

DS-GA 3001.008 Modelling time series data

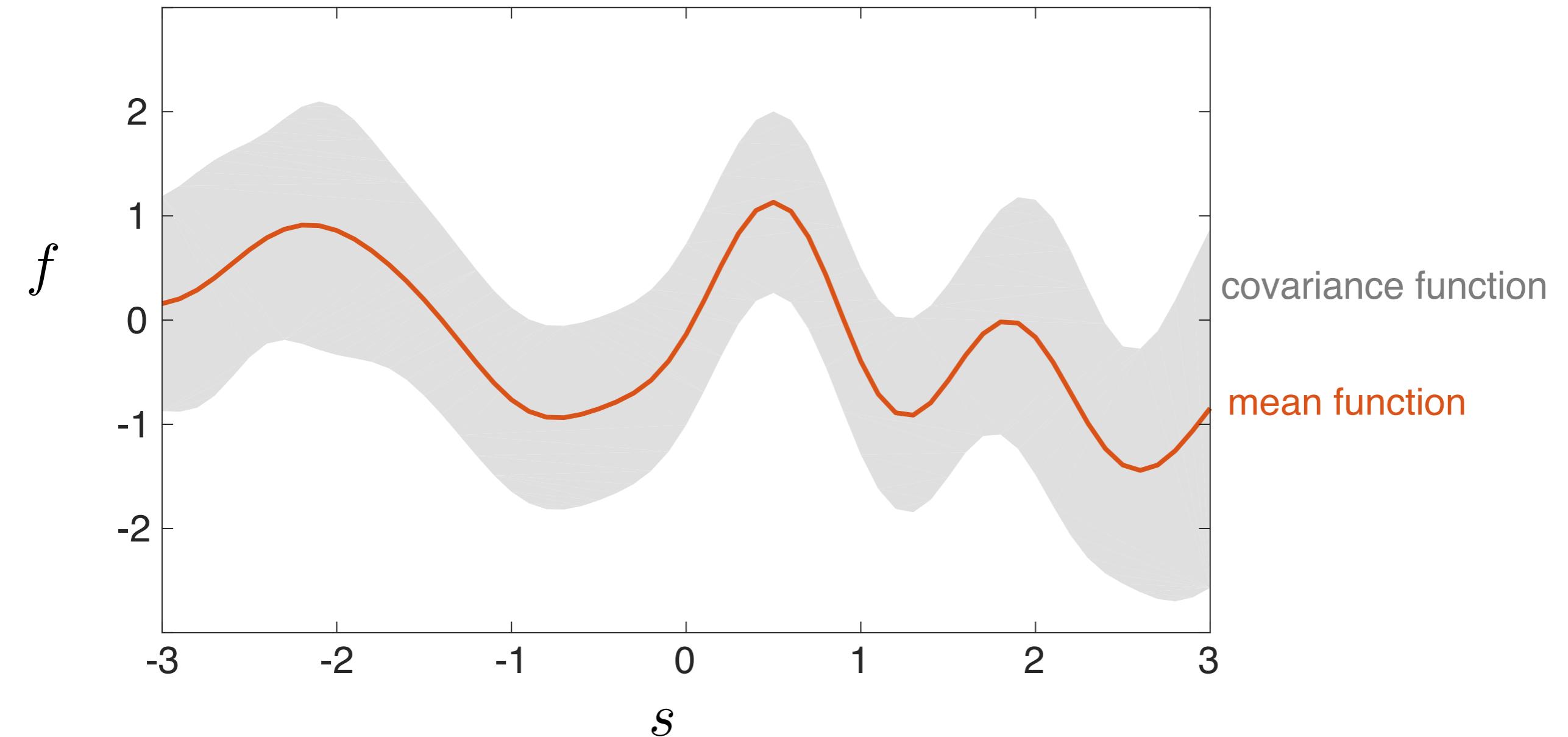
L9. An intro to Gaussian Processes

Instructor: Cristina Savin

NYU, CNS & CDS

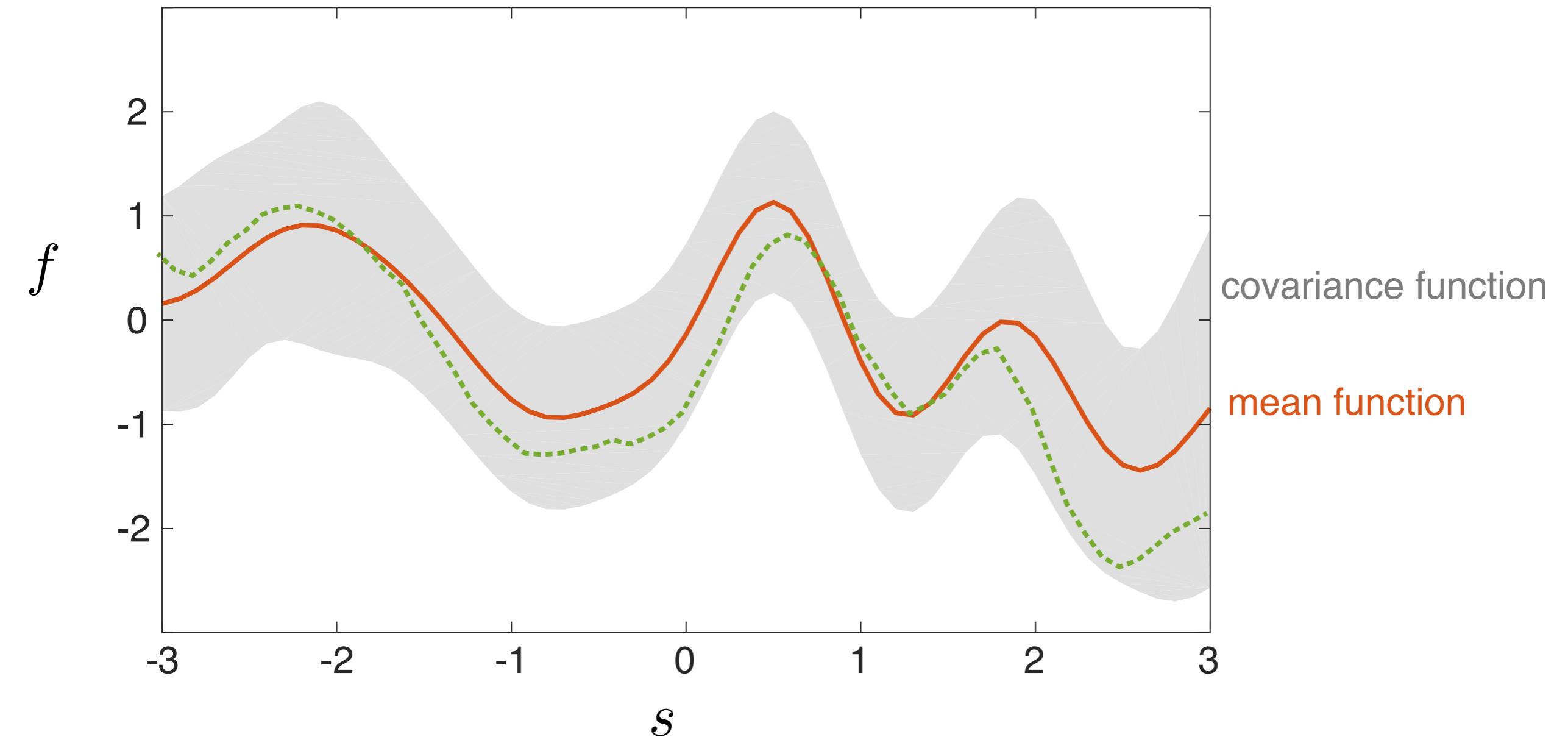
Probabilistic inference with functions

$$f \sim \text{GP} (f; \mu(s), k(s_1, s_2))$$



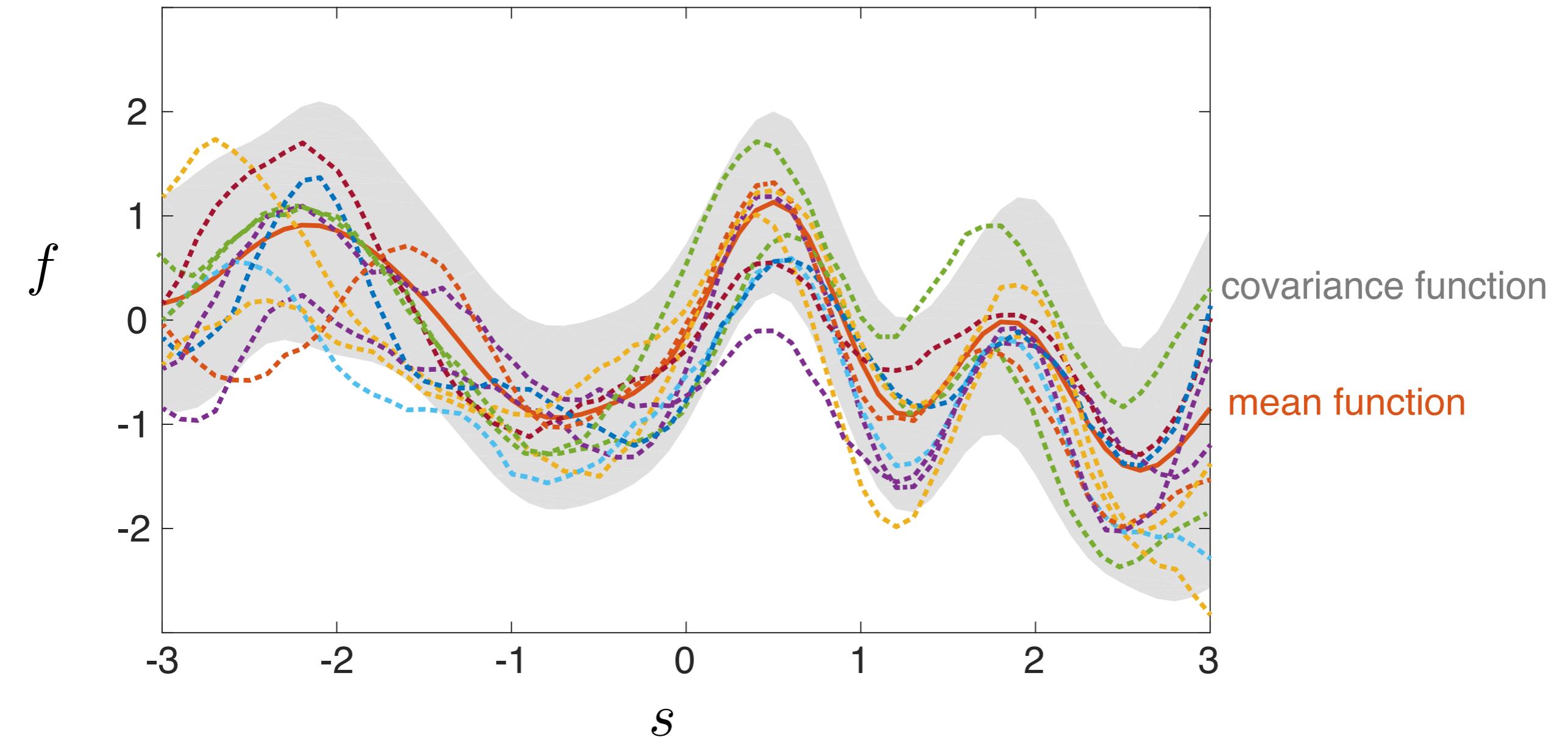
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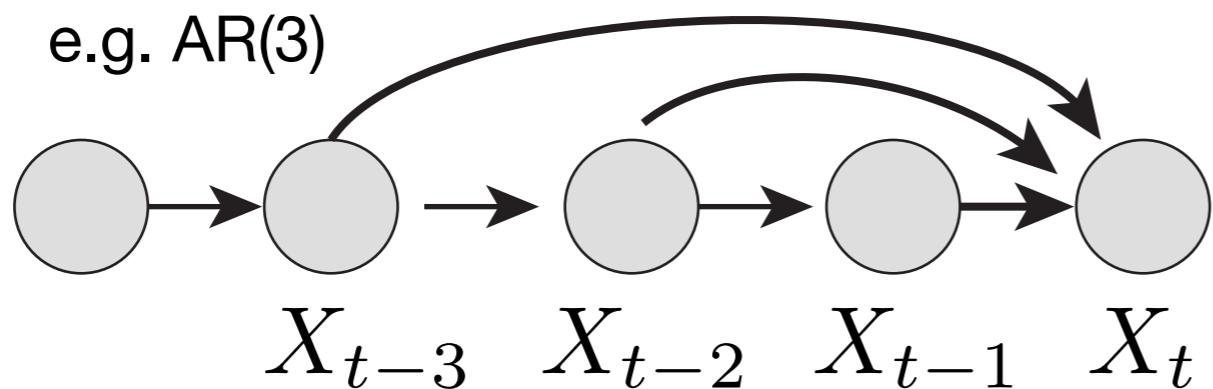
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Big picture

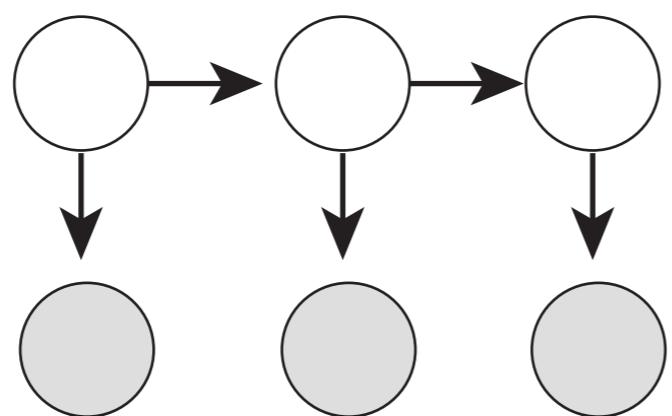
ARIMA: directly model data statistics



simple dependencies

linear prediction

Latent state models: introduce latent variables



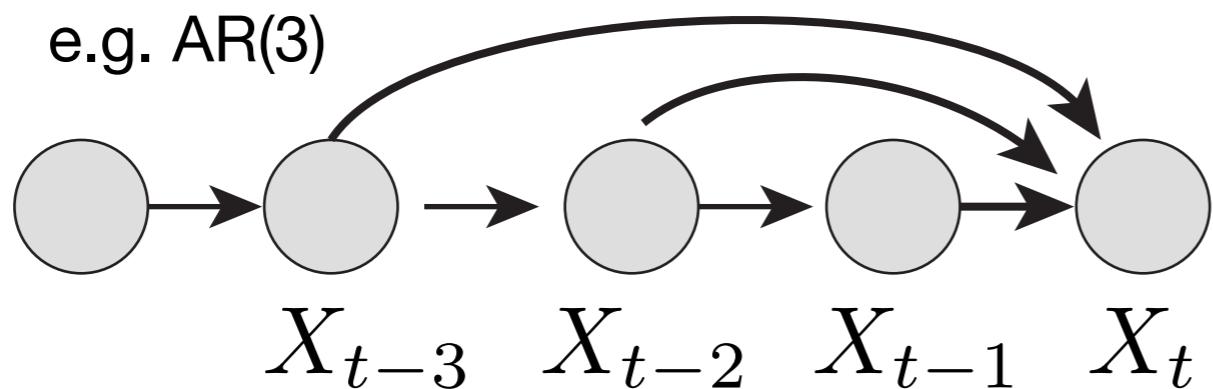
more complex dependencies

Markov dynamics in latent space

more complicated prediction

Big picture

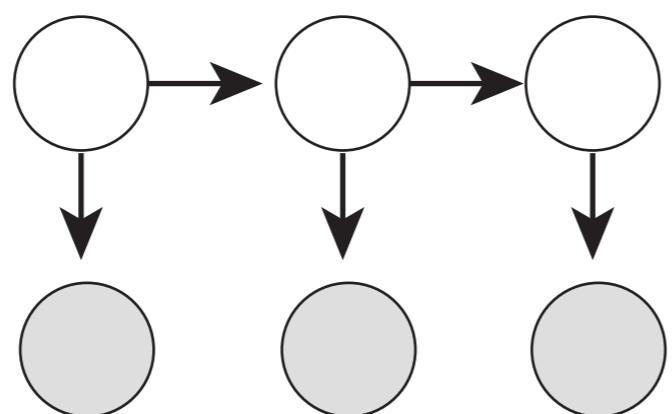
ARIMA: directly model data statistics



simple dependencies
linear prediction

GP: complex functional dependencies

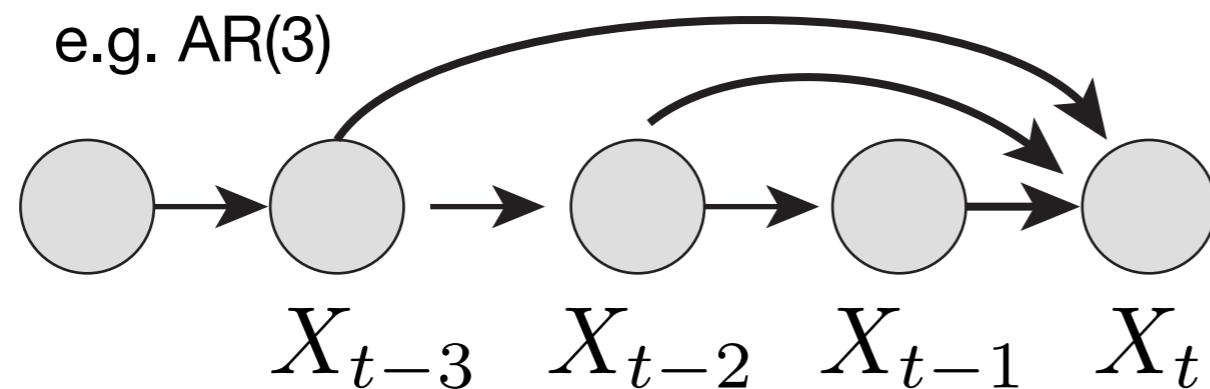
Latent state models: introduce latent variables



more complex dependencies
Markov dynamics in latent space
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Big picture

