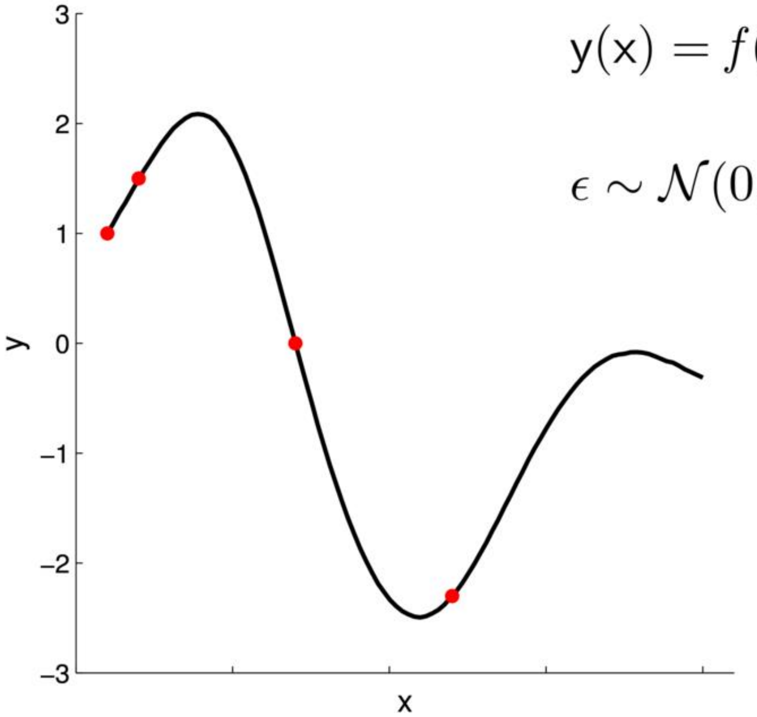
$\Sigma =$ 



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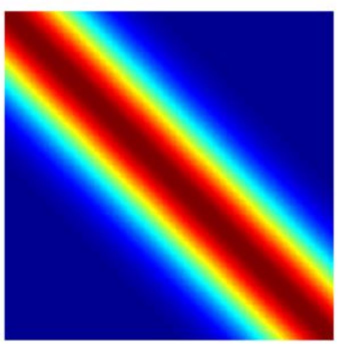
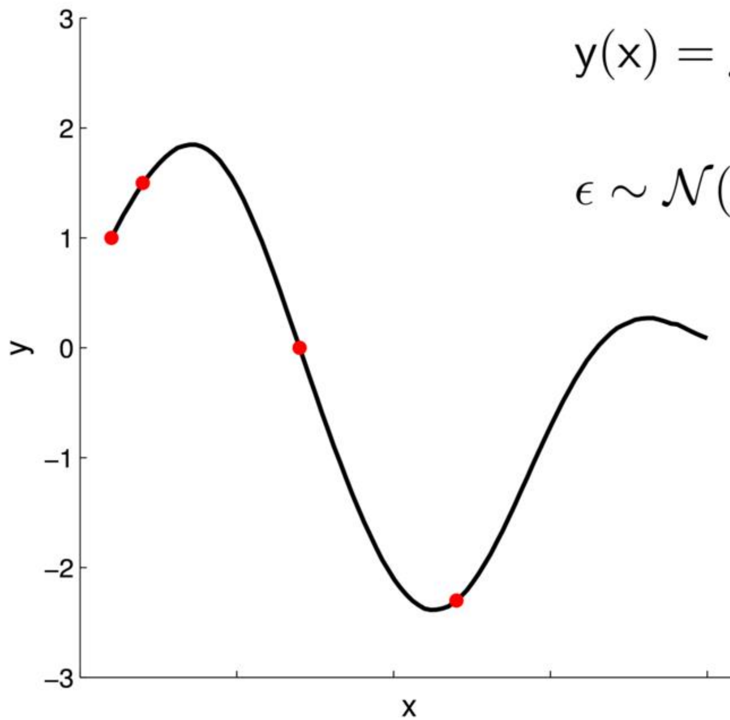
$\Sigma =$ 



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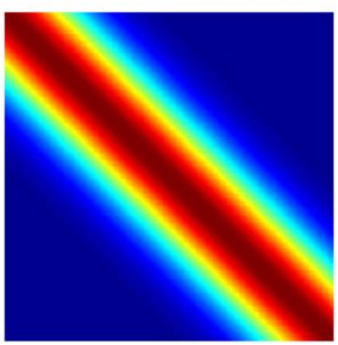
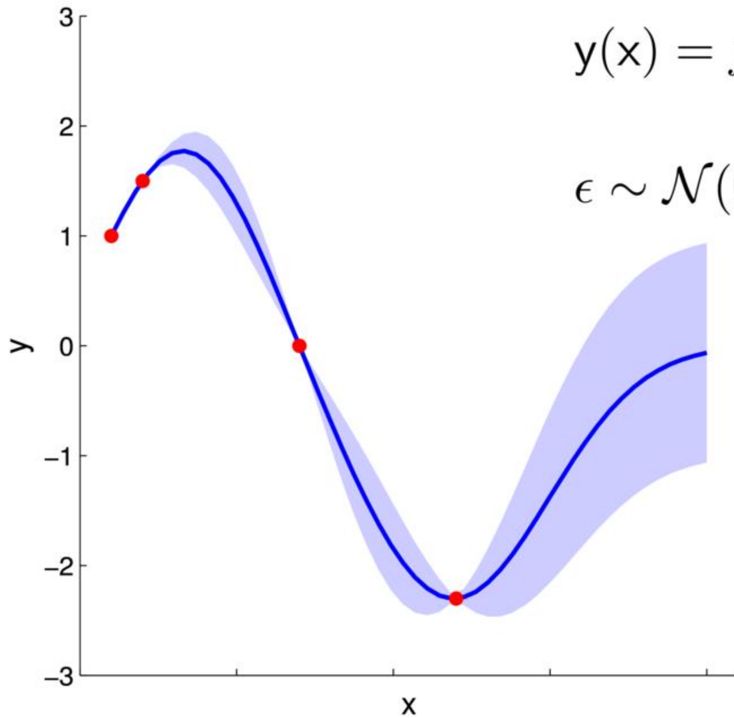
$\Sigma =$ 



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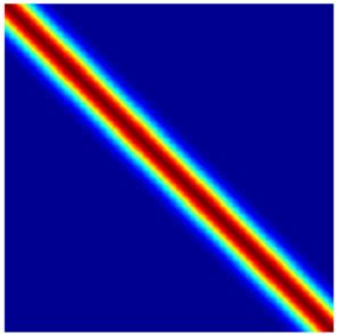
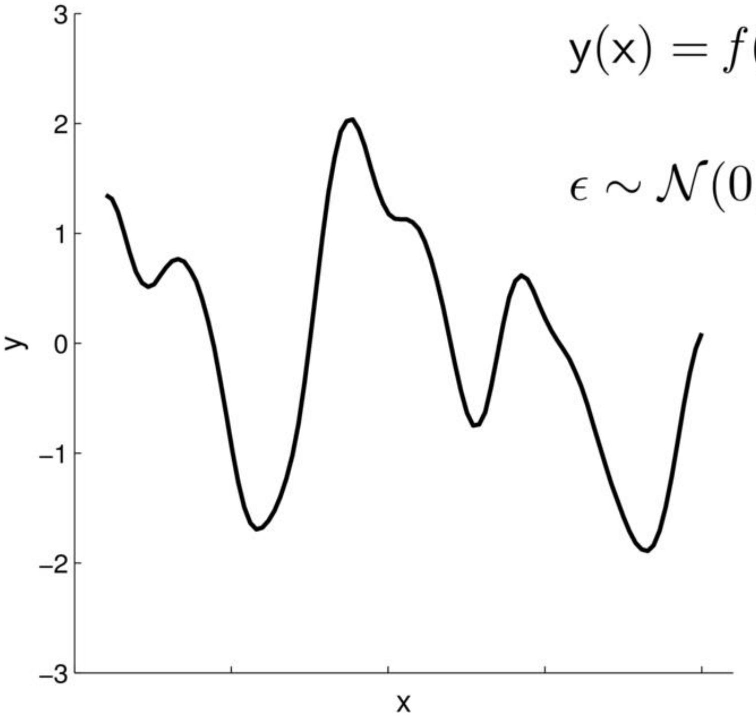
$\Sigma =$ 



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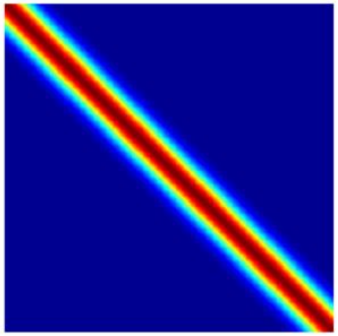
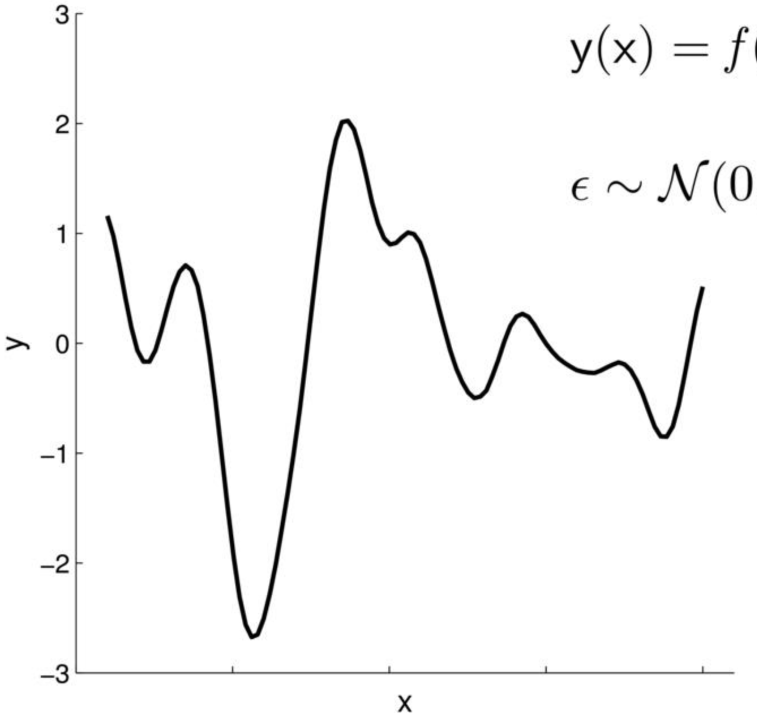
$\Sigma =$ 



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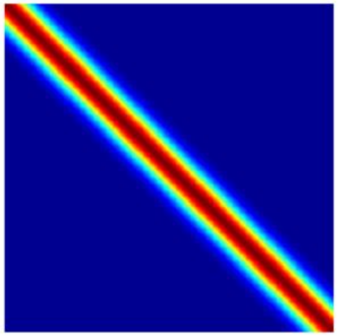
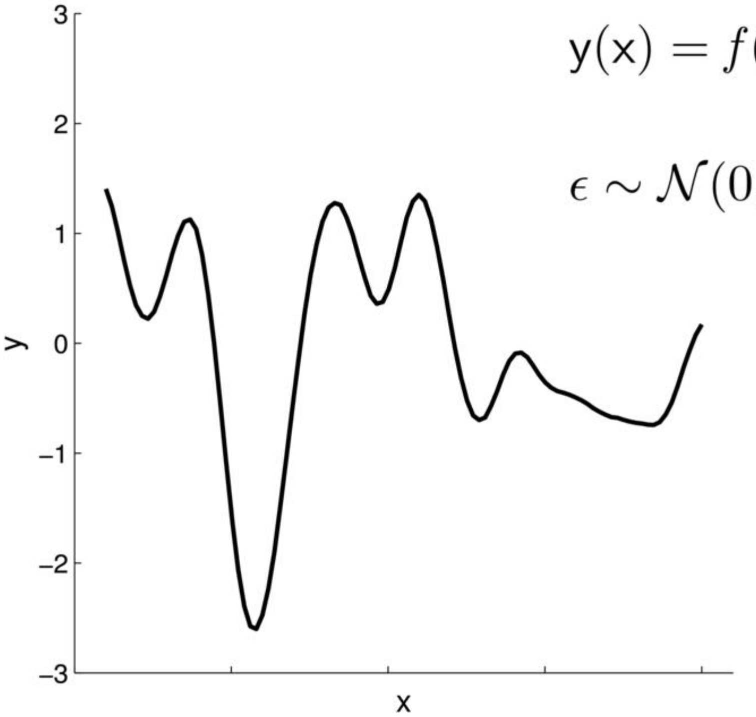
$\Sigma =$ 



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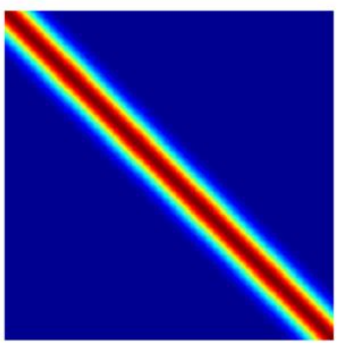
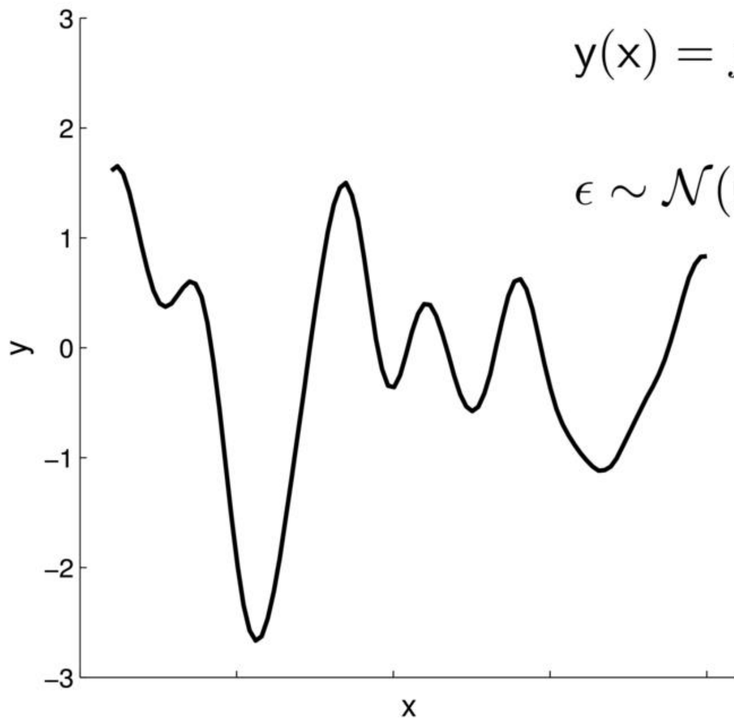
$\Sigma =$ 



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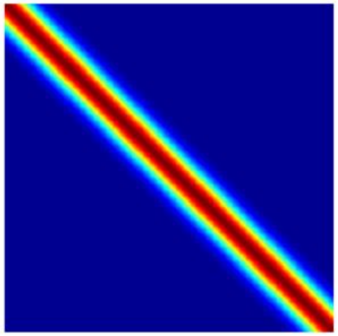
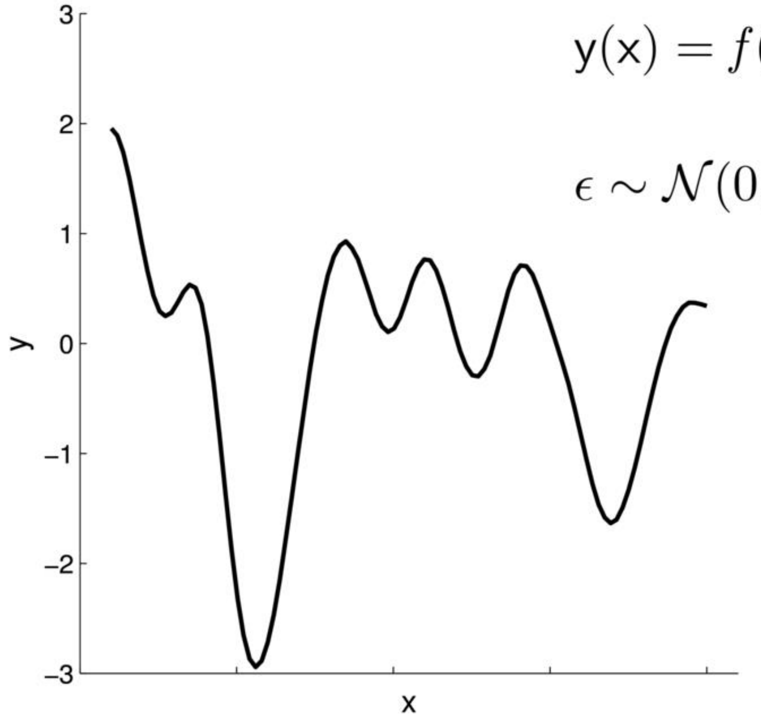
$\Sigma =$ 



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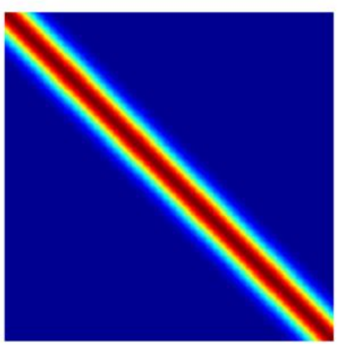
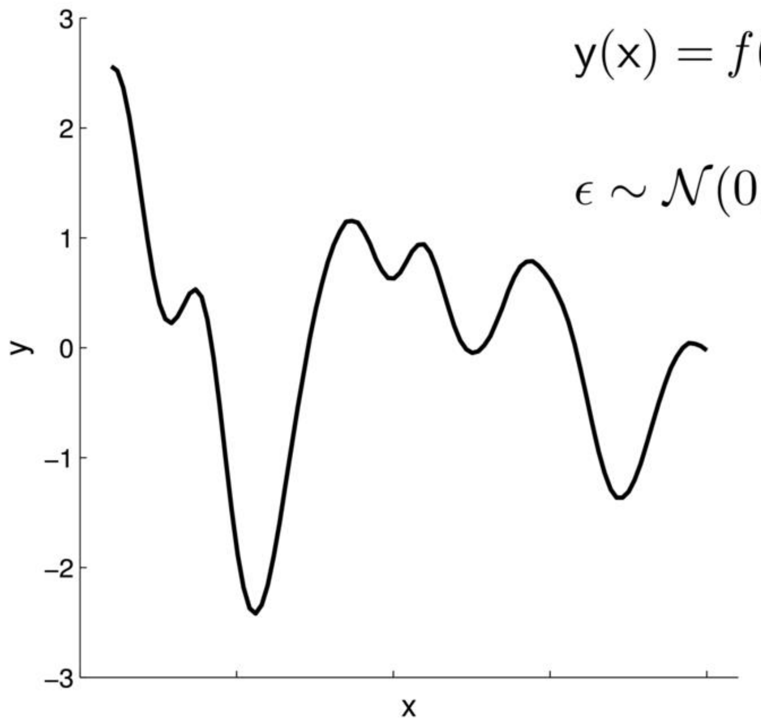
$\Sigma =$ 



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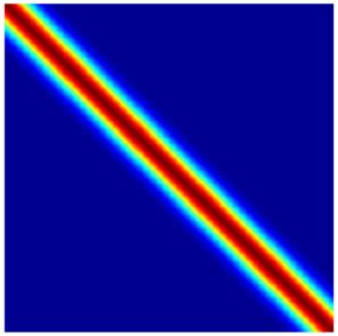
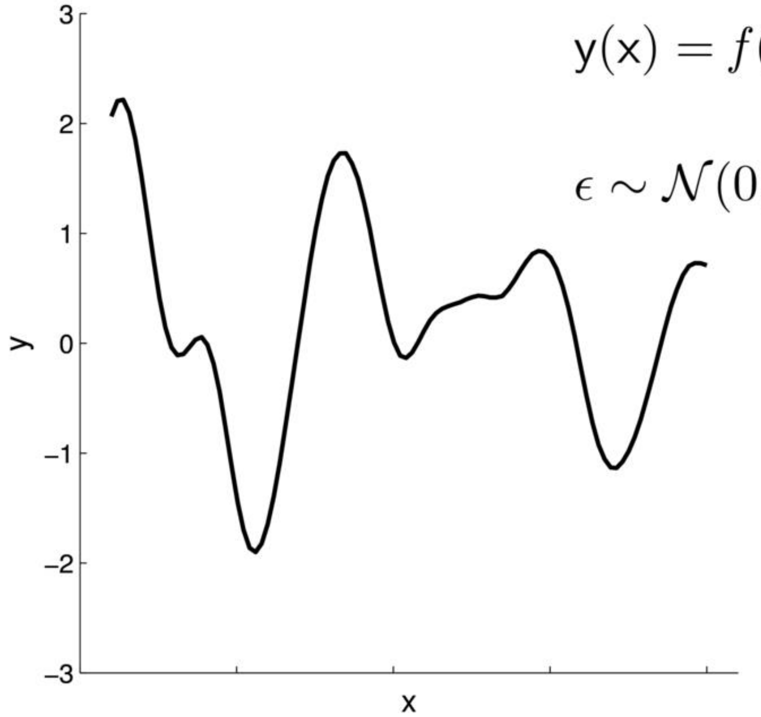
$\Sigma =$ 



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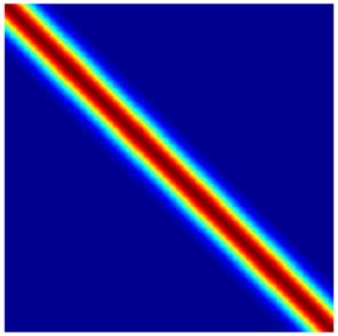
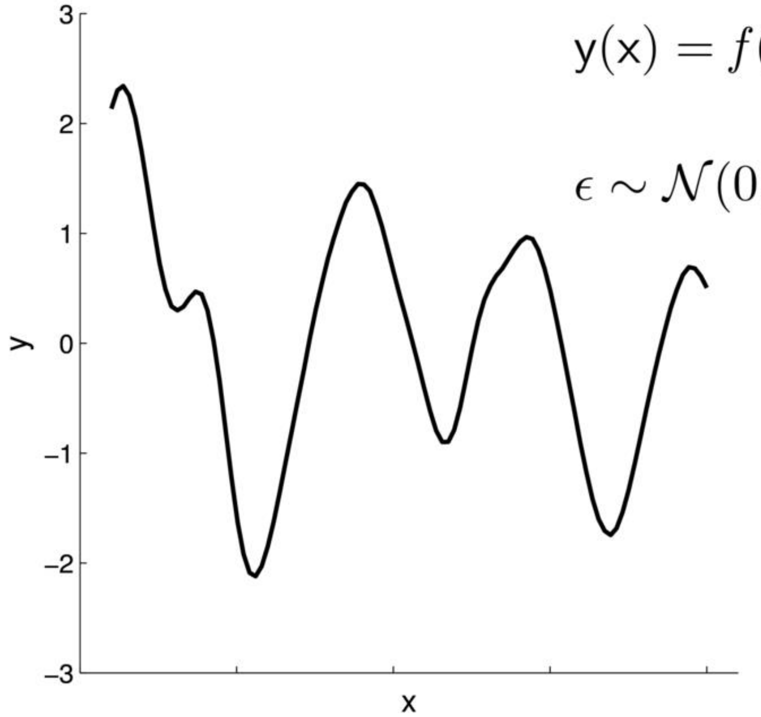
$\Sigma =$ 



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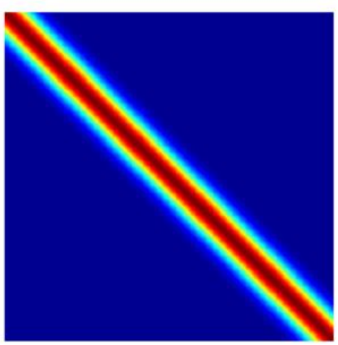
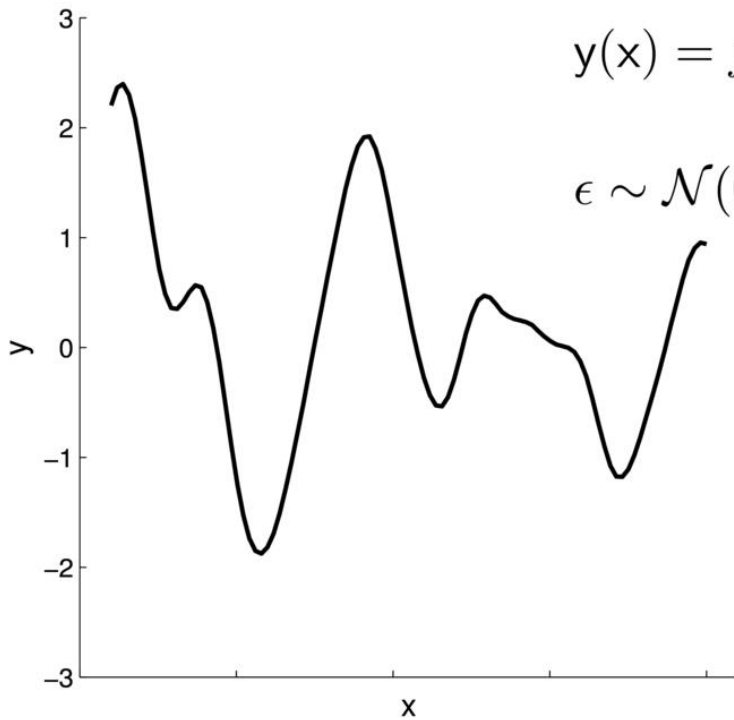
$\Sigma =$ 



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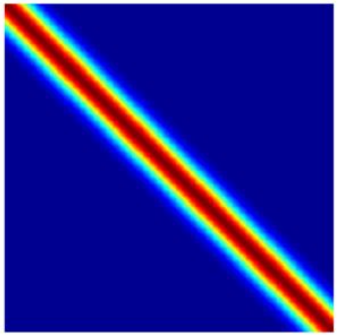
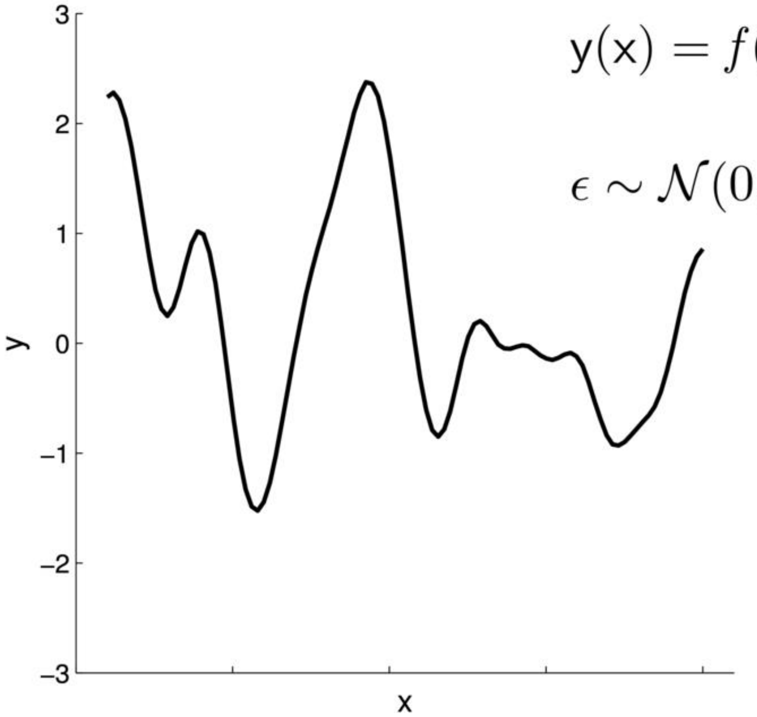
$\Sigma =$ 



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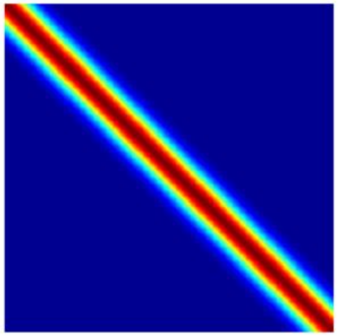
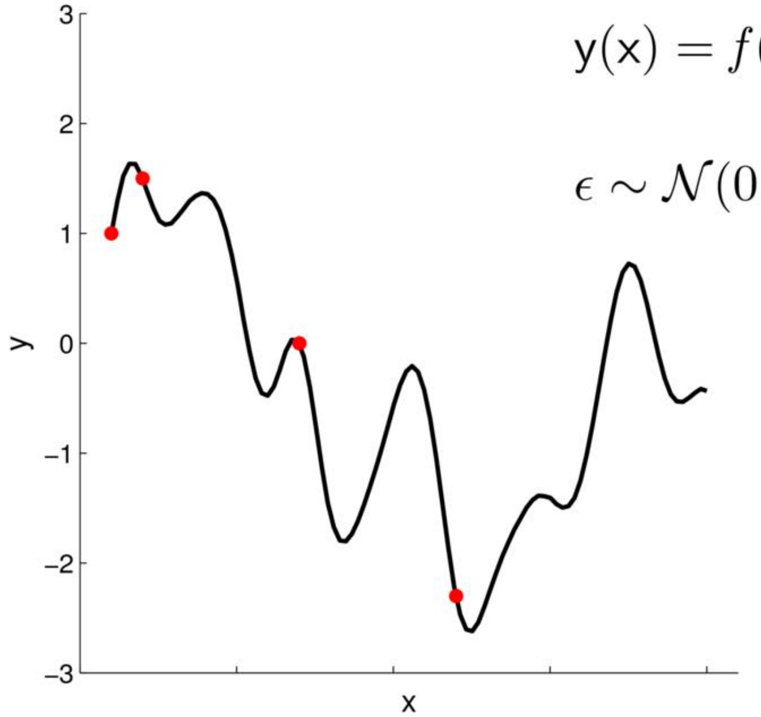
$\Sigma =$ 



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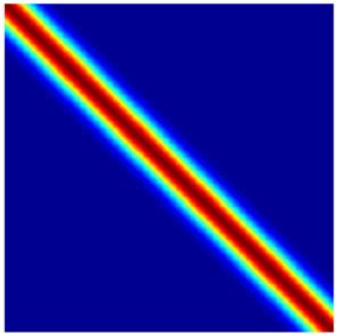
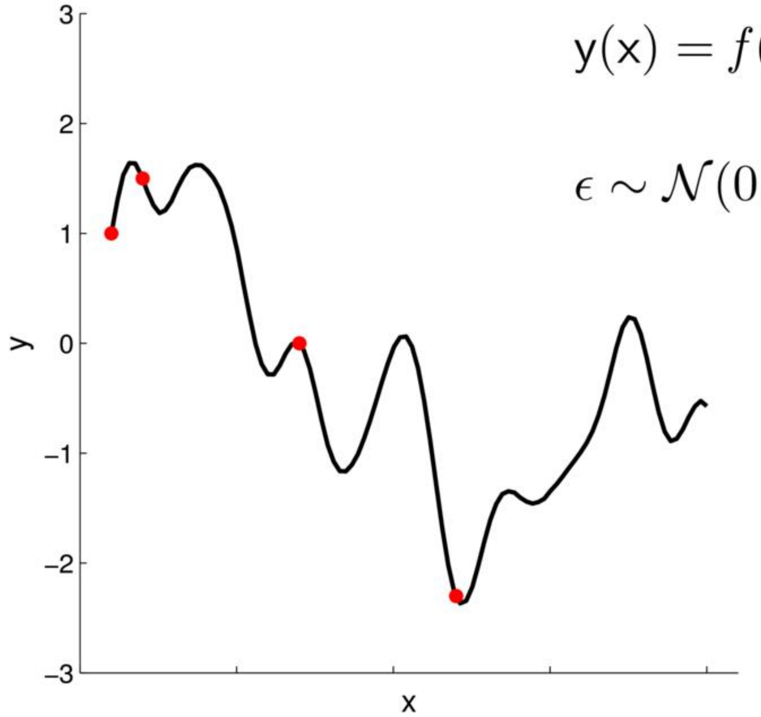
$\Sigma =$ 



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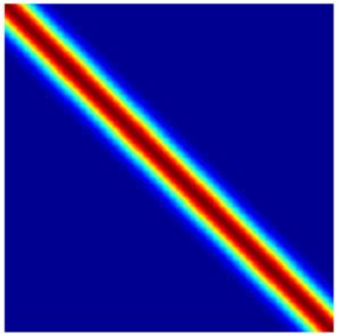
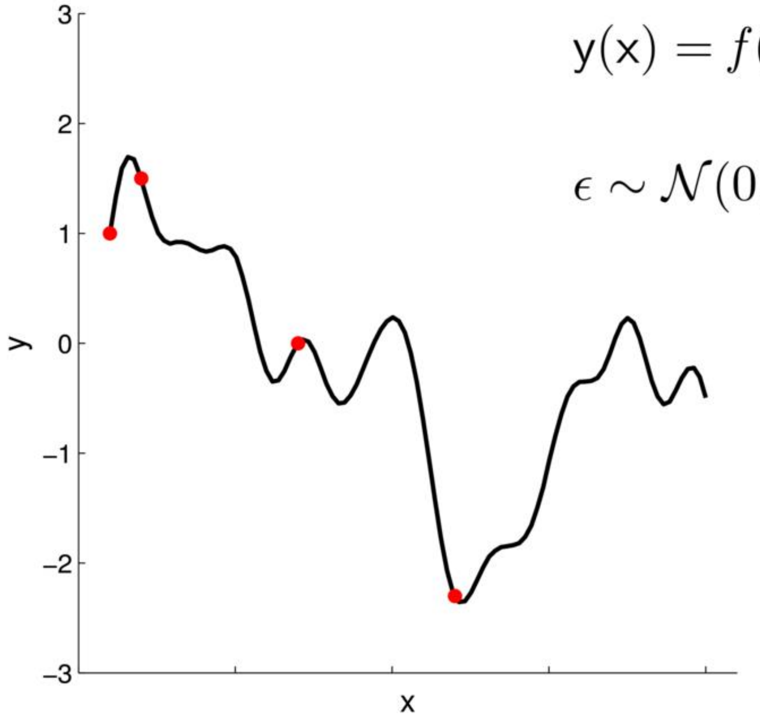
$\Sigma =$ 



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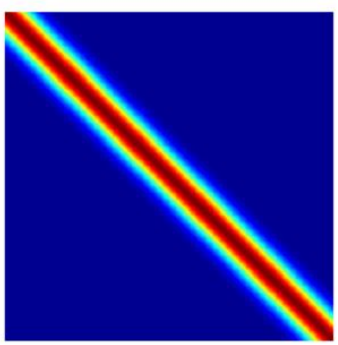
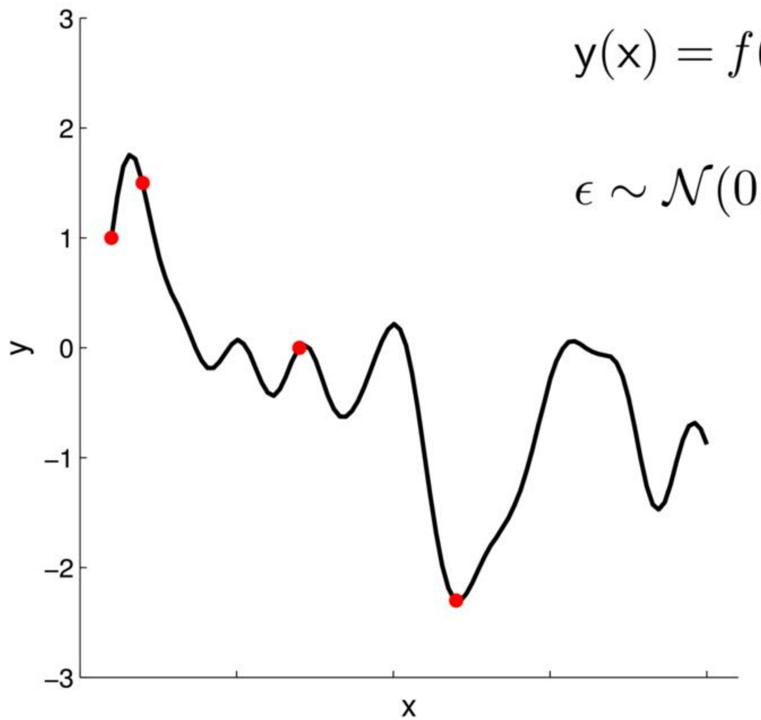
$\Sigma =$ 



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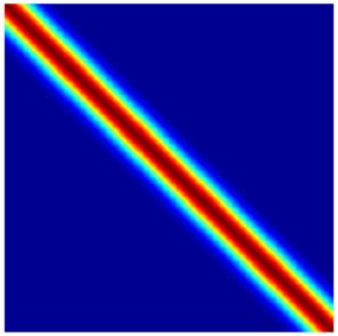
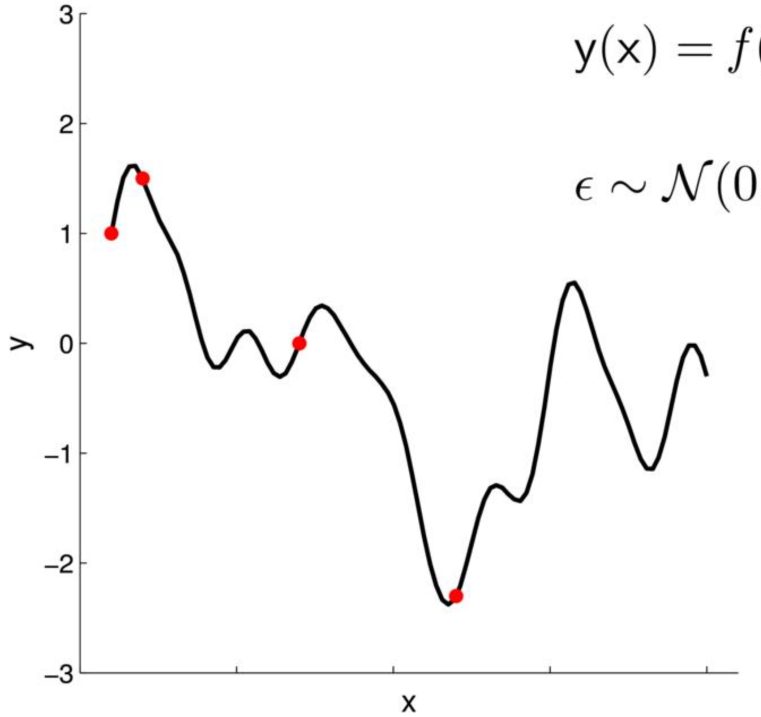
$\Sigma =$ 