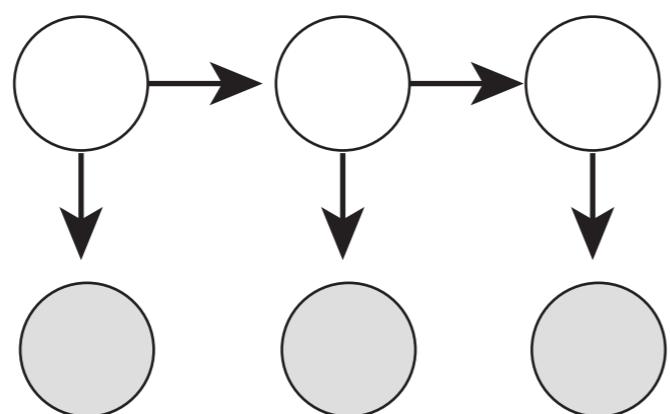
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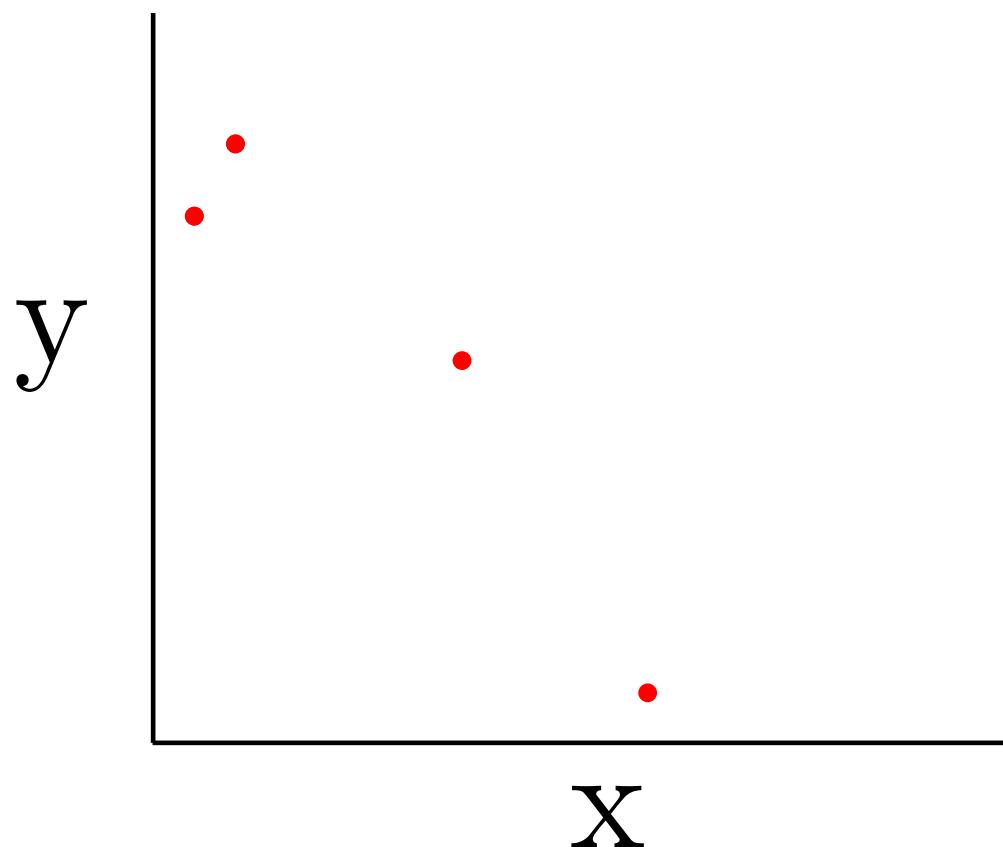
Latent state models: introduce latent variables



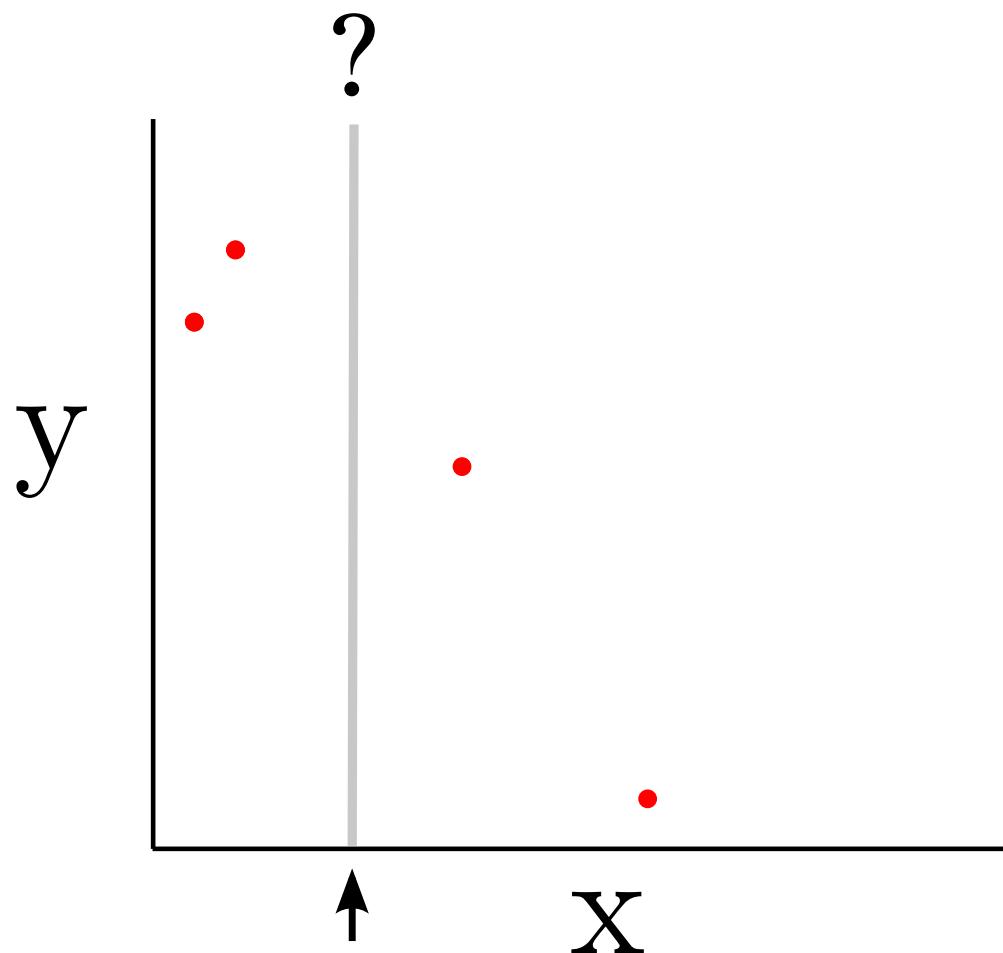
more complex dependencies
Markov dynamics in latent space
more complicated prediction

GP: complex latent dynamics

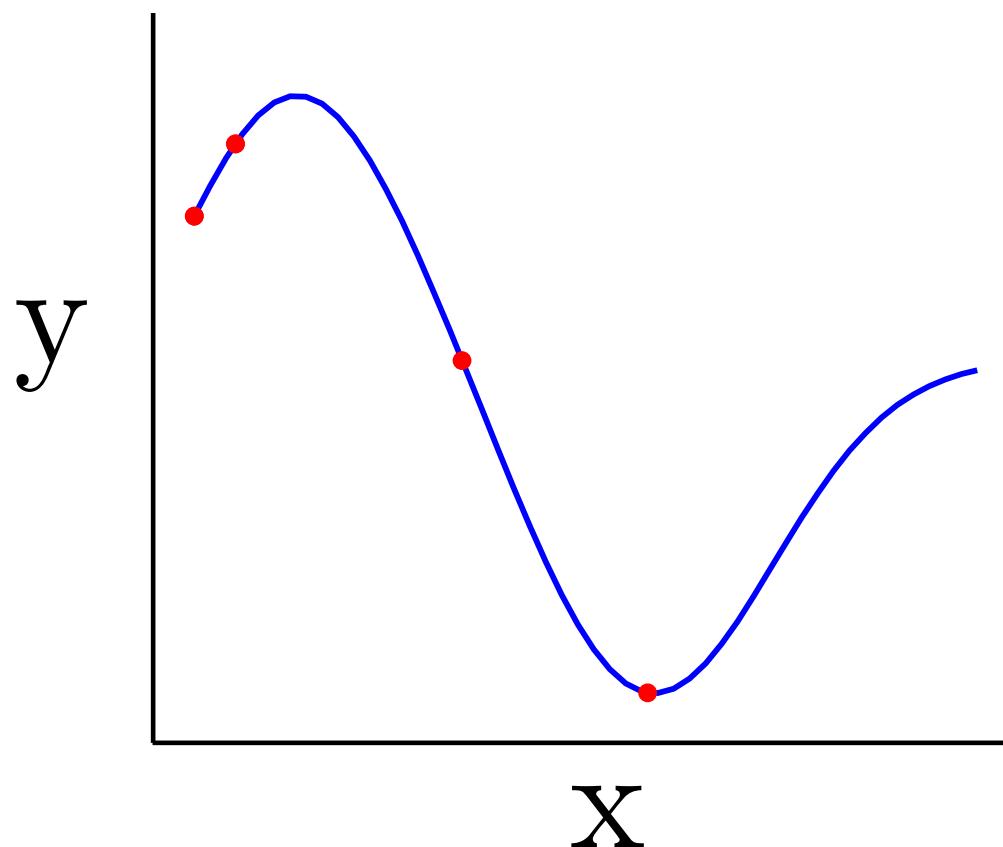
Motivation: non-linear regression



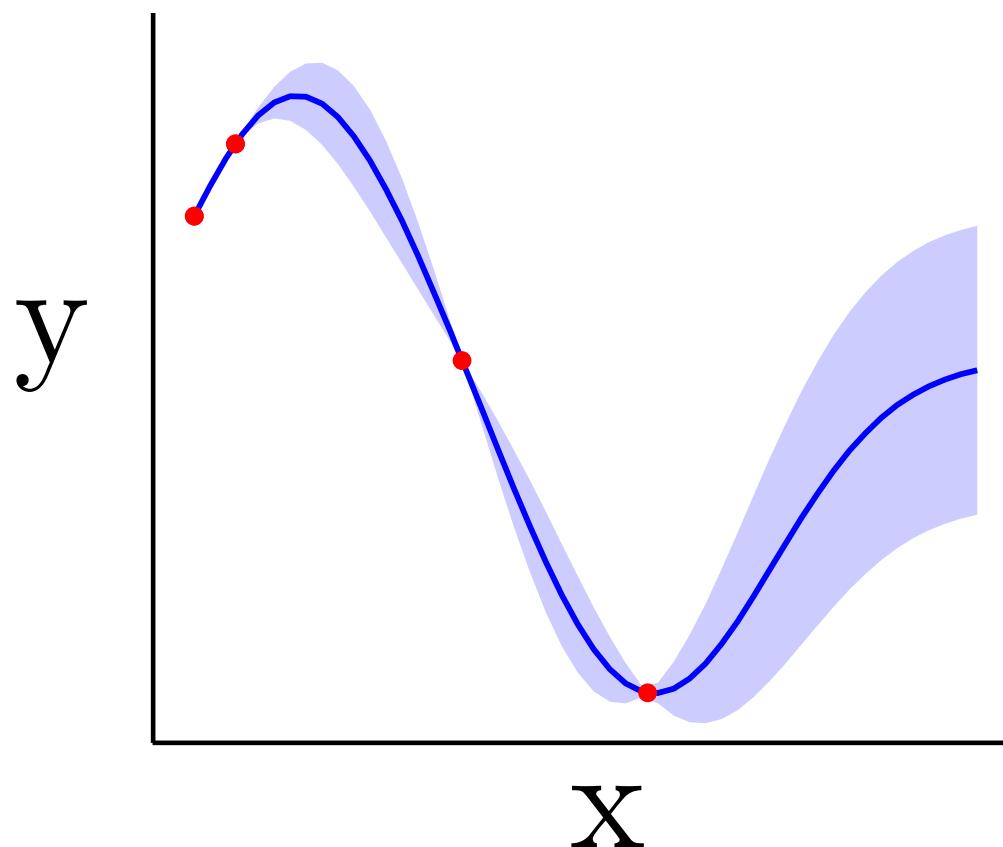
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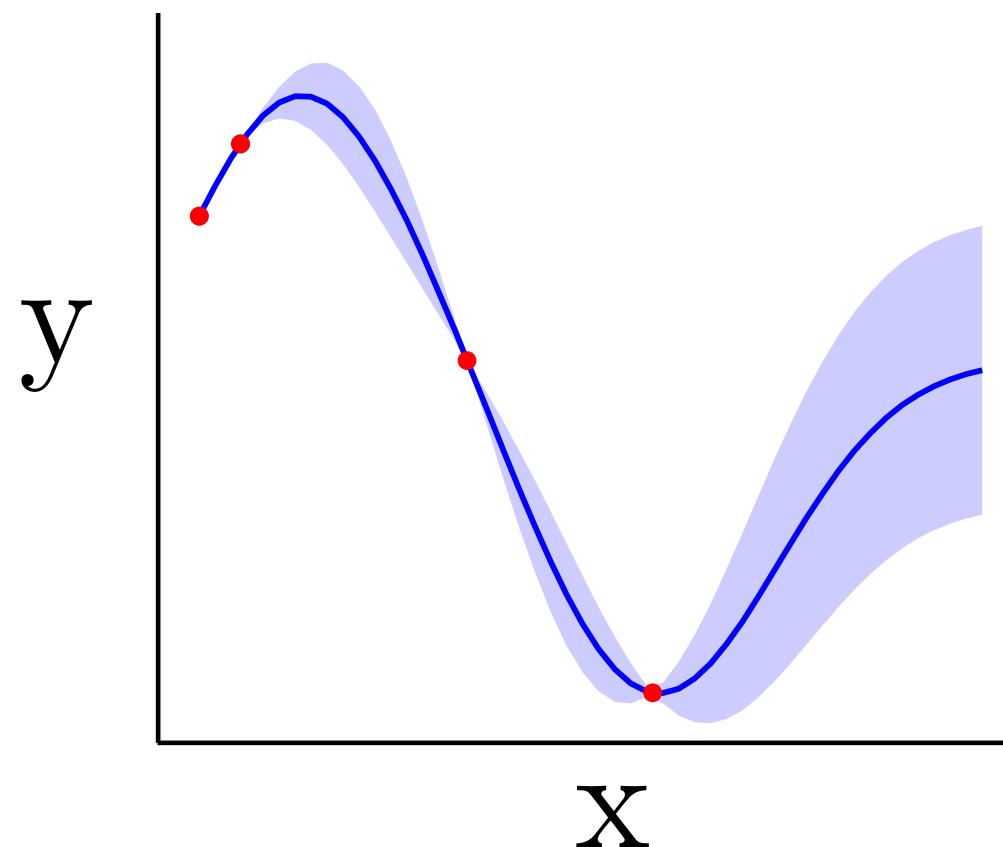