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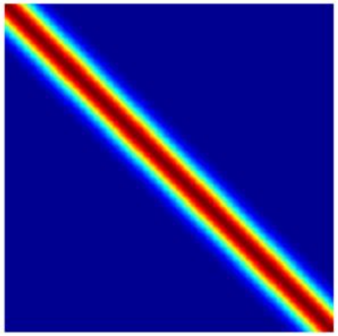
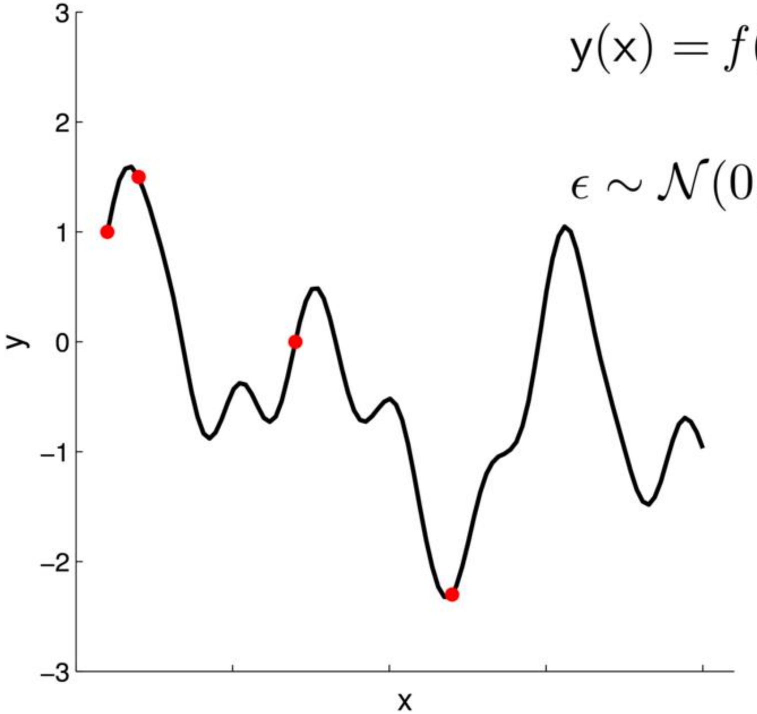
$\Sigma =$ 



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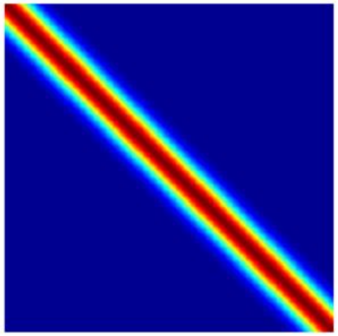
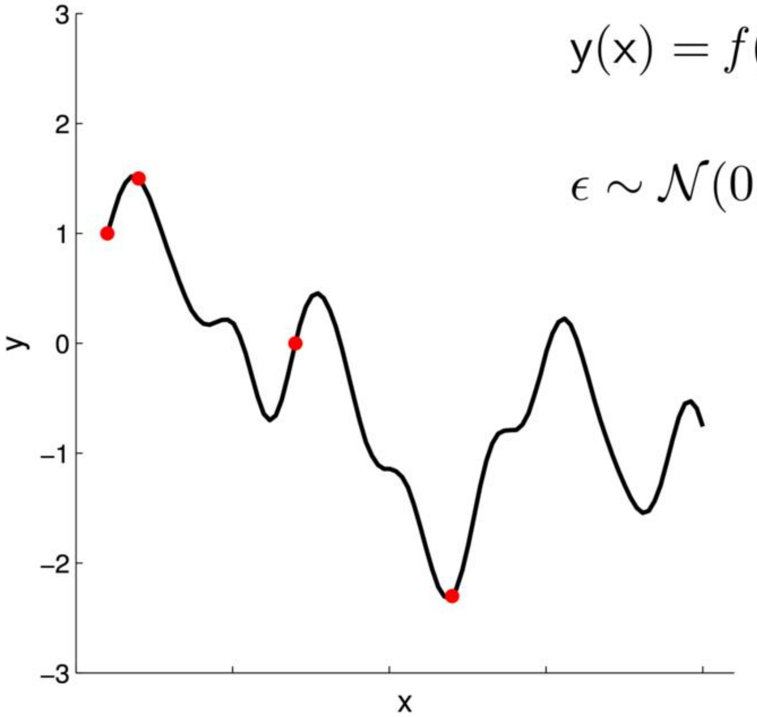
$\Sigma =$ 



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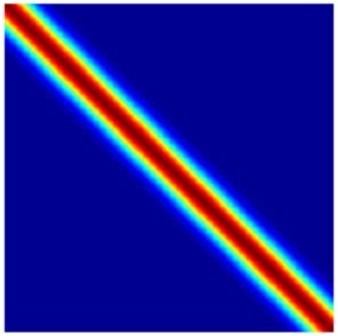
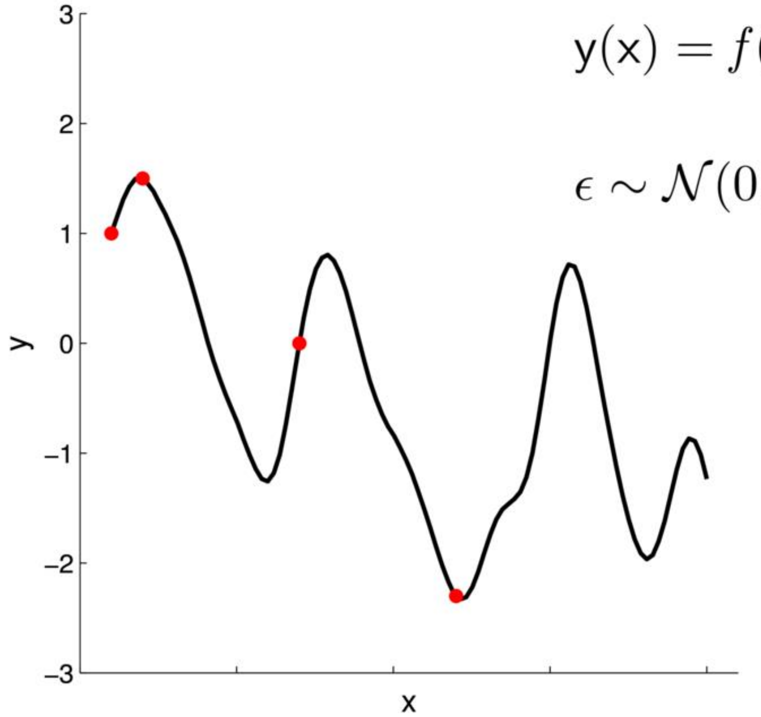
$\Sigma =$ 



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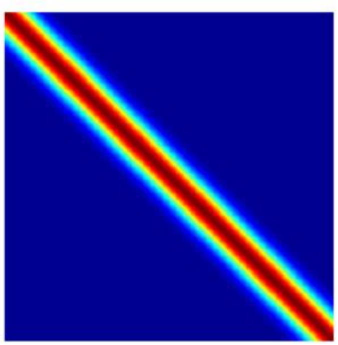
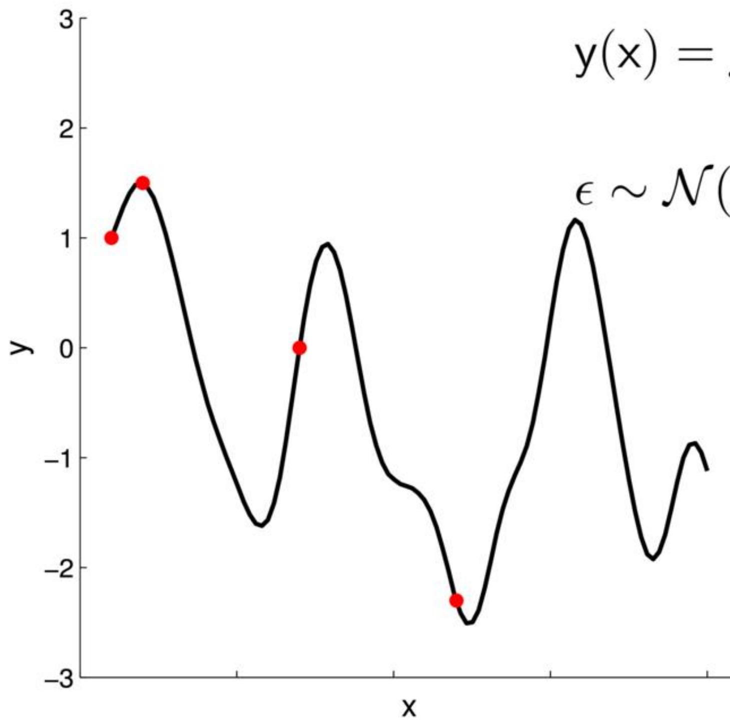
$\Sigma =$ 



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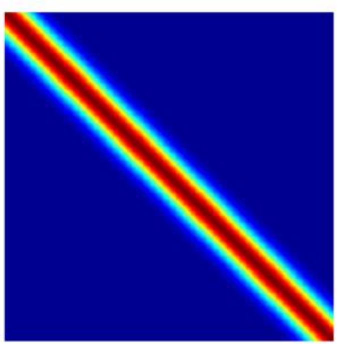
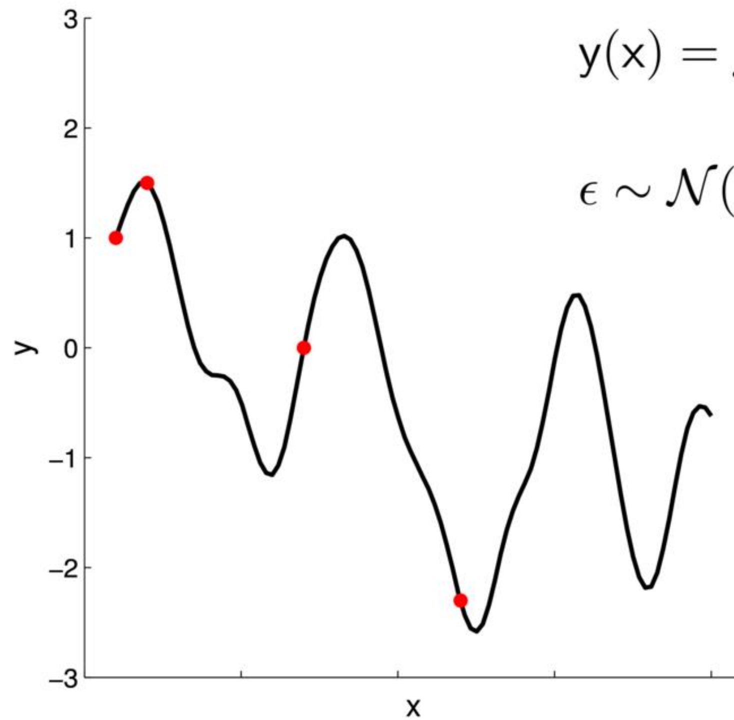
$\Sigma =$ 



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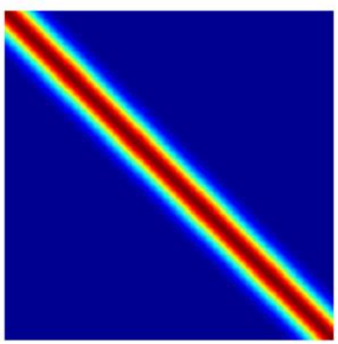
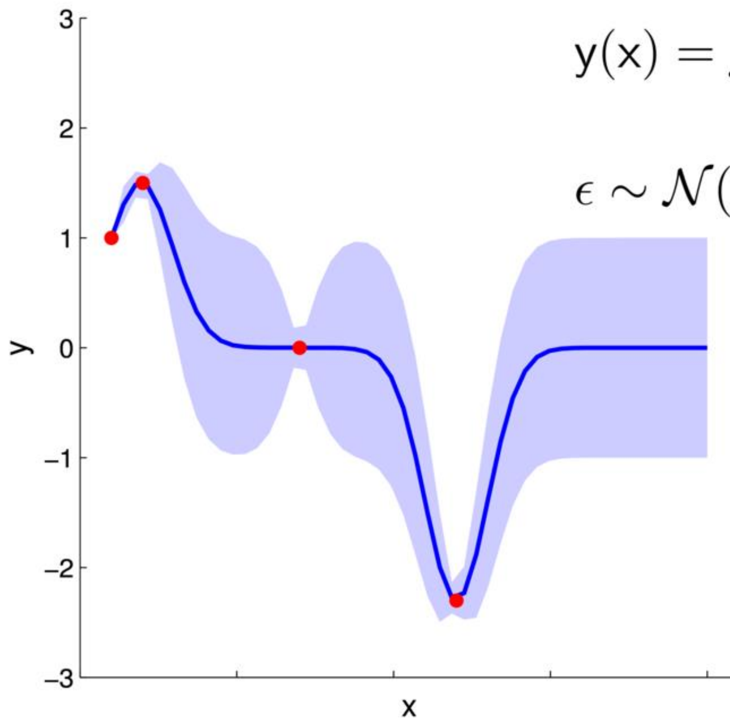
$\Sigma =$ 



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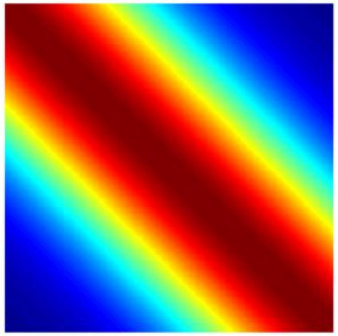
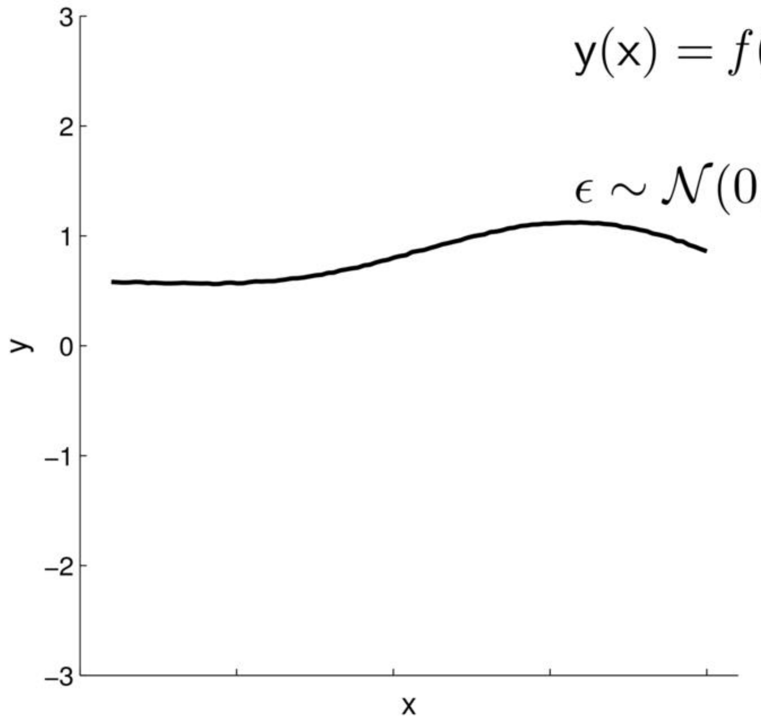
$\Sigma =$ 



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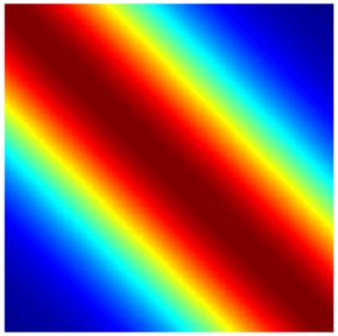
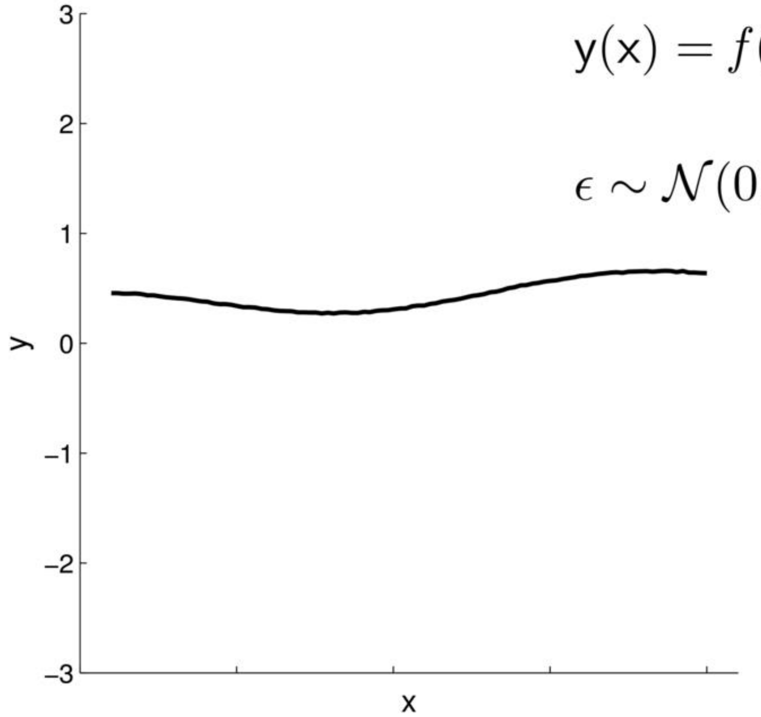
$\Sigma =$ 



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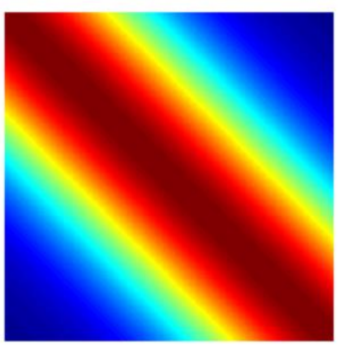

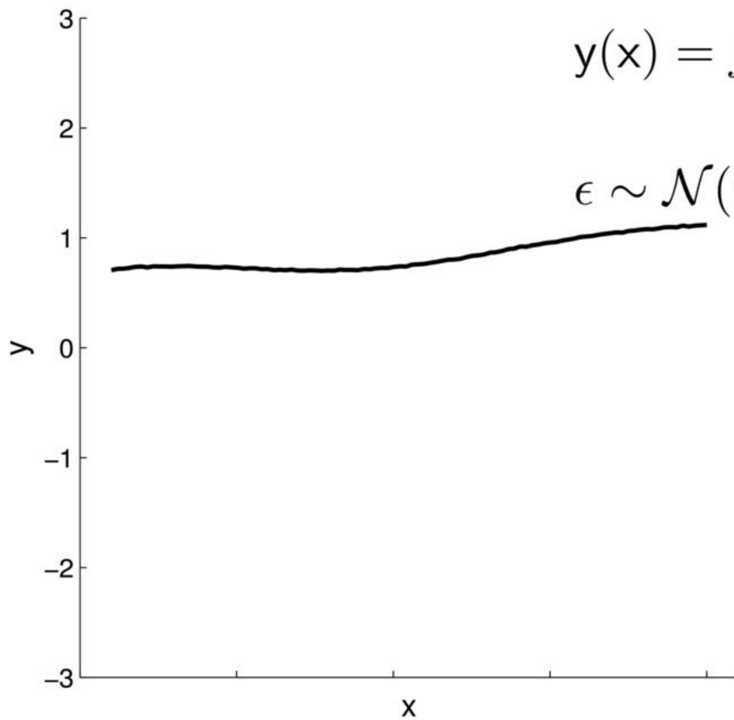

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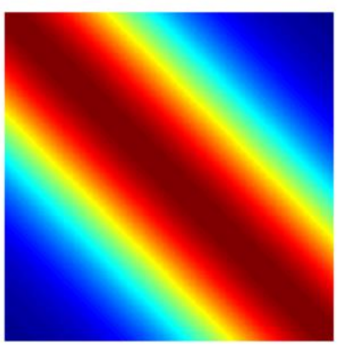

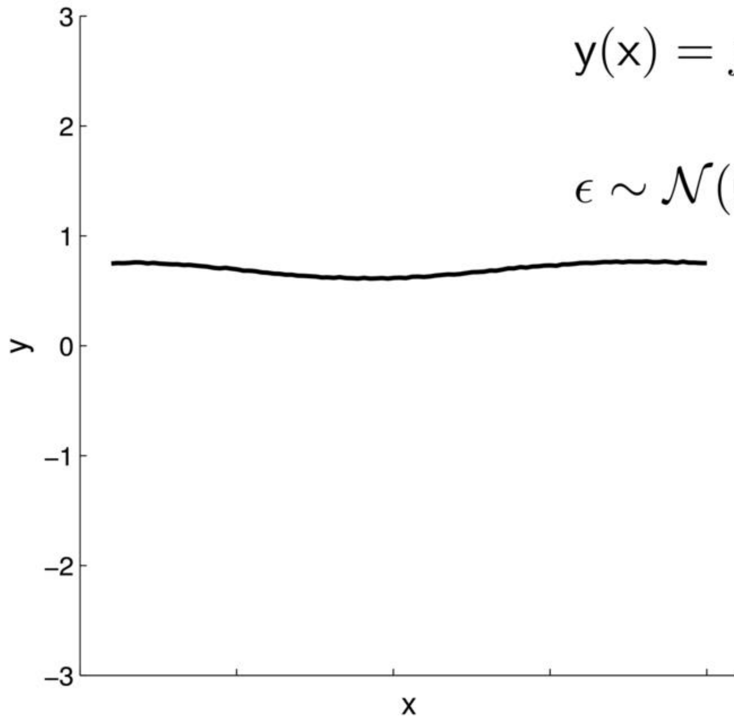

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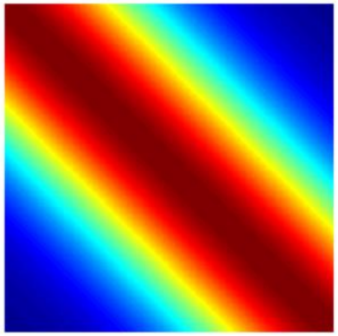

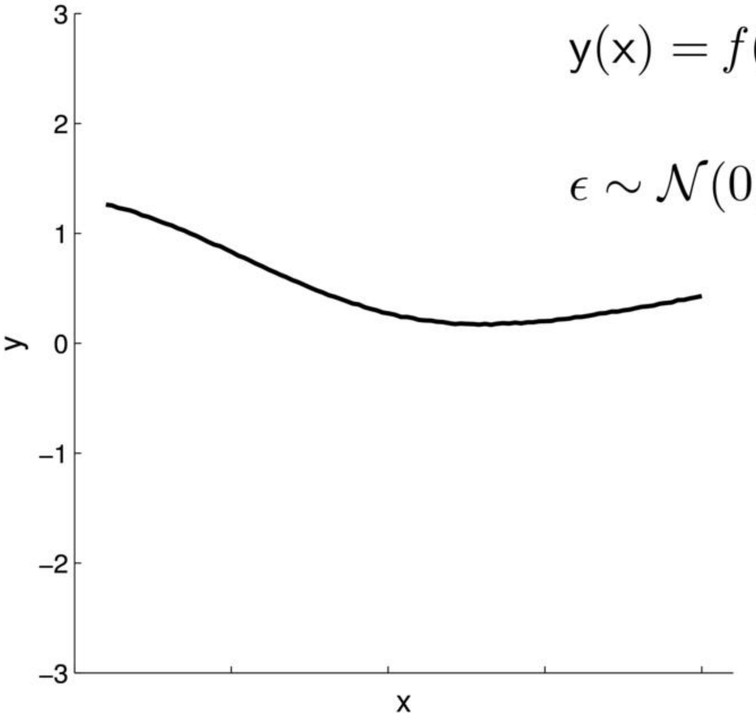

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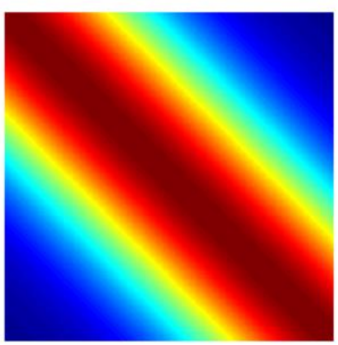
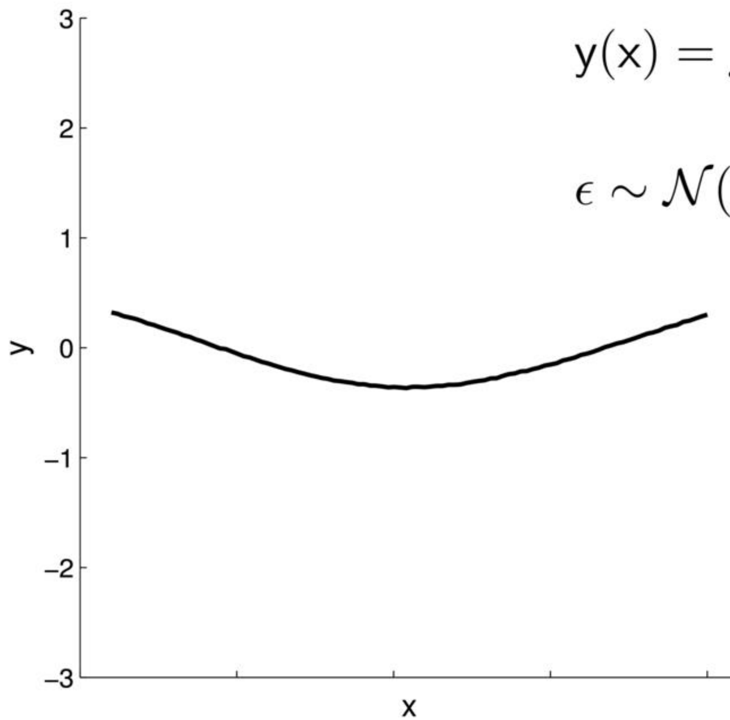
$\Sigma =$ 



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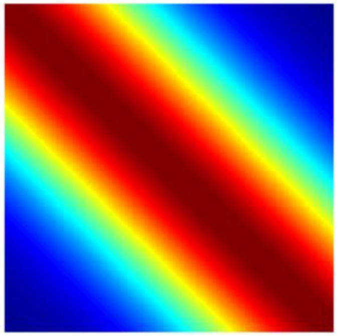
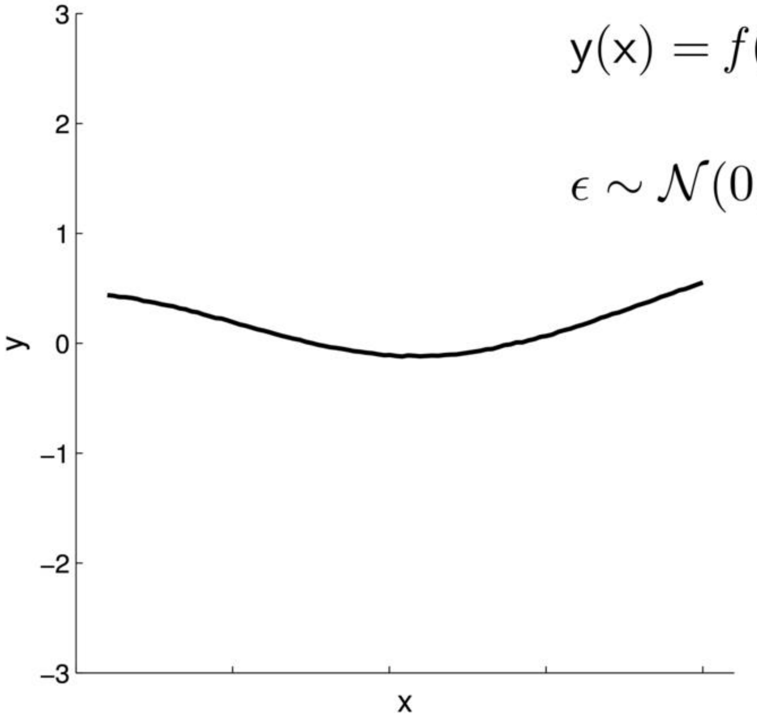
$\Sigma =$ 



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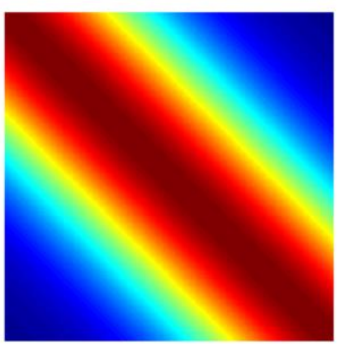

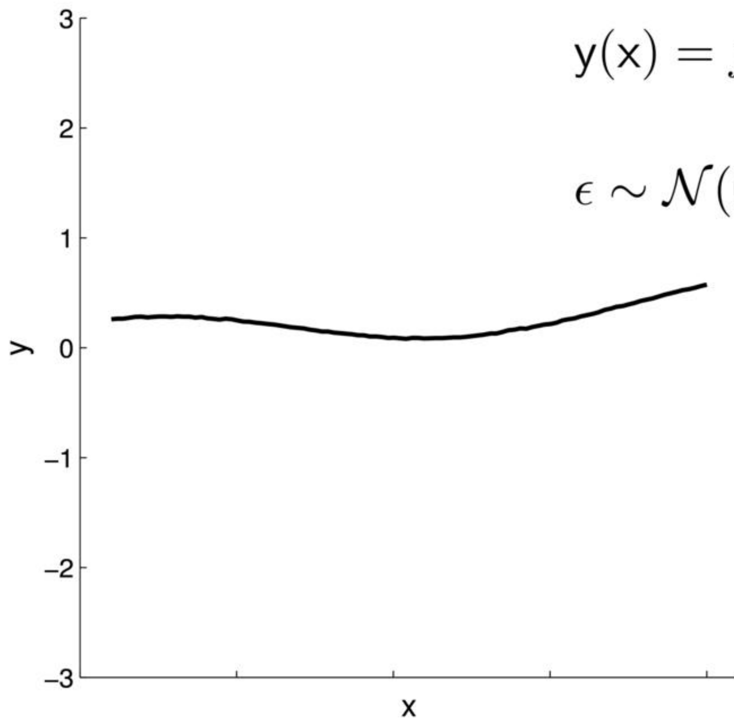

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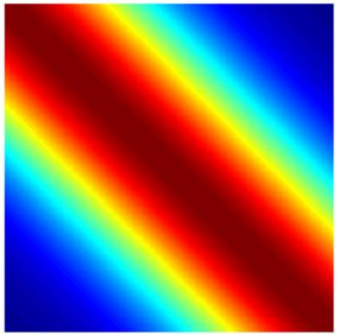
$\Sigma =$ 

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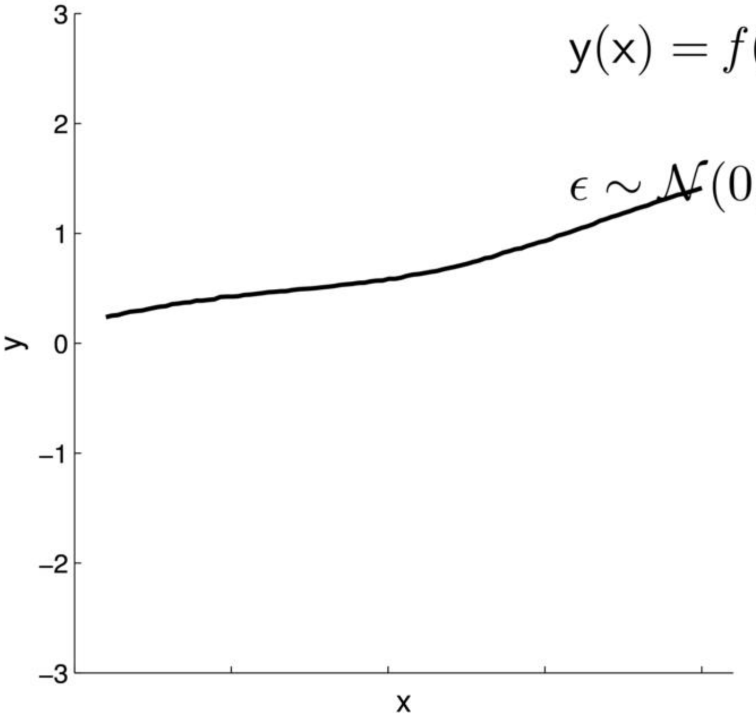

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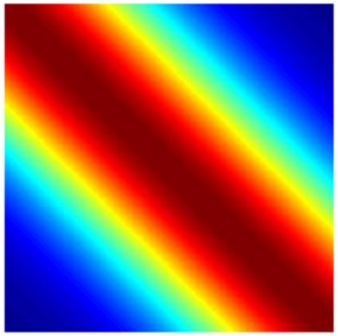
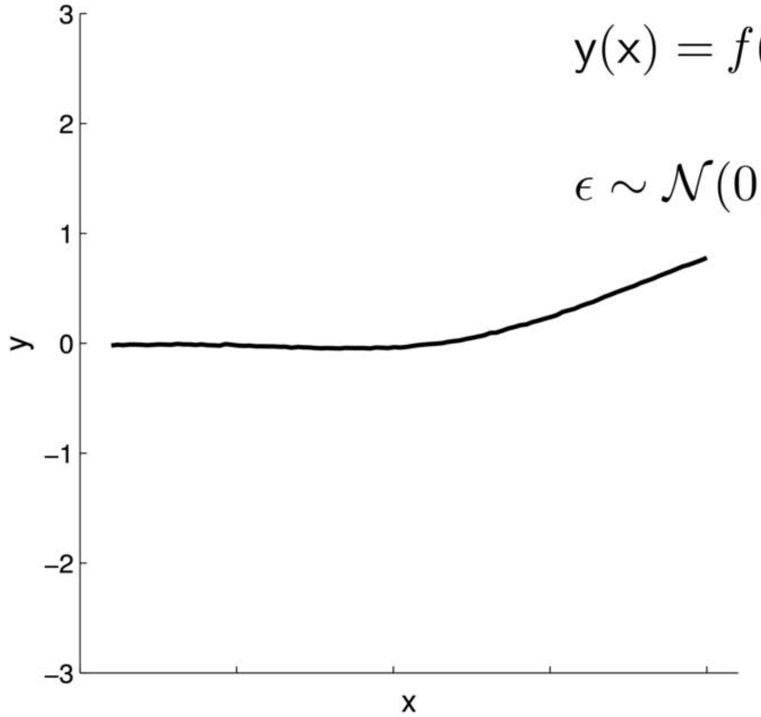
$\Sigma =$ 



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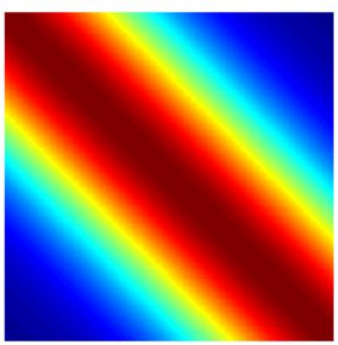
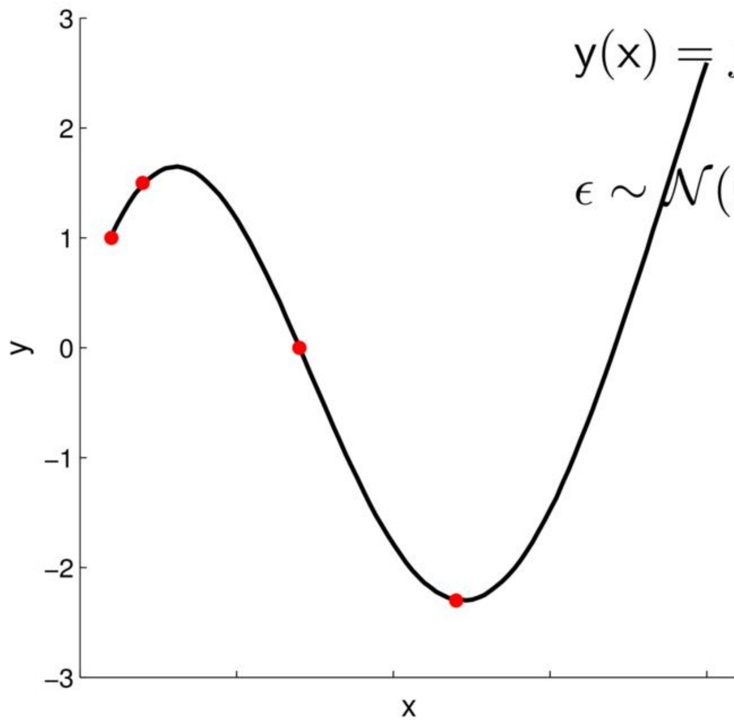
$\Sigma =$ 