Motivation: non-linear regression



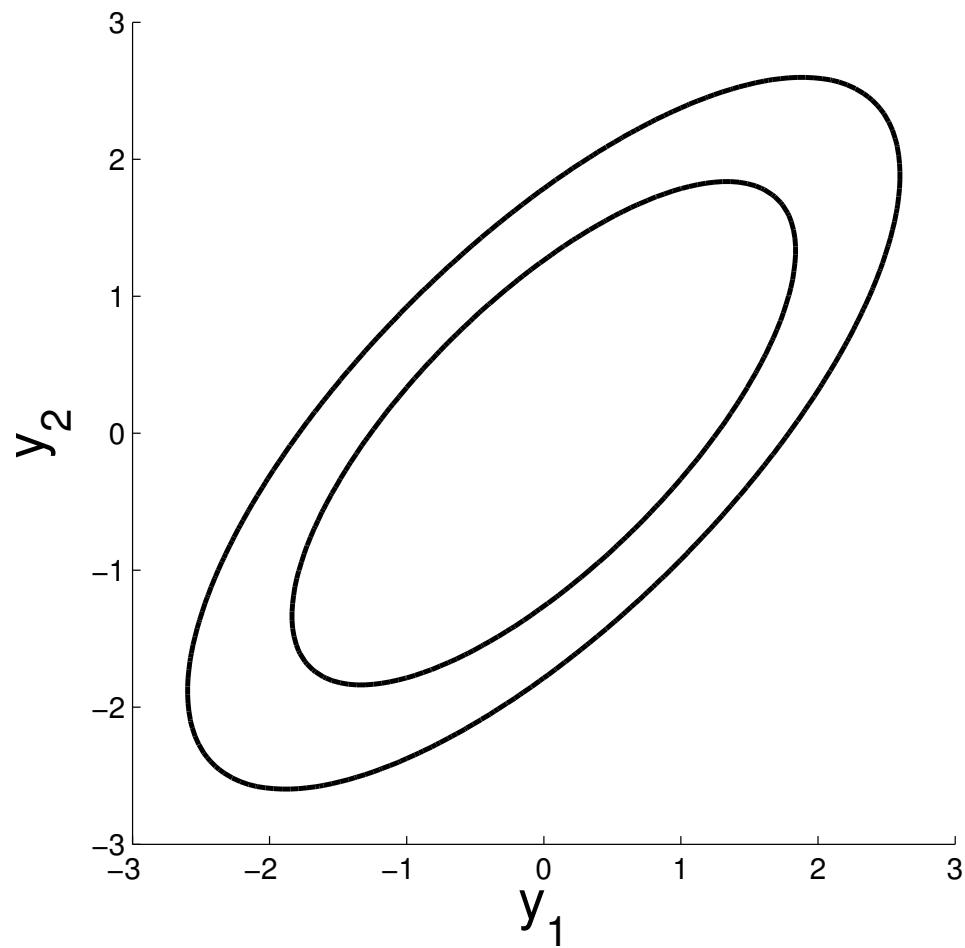
Motivation: non-linear regression

Can we do this with a plain old Gaussian?



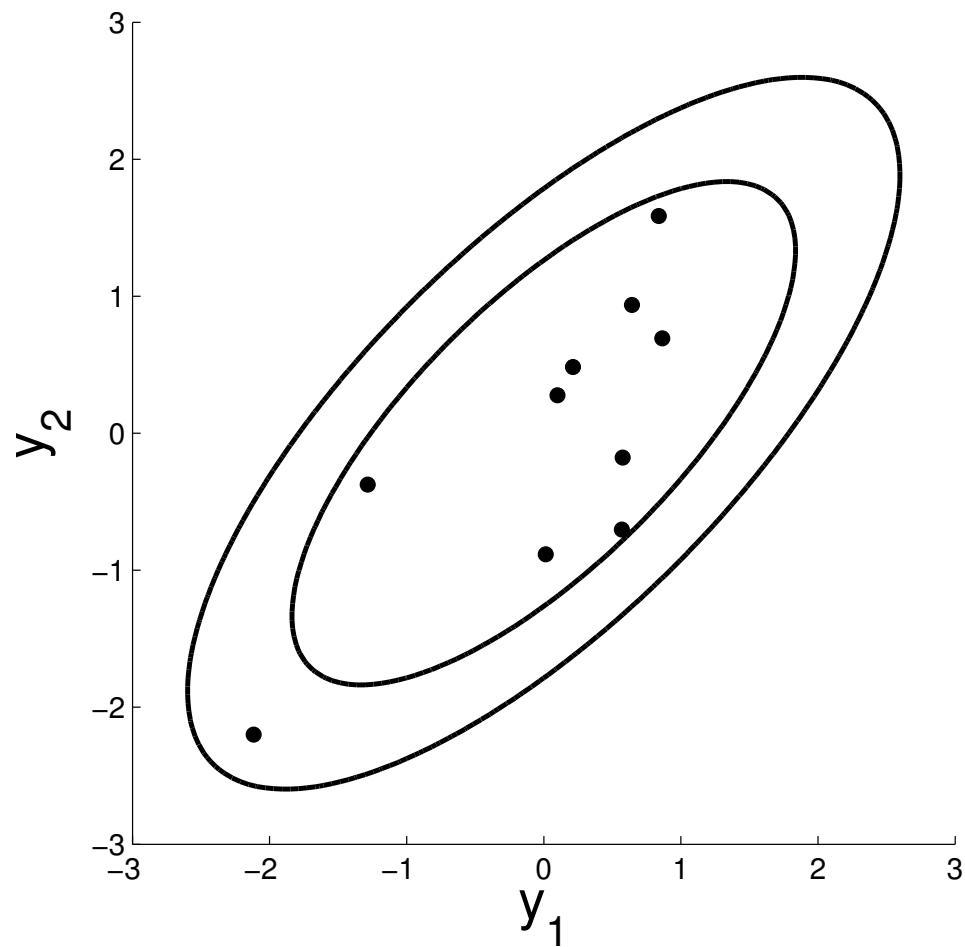
Gaussian distribution

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



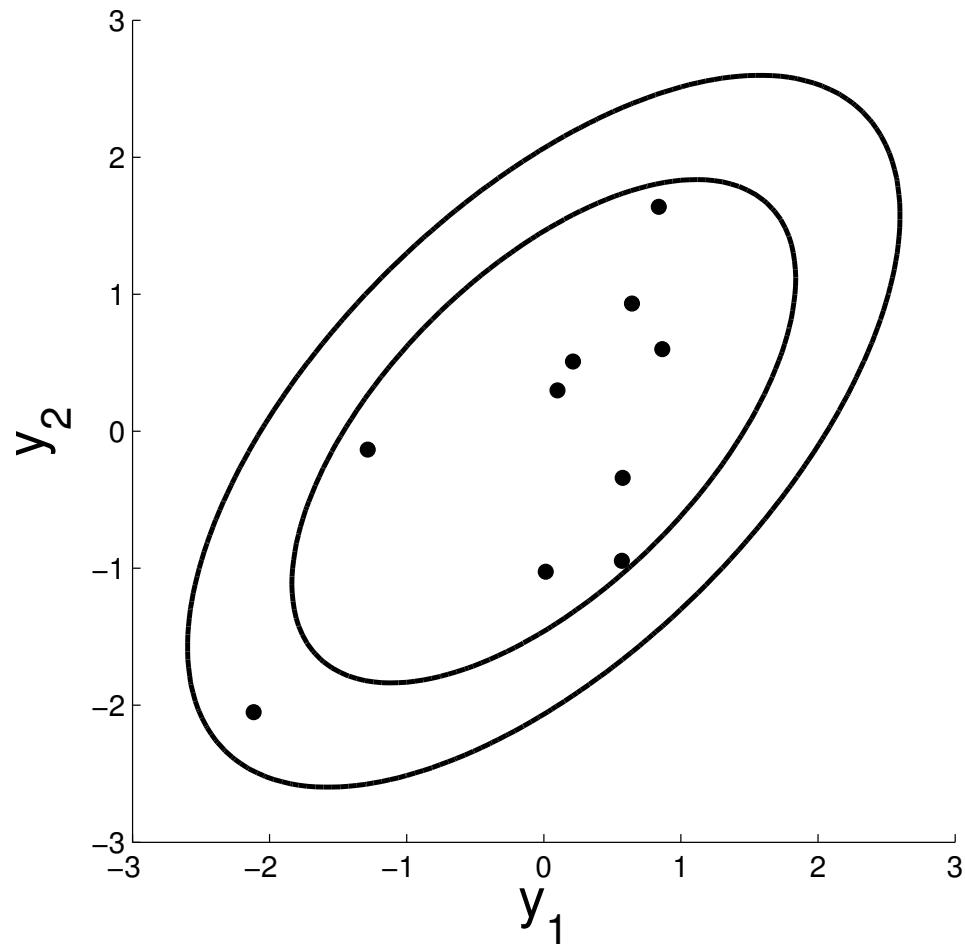
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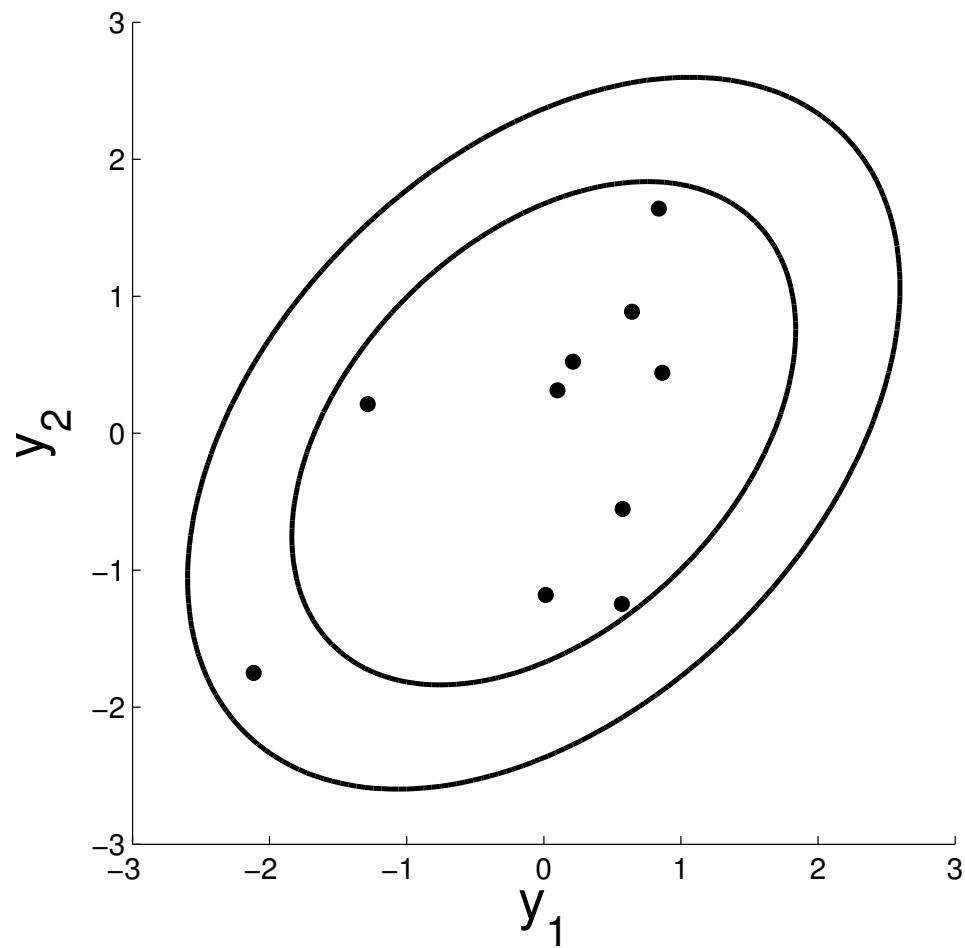
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$$p(\mathbf{y}|\Sigma) \propto \exp\left(-\frac{1}{2}\mathbf{y}^\top \Sigma^{-1} \mathbf{y}\right)$$
$$\Sigma = \begin{bmatrix} 1 & .6 \\ .6 & 1 \end{bmatrix}$$



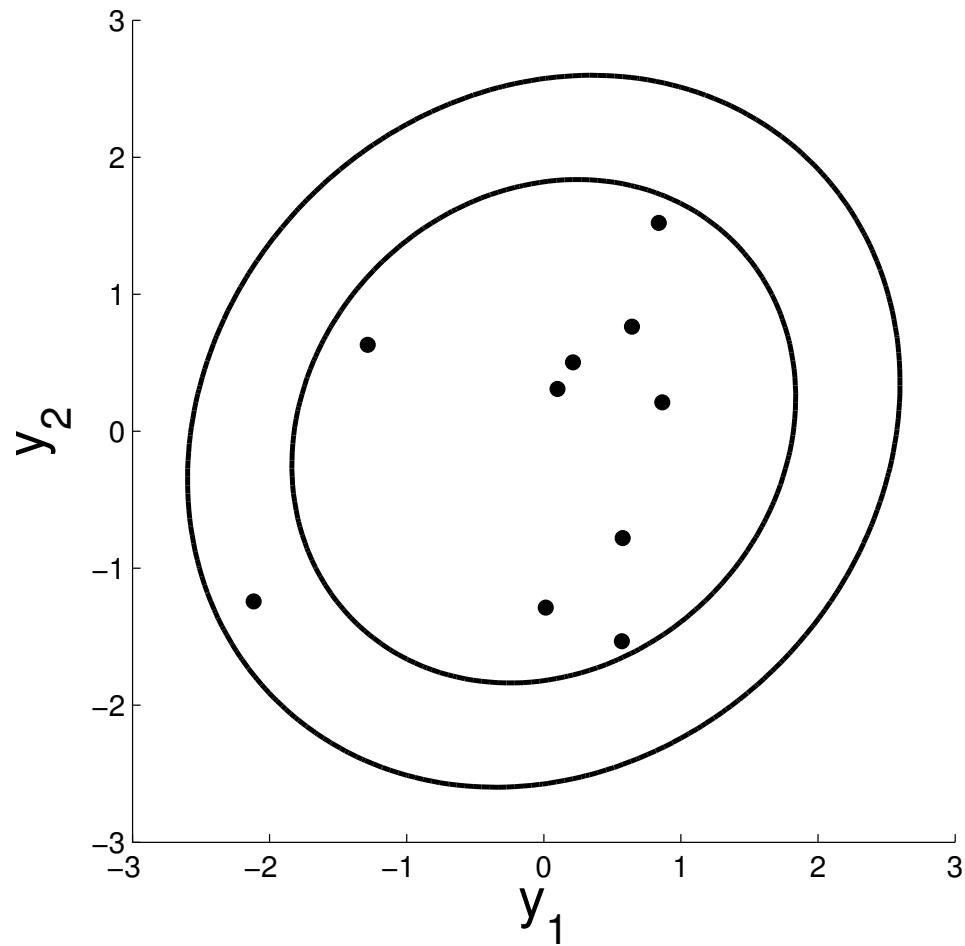
Gaussian distribution

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



Gaussian distribution

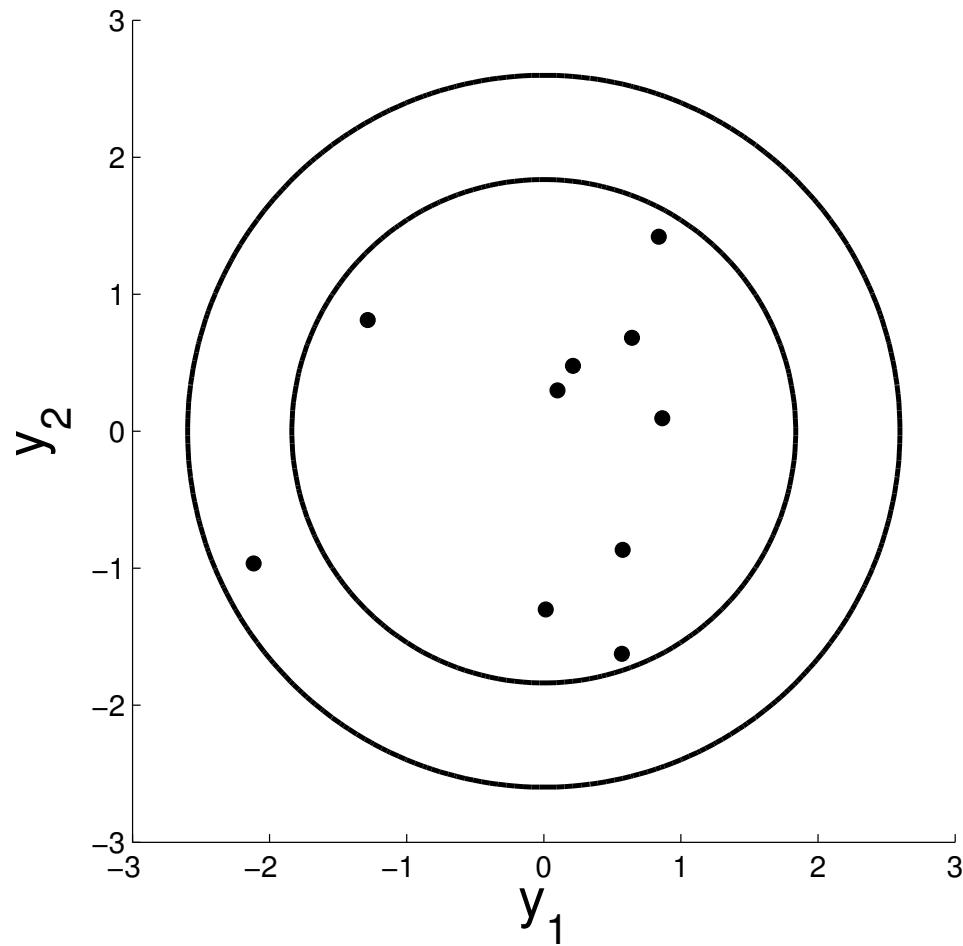
$$p(\mathbf{y}|\Sigma) \propto \exp\left(-\frac{1}{2}\mathbf{y}^\top \Sigma^{-1} \mathbf{y}\right)$$
$$\Sigma = \begin{bmatrix} 1 & .1 \\ .1 & 1 \end{bmatrix}$$