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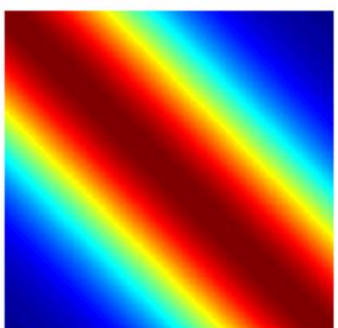
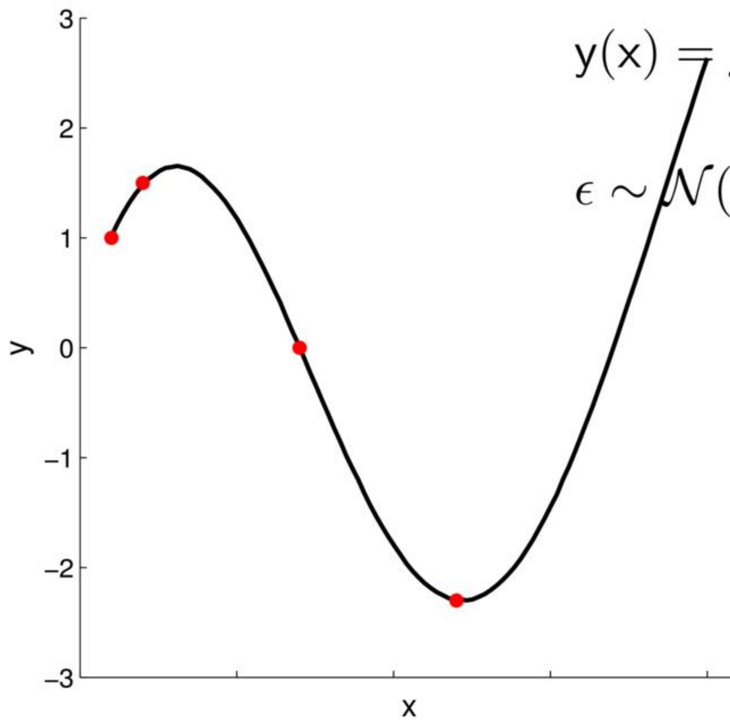
$\Sigma =$ 



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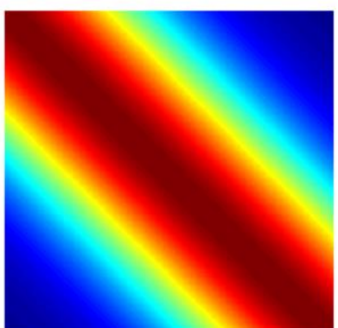
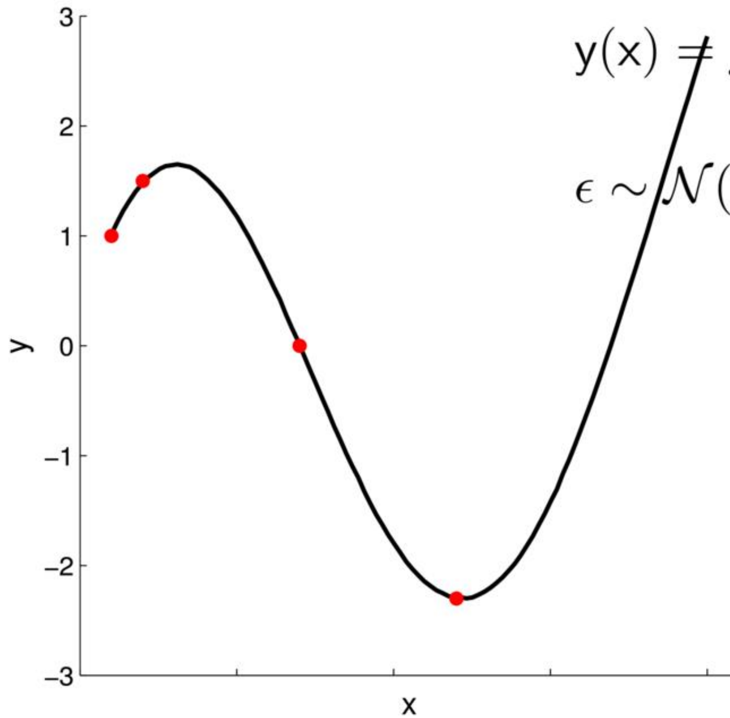
$\Sigma =$ 



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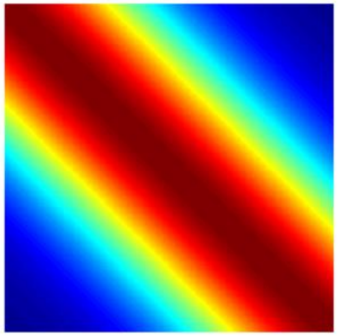
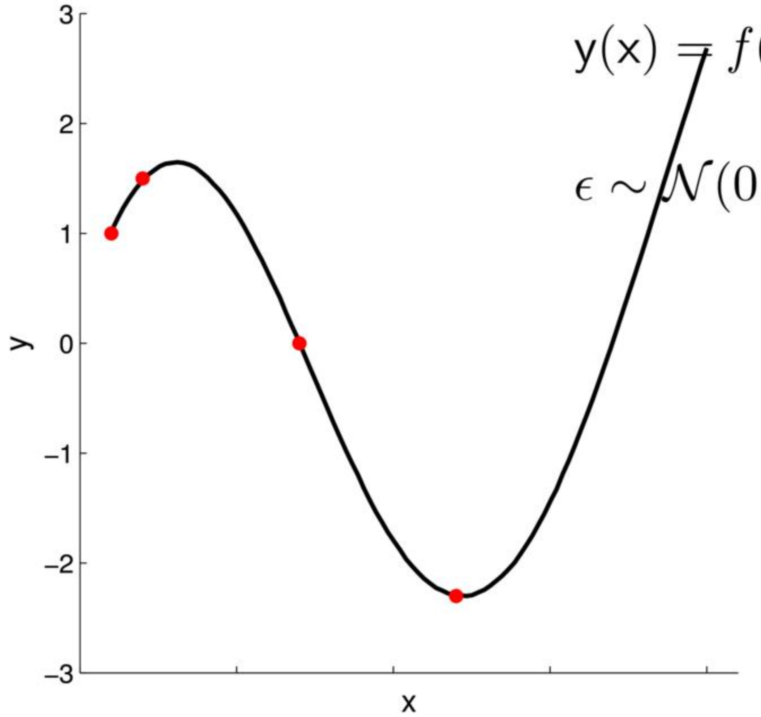
$\Sigma =$ 



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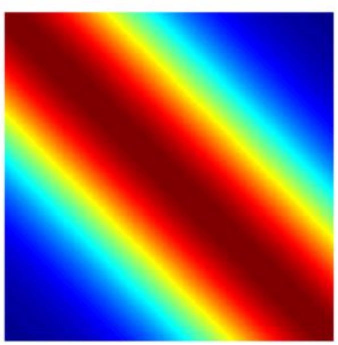
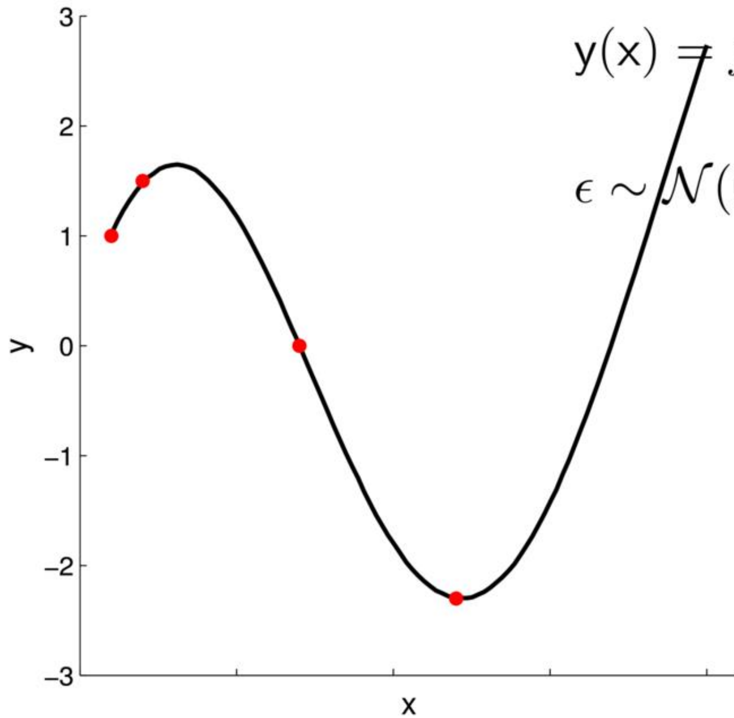
$\Sigma =$ 



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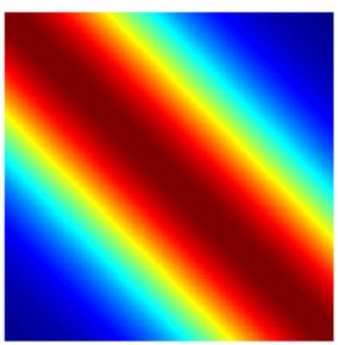

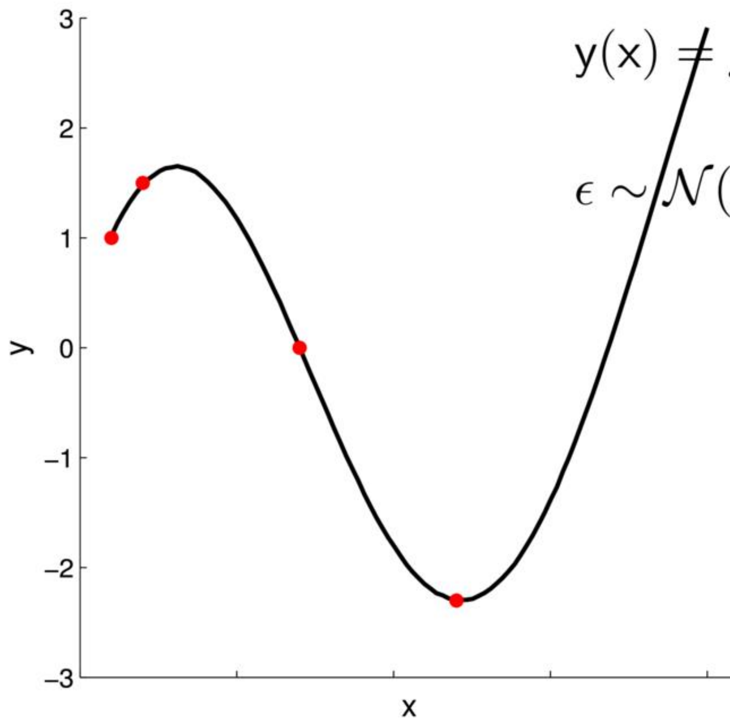

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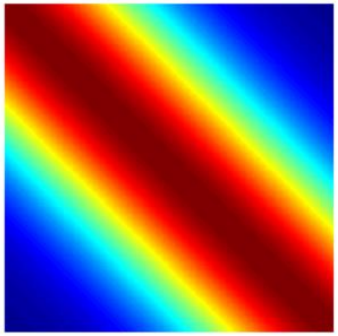
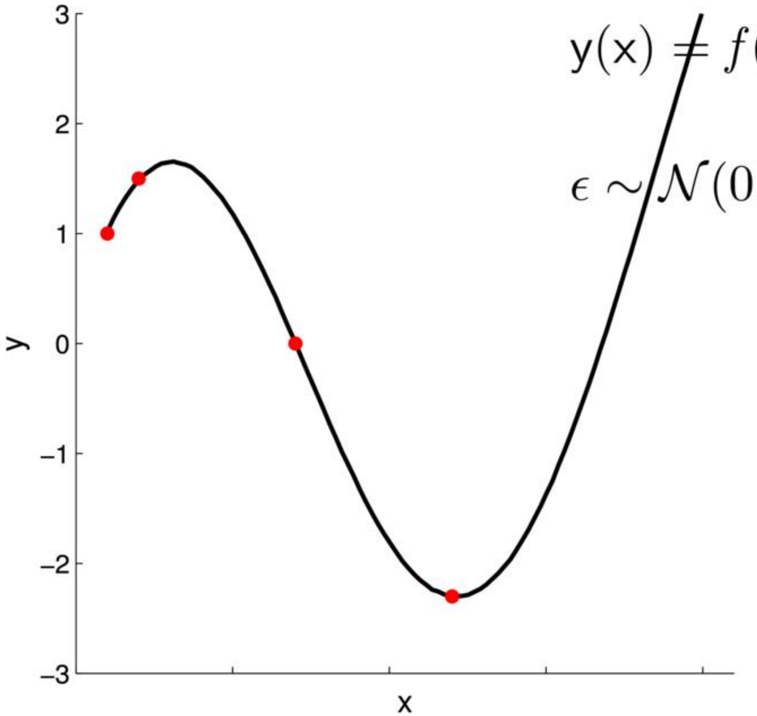
$\Sigma =$ 



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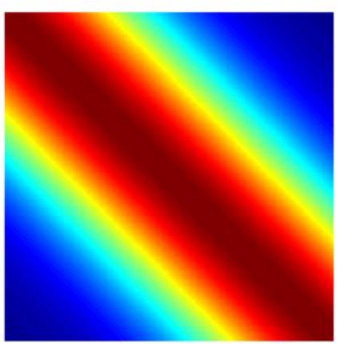
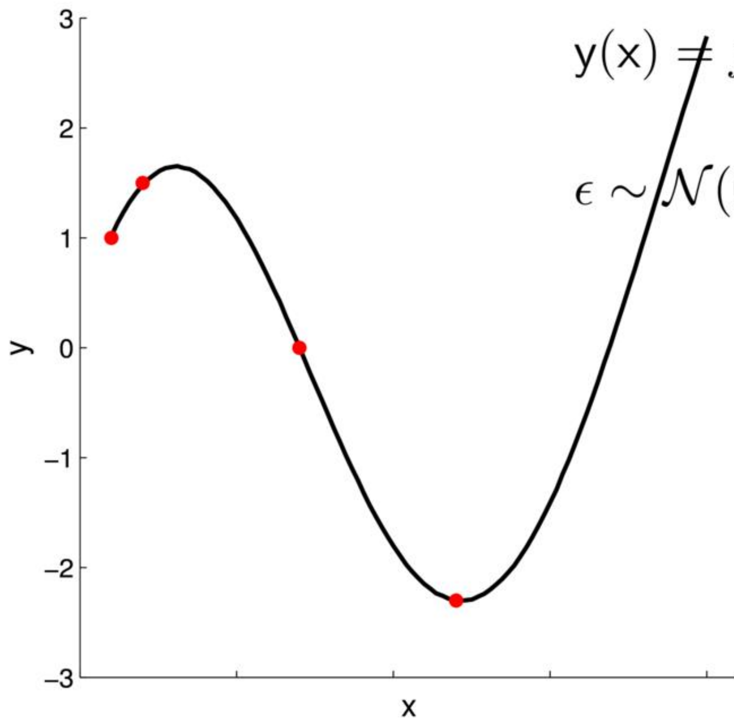
$\Sigma =$ 



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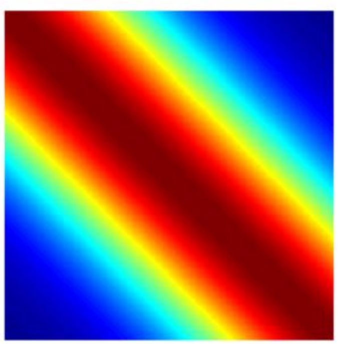
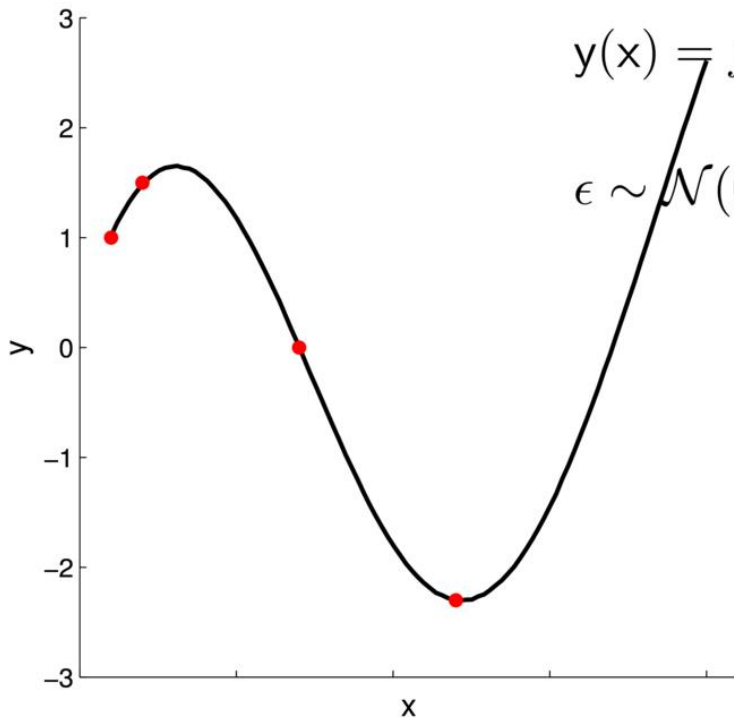
$\Sigma =$ 



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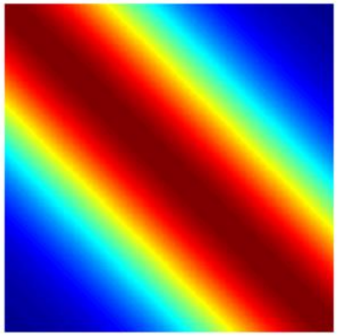
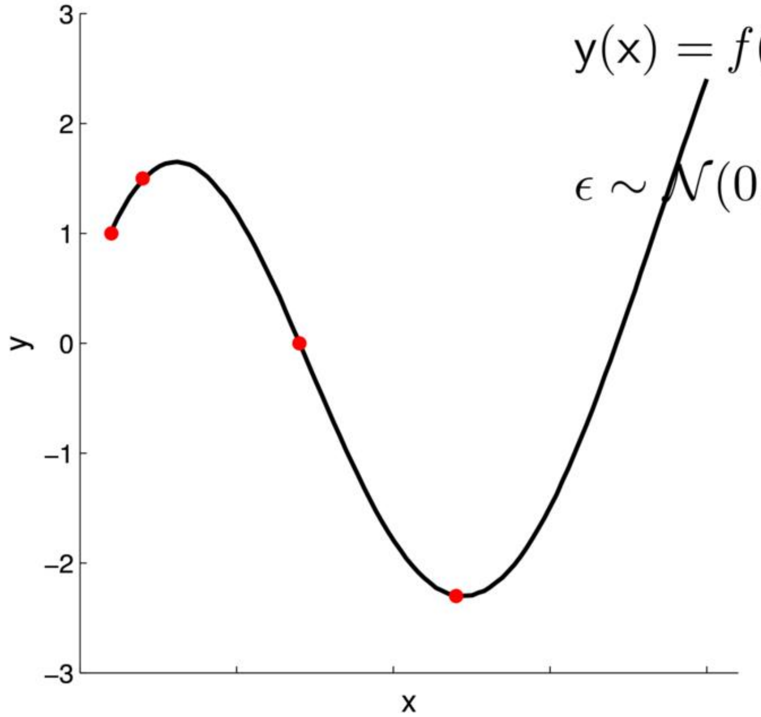
$\Sigma =$ 



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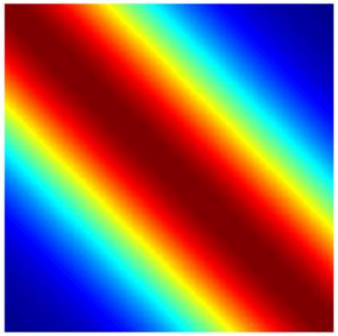

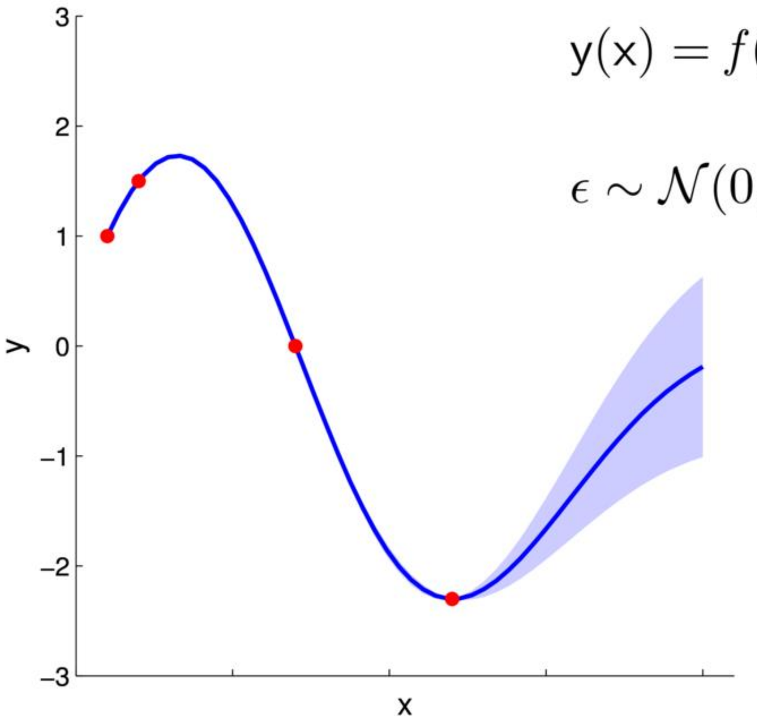

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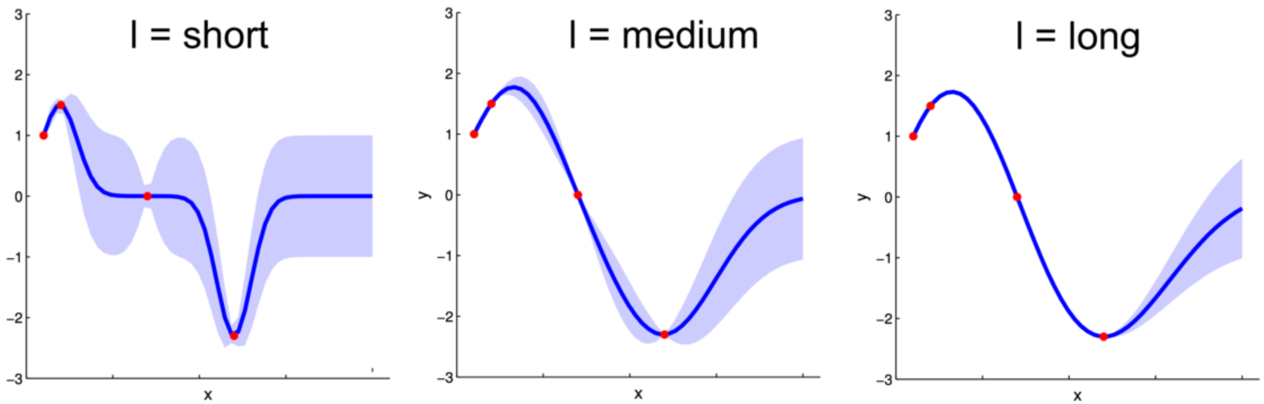
  - l controls the horizontal length-scale
  - σ^2 controls the vertical scale of the data
- $\Longrightarrow$ need automatic learning of hyper-parameters from data



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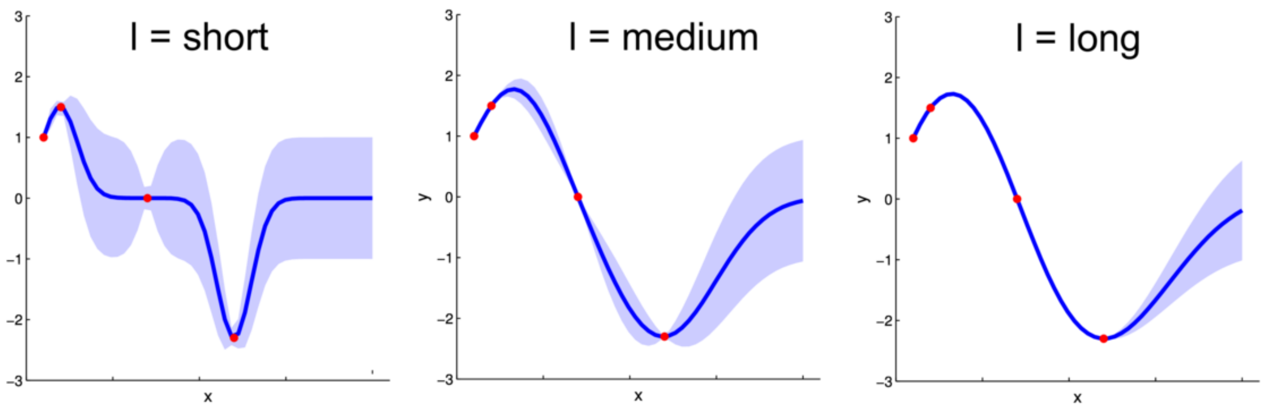
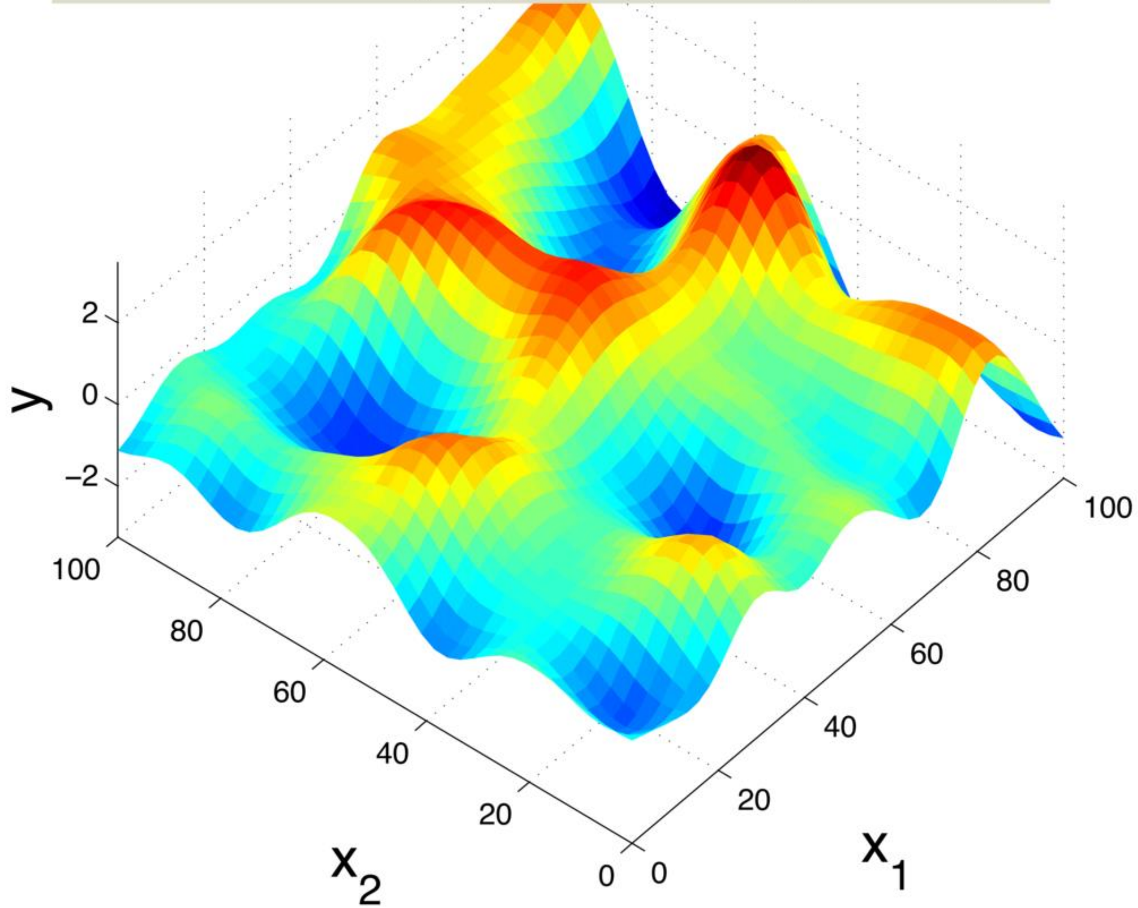
$$\arg\max_{l,\sigma^2} \log p(\mathbf{y} \mid \theta)$$

🡸 More on this later.



Higher Dimensional Input Spaces

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



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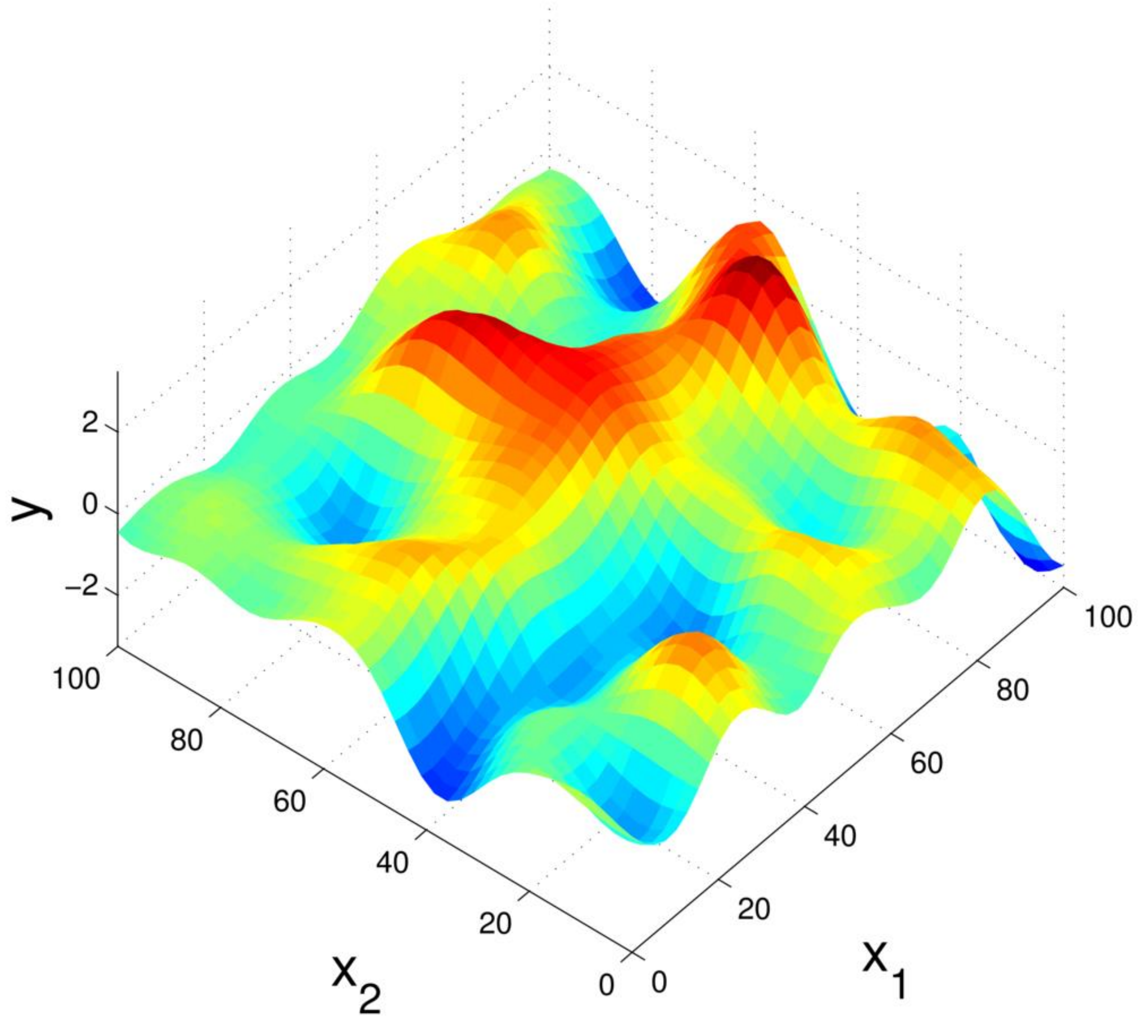

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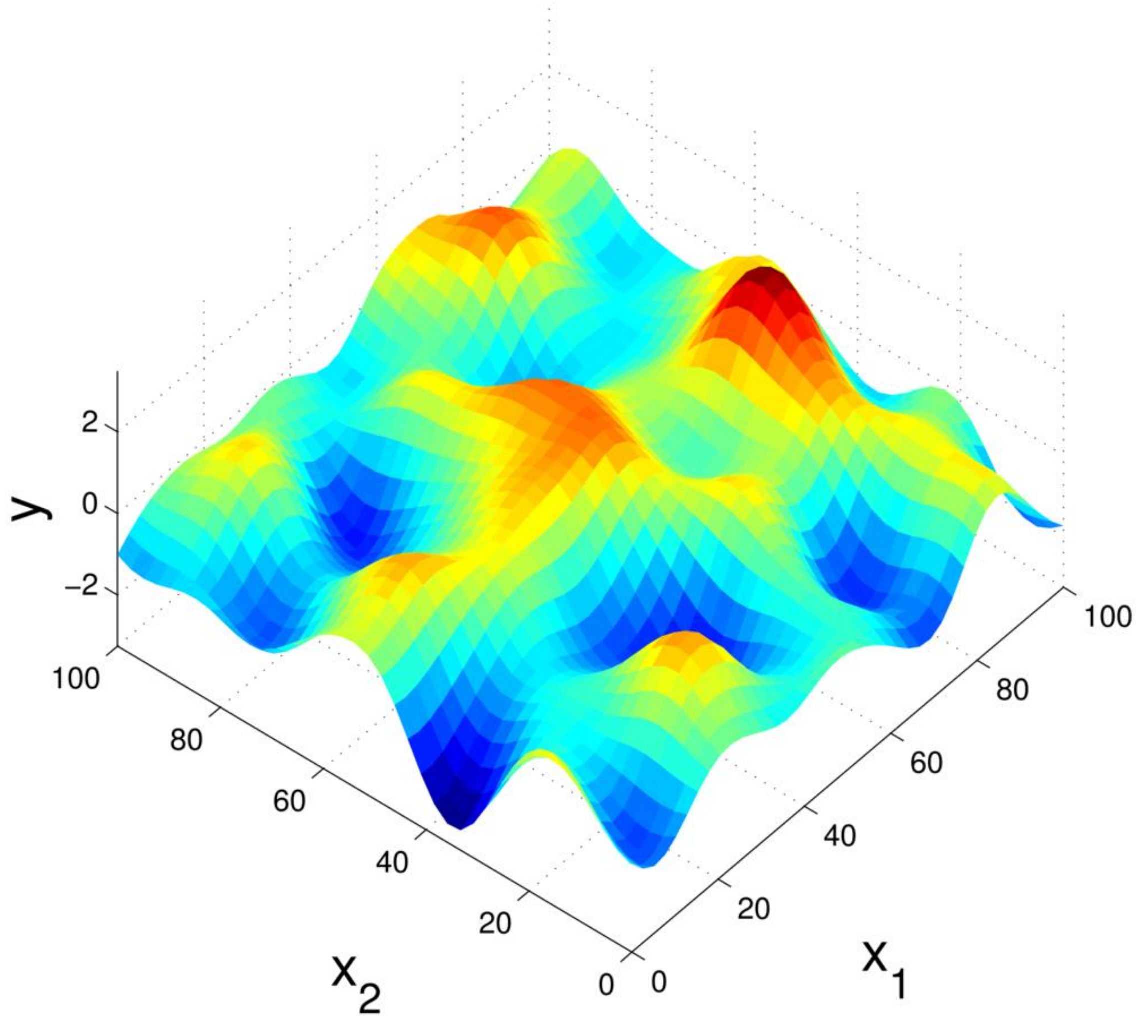

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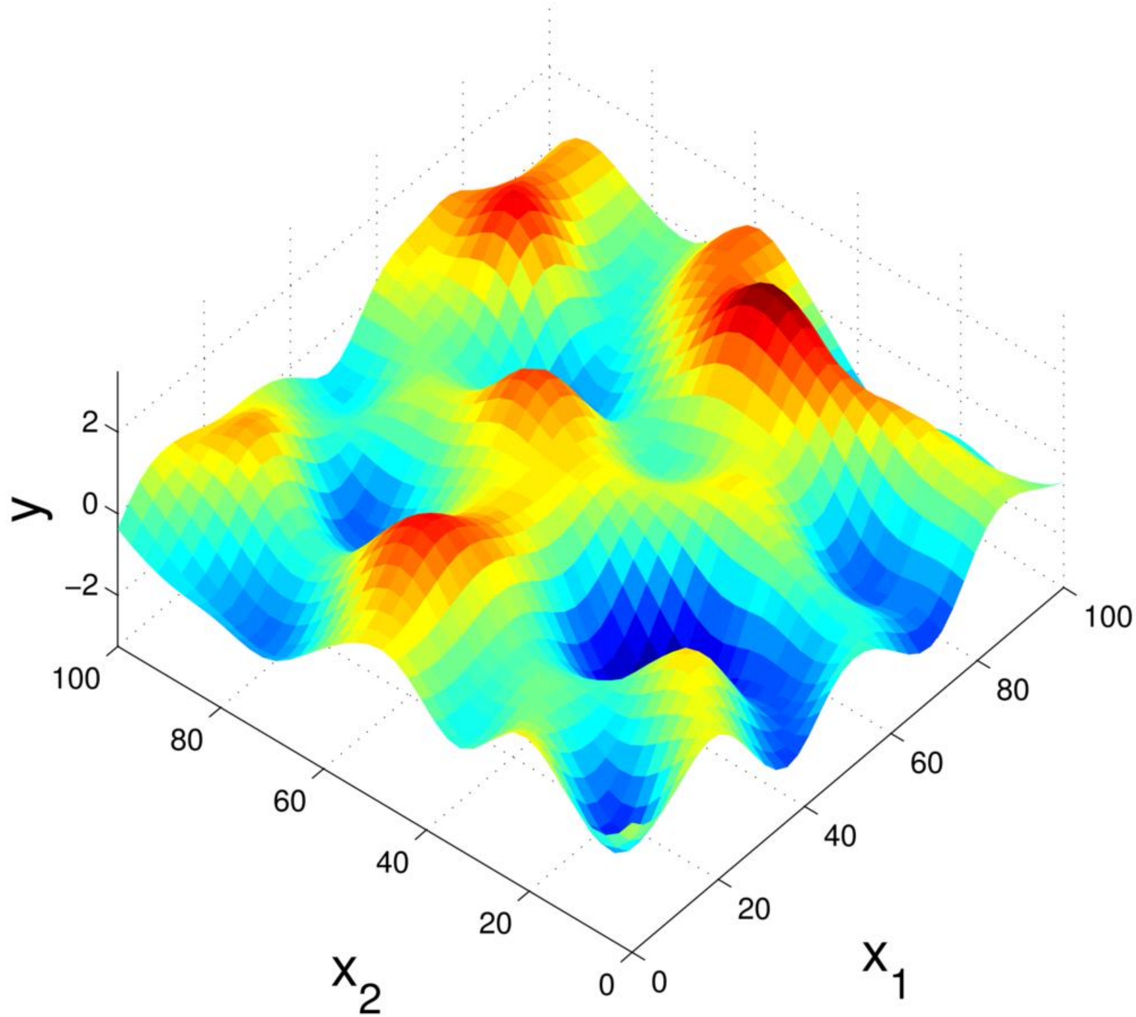