Gaussian distribution

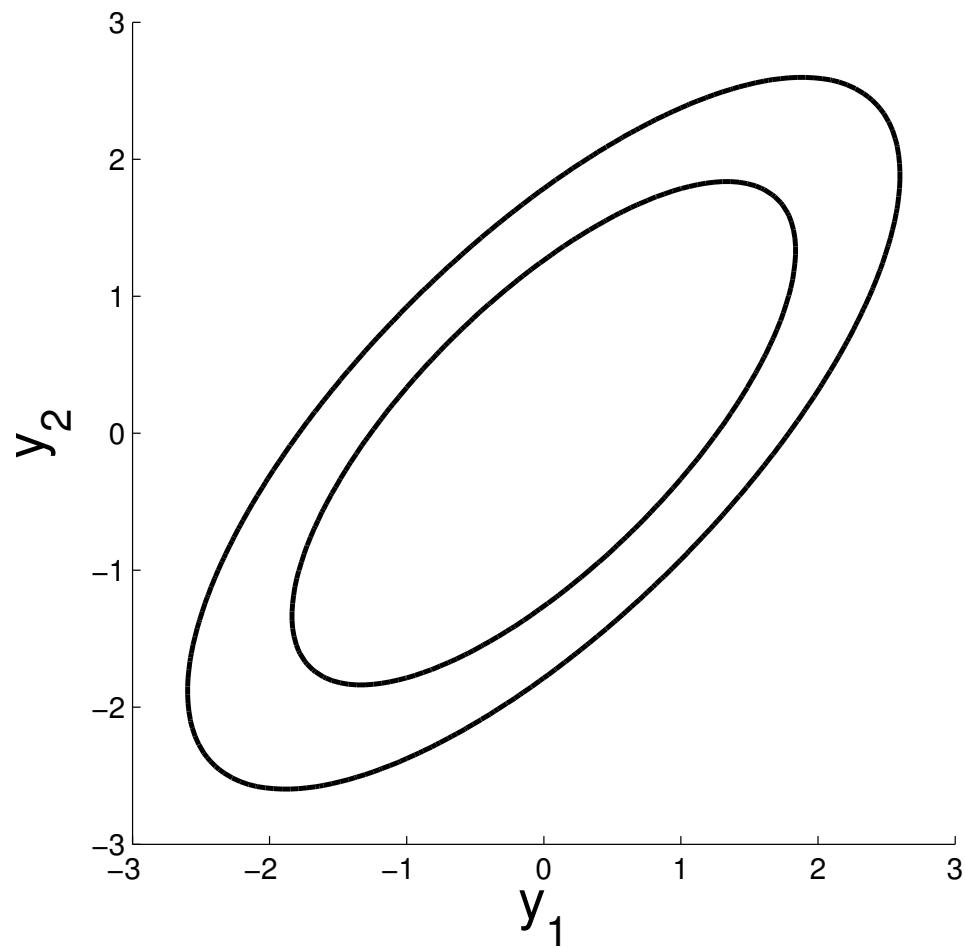
$$p(\mathbf{y}|\Sigma) \propto \exp\left(-\frac{1}{2}\mathbf{y}^\top \Sigma^{-1} \mathbf{y}\right)$$

$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



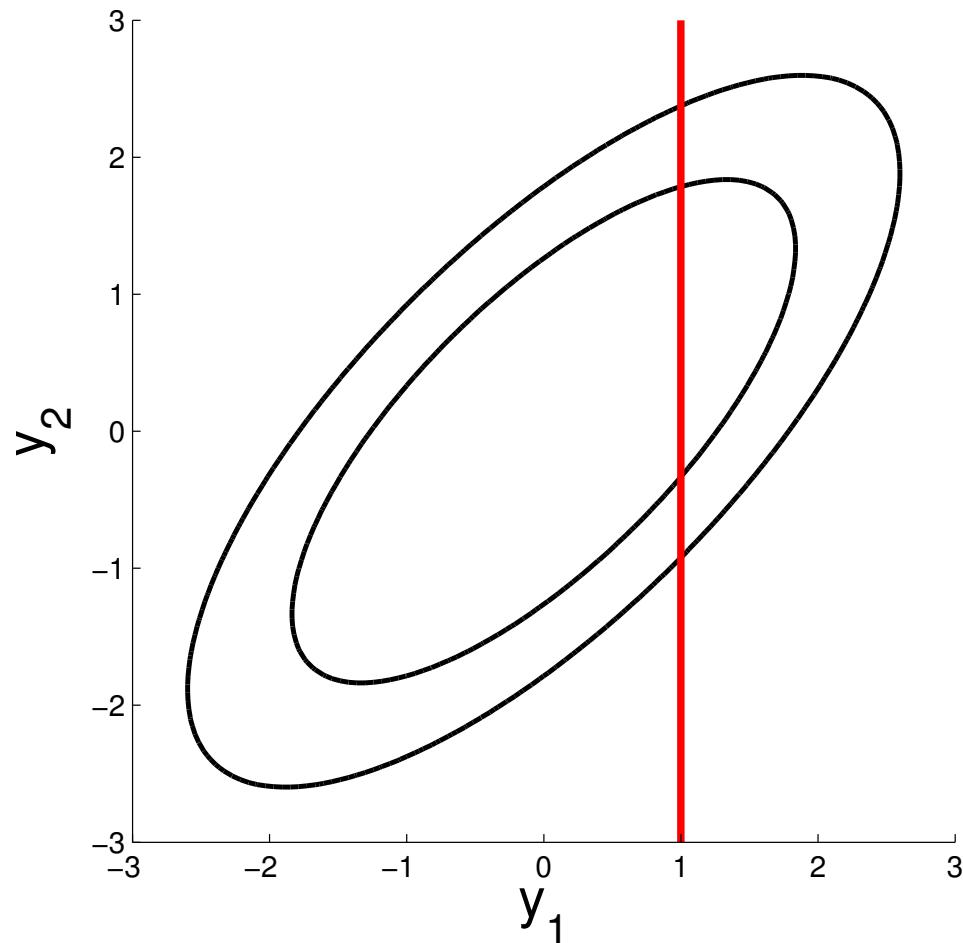
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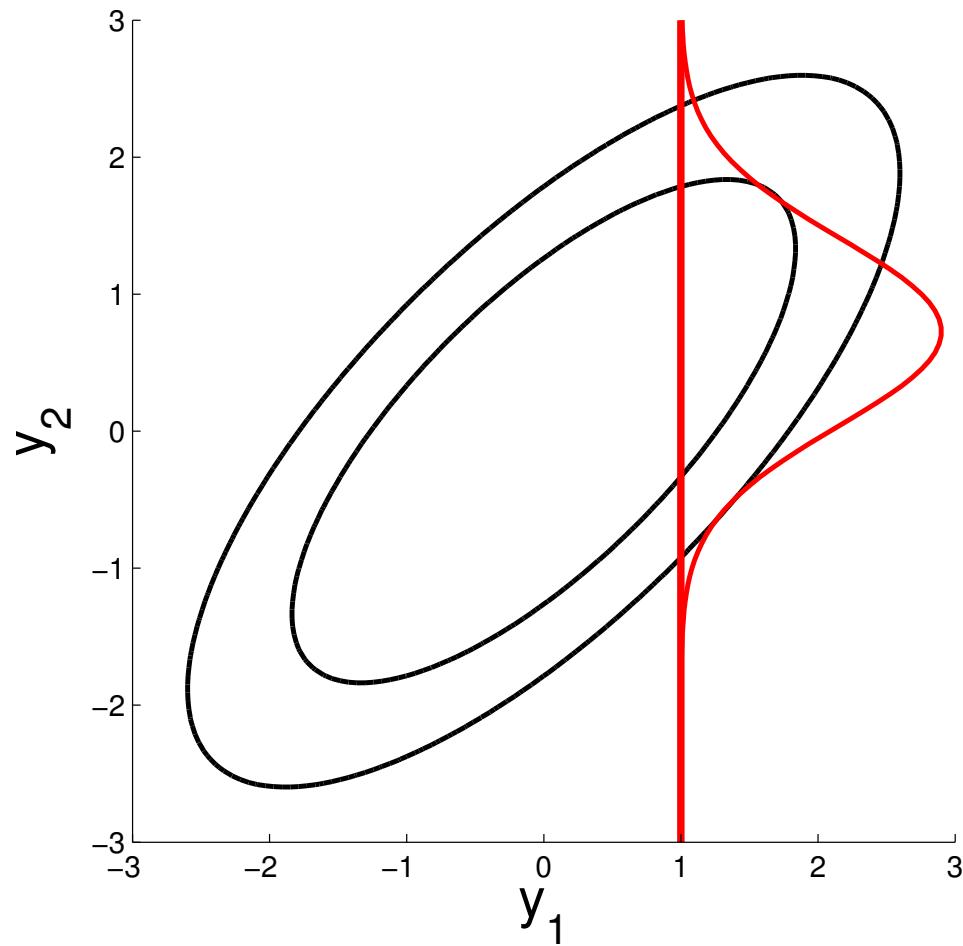
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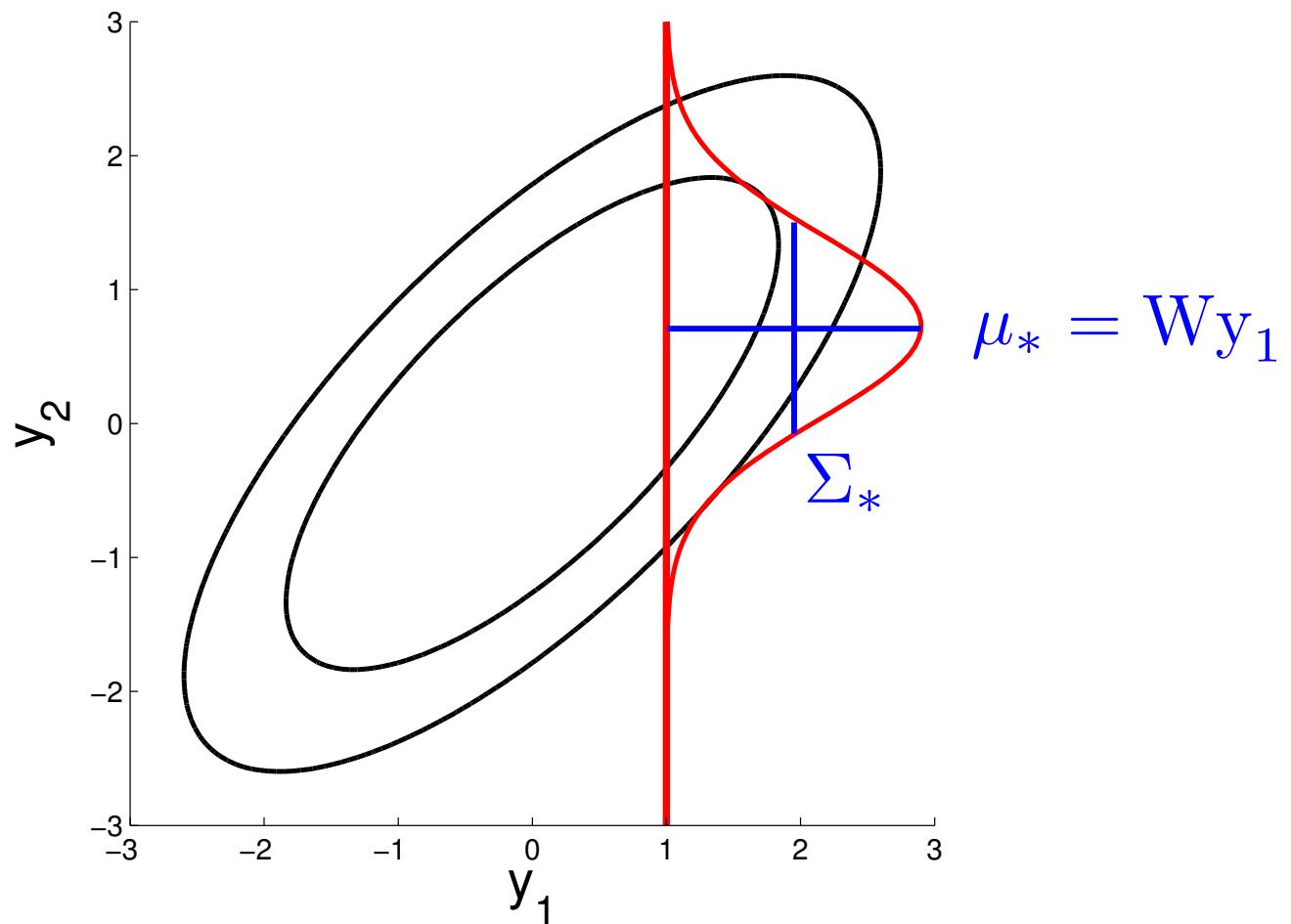
Gaussian distribution

$$p(\mathbf{y}_2|\mathbf{y}_1, \Sigma) \propto \exp\left(-\frac{1}{2}(\mathbf{y}_2 - \boldsymbol{\mu}_*) \boldsymbol{\Sigma}_*^{-1} (\mathbf{y}_2 - \boldsymbol{\mu}_*)\right)$$



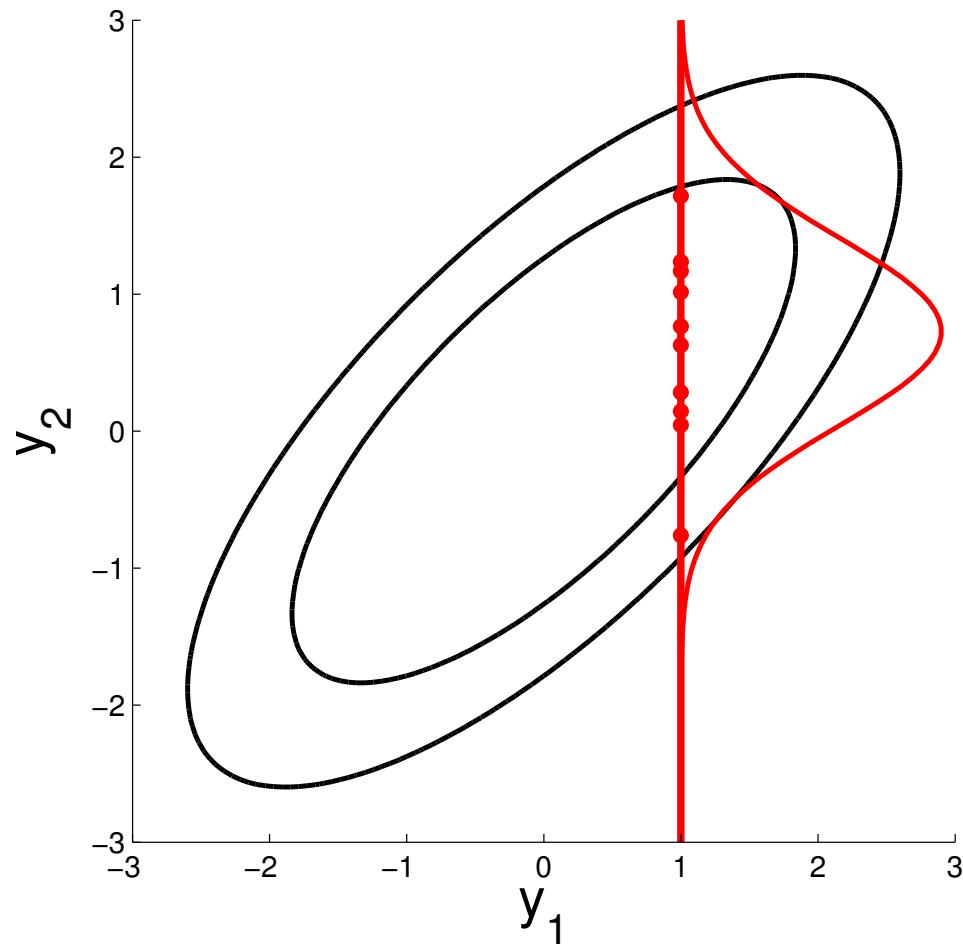
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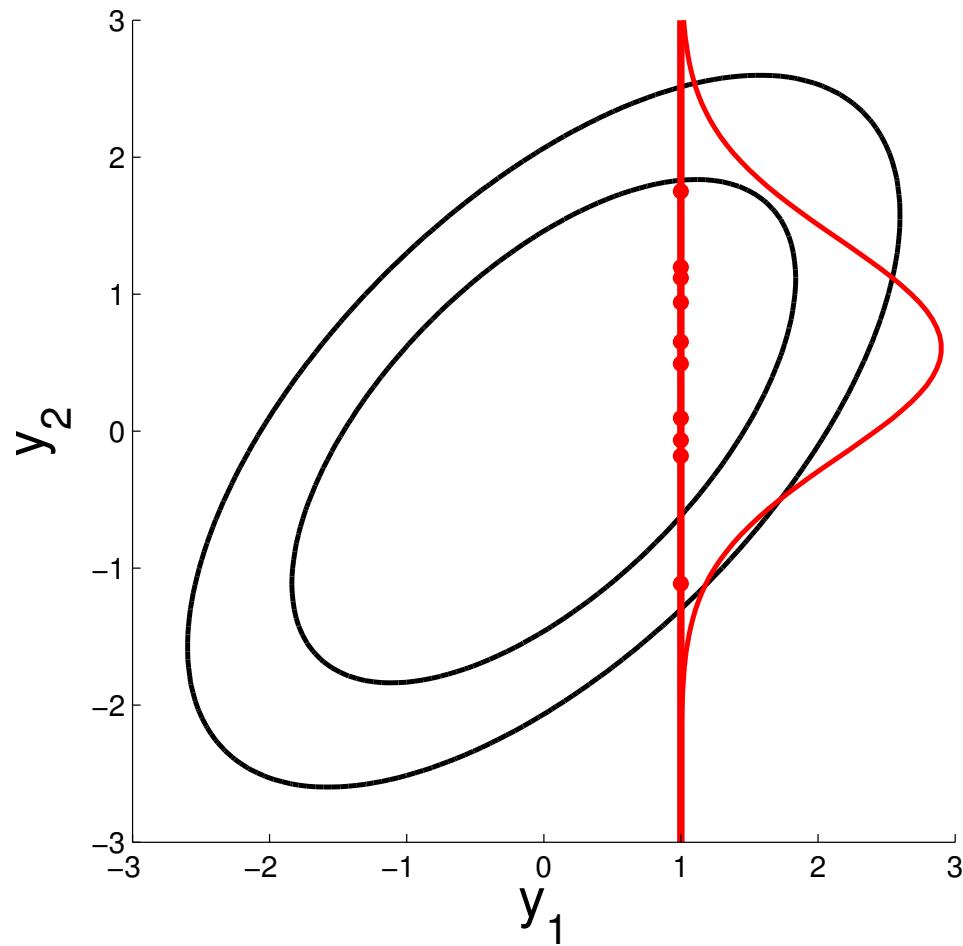
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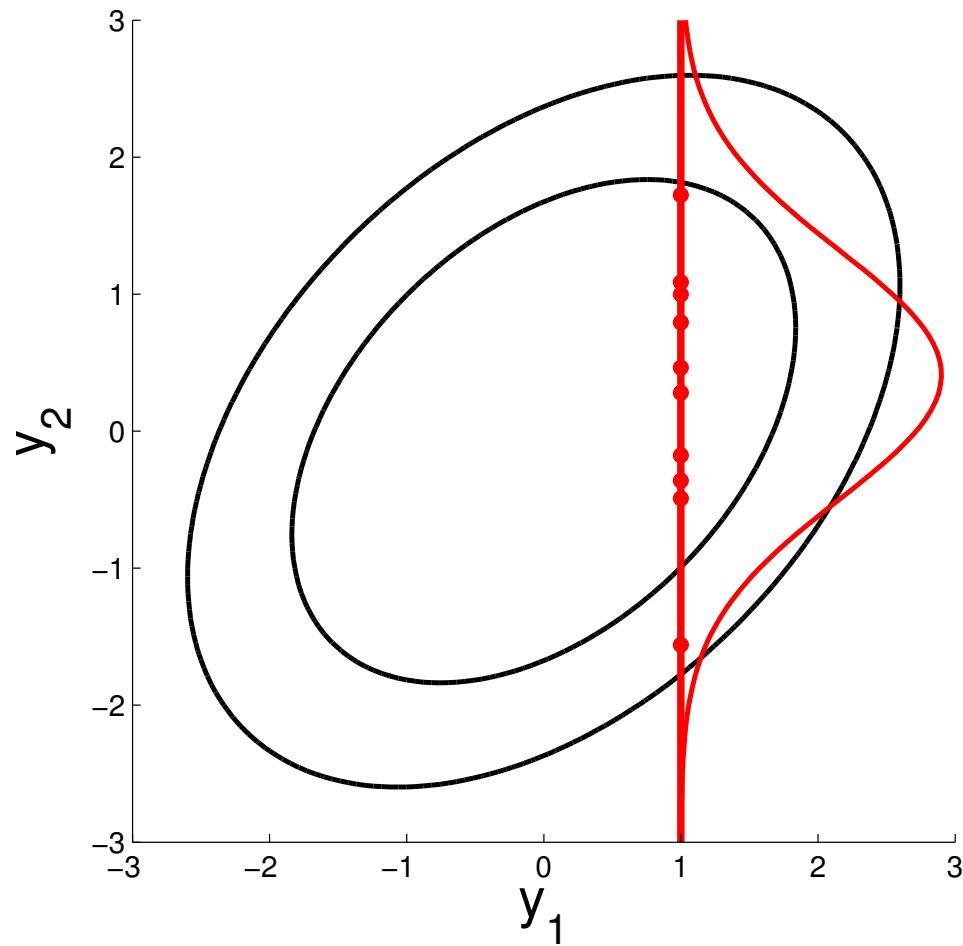
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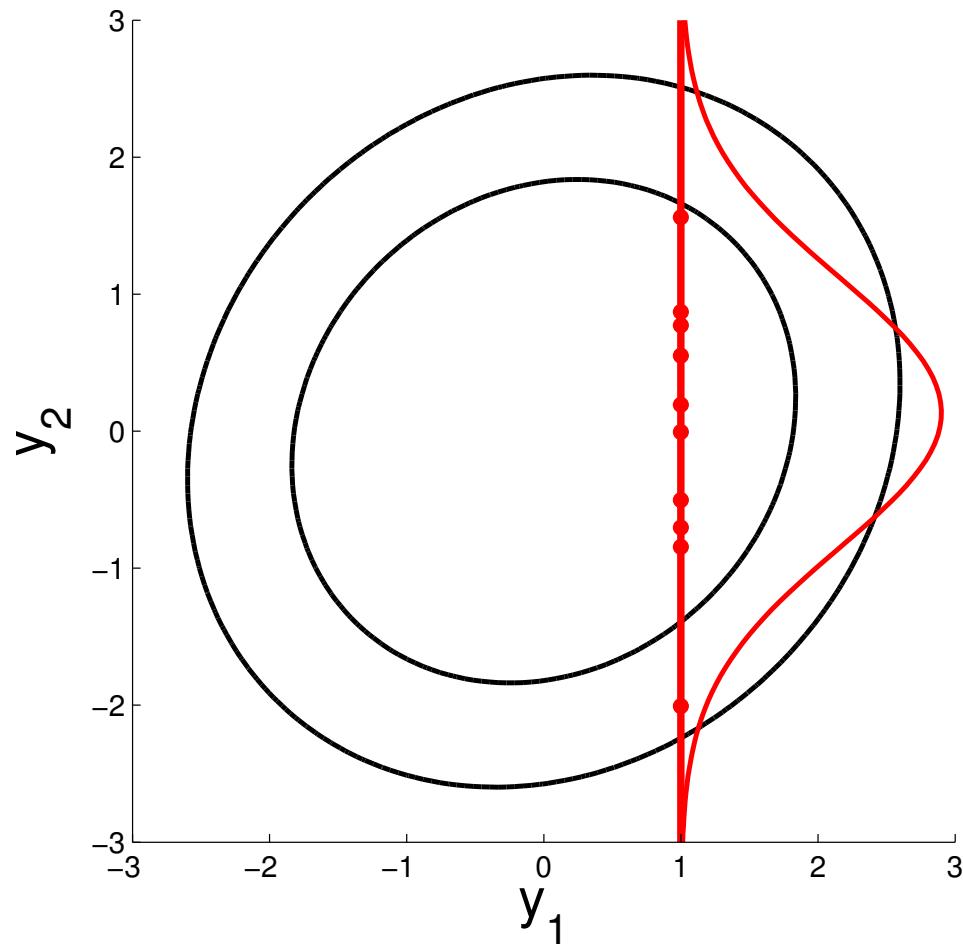
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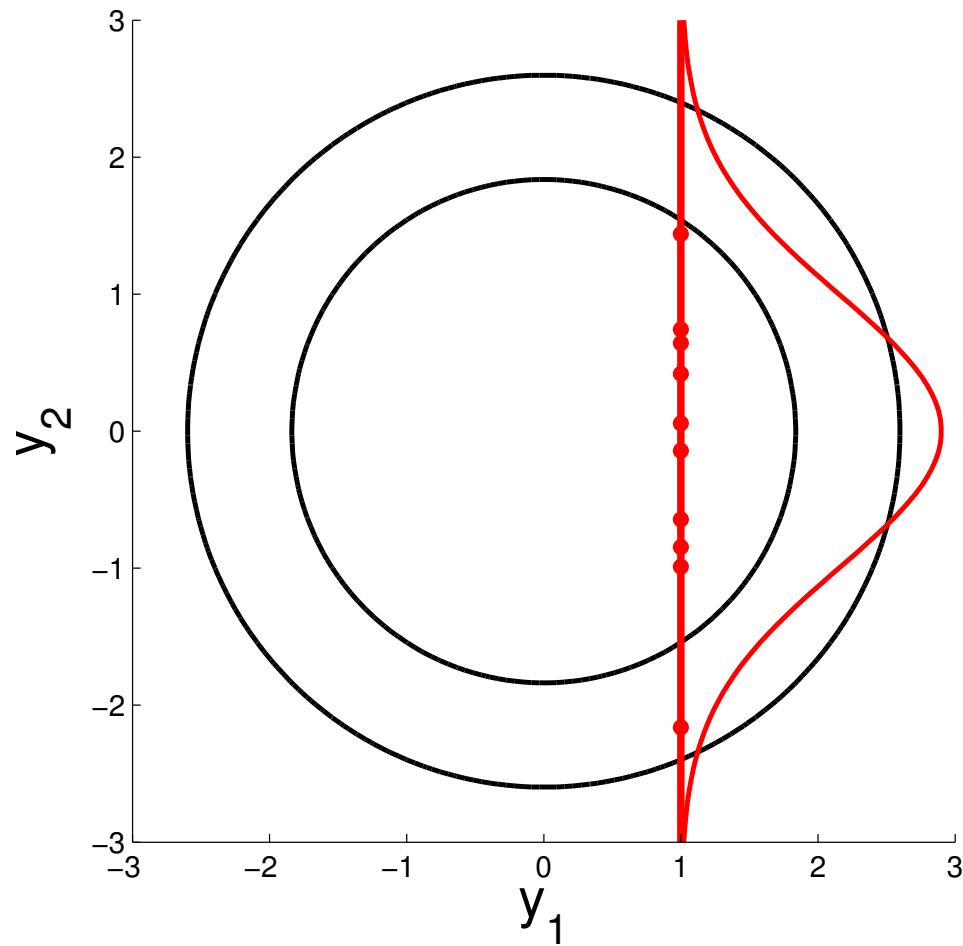
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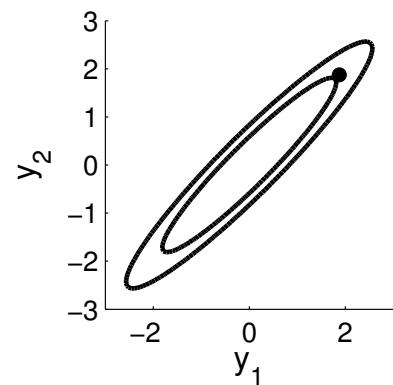


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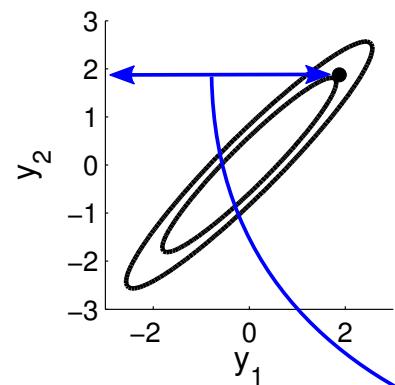