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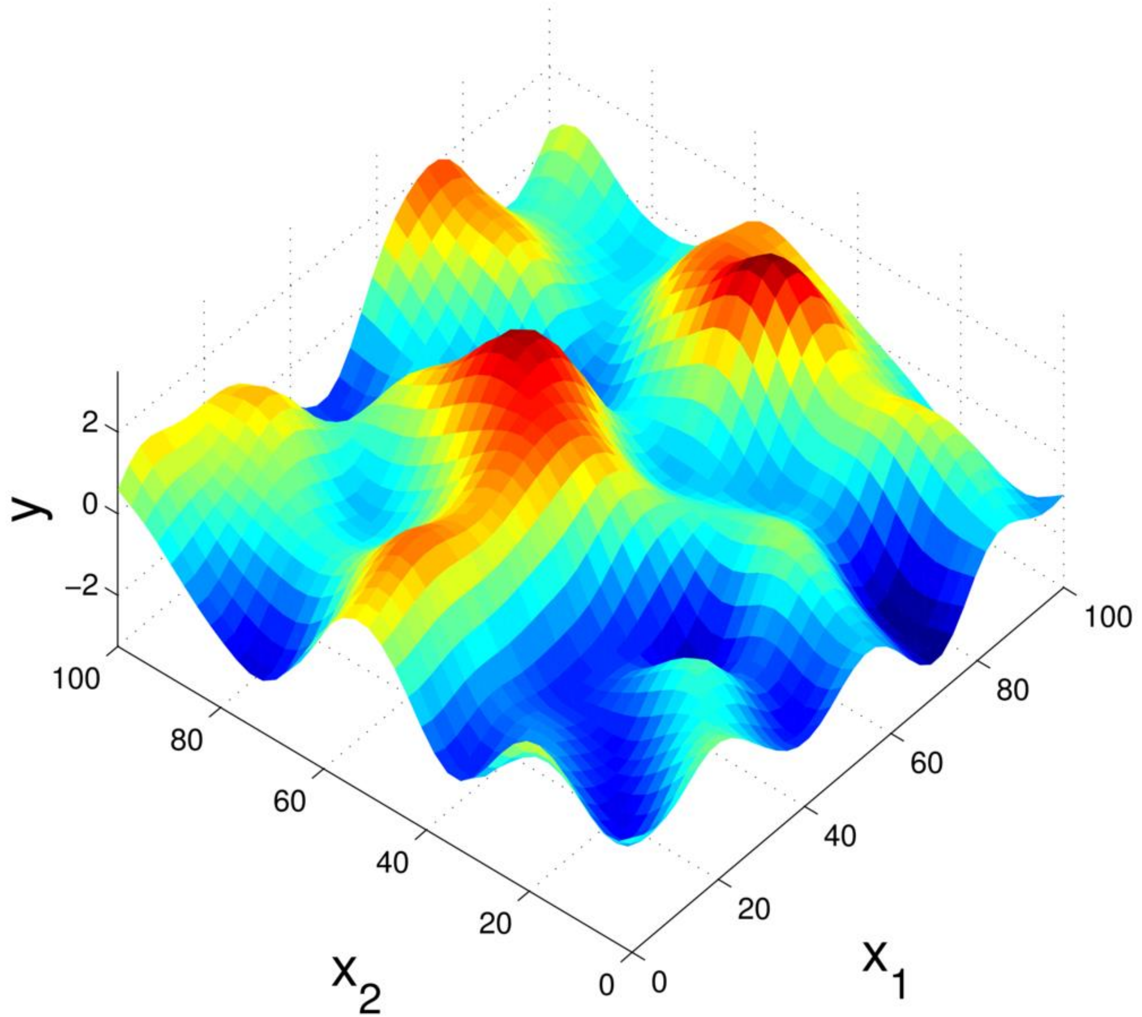

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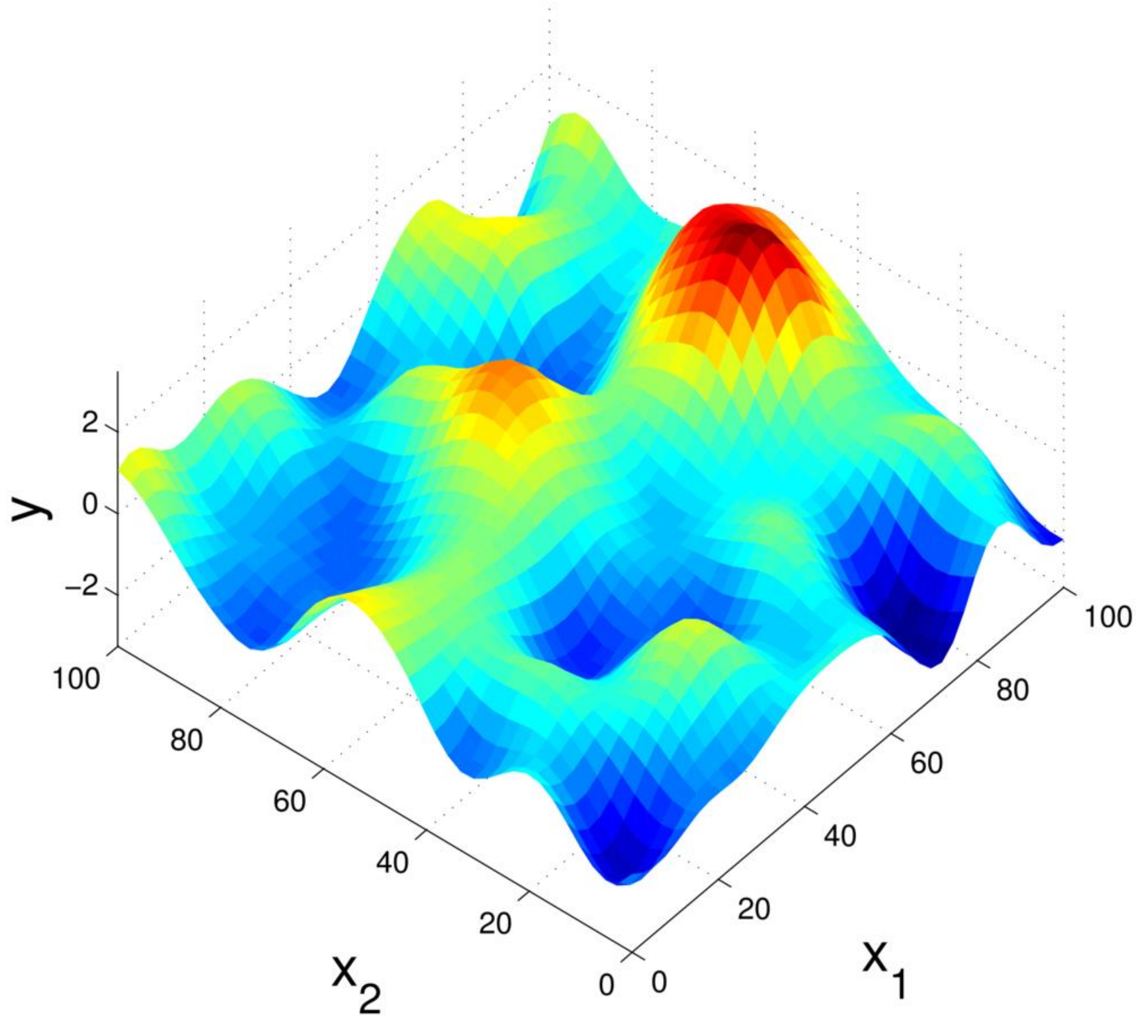

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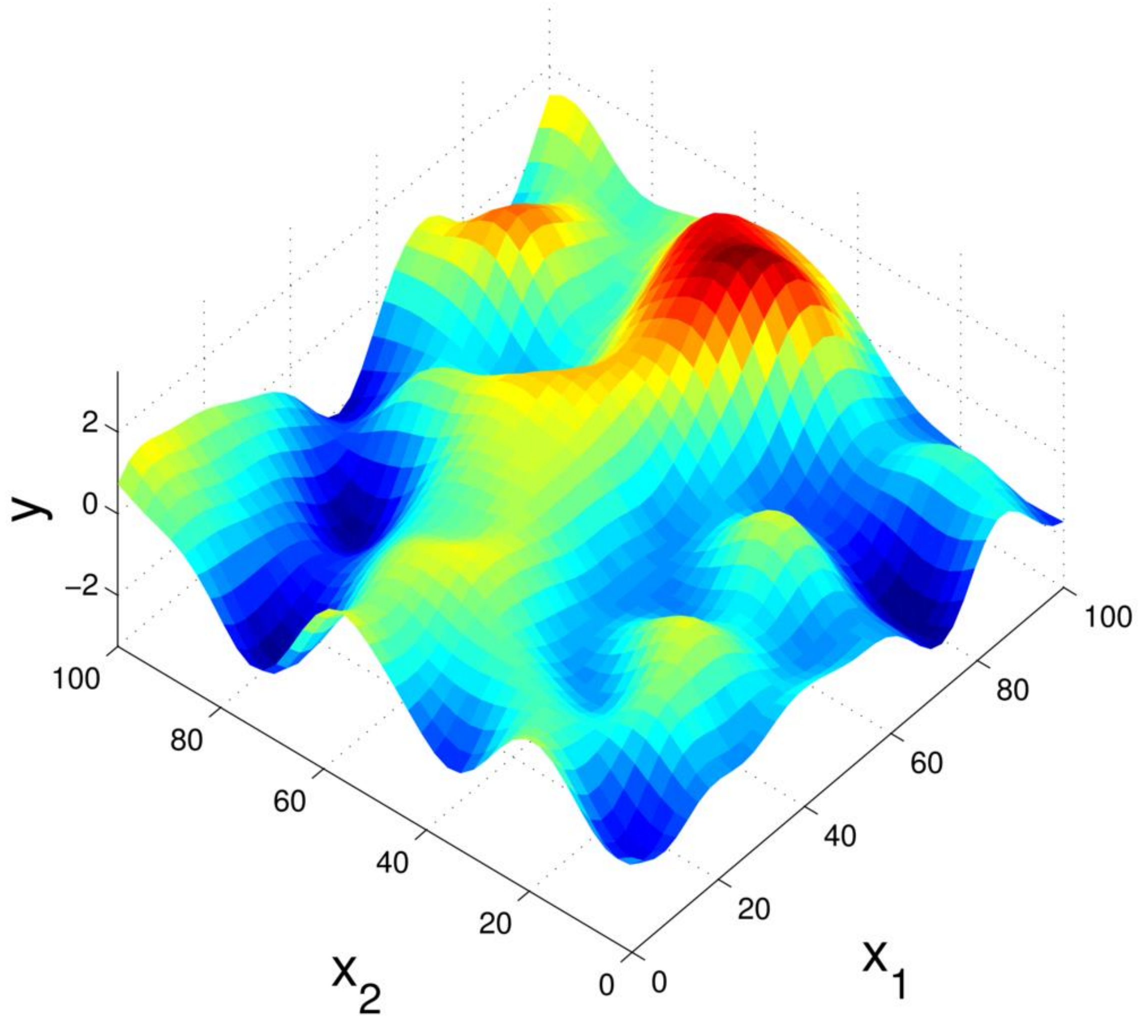

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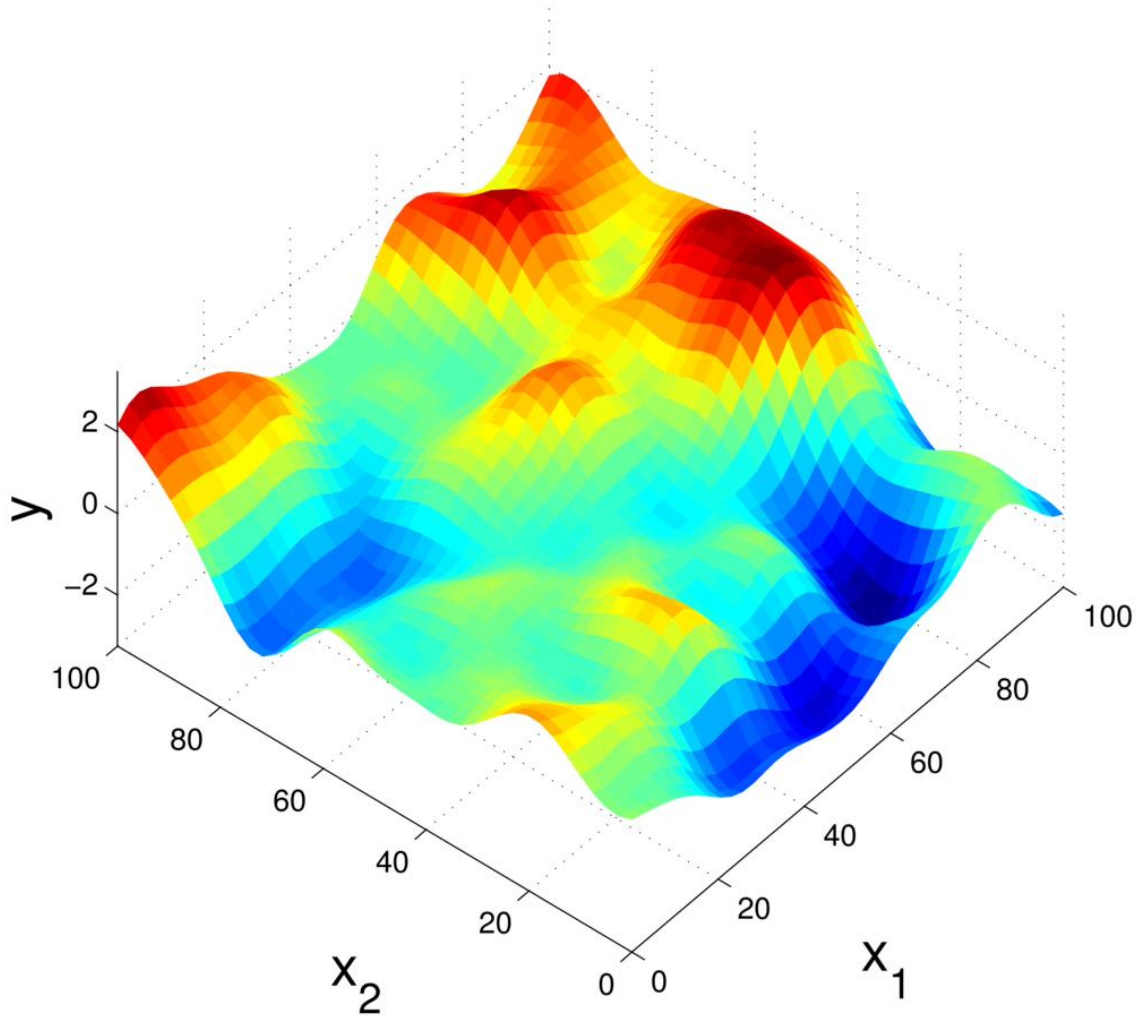

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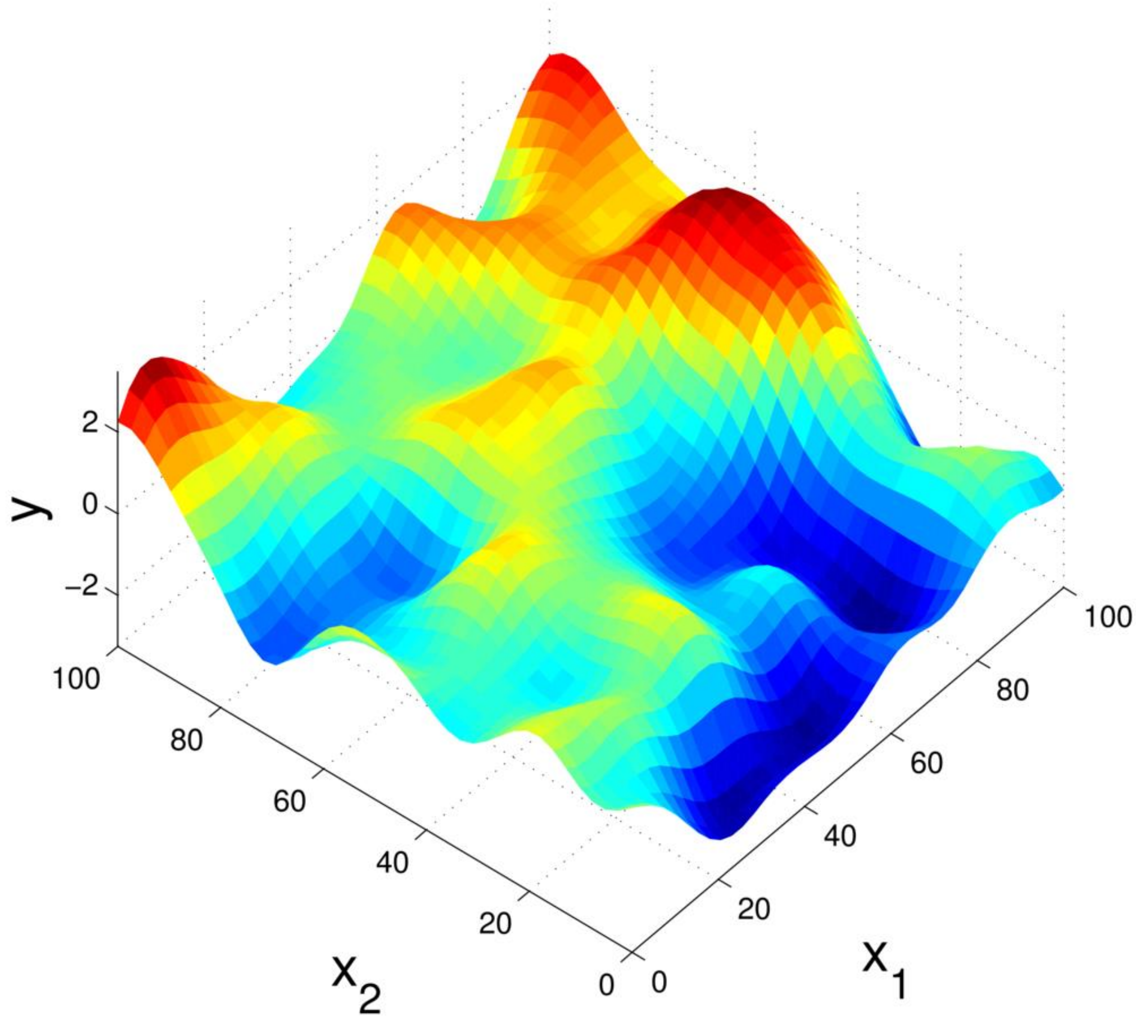

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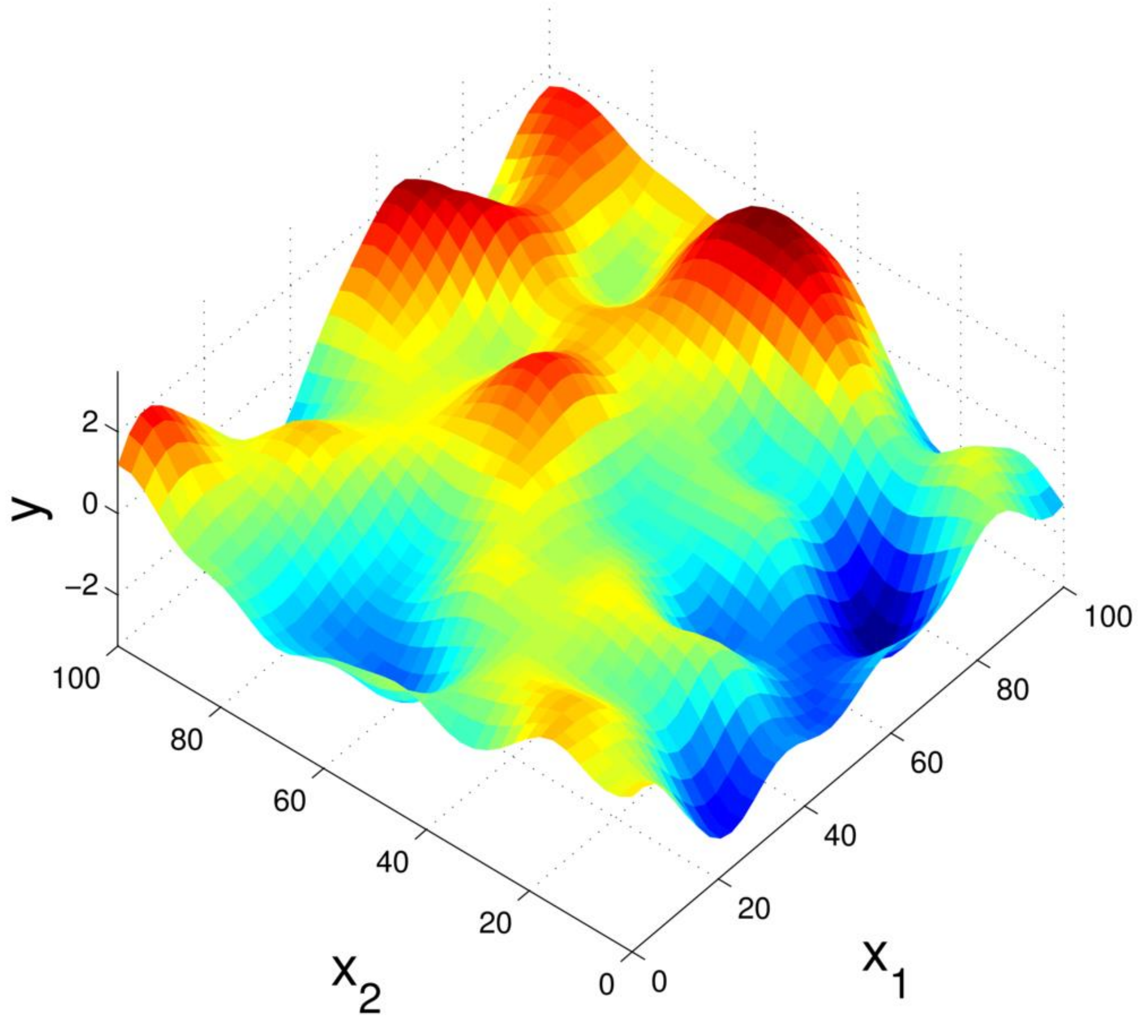

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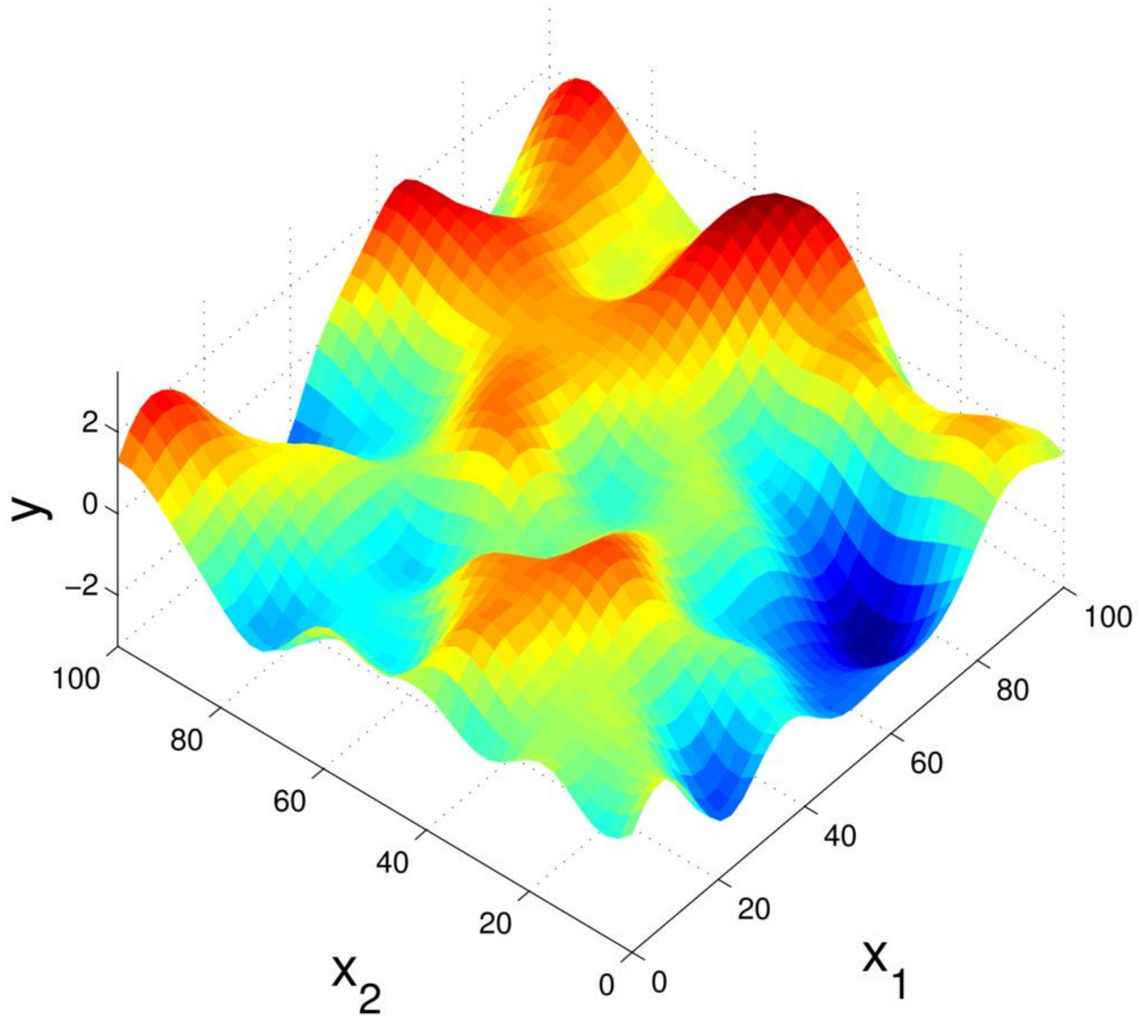

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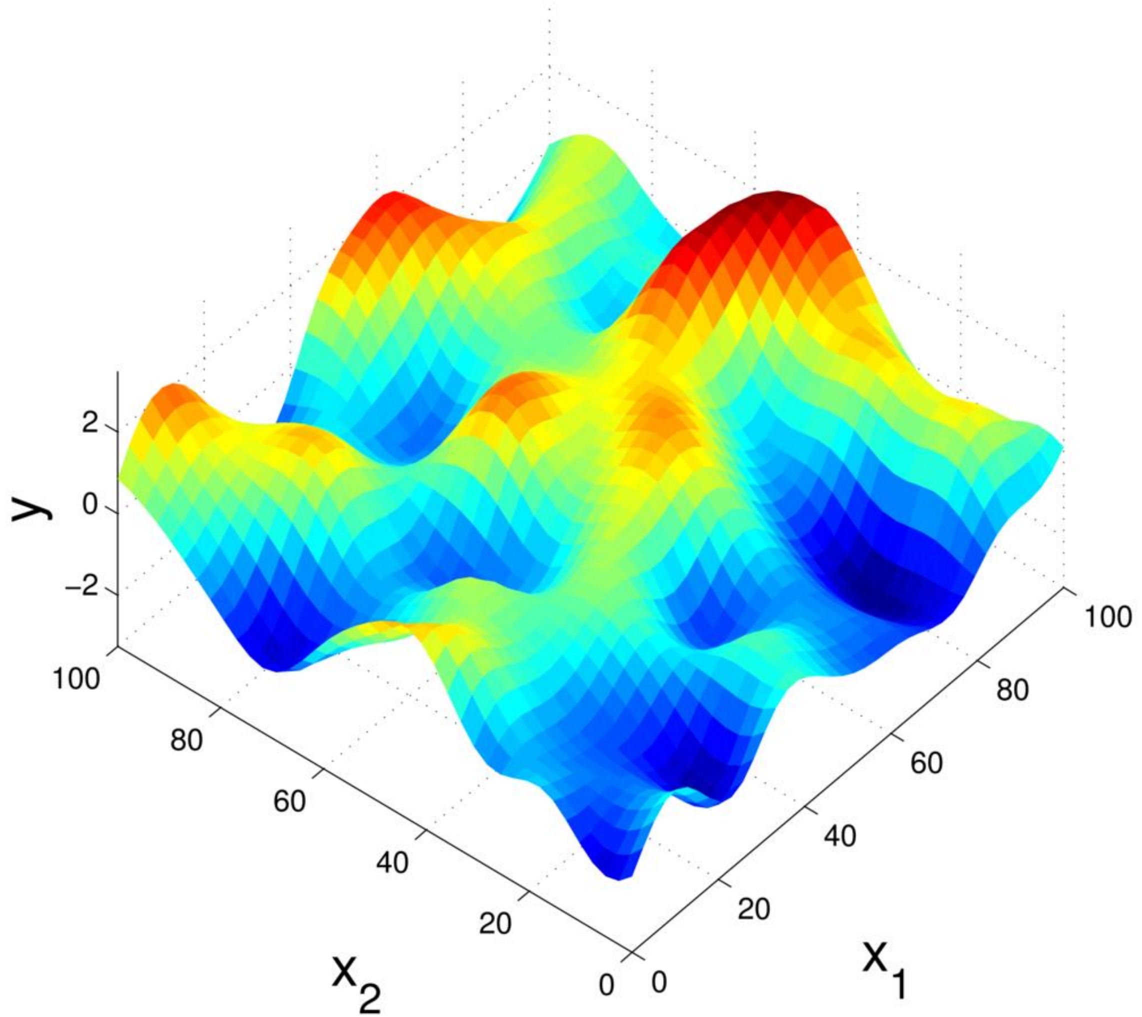

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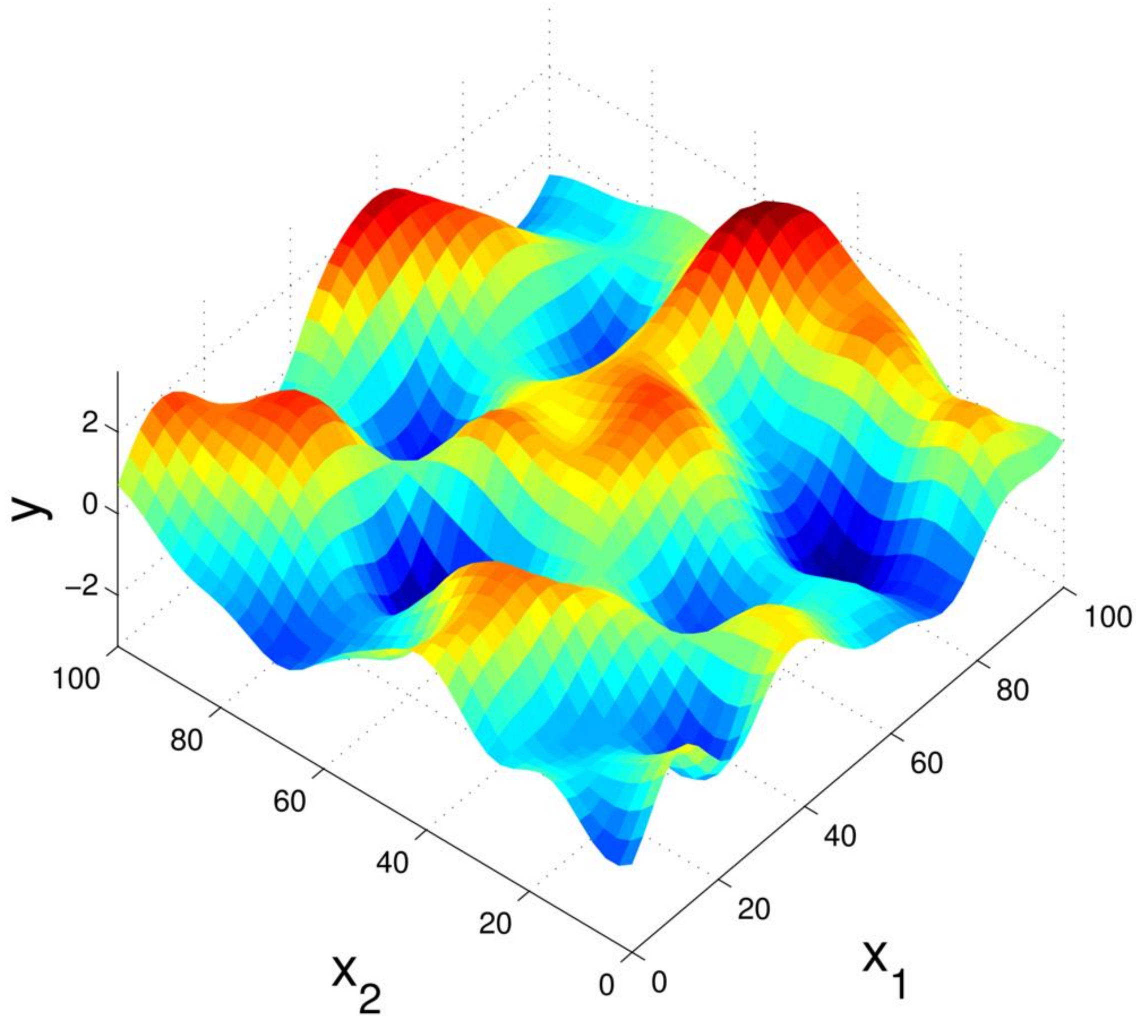

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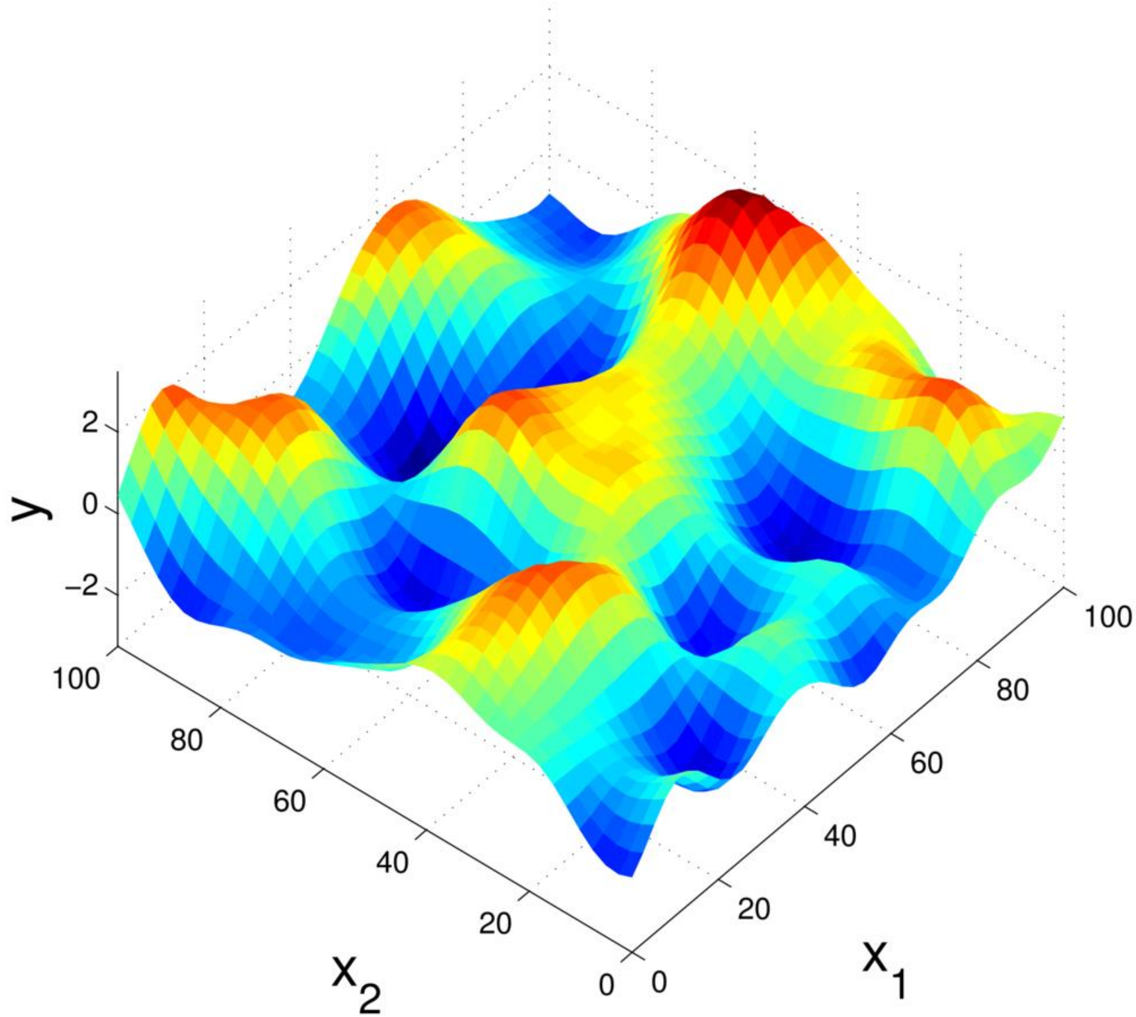

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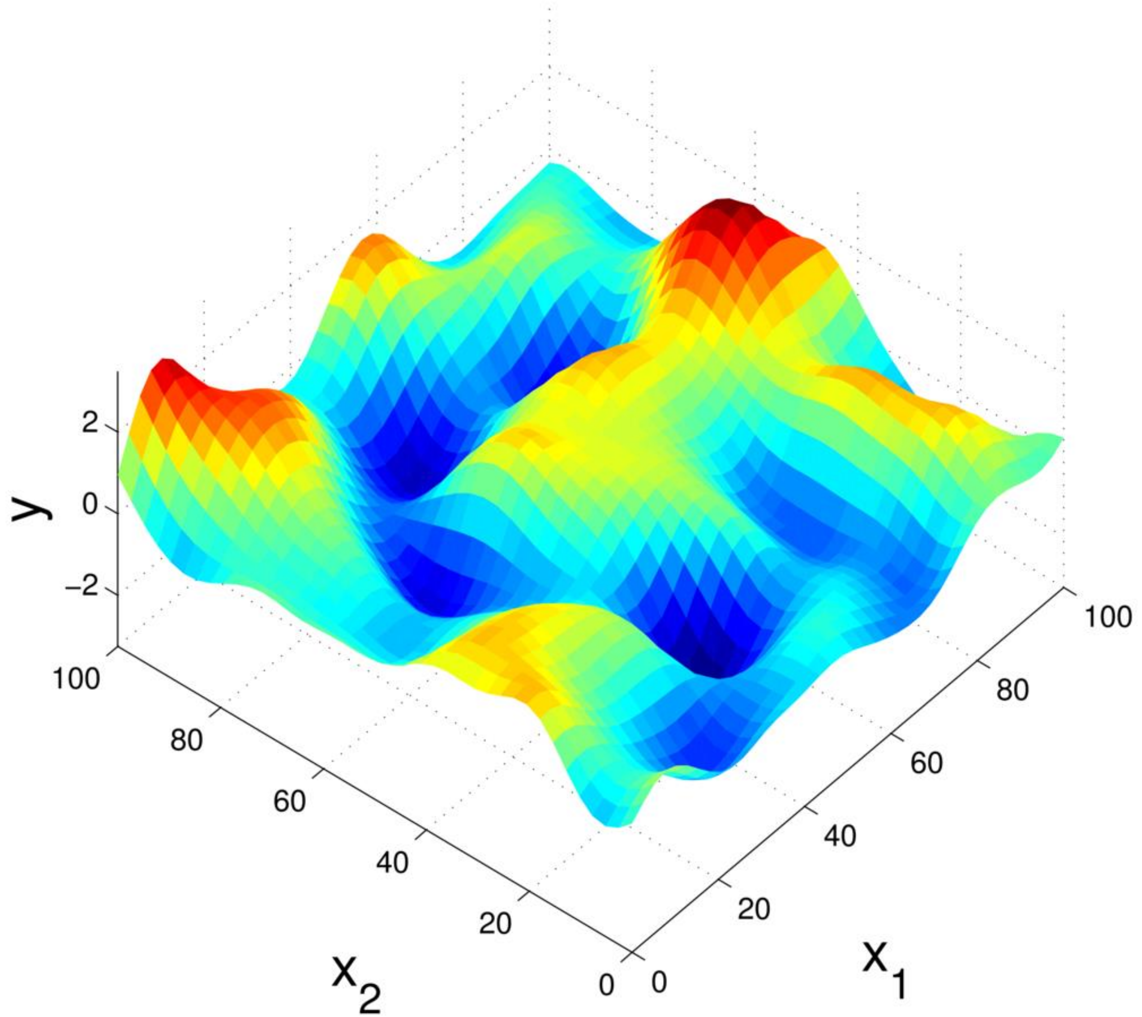


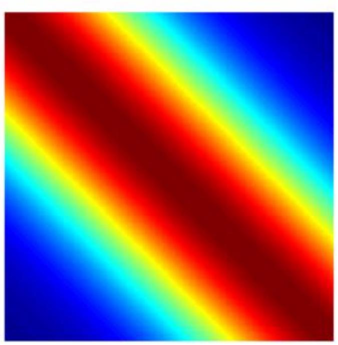
What effect do the Hyper-parameter have?