New visualisation

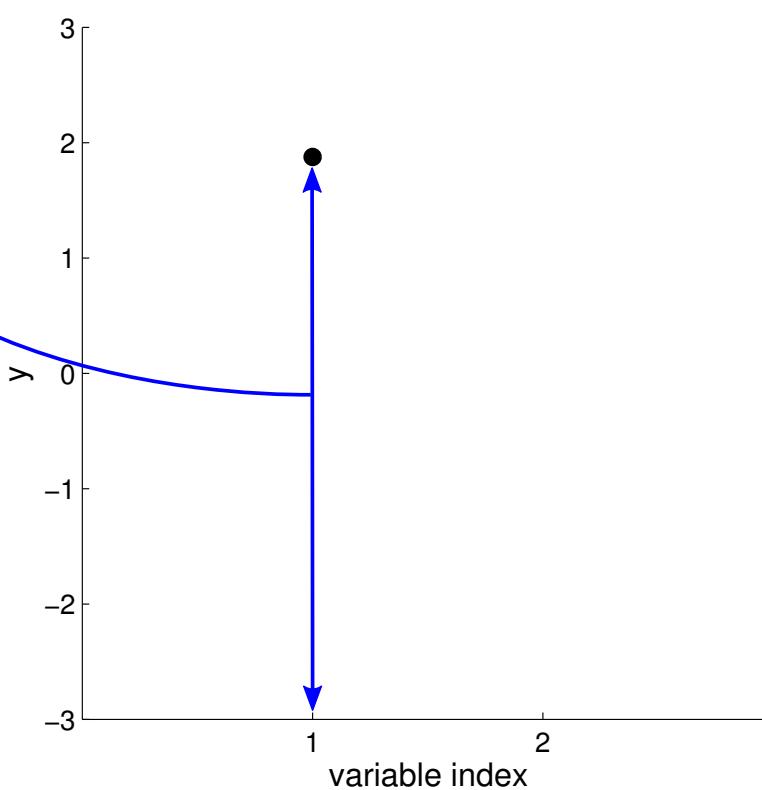


$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$

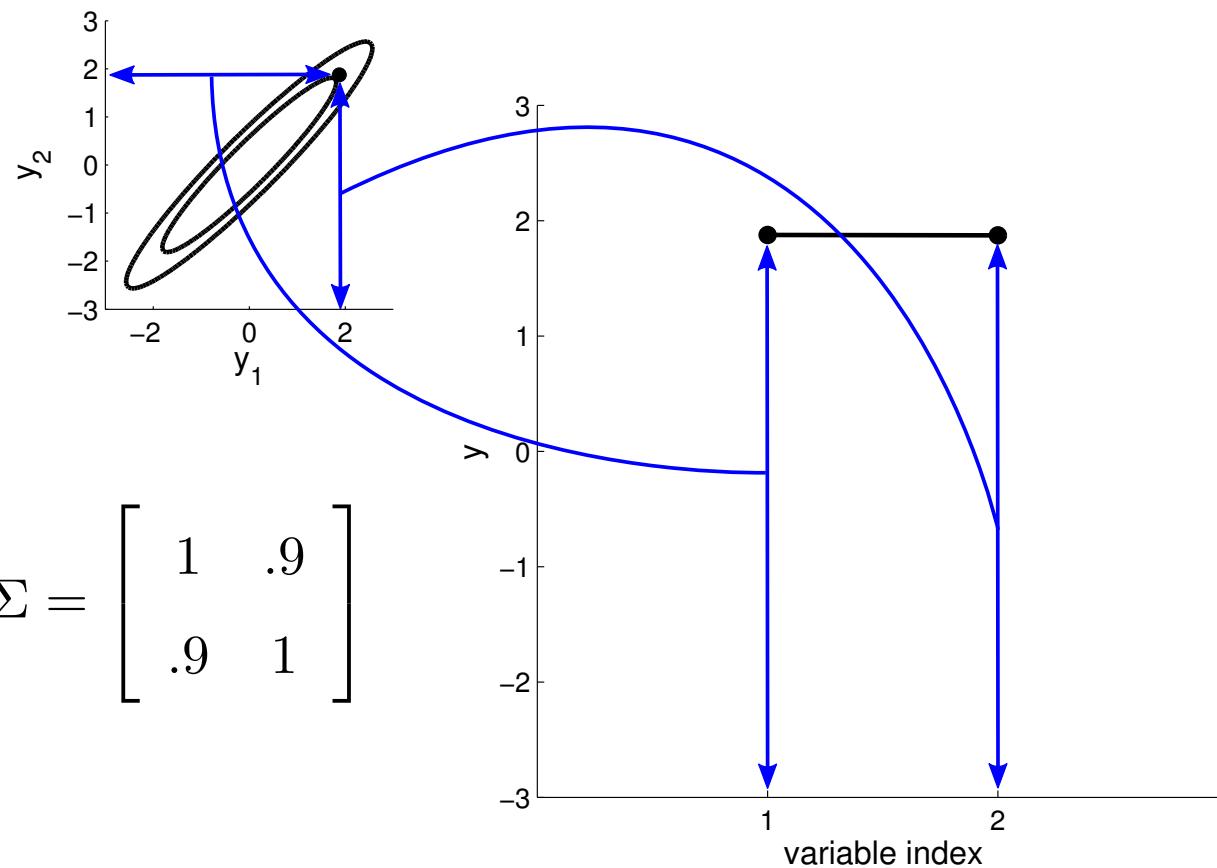
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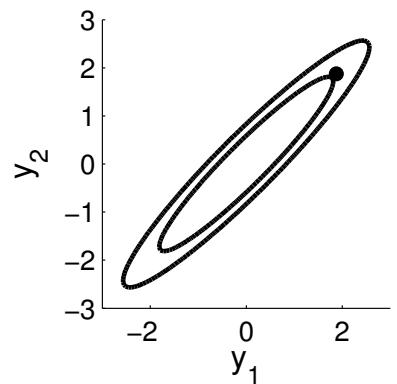
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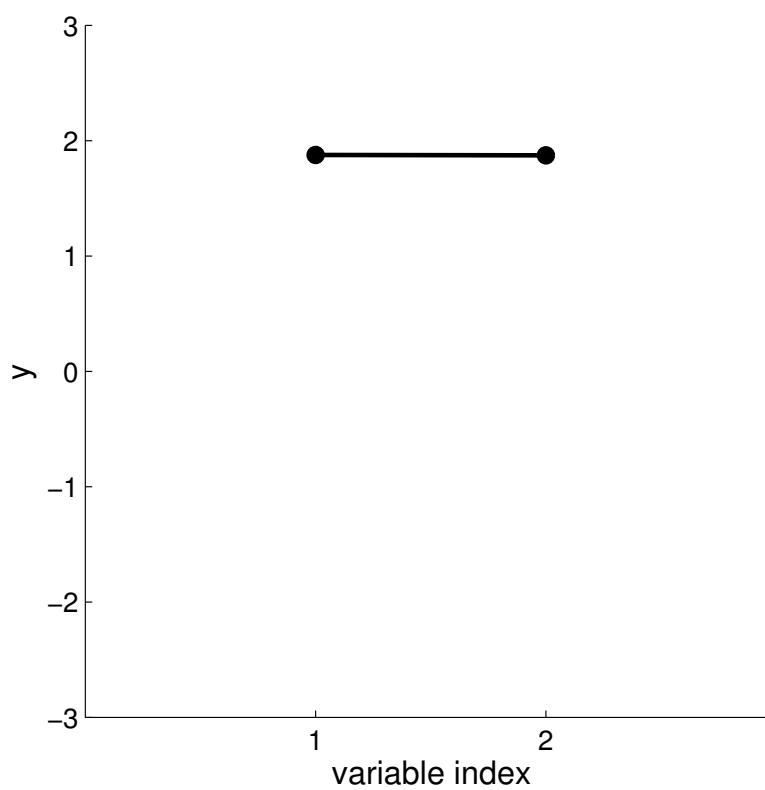
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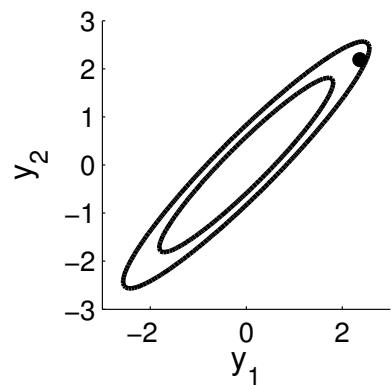
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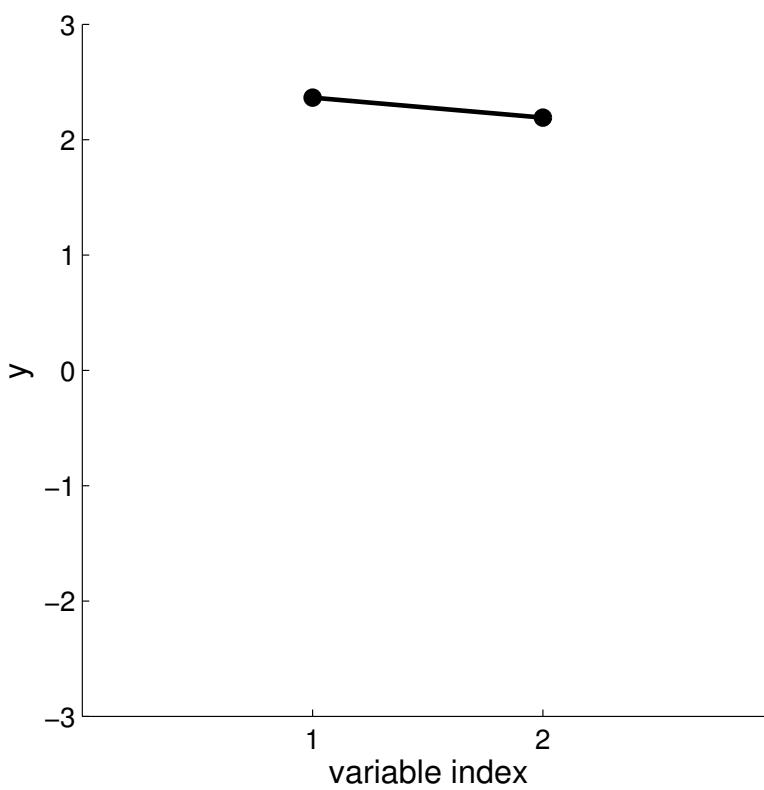
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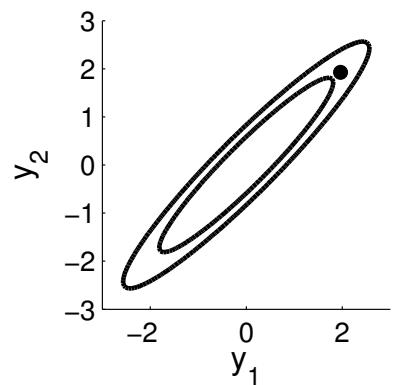
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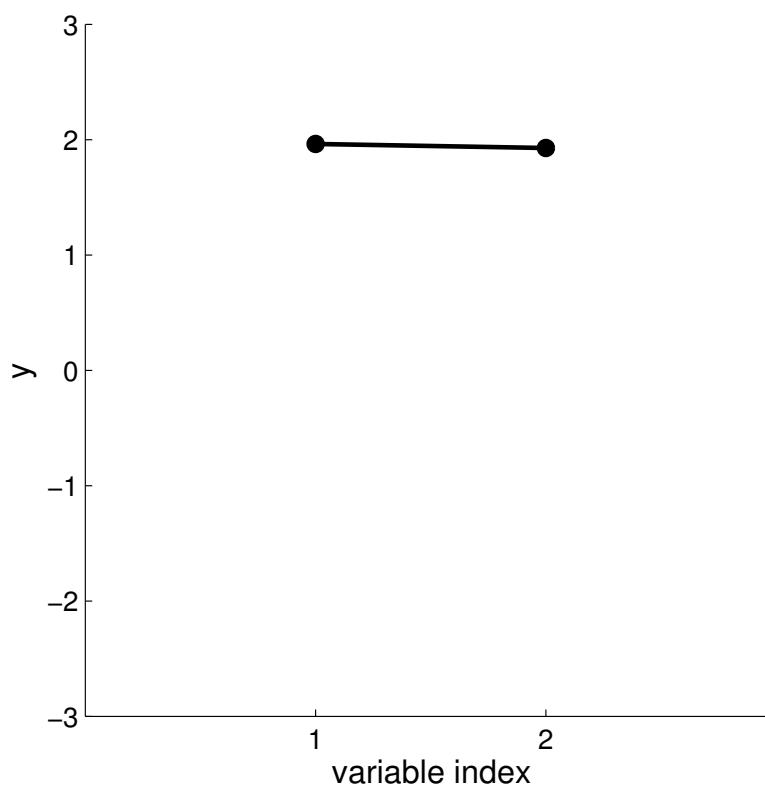
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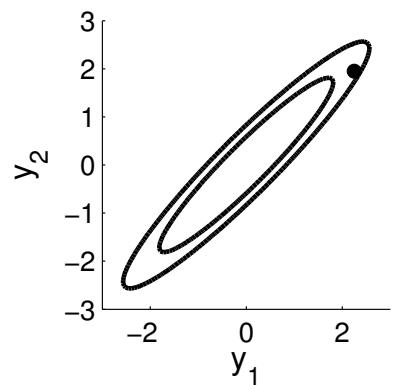
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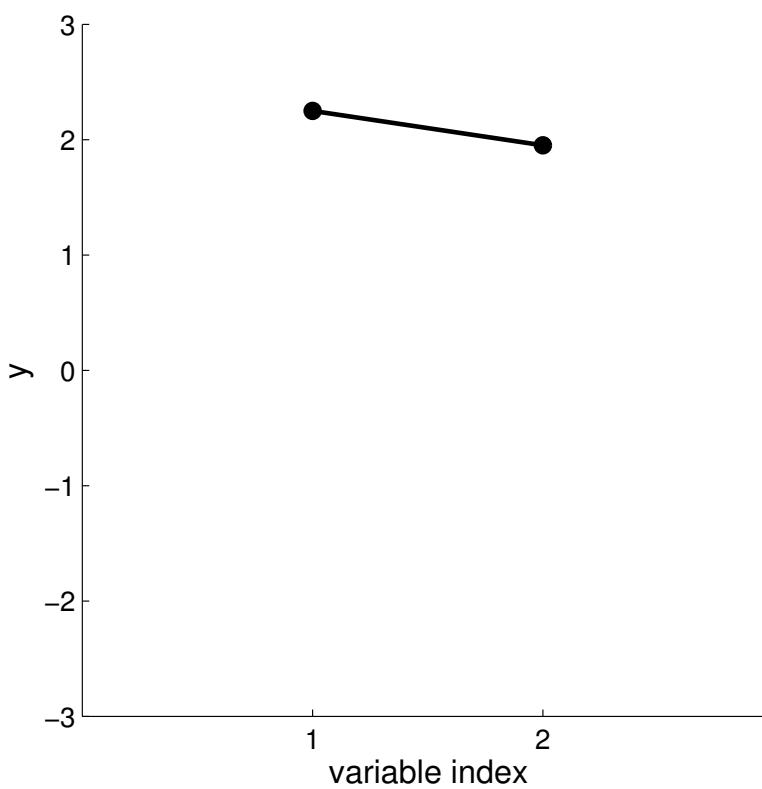
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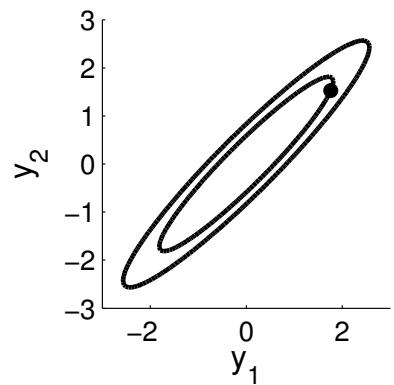
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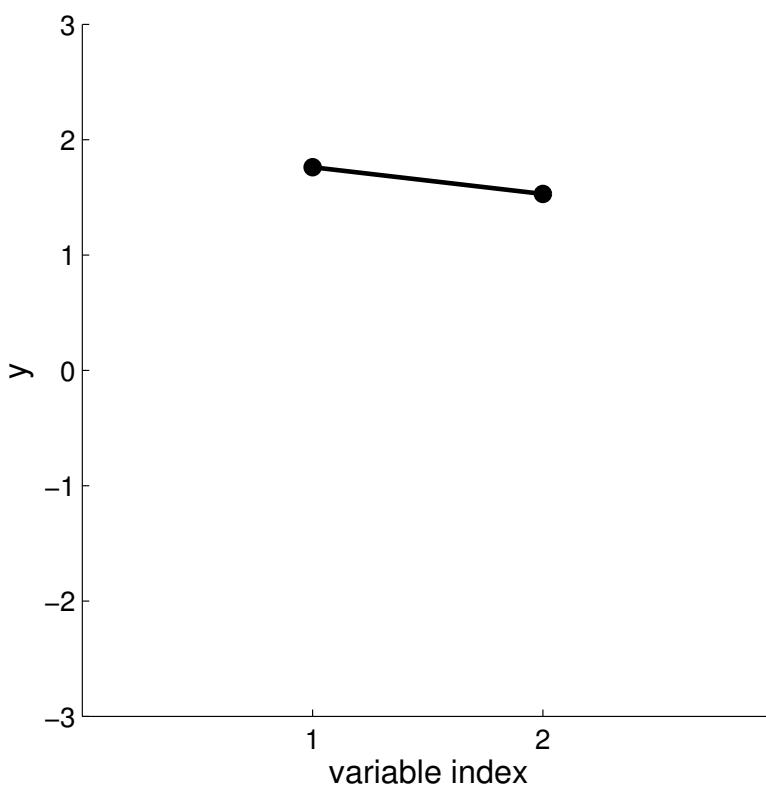
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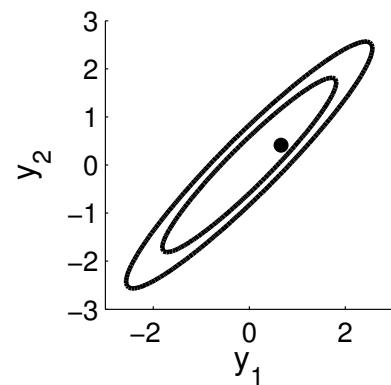
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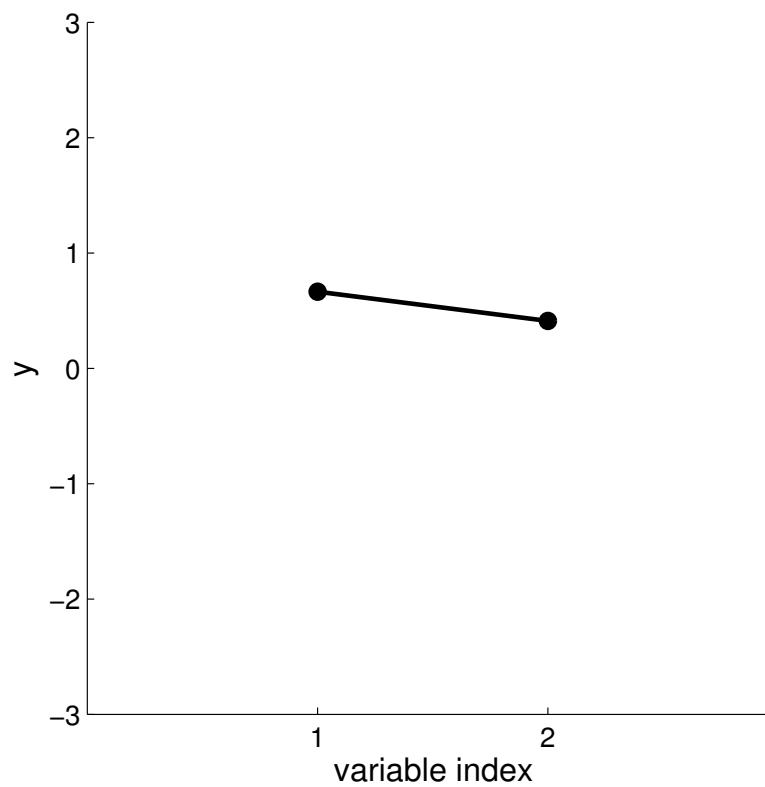