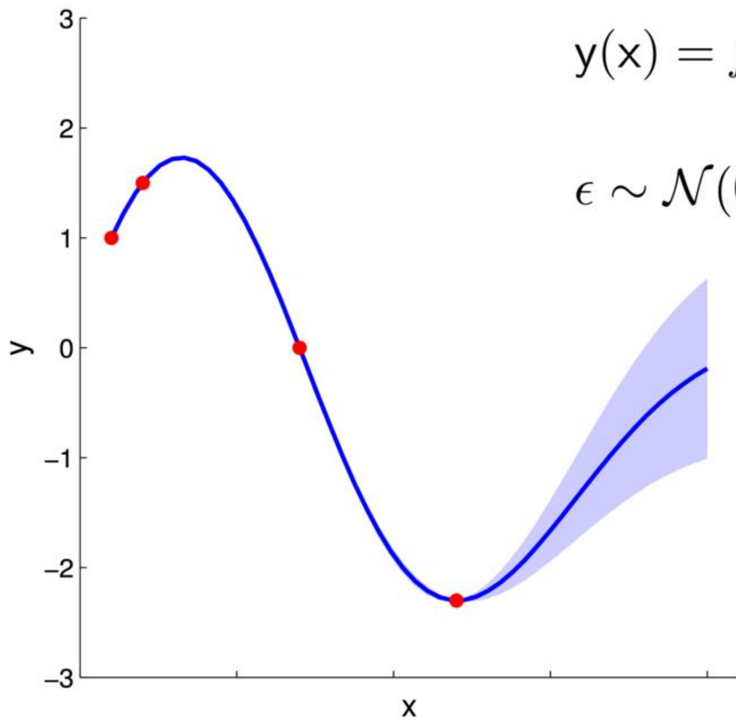
Non-parametric (∞-parametric)

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

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

$$\mathrm{K}(\mathrm{x}_1, \mathrm{x}_2) = \sigma^2 e^{-\frac{1}{2l^2}(\mathrm{x}_1 - \mathrm{x}_2)^2}$$

$\Sigma =$ 



Parametric model

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

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

What effect do the Hyper-parameter have?

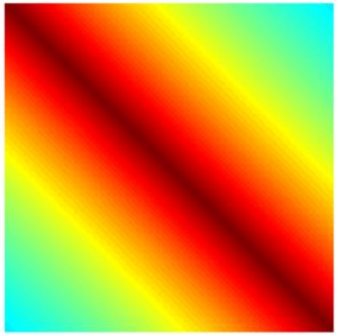
$$K(x_1, x_2) = \sigma^2 \exp\left(-\frac{1}{2l^2}|x_1 - x_2|\right)$$

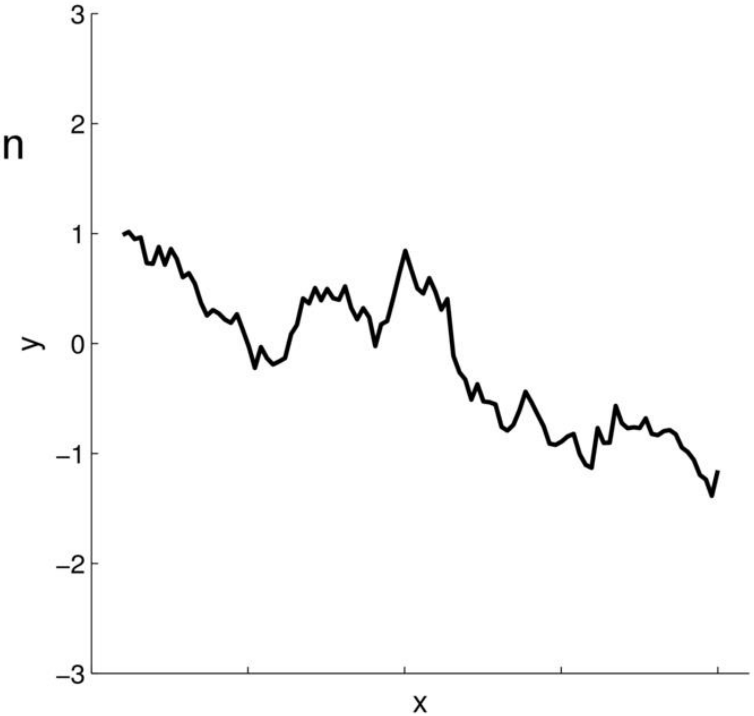
Laplacian covariance function

Browninan motion

Ornstein-Uhlenbeck

$\Sigma =$





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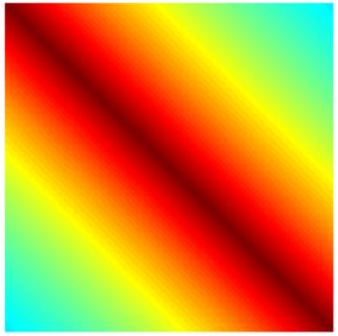
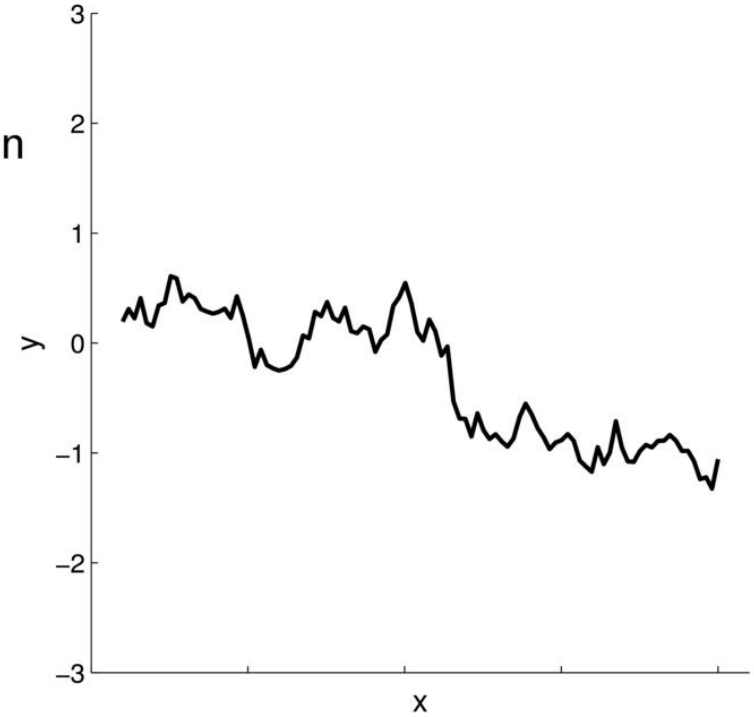
$\Sigma =$ 



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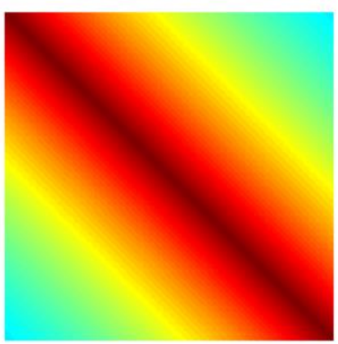

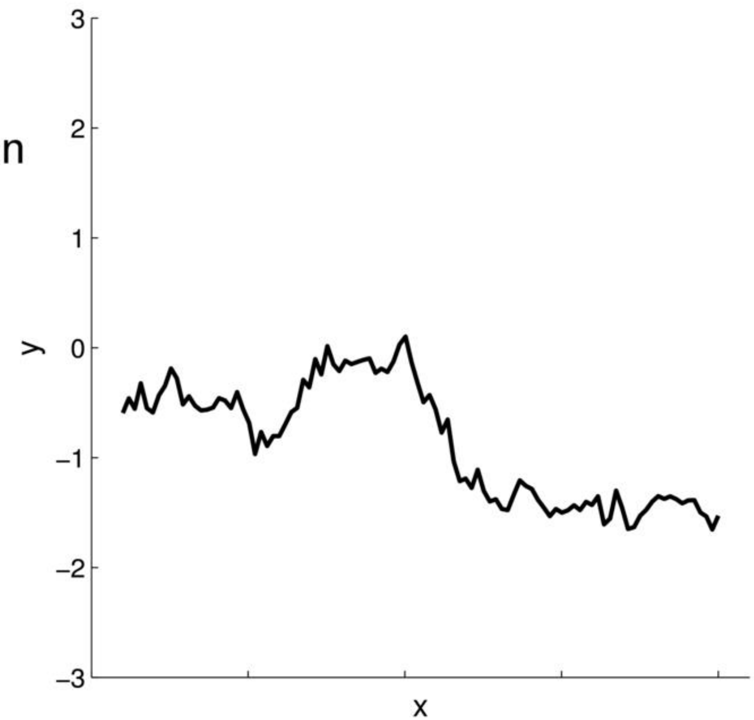

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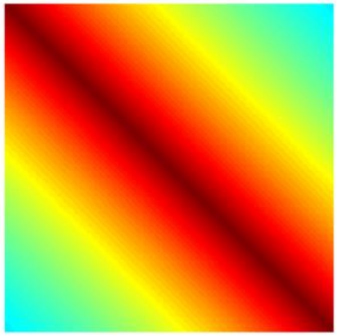

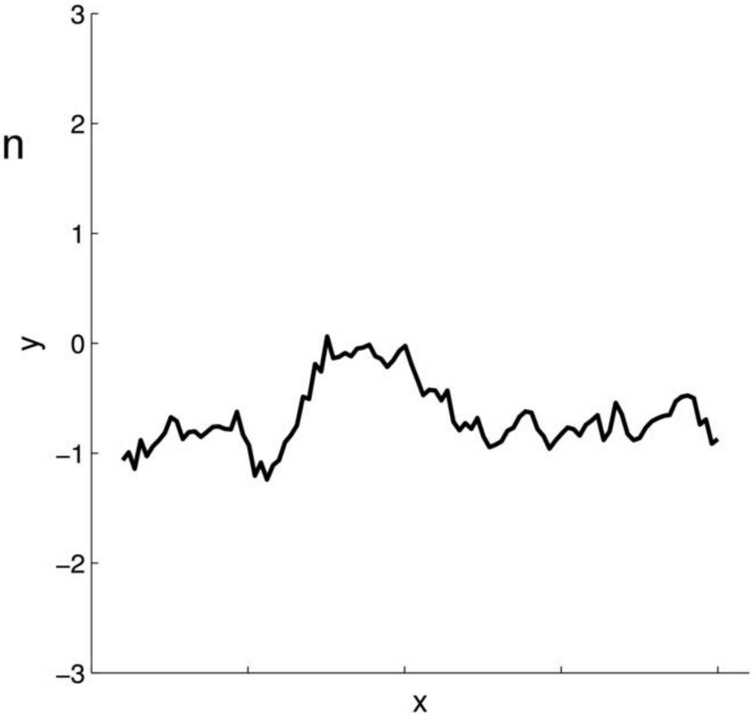

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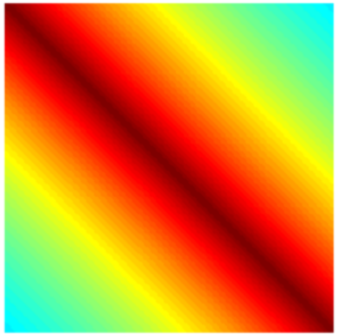

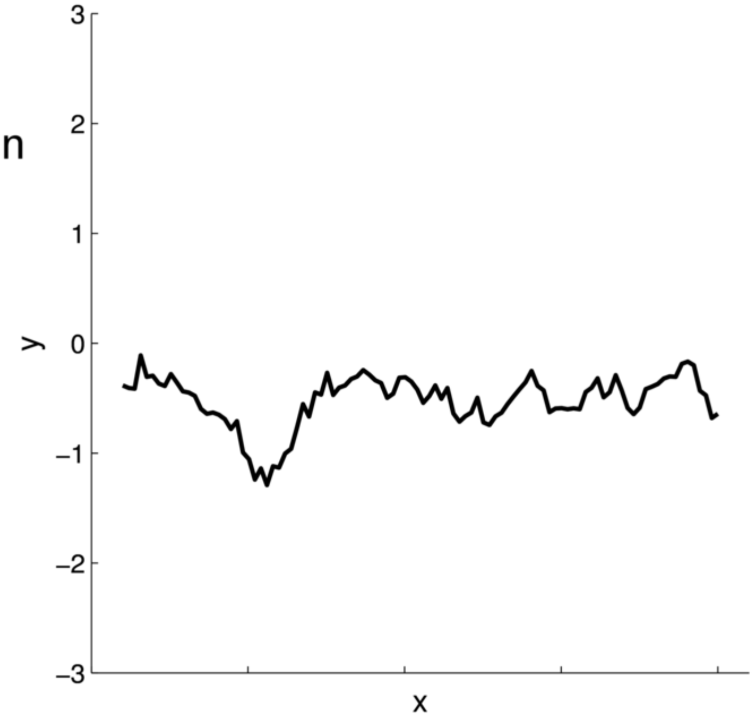

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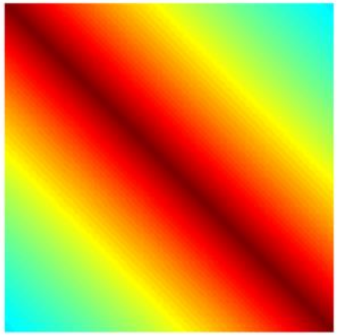

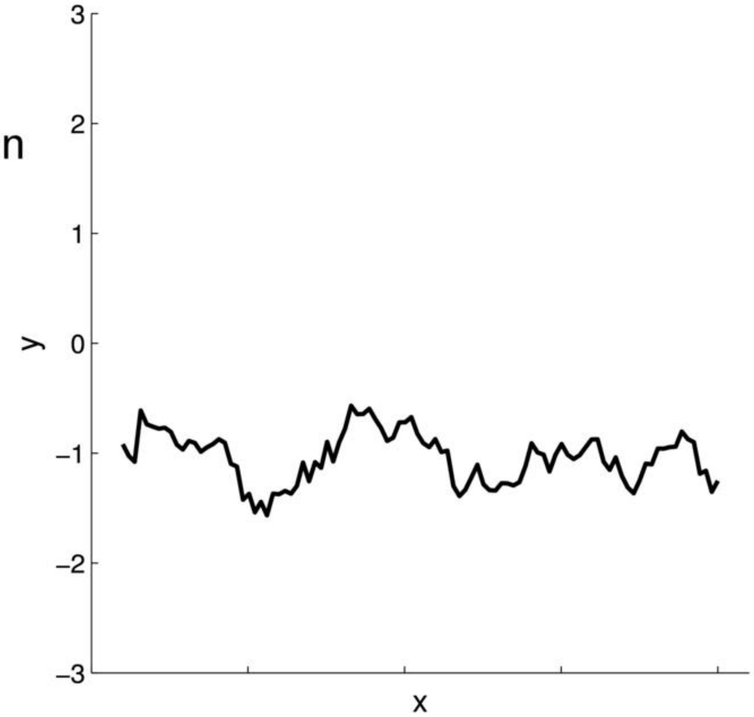

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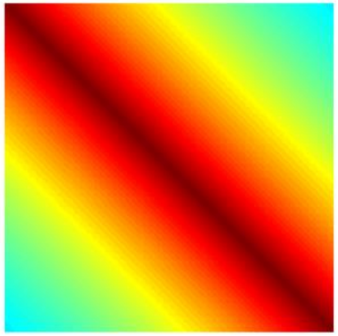
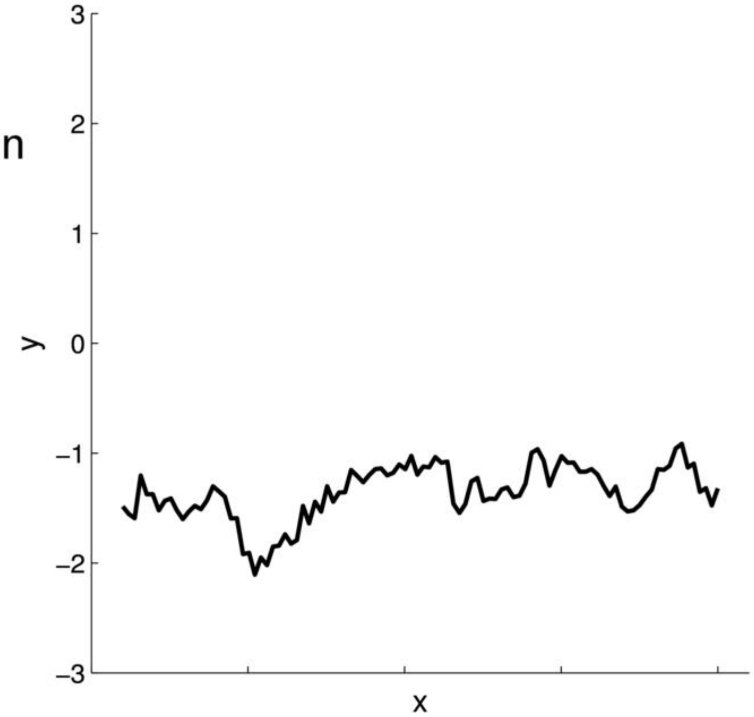
$\Sigma =$ 



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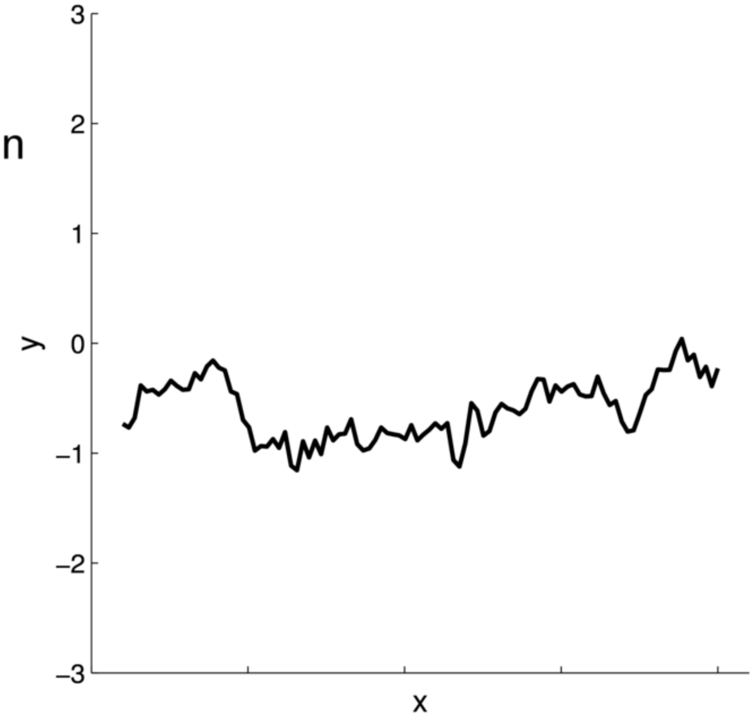
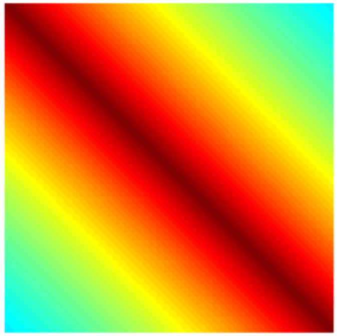


$\Sigma =$ 

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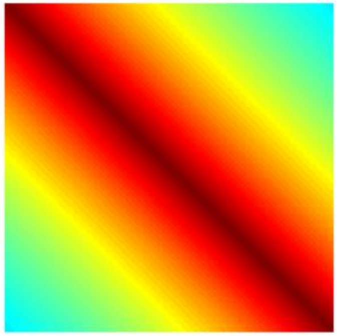

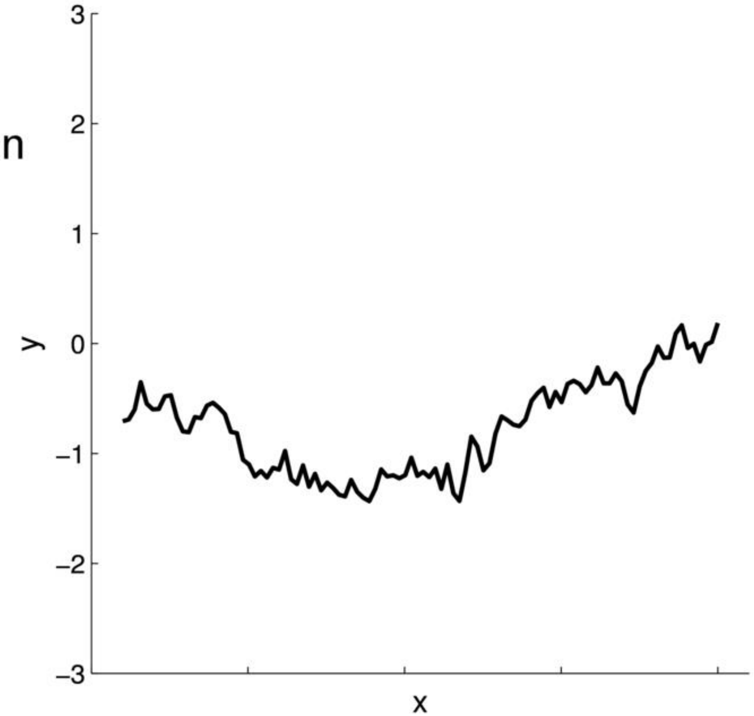

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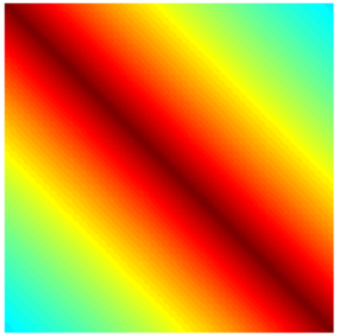
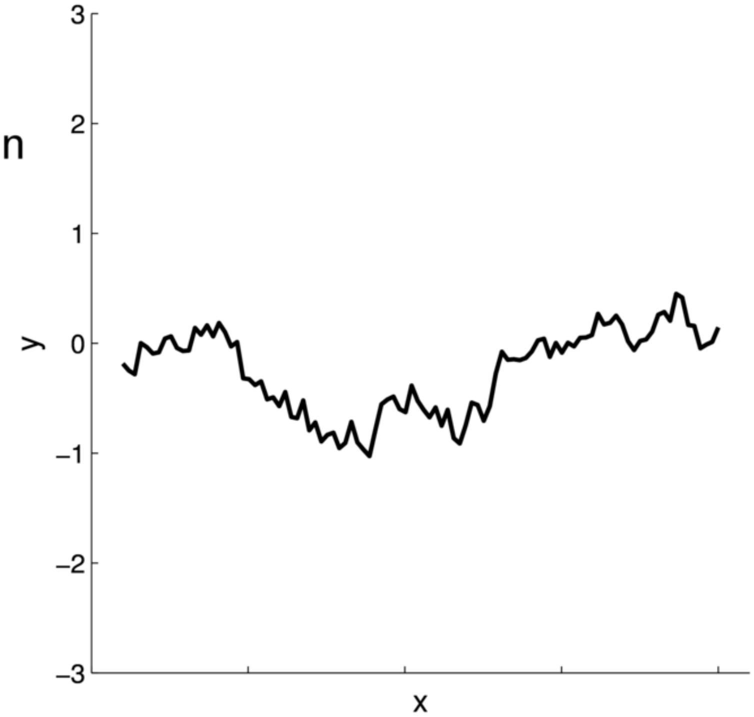
$\Sigma =$ 



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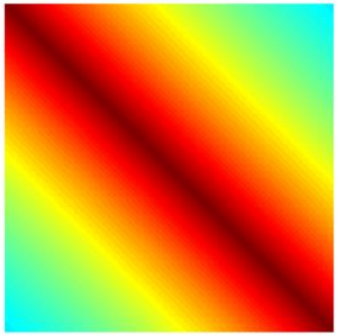

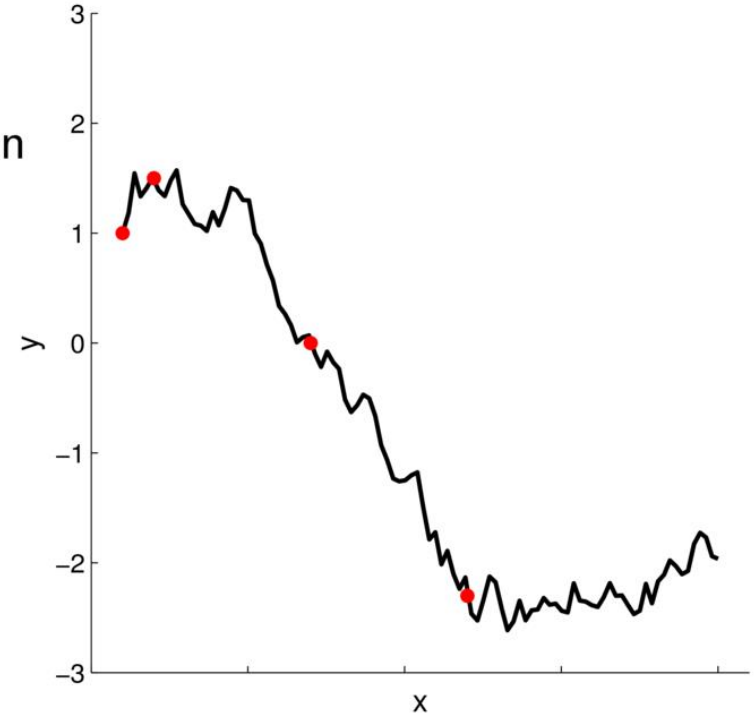

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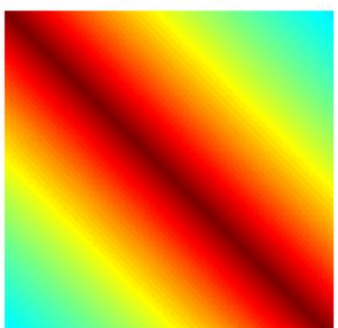
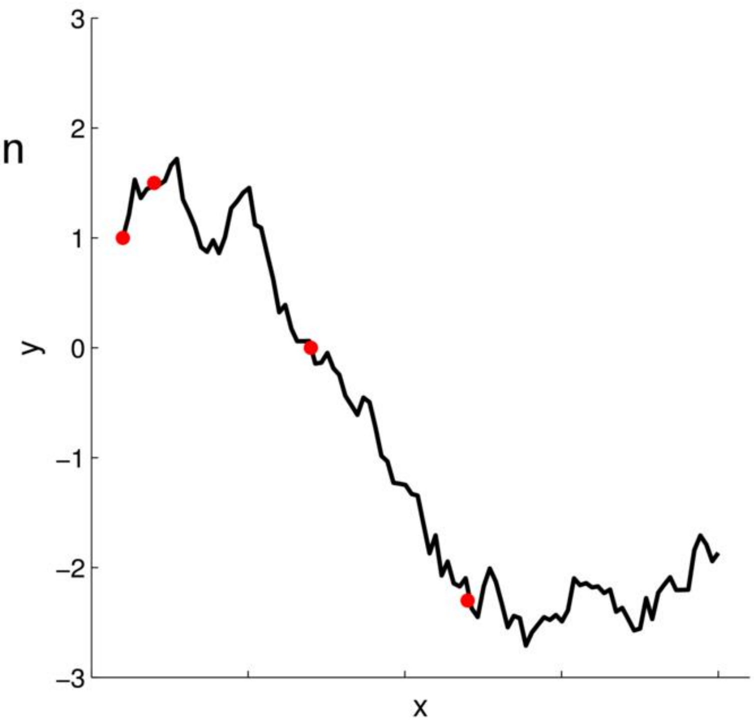
$\Sigma =$ 



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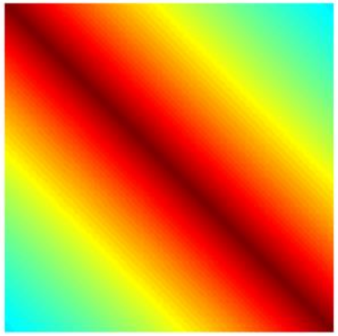
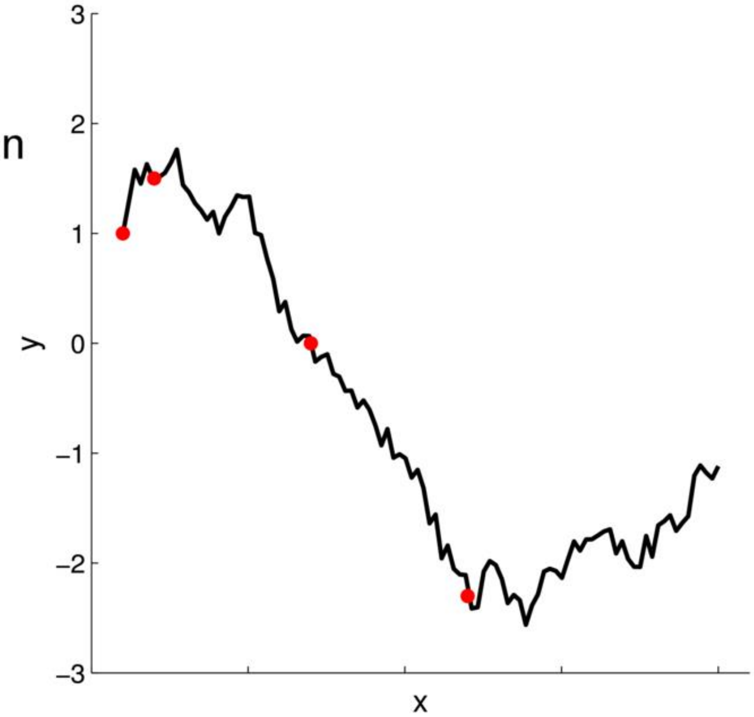
$\Sigma =$ 



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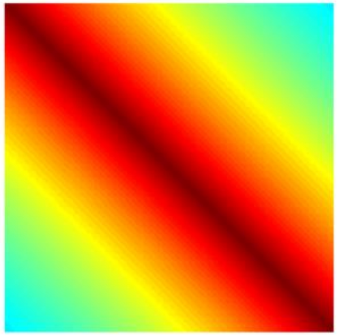
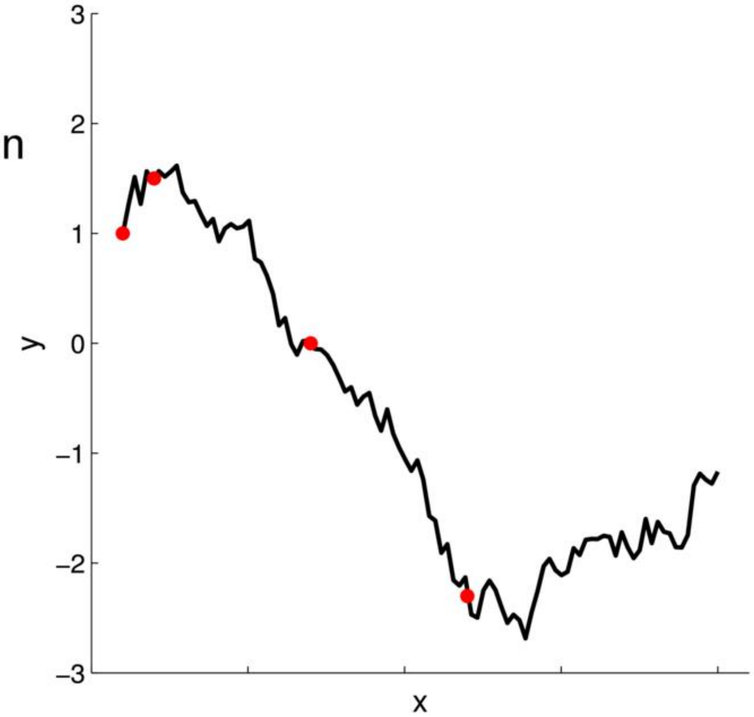
$\Sigma =$ 



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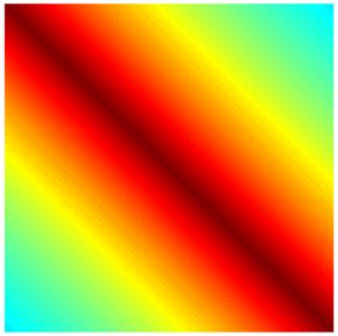

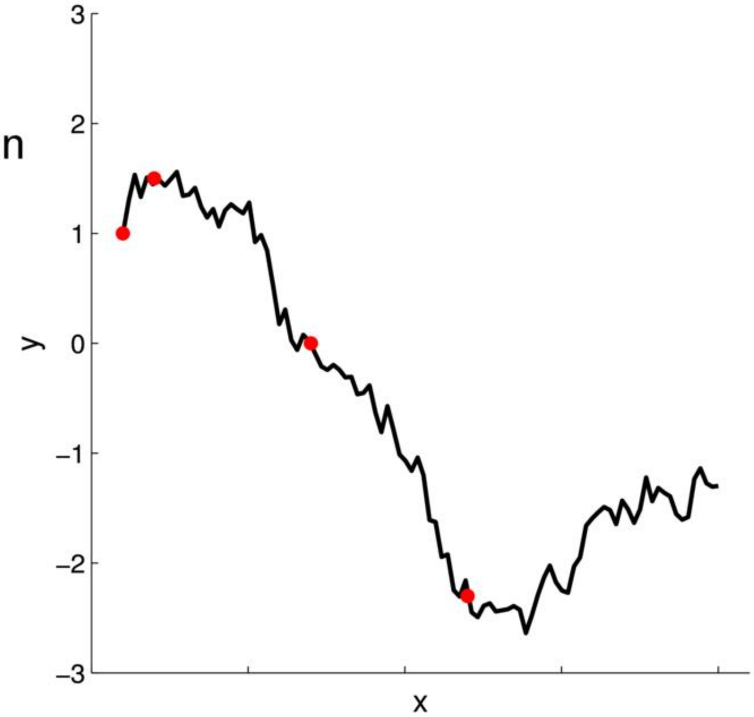

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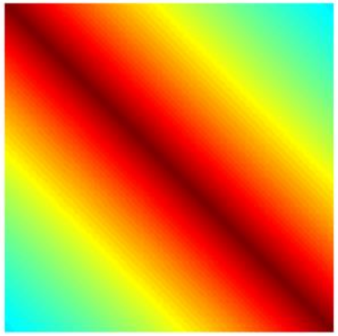

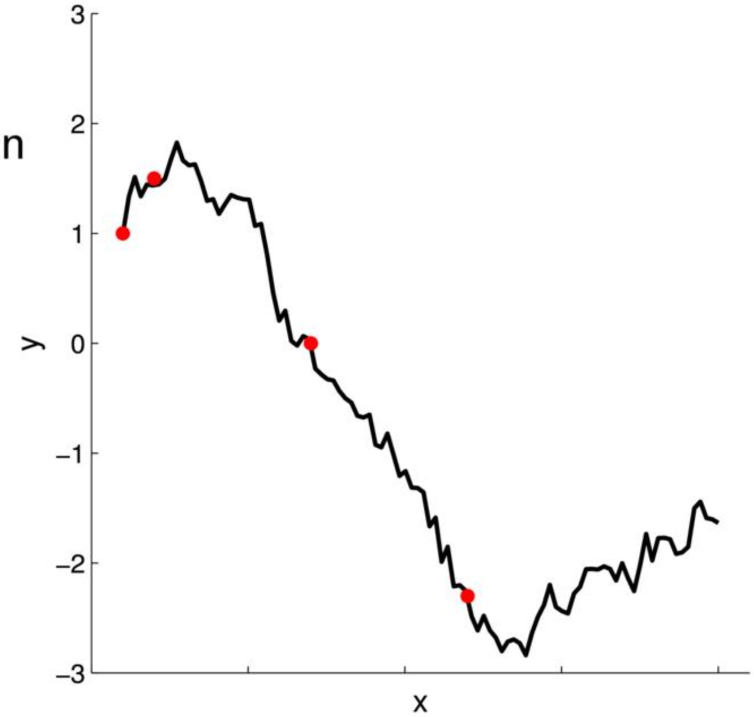

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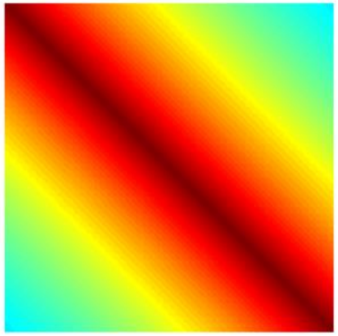

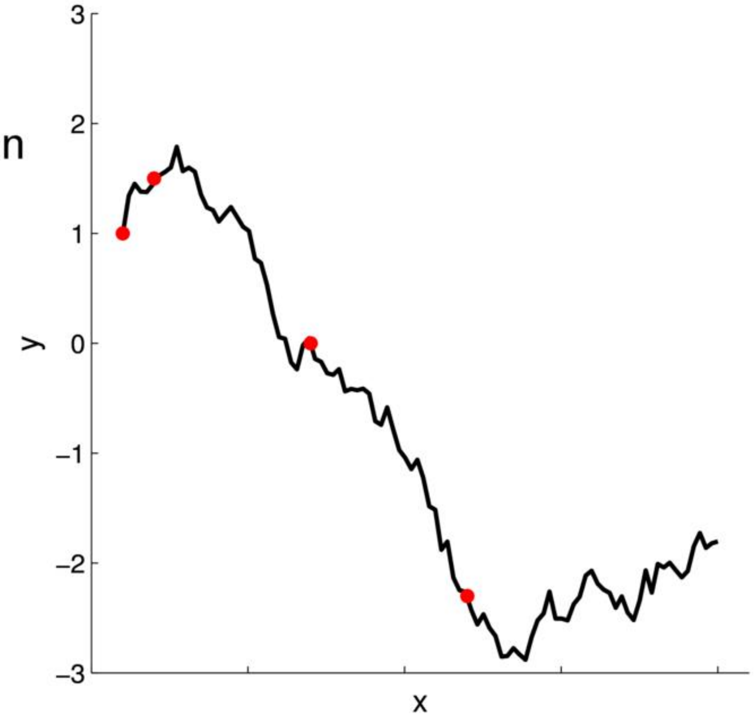

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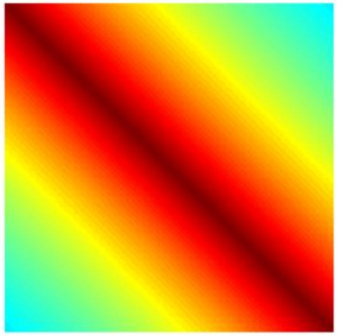

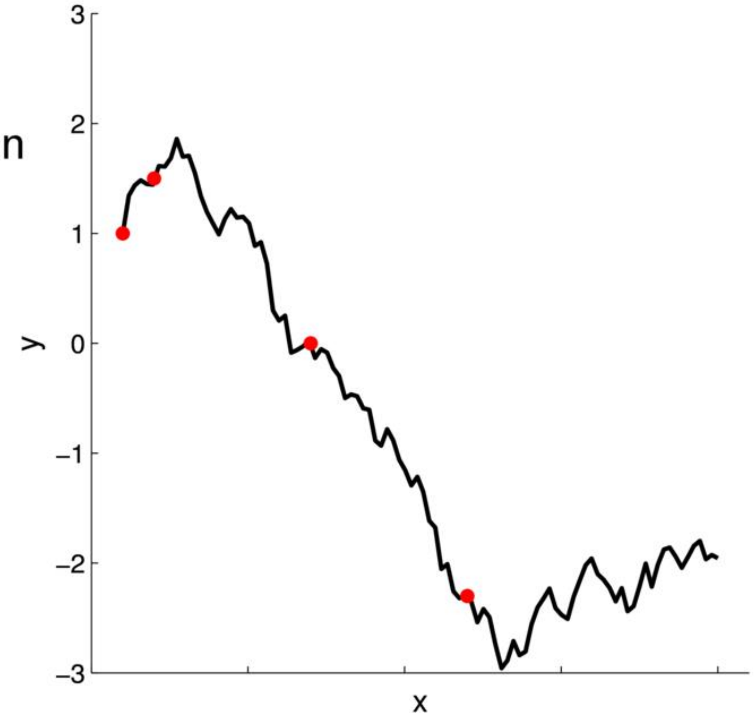

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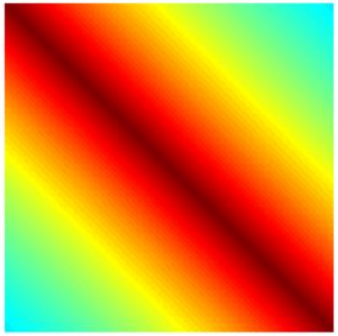

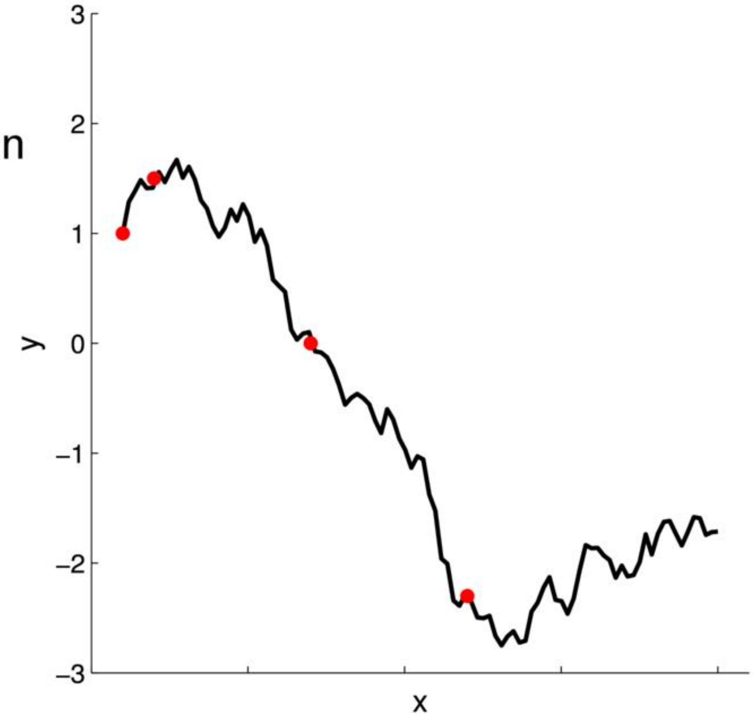

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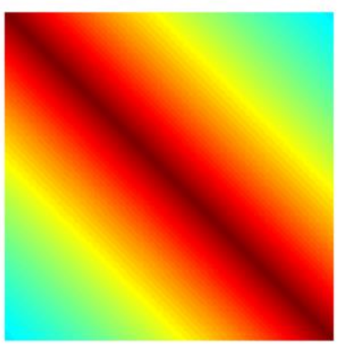
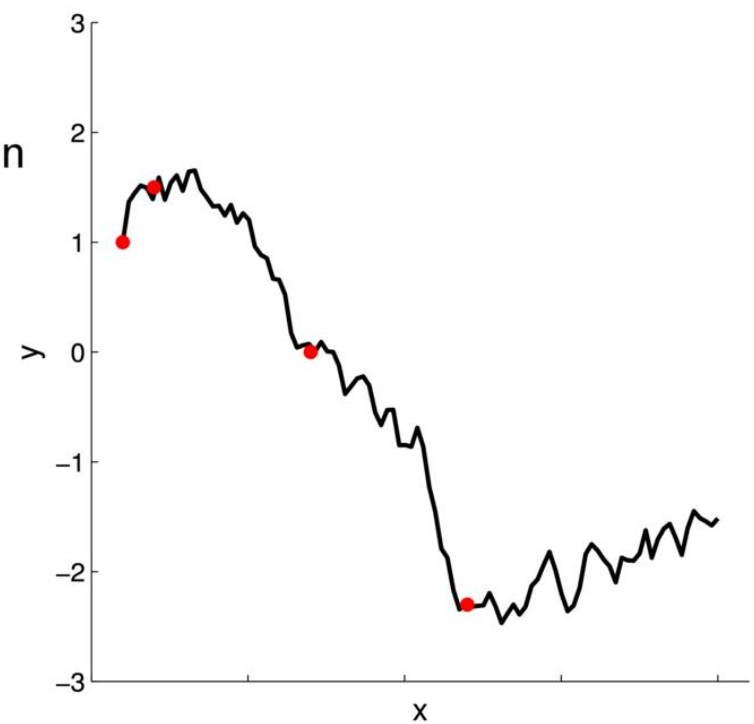
$\Sigma =$ 



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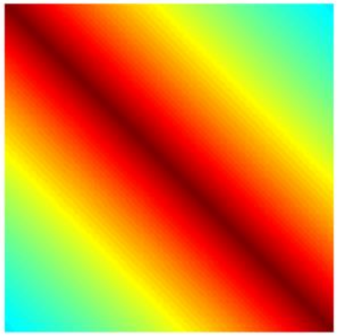
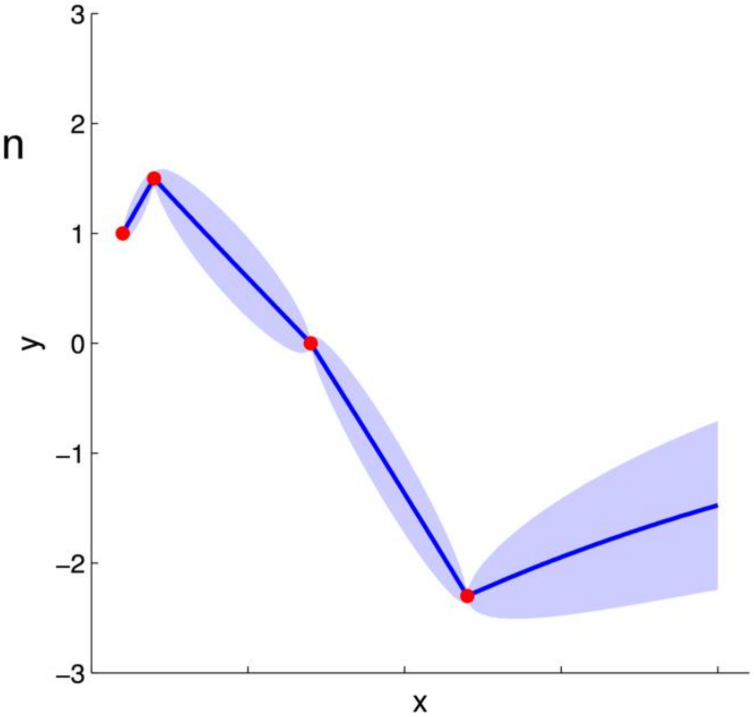
$\Sigma =$ 



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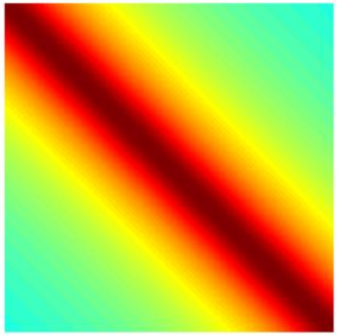
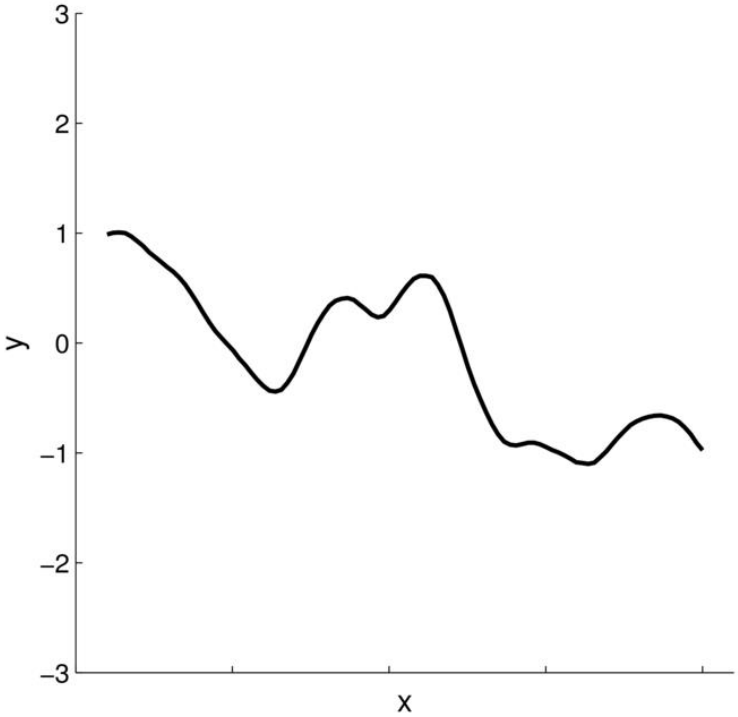
Rational Quadratic

$\Sigma =$





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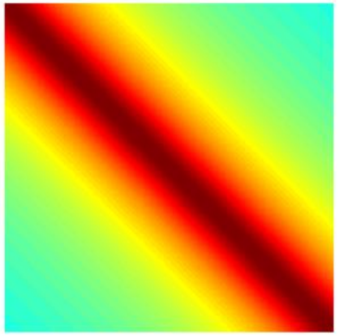
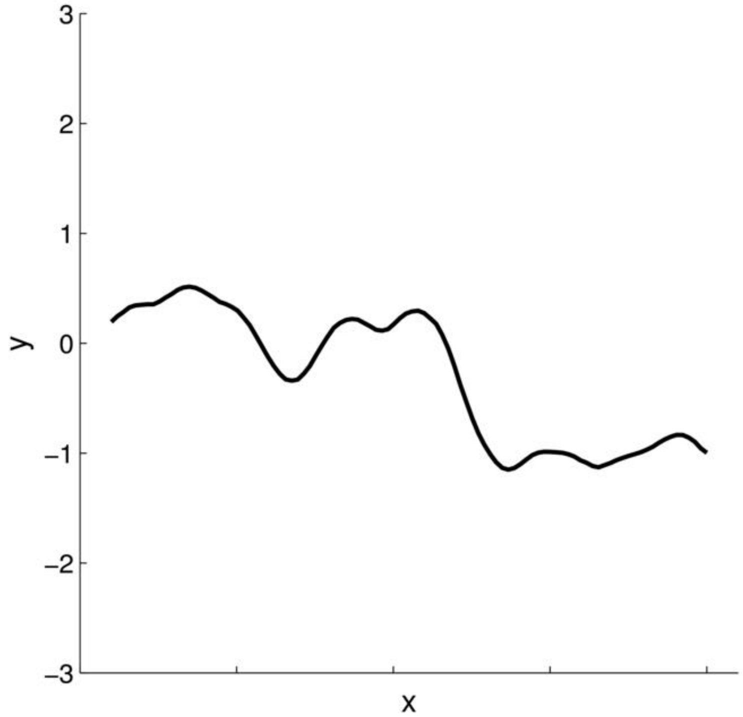
$\Sigma =$ 



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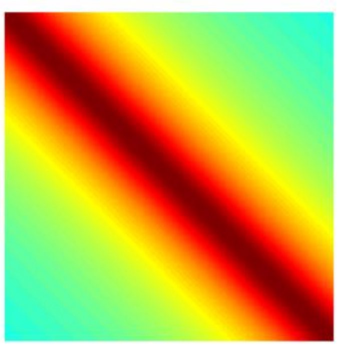

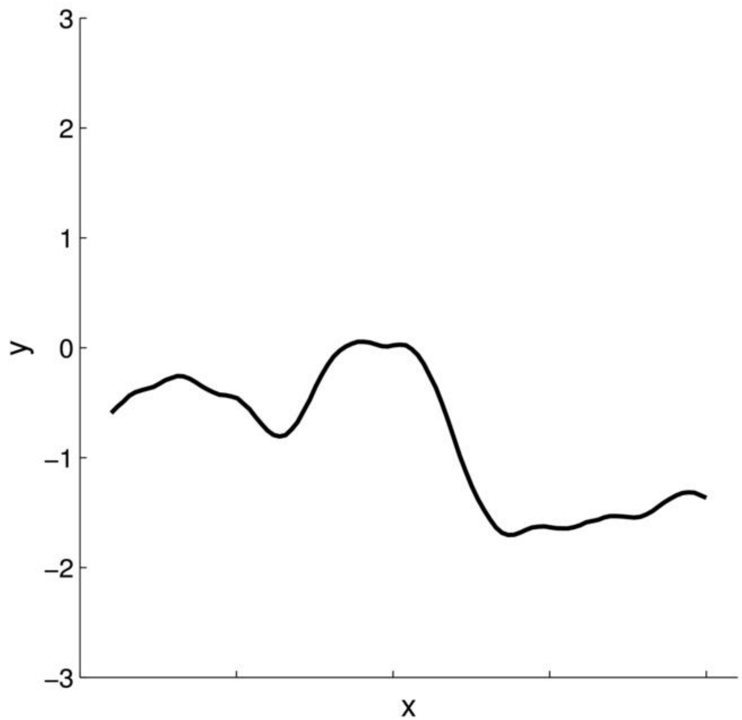

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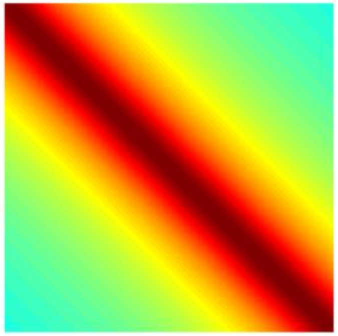
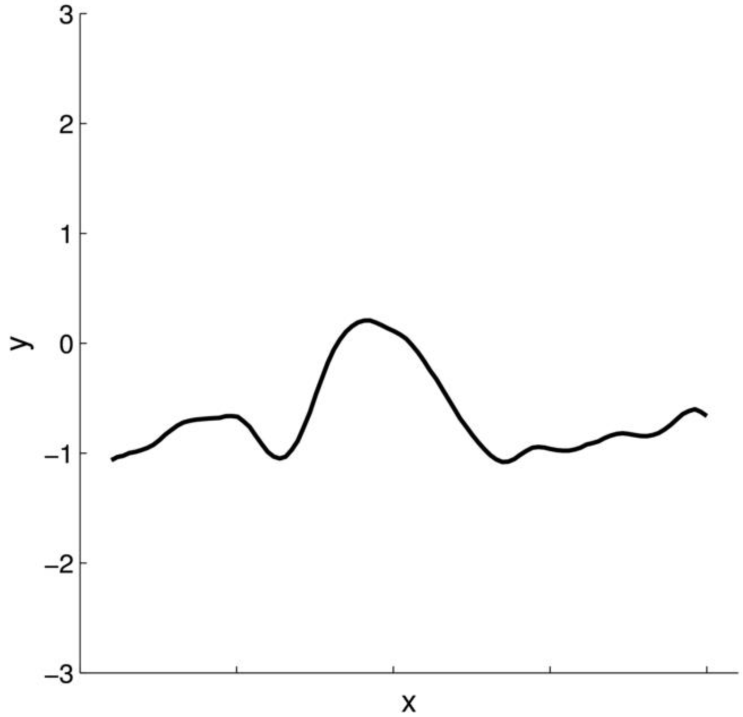
$\Sigma =$ 



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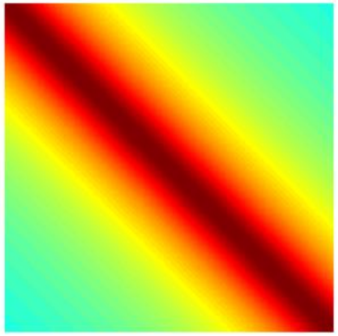
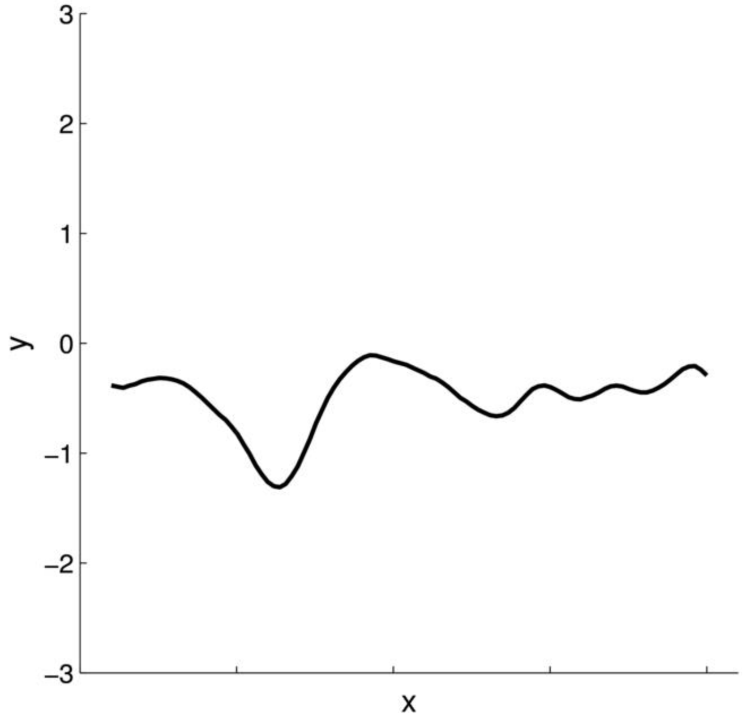
$\Sigma =$ 



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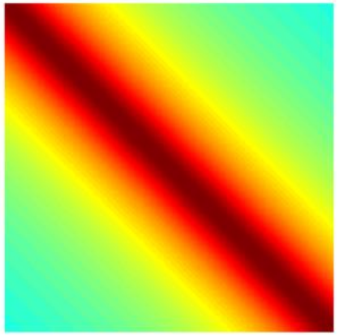
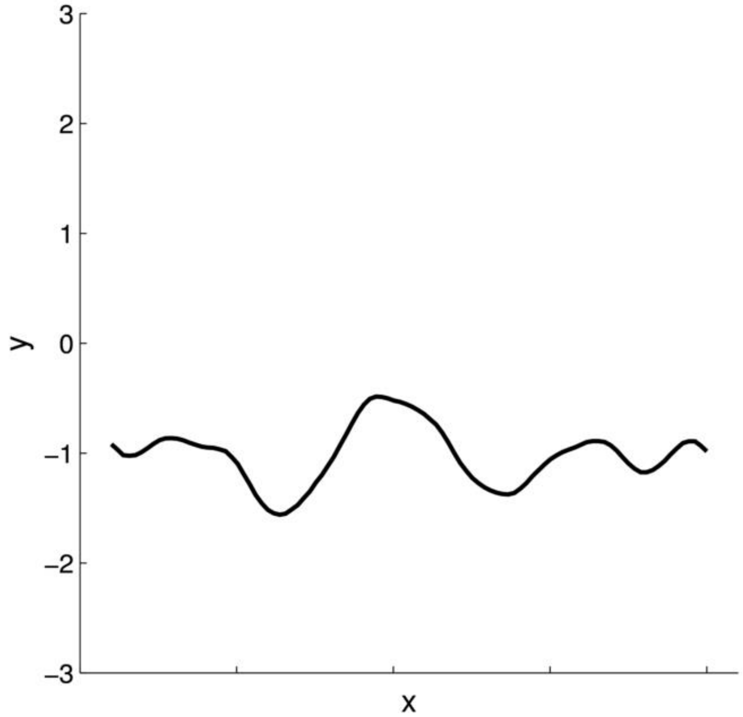
$\Sigma =$ 



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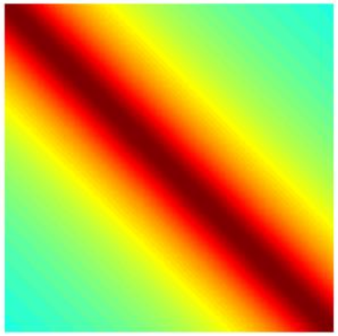

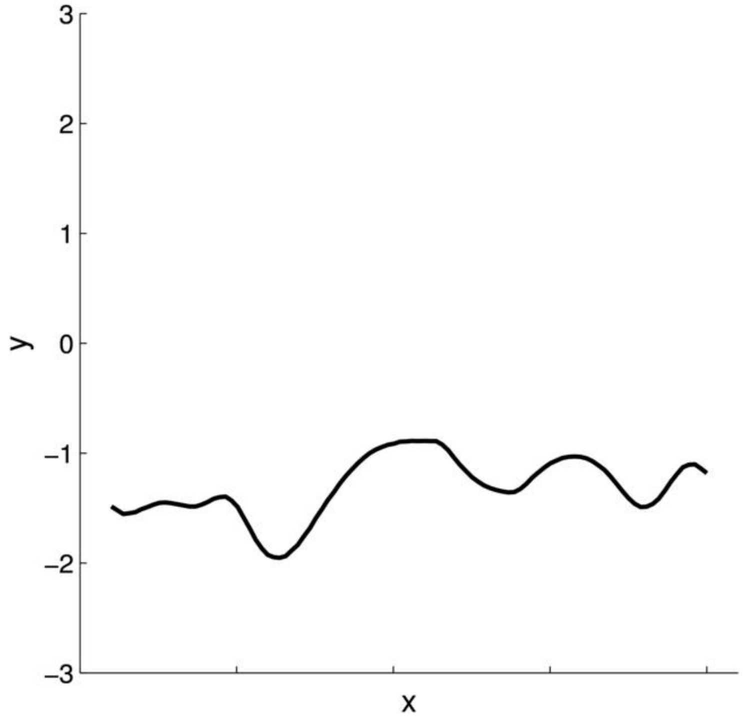

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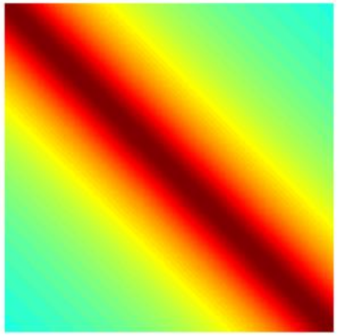
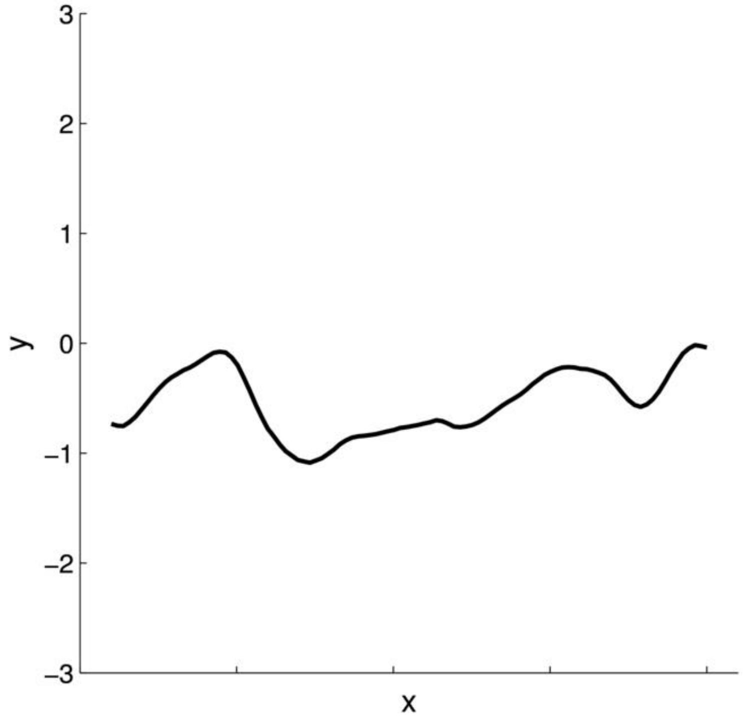
$\Sigma =$ 



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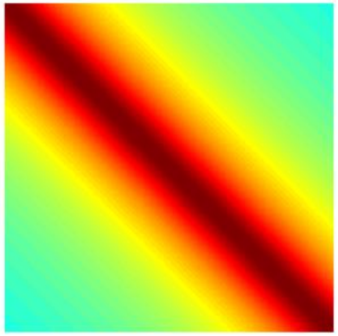
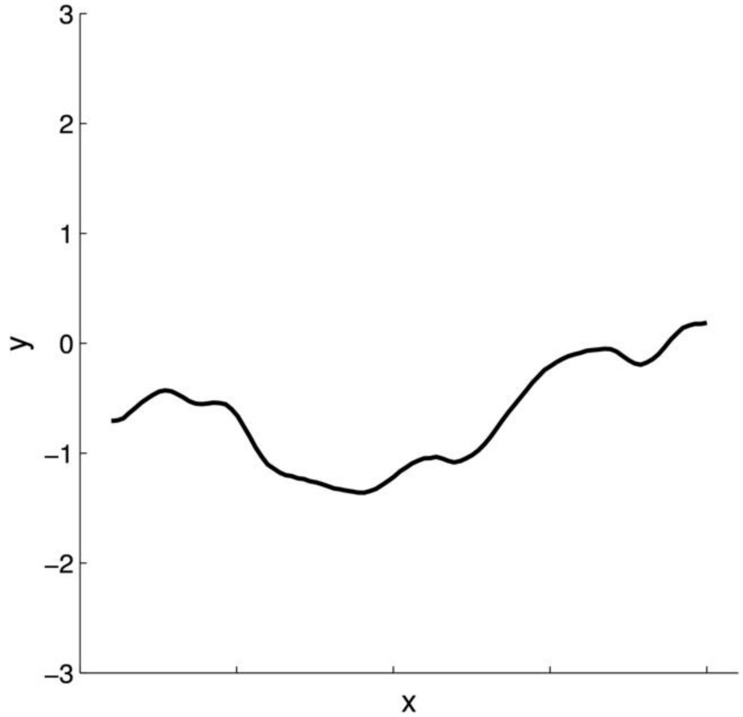
$\Sigma =$ 



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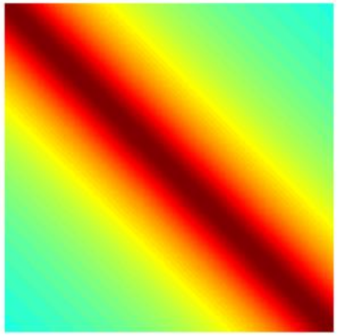
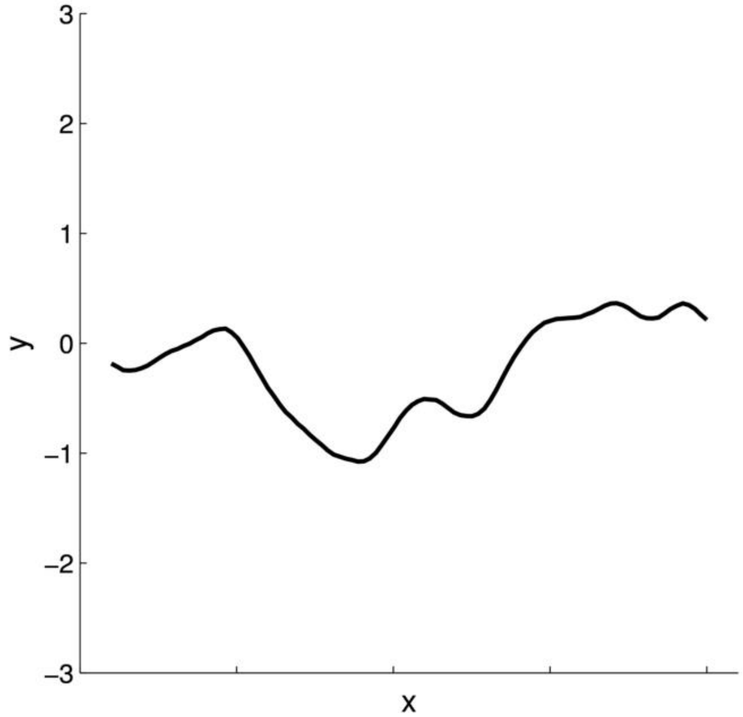
$\Sigma =$ 



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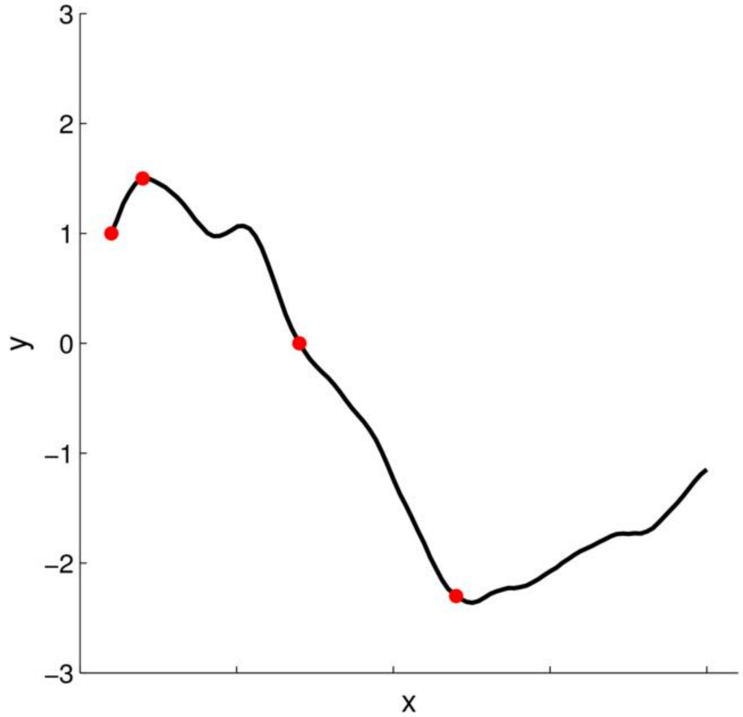
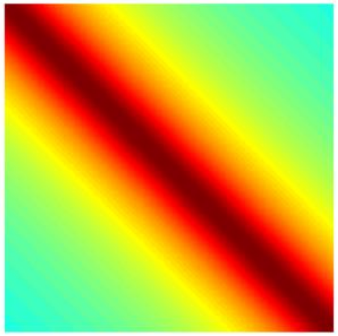


$\Sigma =$ 

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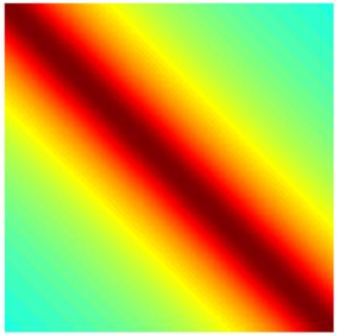
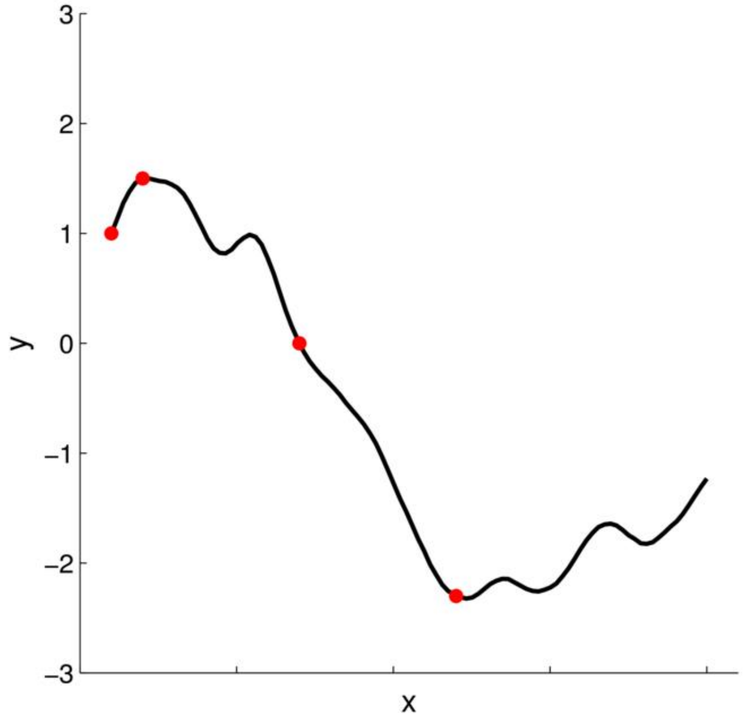
$\Sigma =$ 