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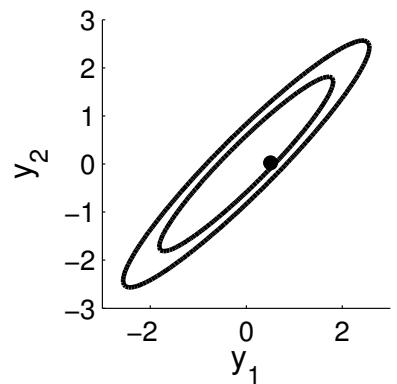
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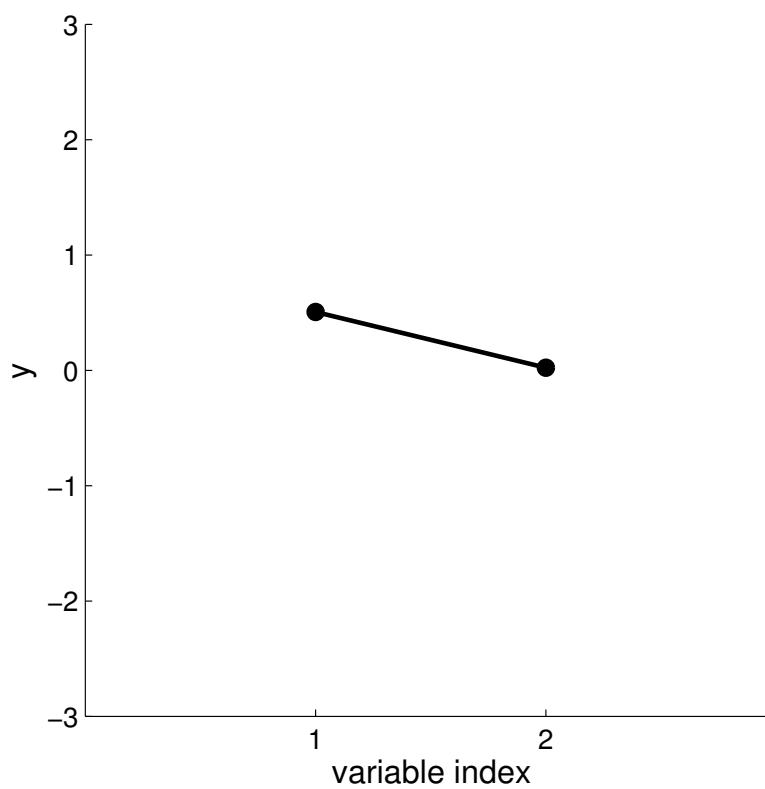
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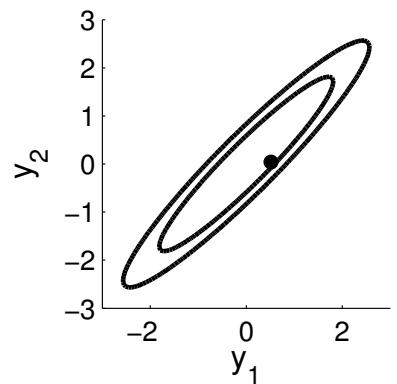
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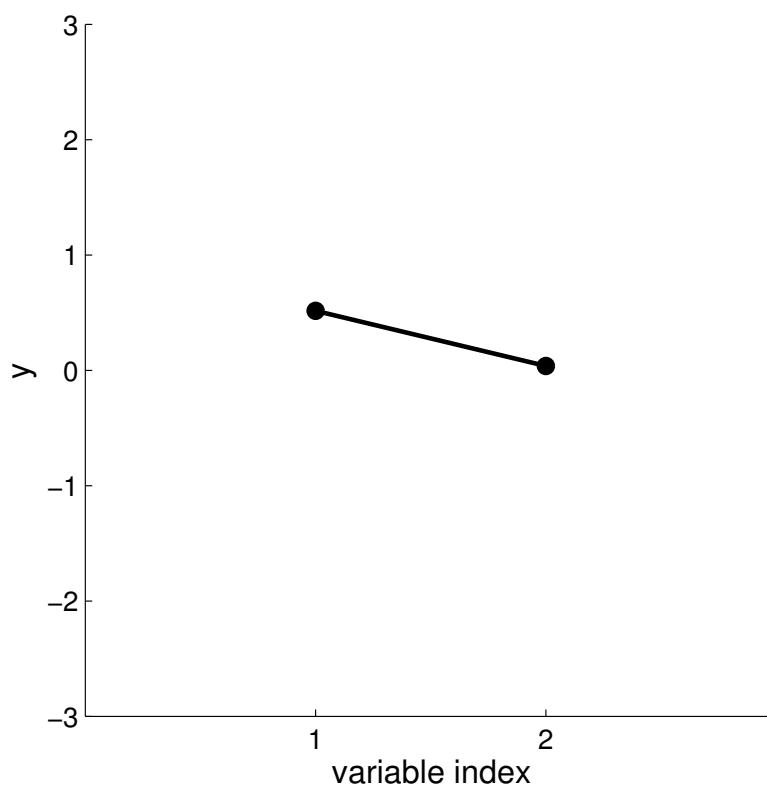
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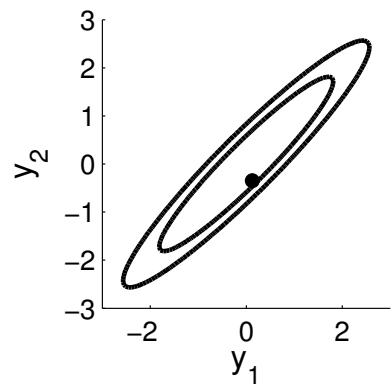
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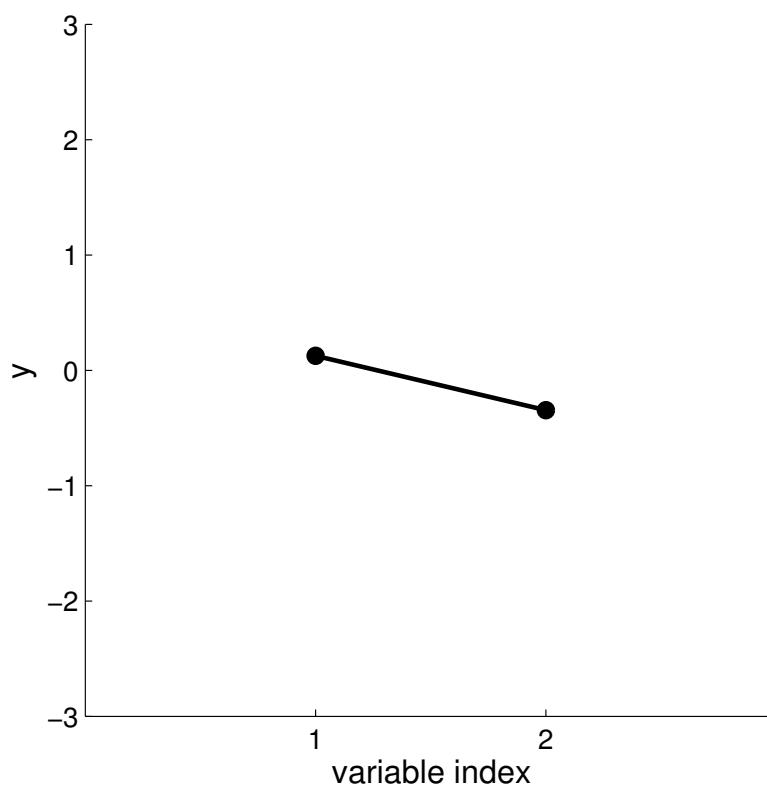
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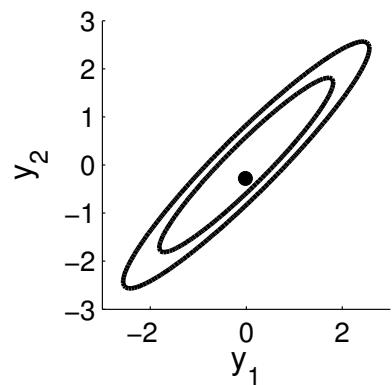
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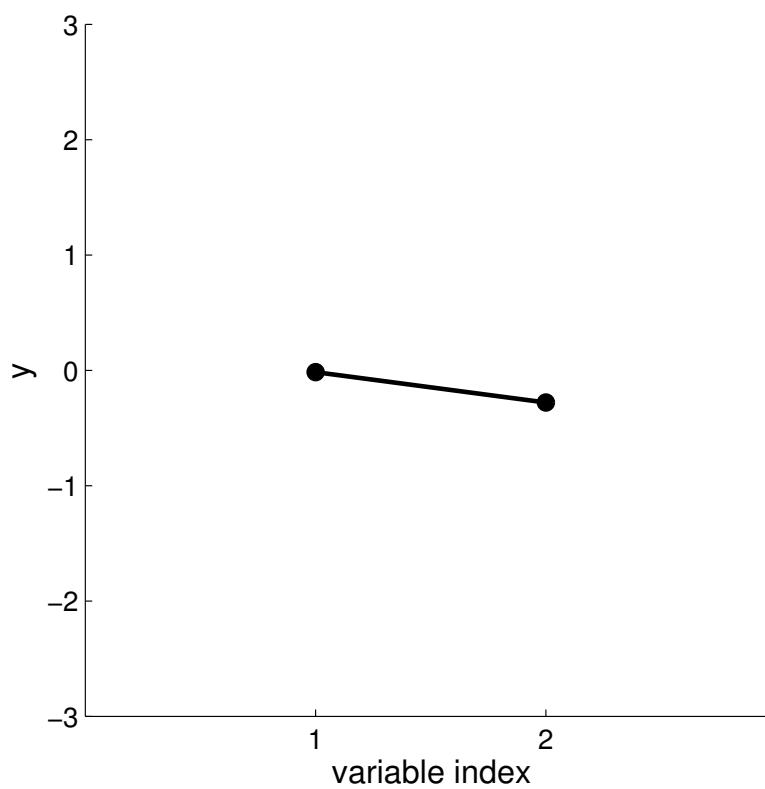
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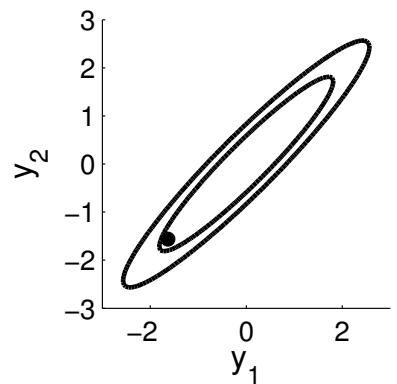
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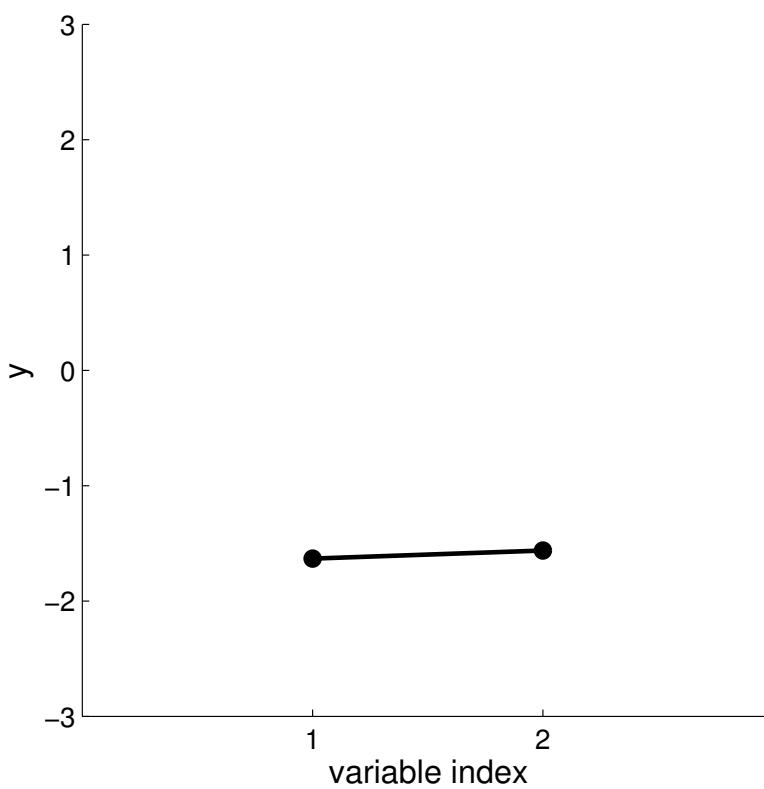
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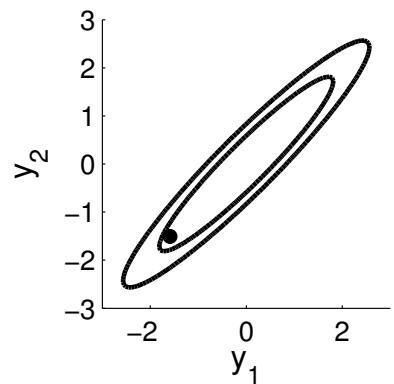
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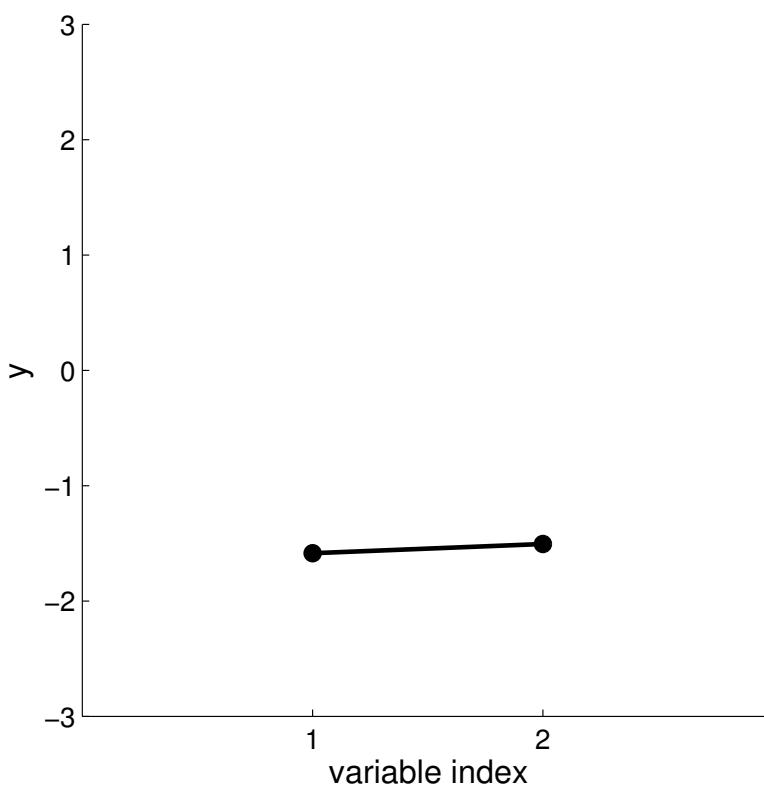
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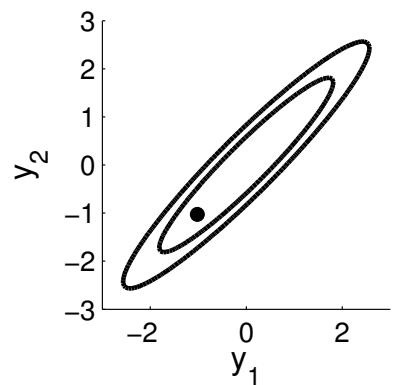
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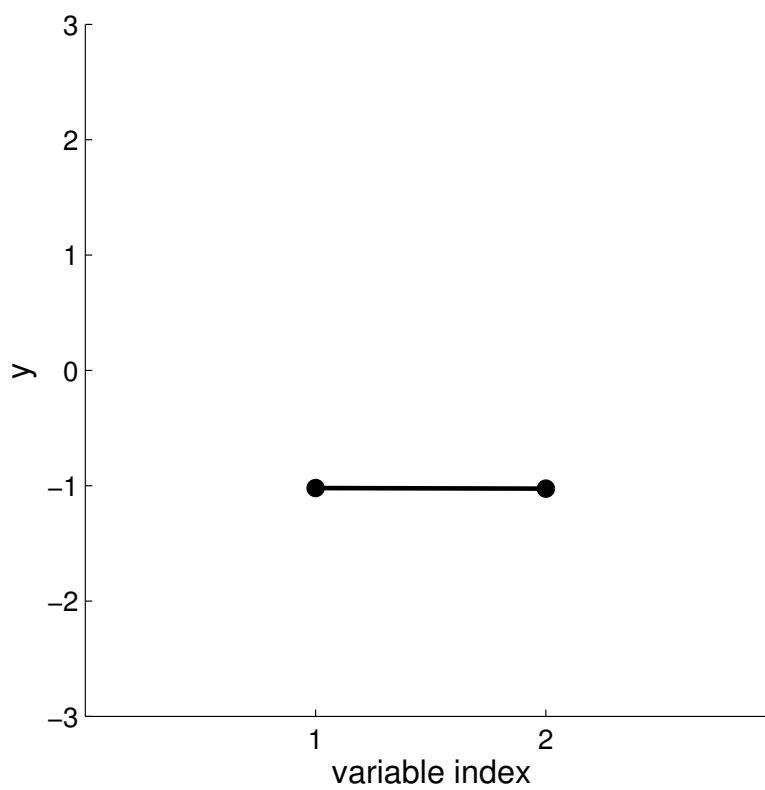