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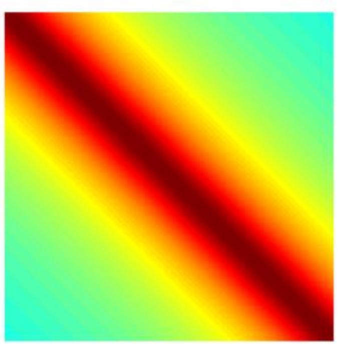

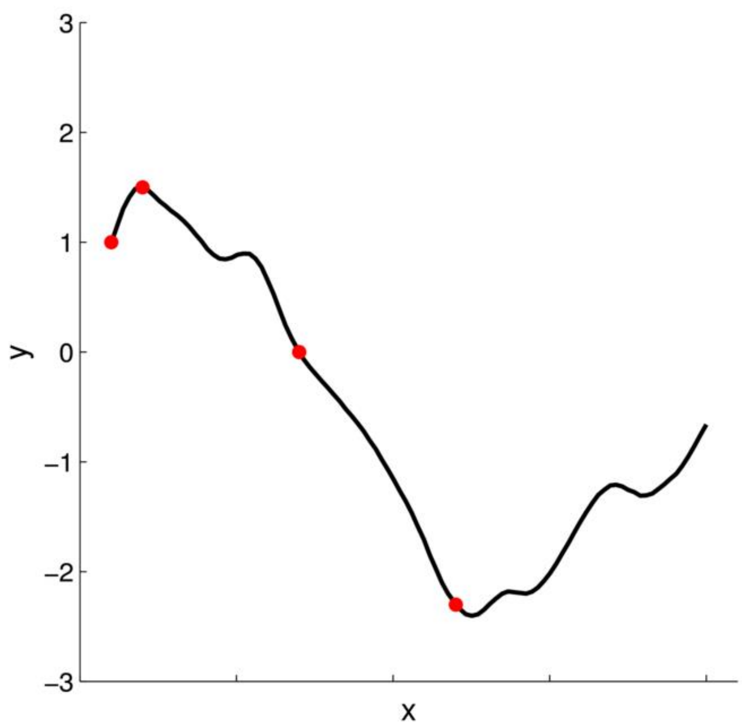

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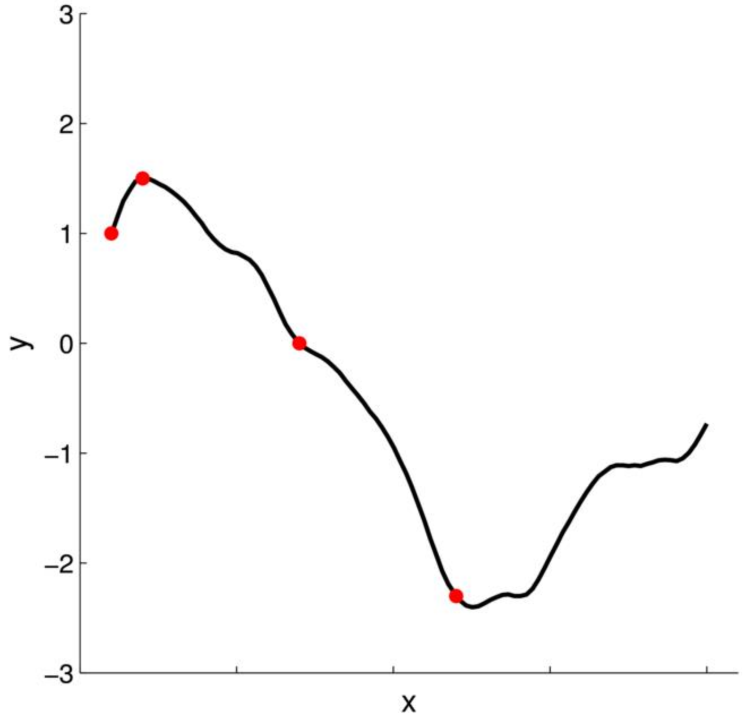

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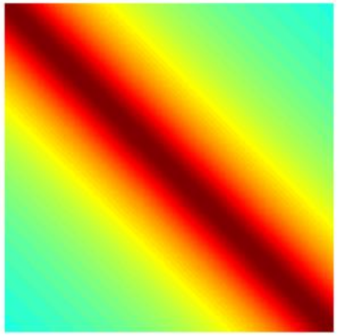

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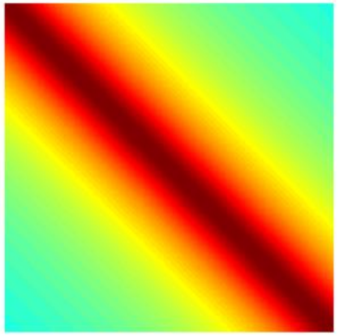

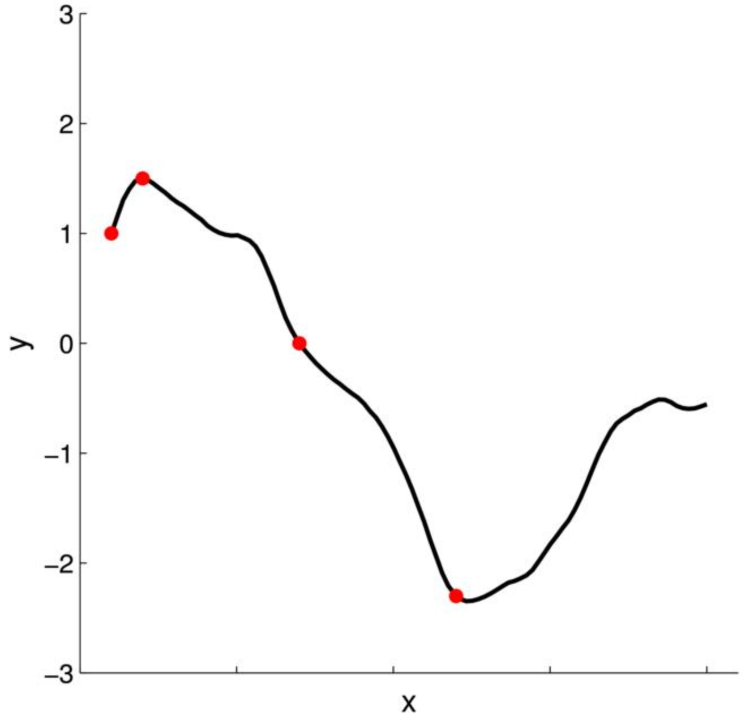

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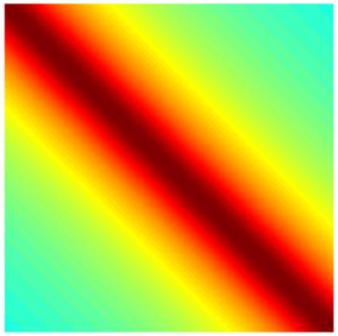

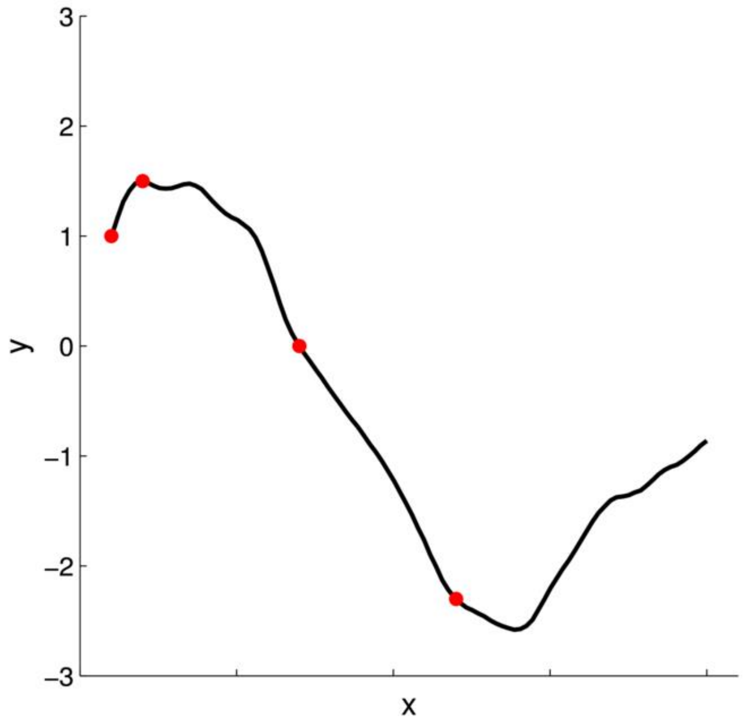

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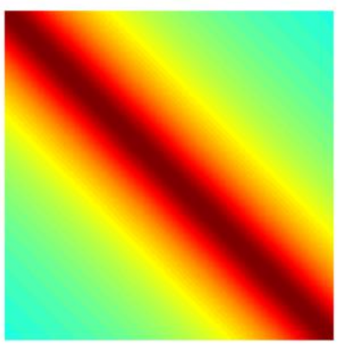

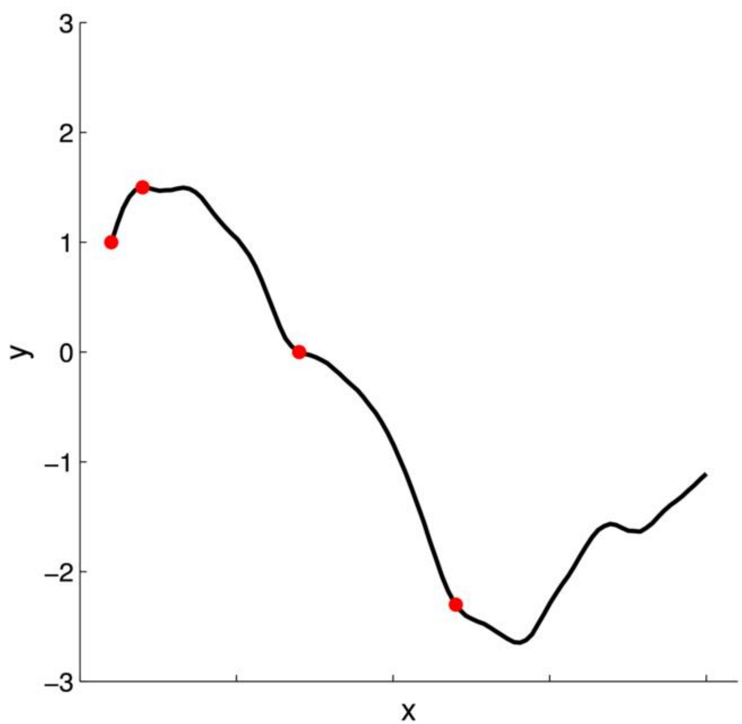

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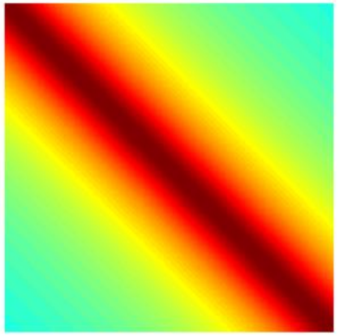
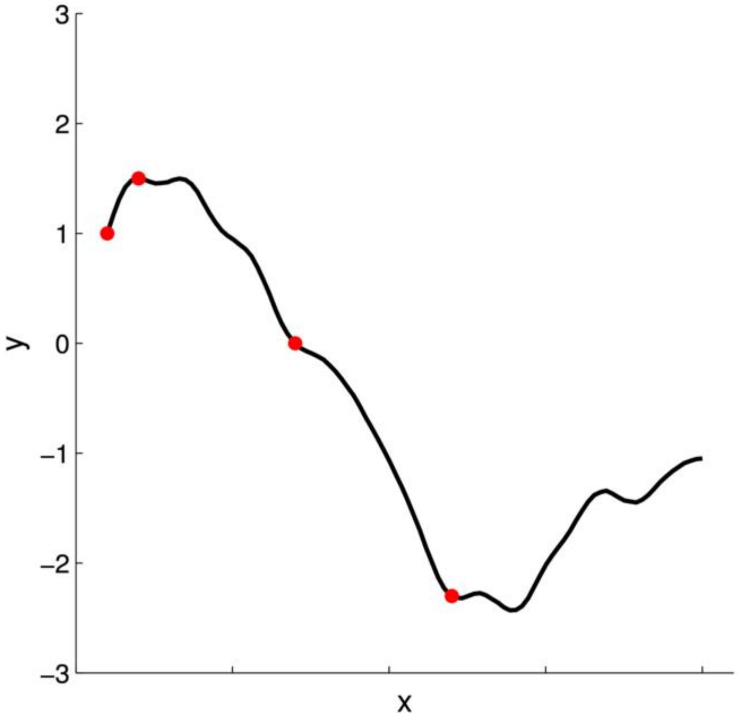
$\Sigma =$ 



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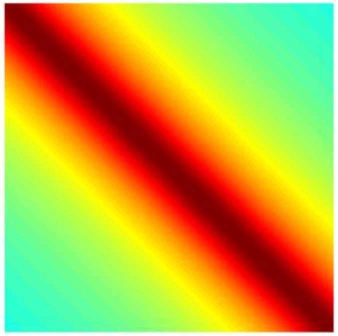

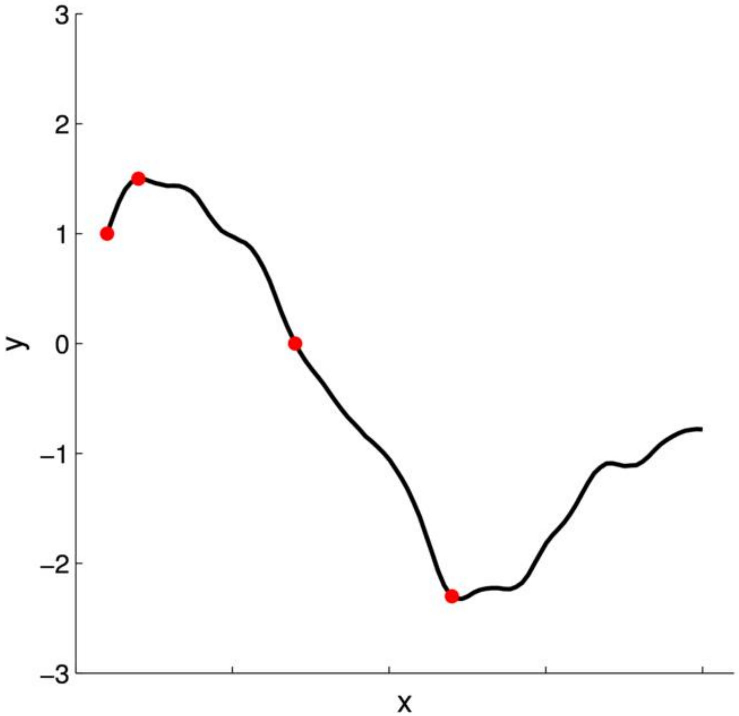

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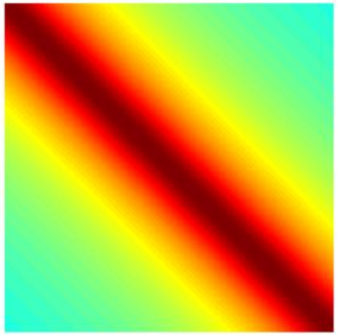
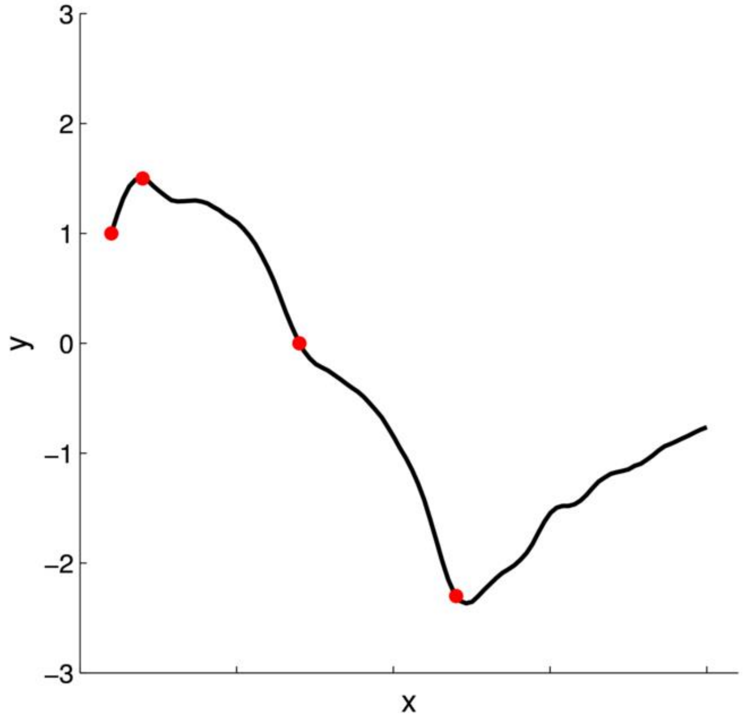
$\Sigma =$ 



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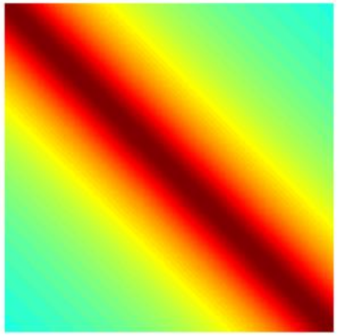
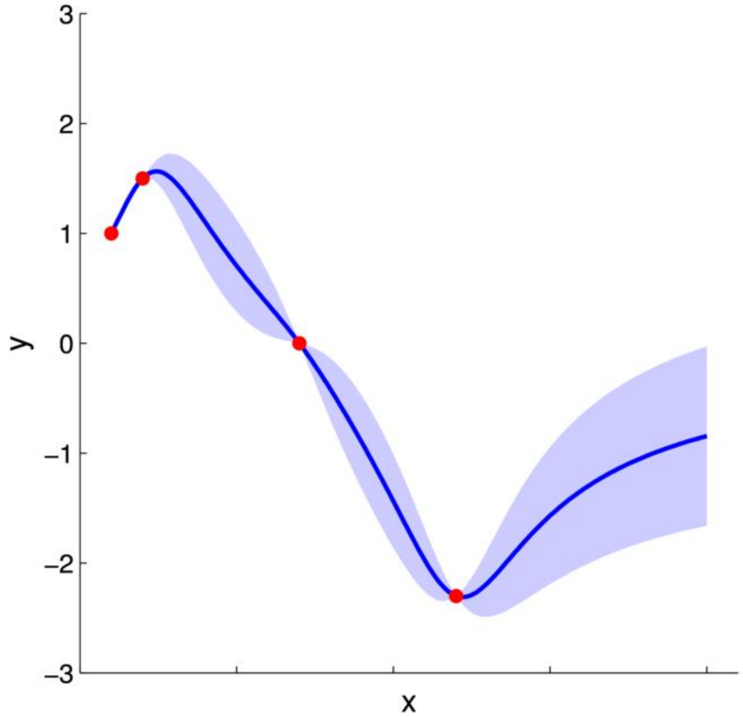
$\Sigma =$ 



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Periodic

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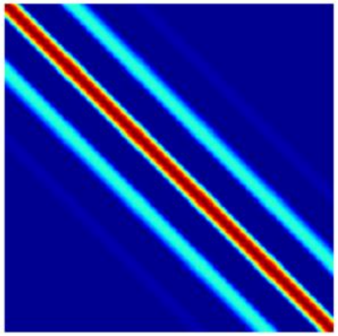
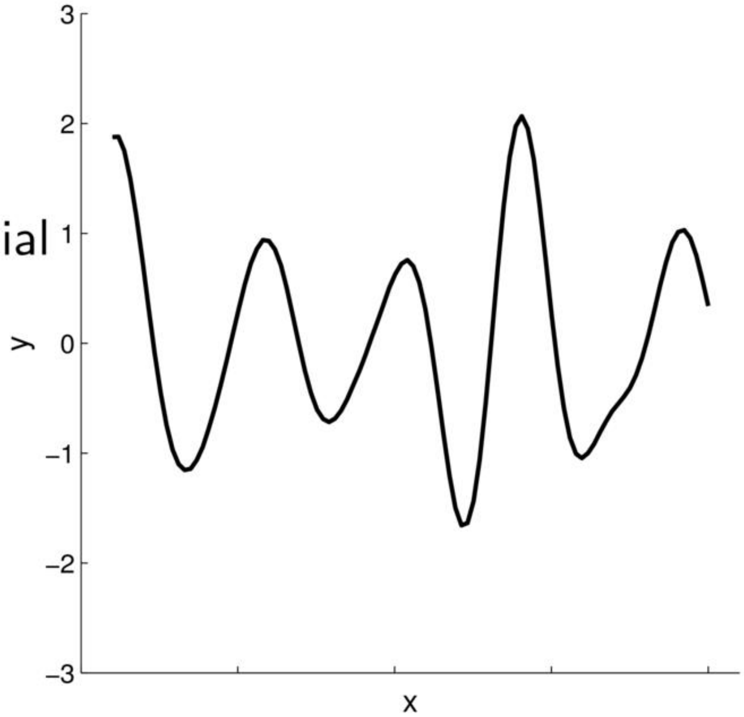
$\Sigma =$ 



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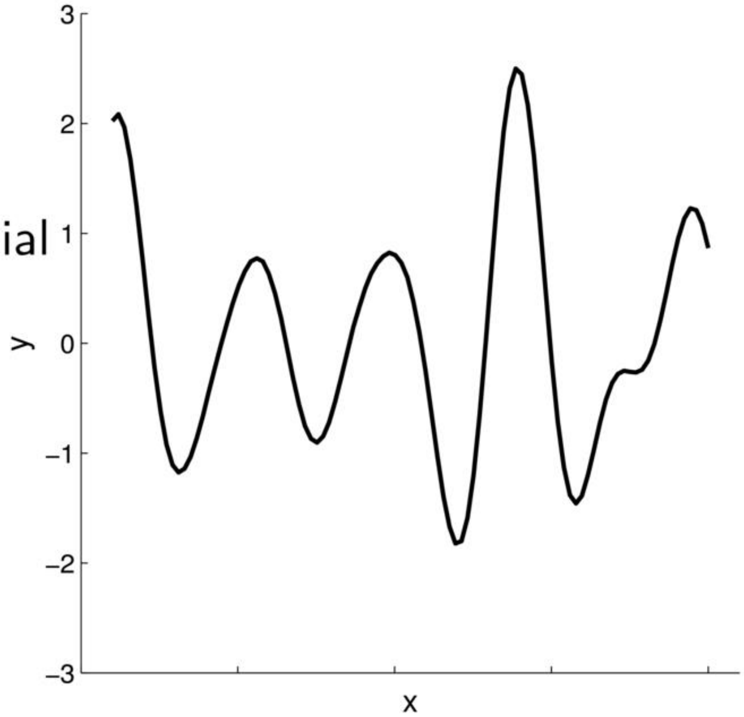
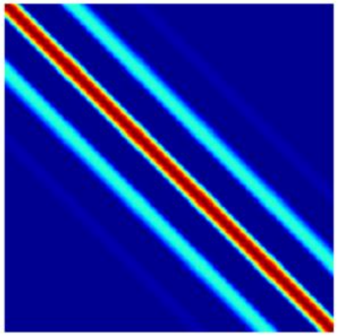


$\Sigma =$ 

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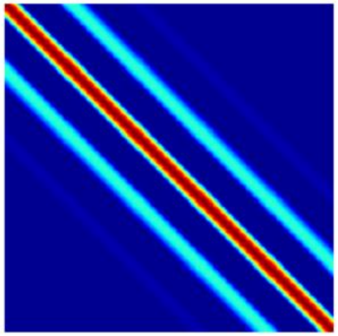

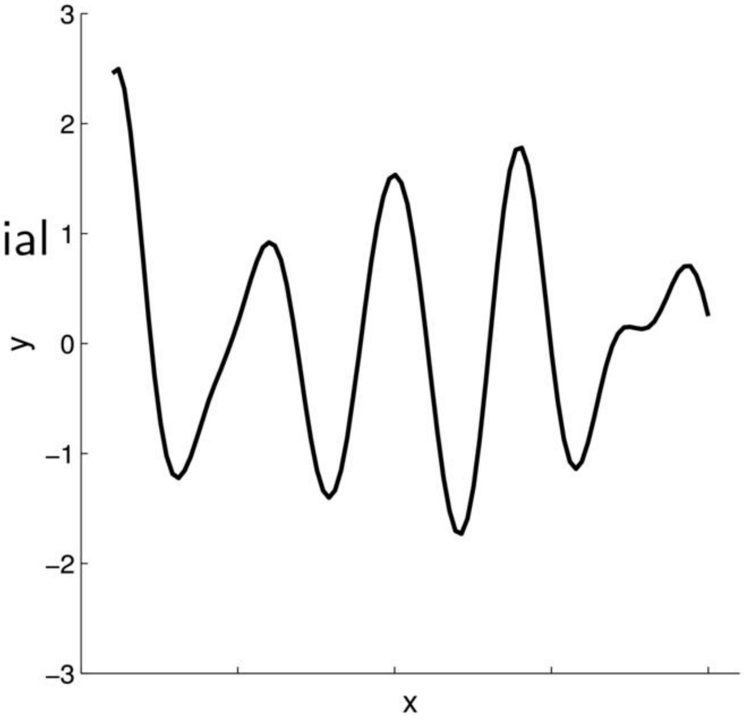

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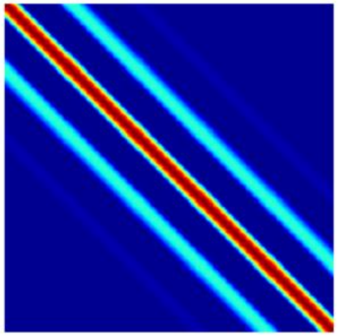

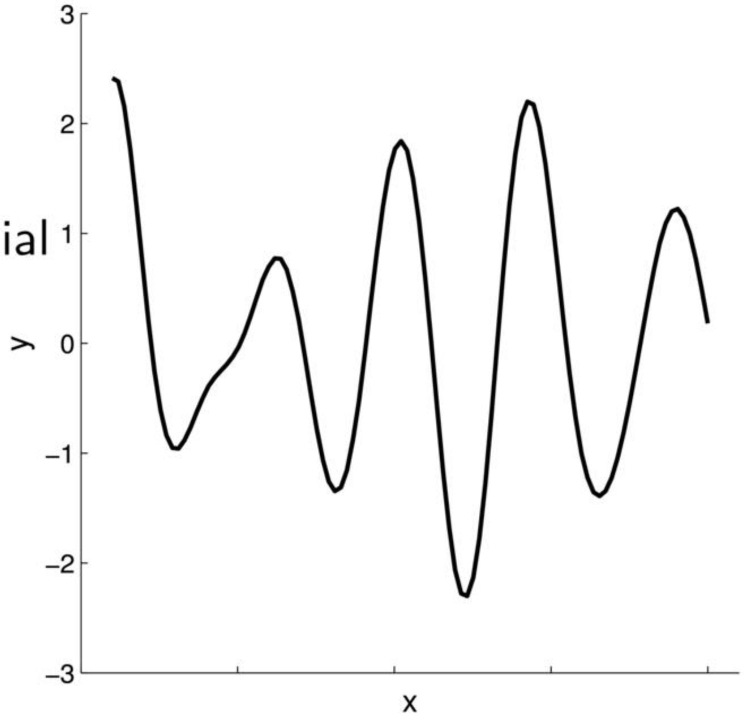

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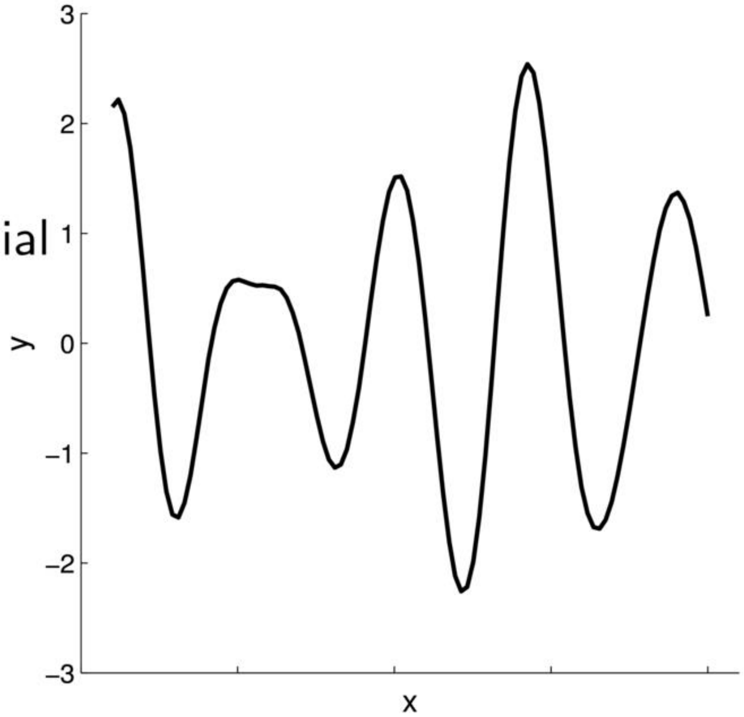
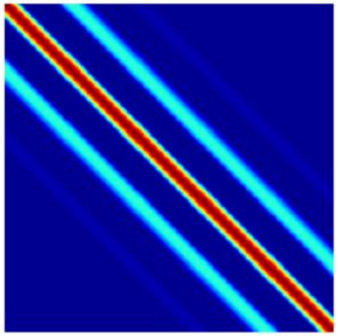


$\Sigma =$ 

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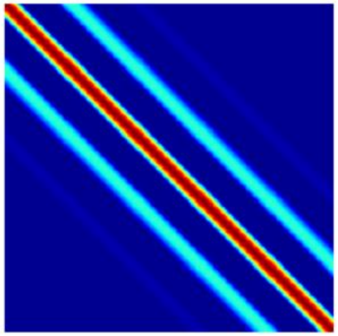
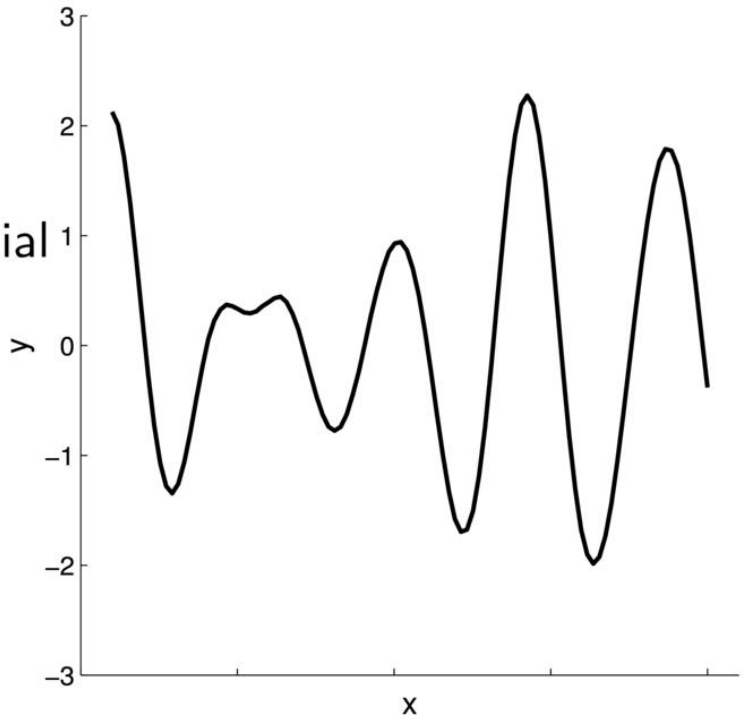
$\Sigma =$ 



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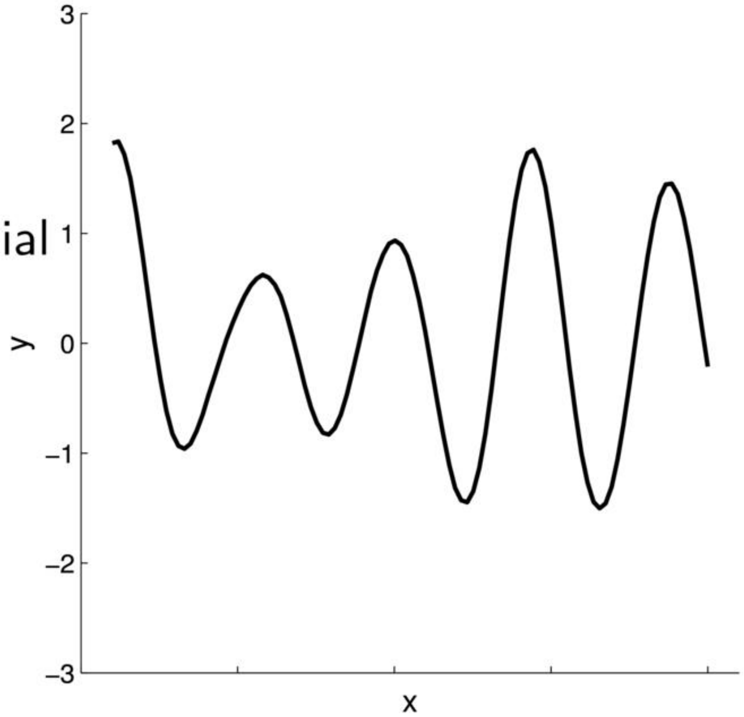
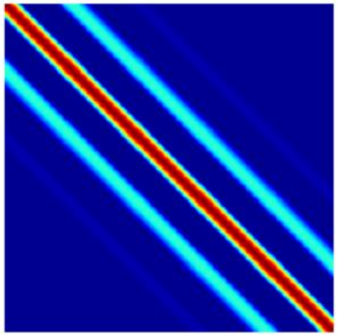


$\Sigma =$ 

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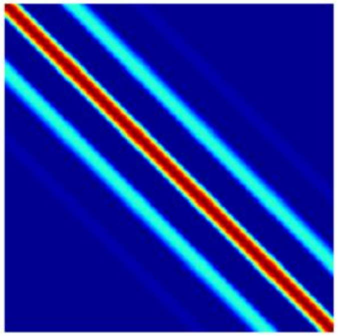

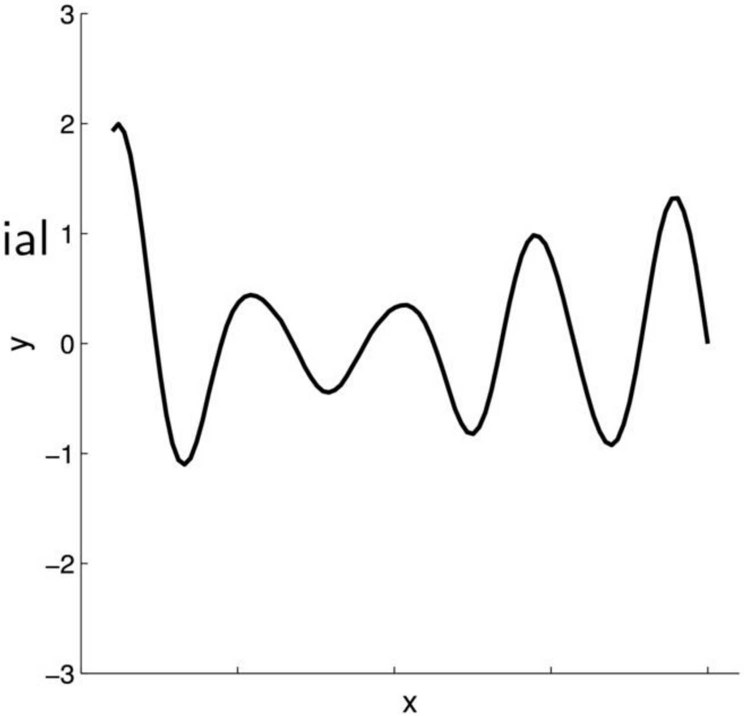

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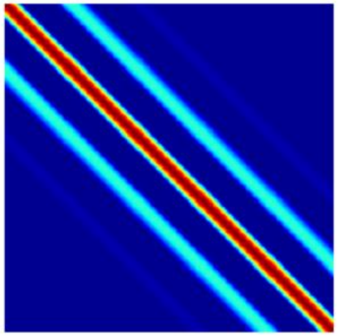

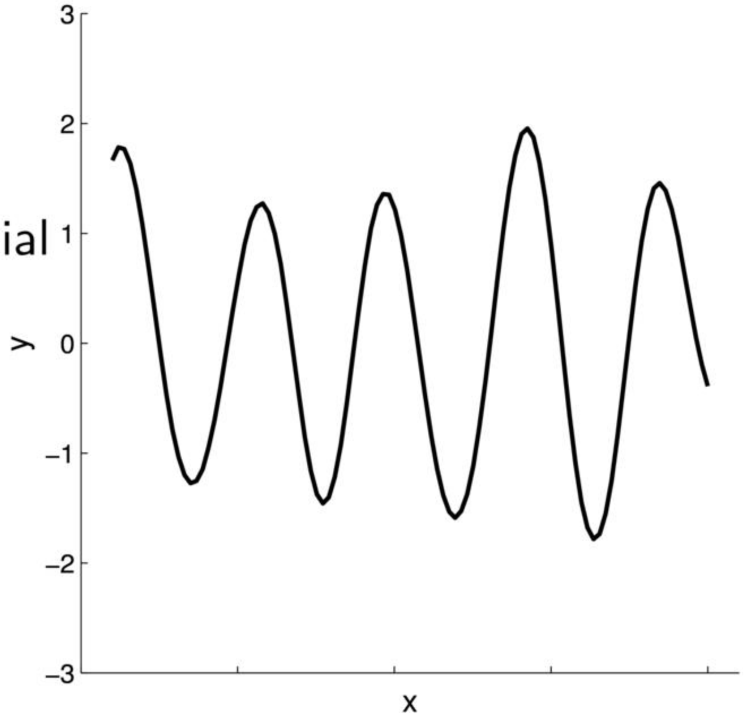

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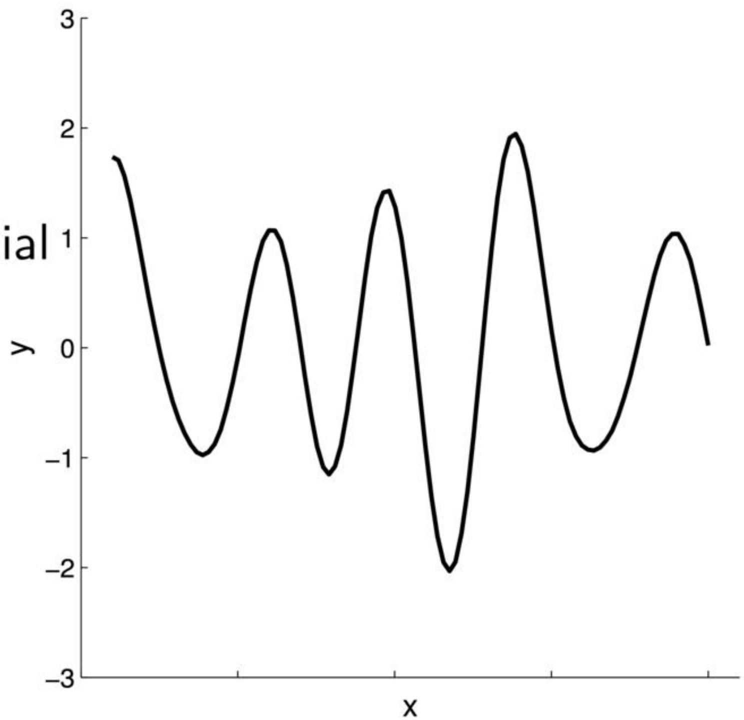

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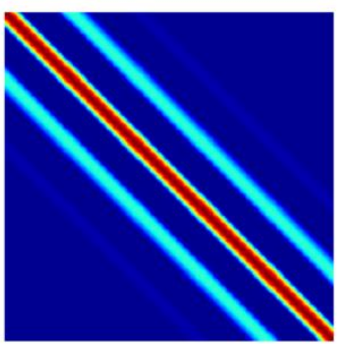

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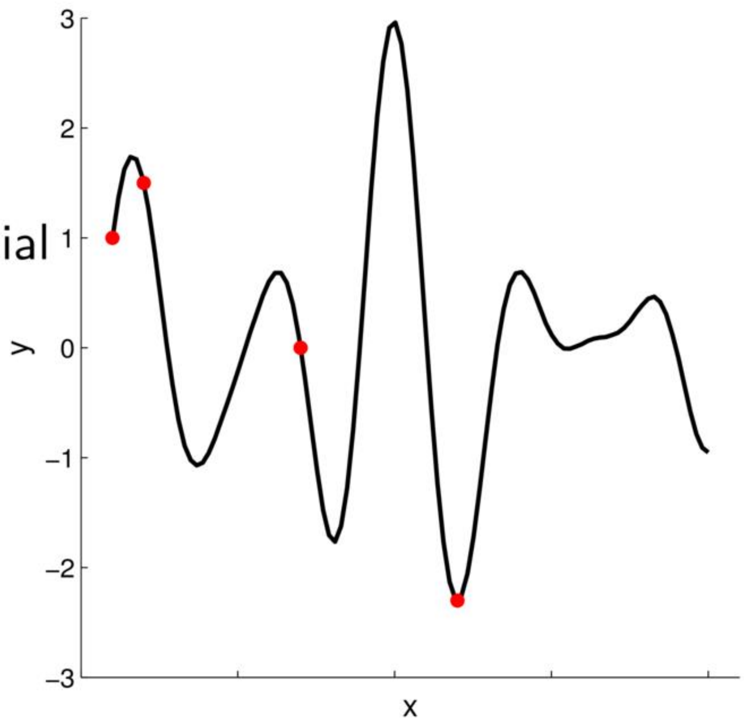
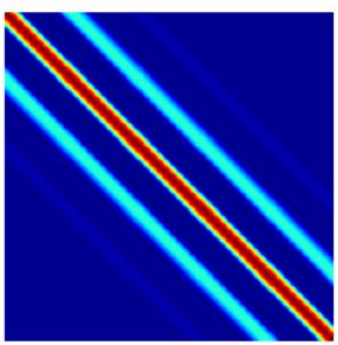


$\Sigma =$ 

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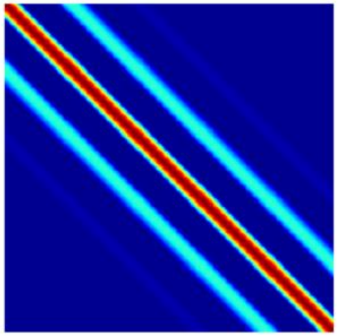
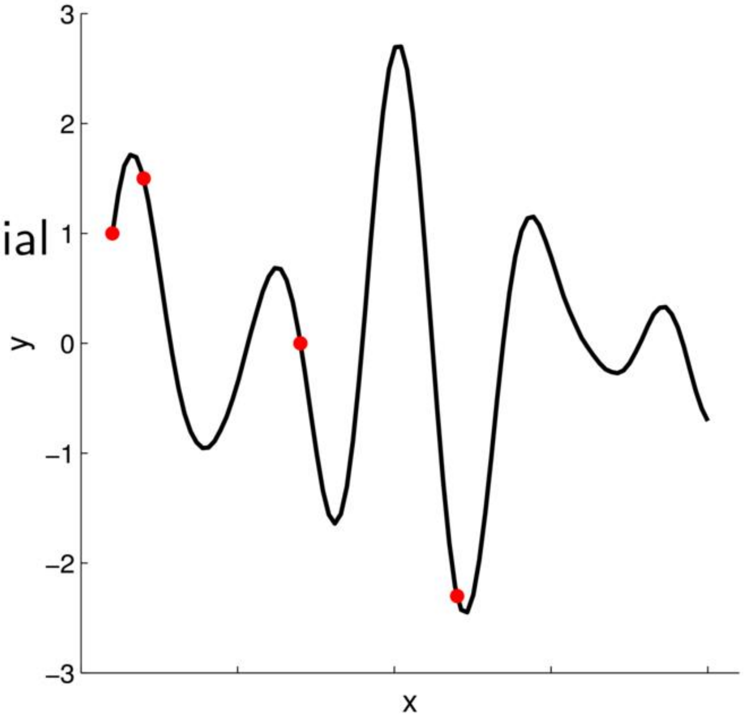
$\Sigma =$ 



What effect do the Hyper-parameter have?

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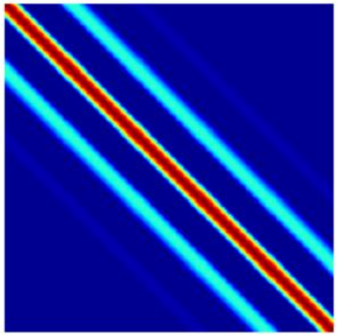

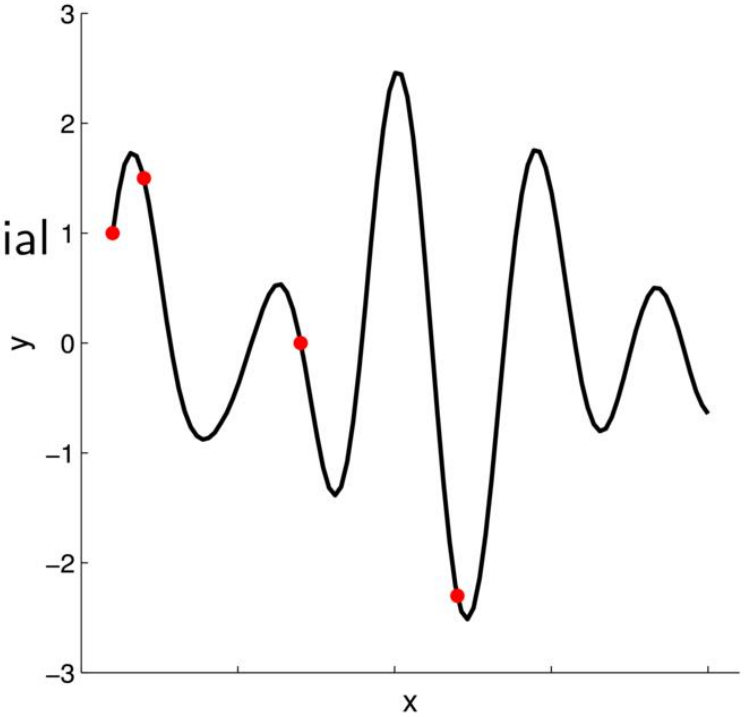

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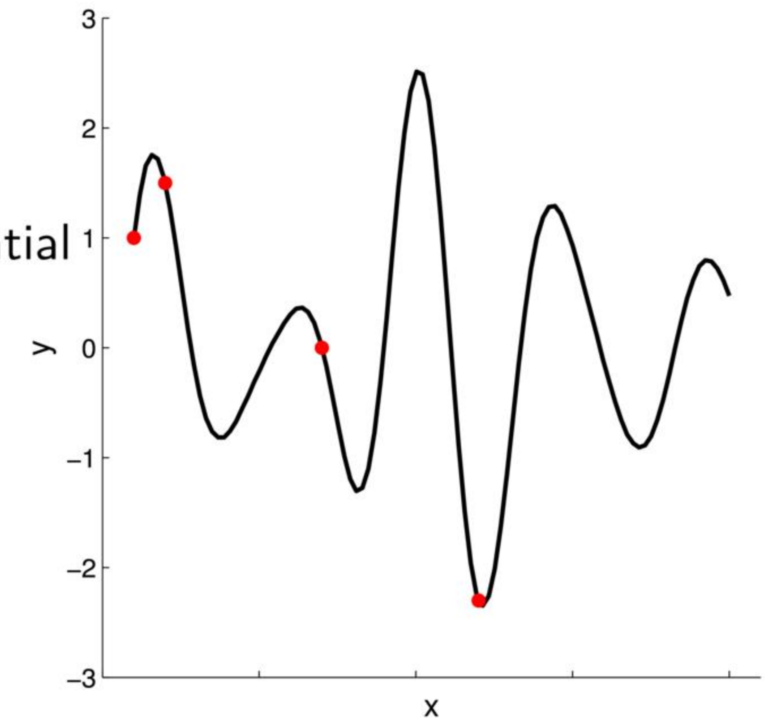

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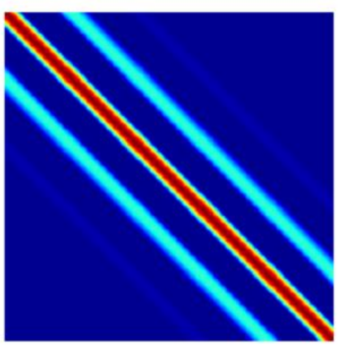

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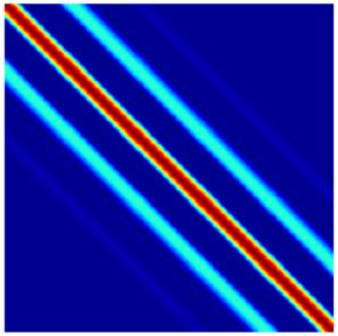
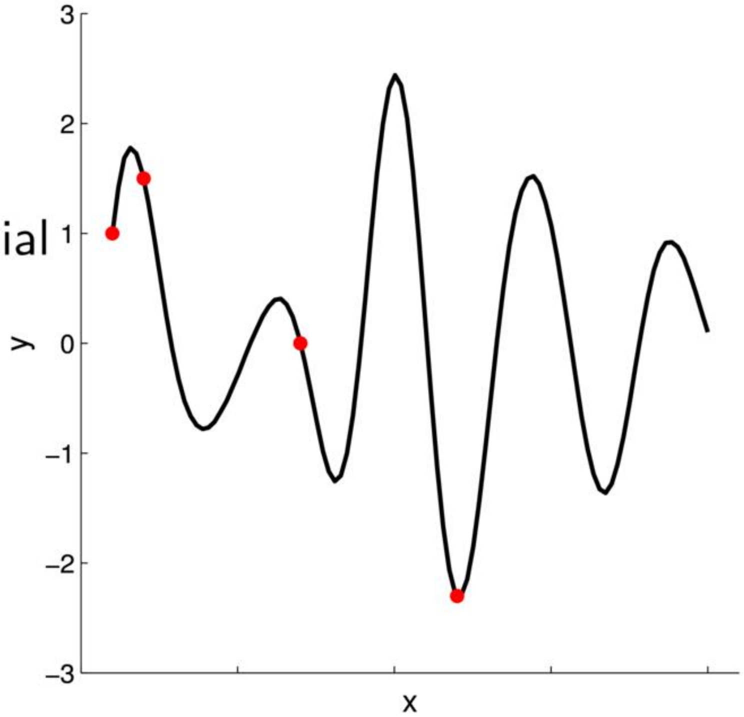
$\Sigma =$ 



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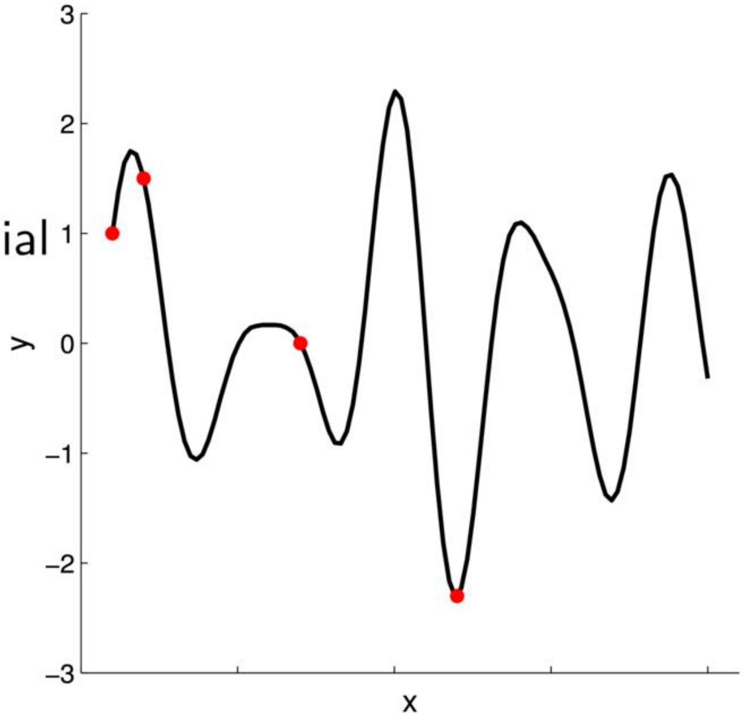
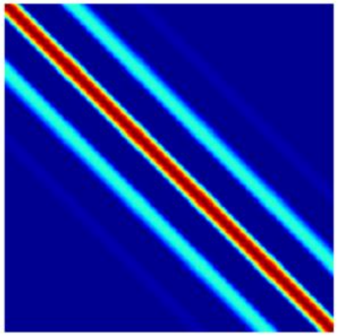


$\Sigma =$ 

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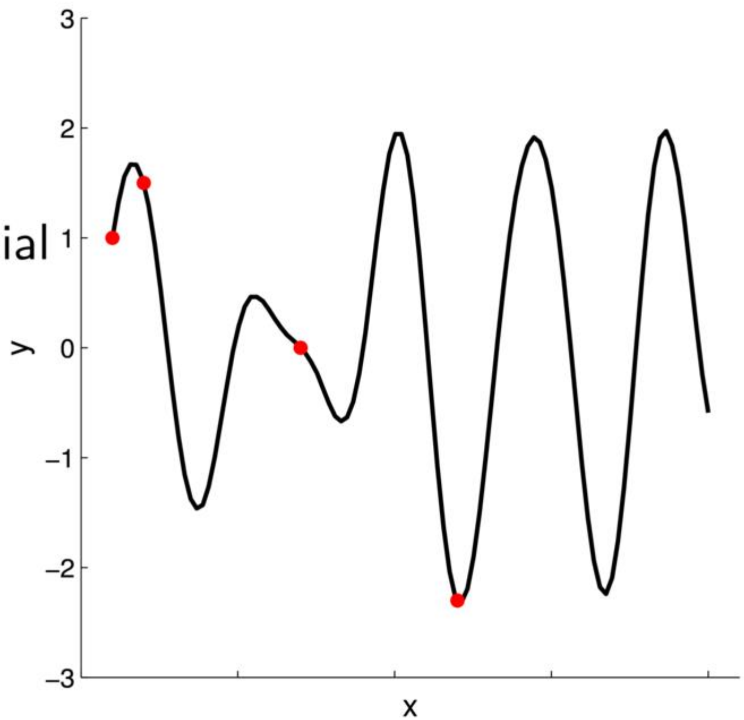

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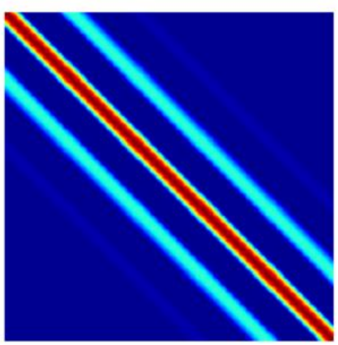

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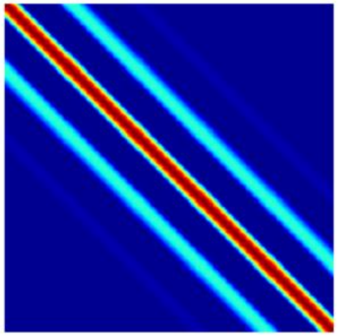
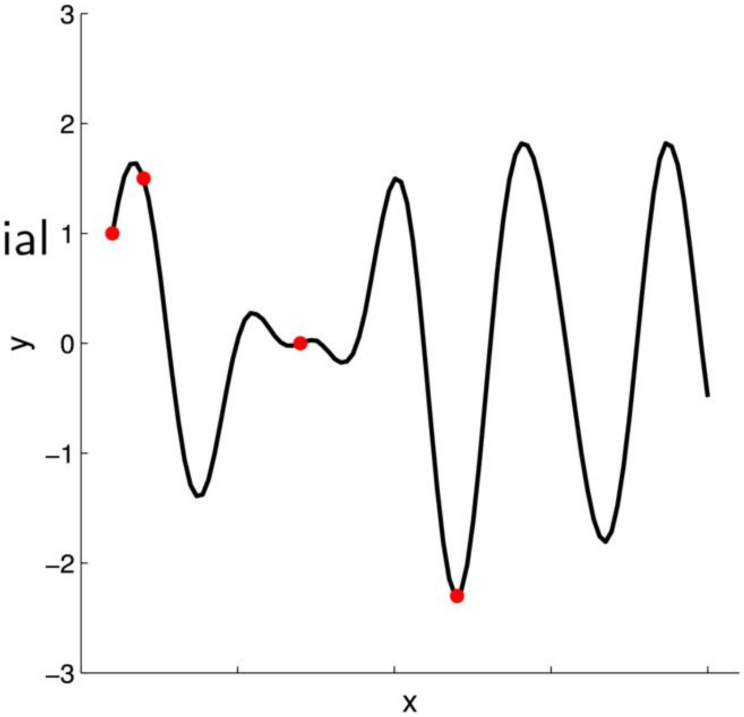
$\Sigma =$ 



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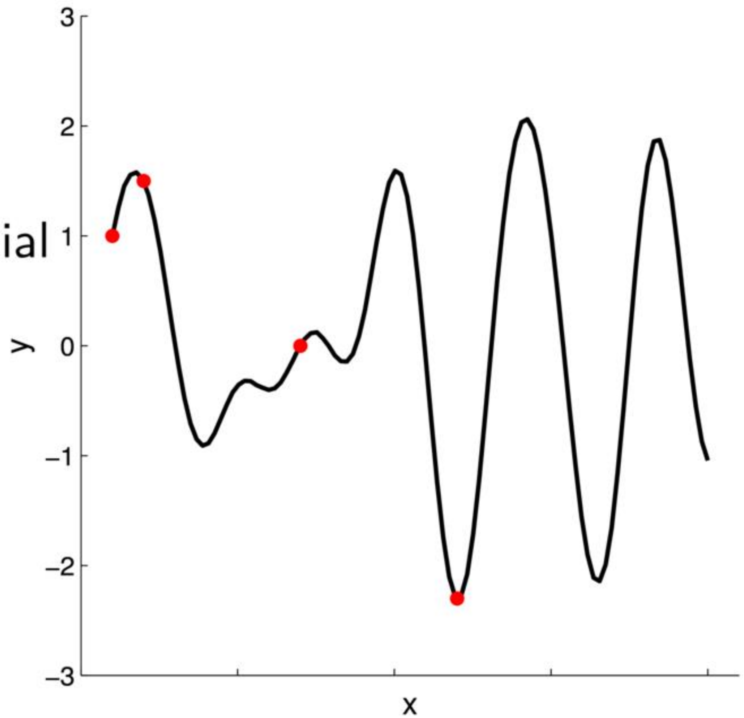

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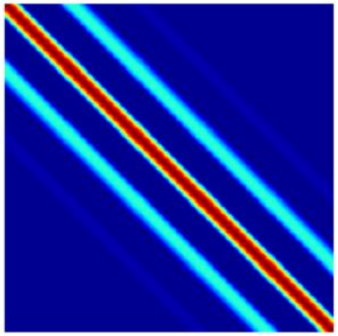

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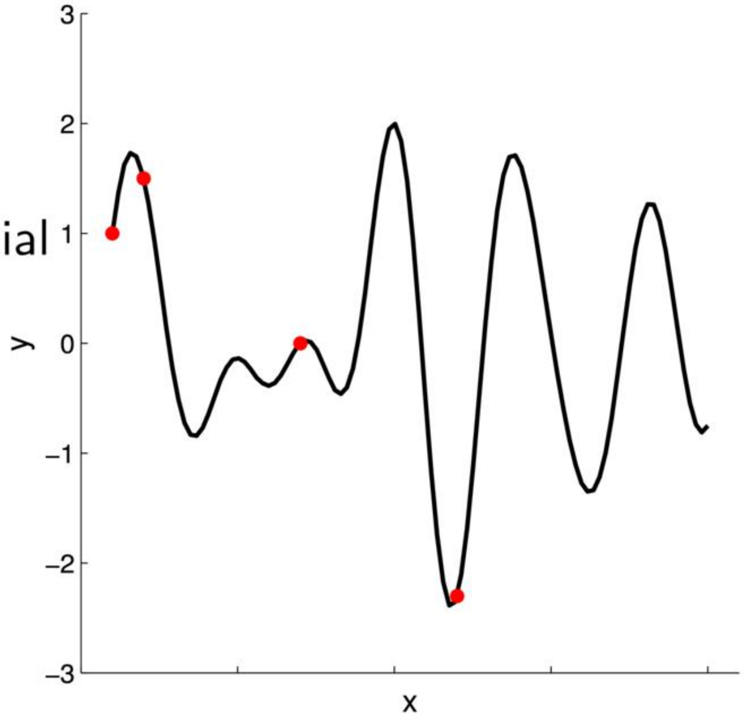
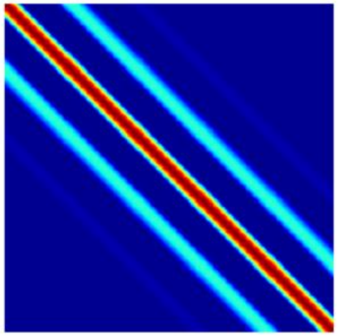


$\Sigma =$ 

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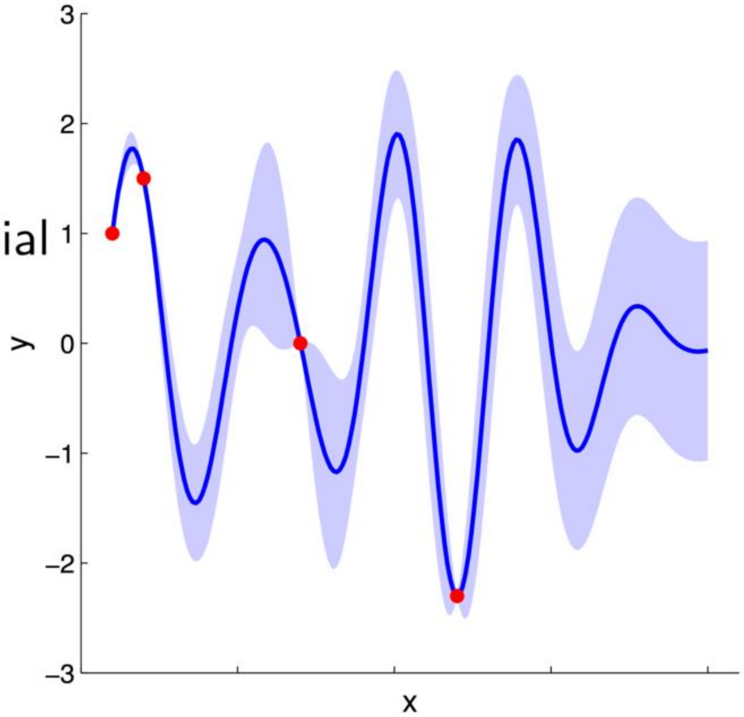
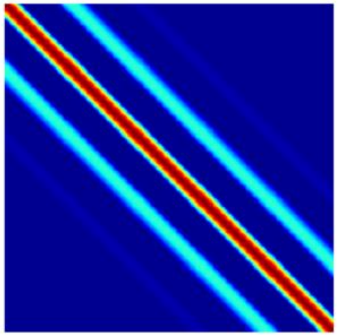
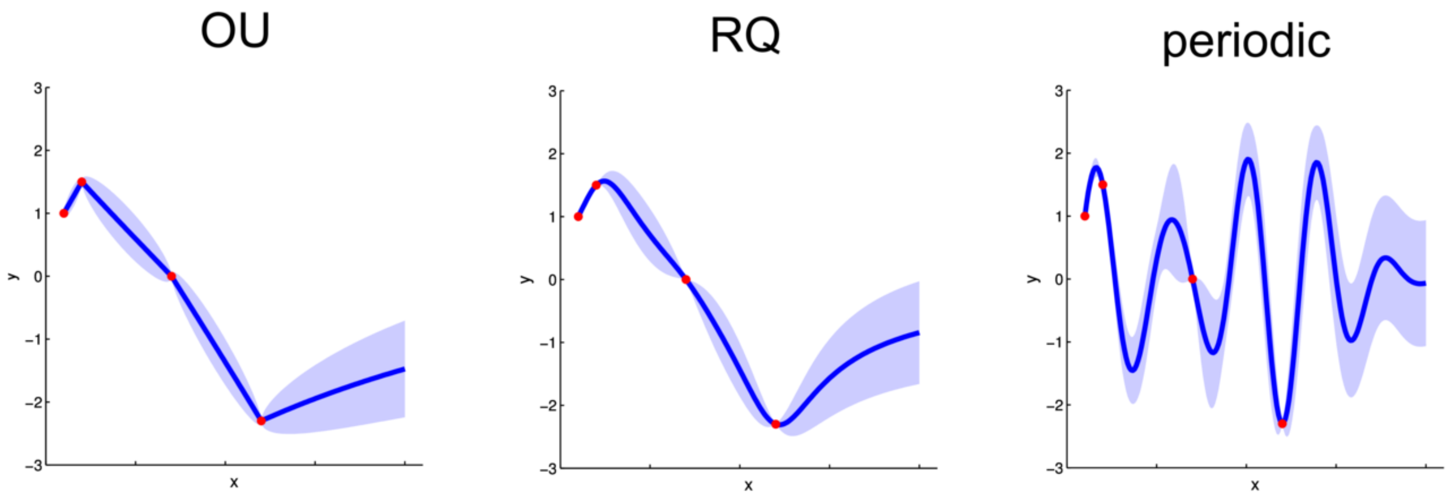


$\Sigma =$ 

The Covariance Function has a Large Effect



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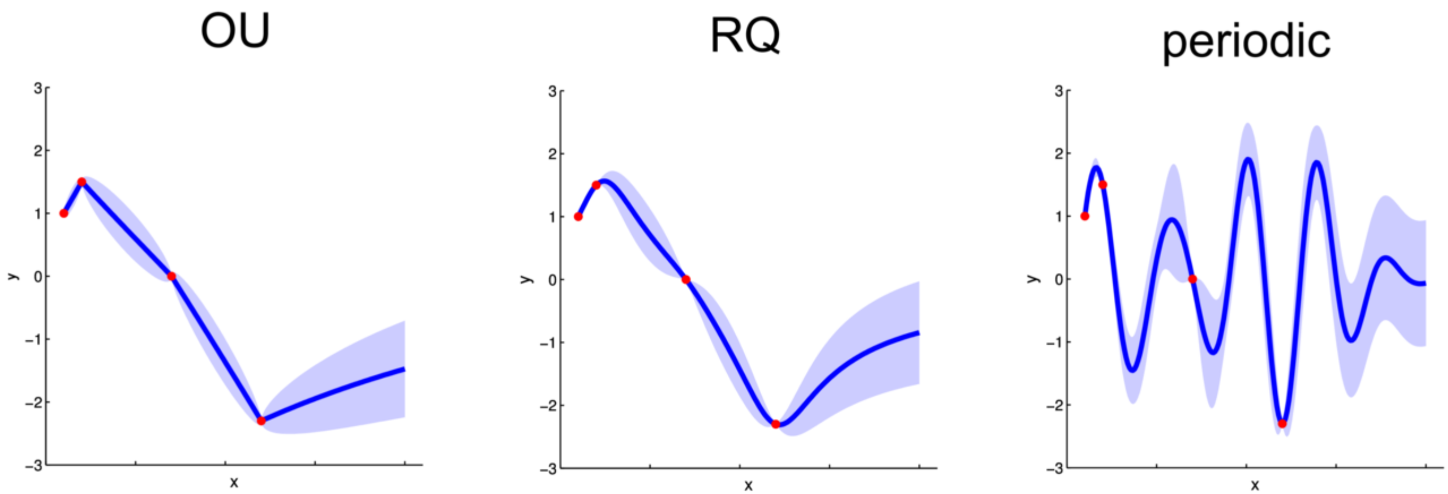

Bayesian model comparison:

$$p(M|\mathbf{y}_{1:N}) = \frac{p(\mathbf{y}_{1:N}|M)p(M)}{\sum_{M'} p(\mathbf{y}_{1:N}|M')p(M')}$$

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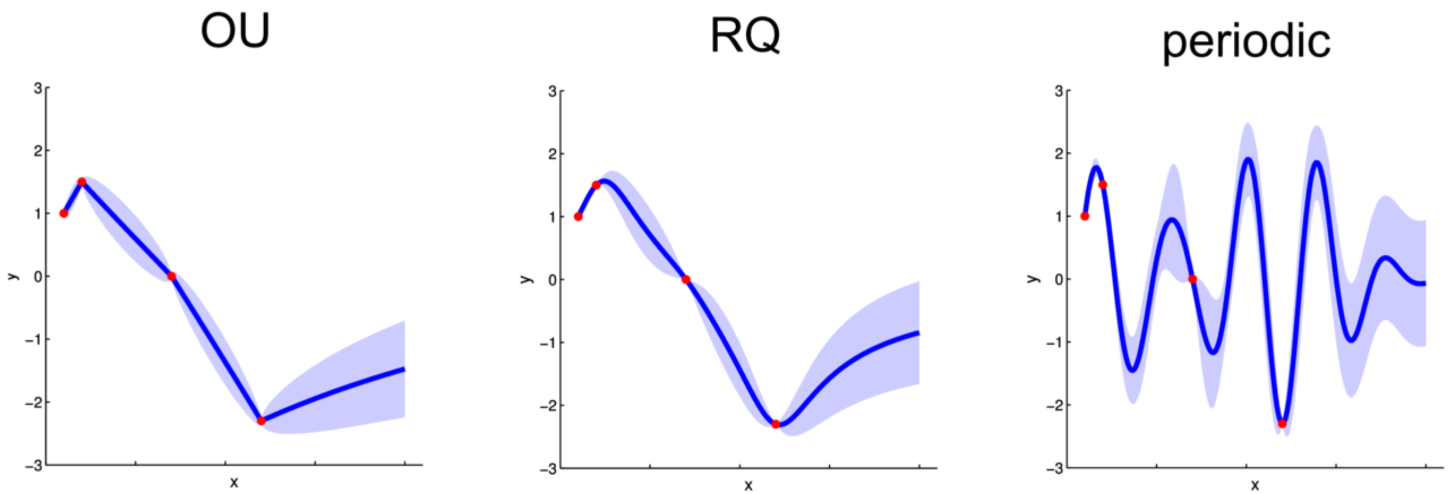

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prior over models

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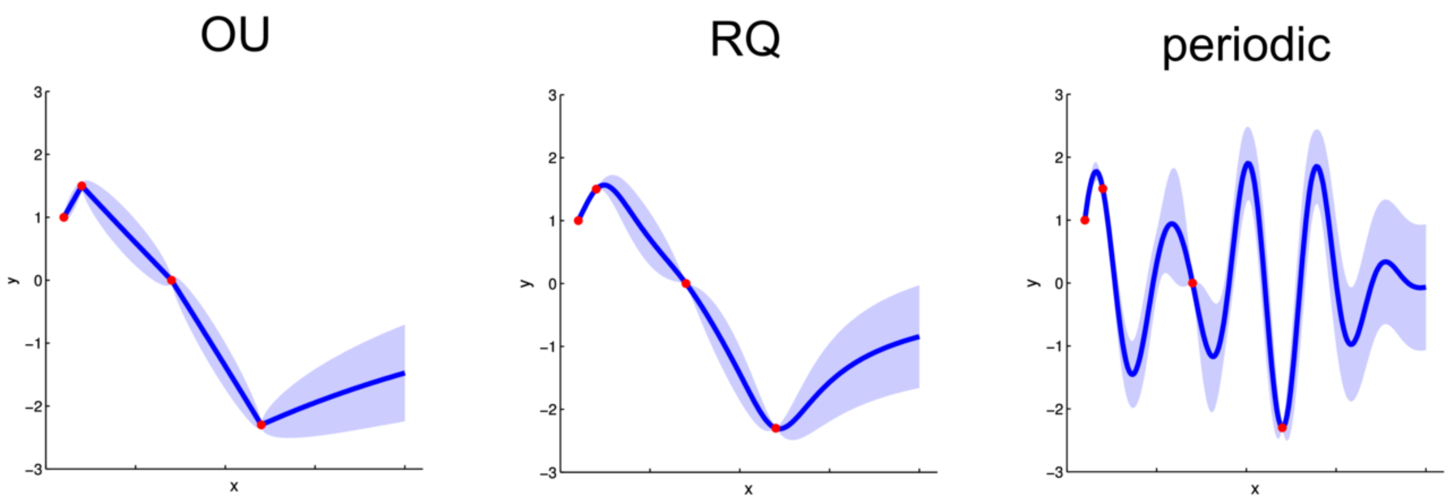

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prior over models

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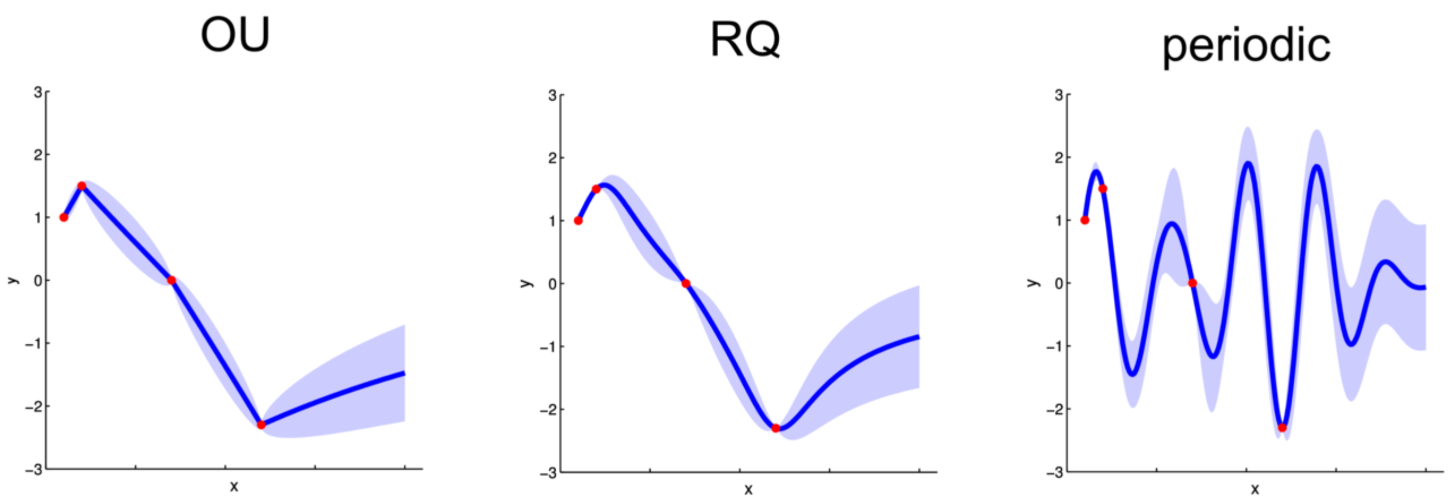

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Health warnings: Hard to compute (need approximations)
Often results are very sensitive to the priors $p(\theta|M)$