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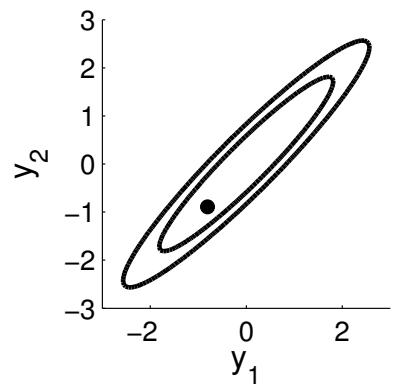
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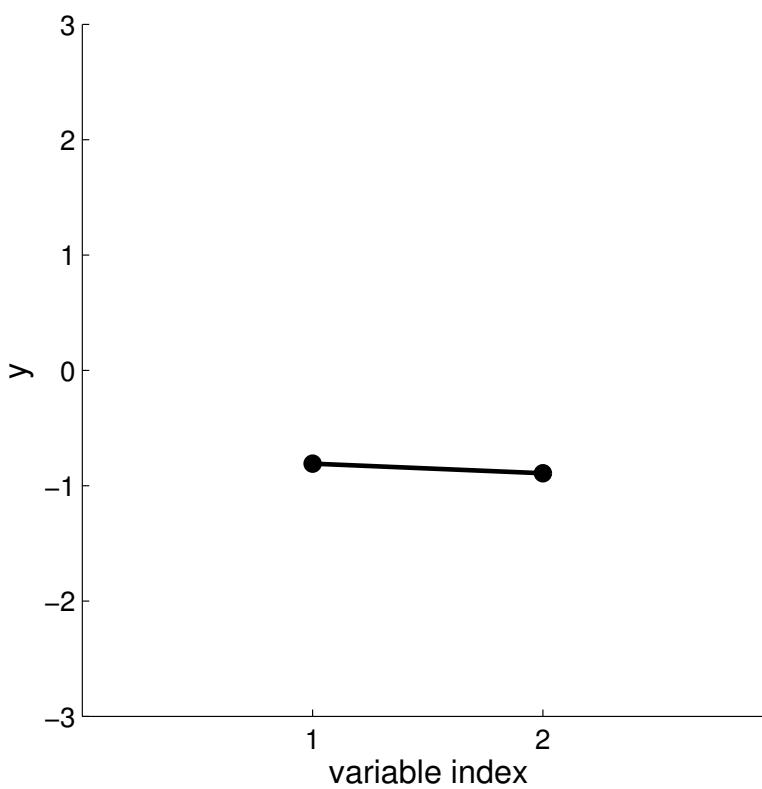
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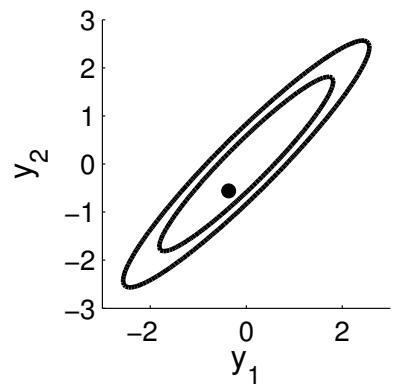
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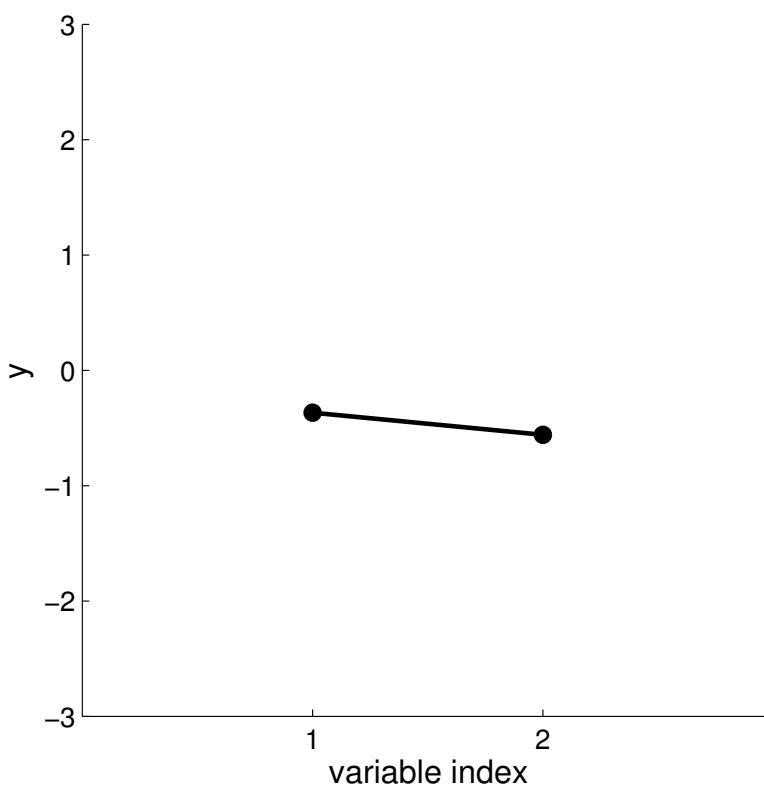
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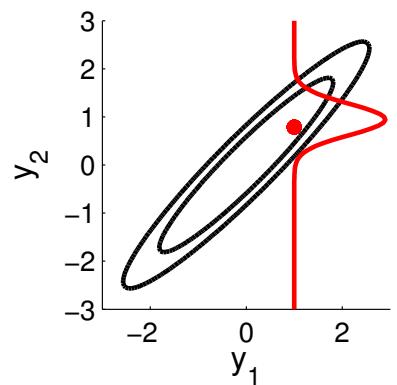
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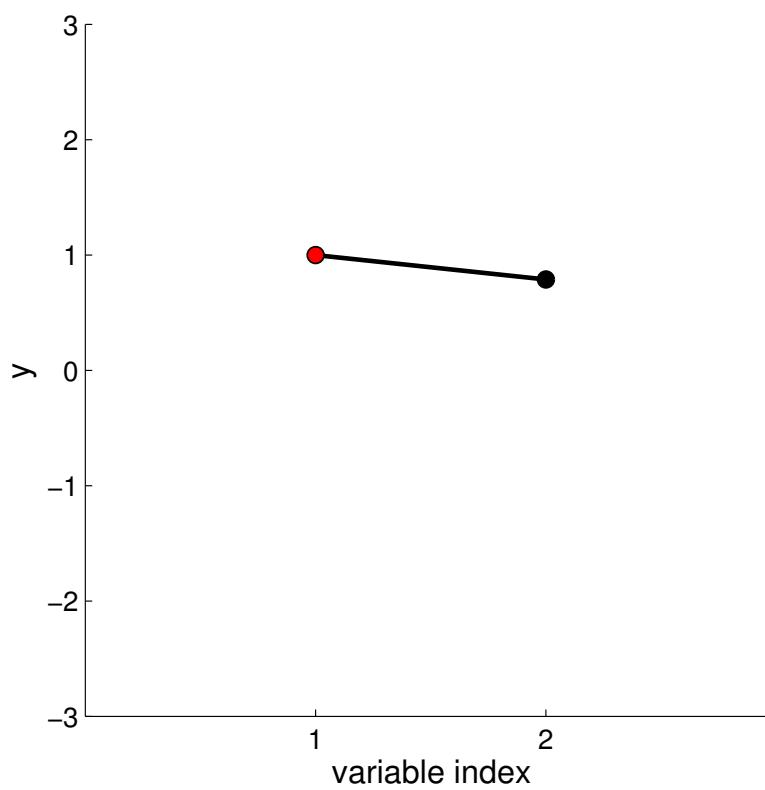
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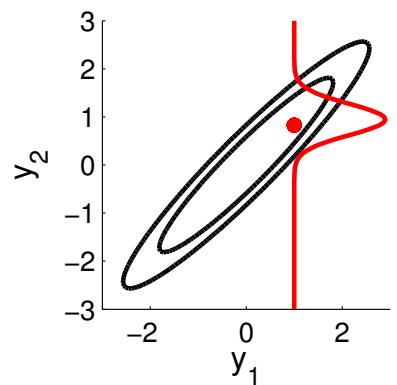
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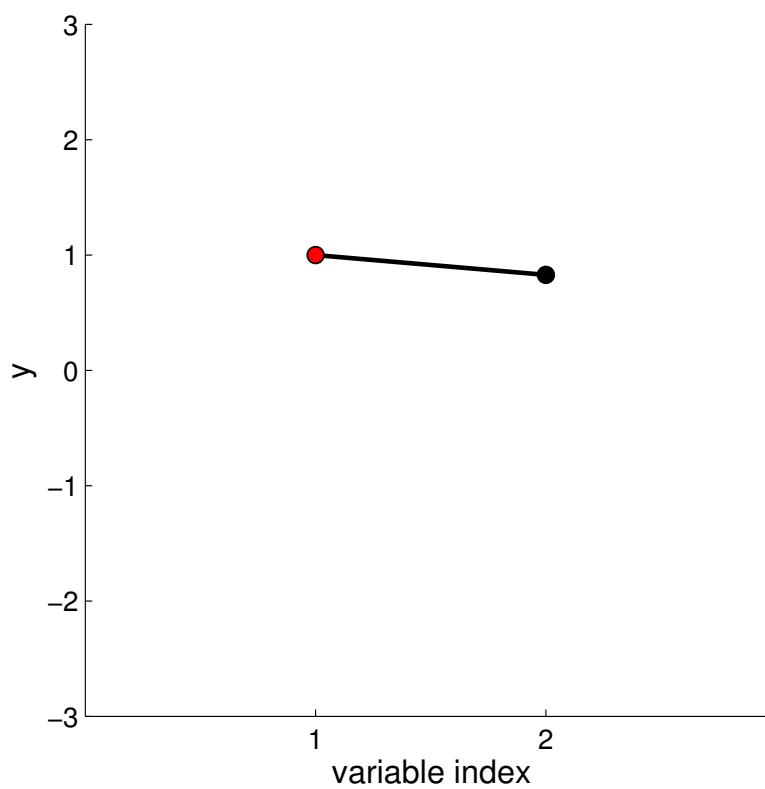
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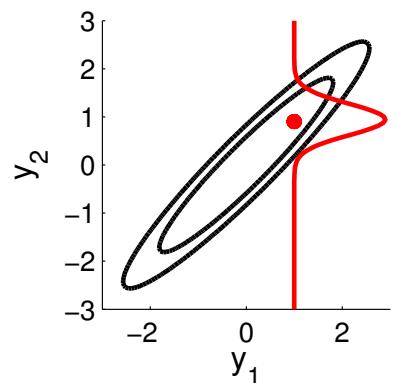
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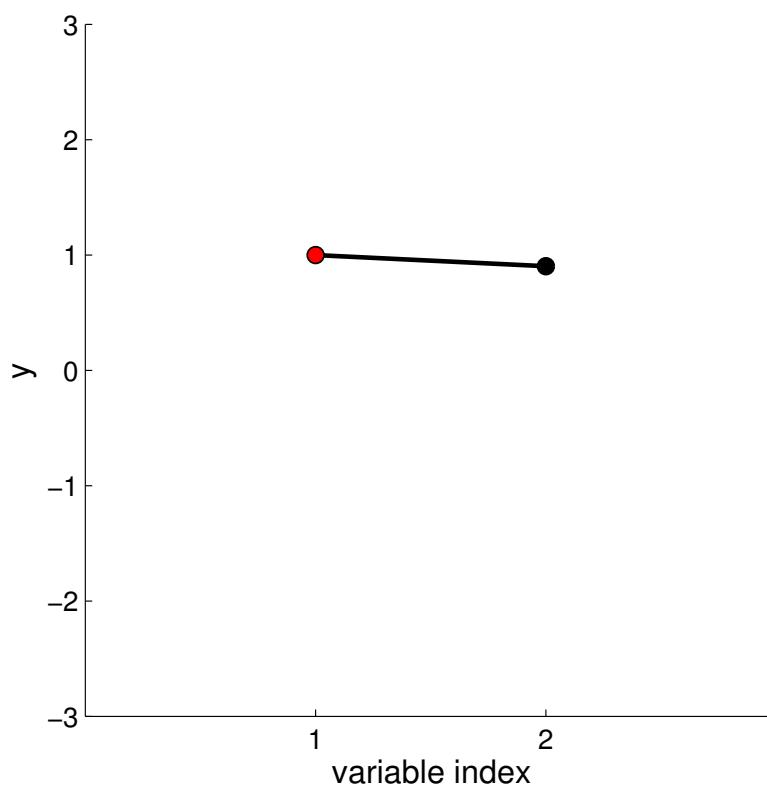
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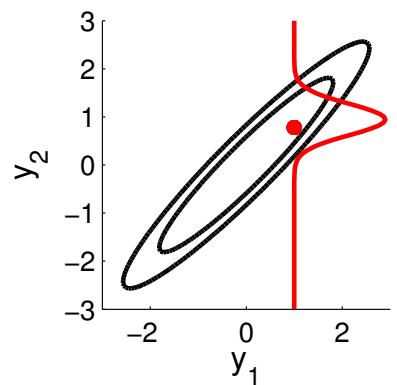
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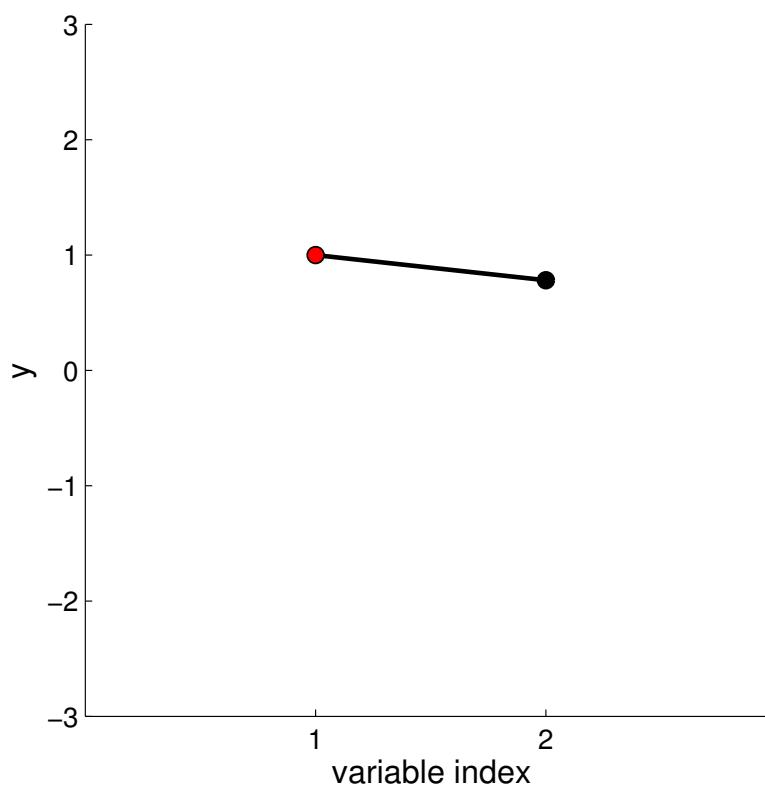
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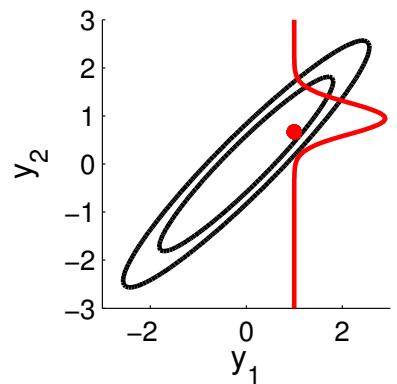
New visualisation



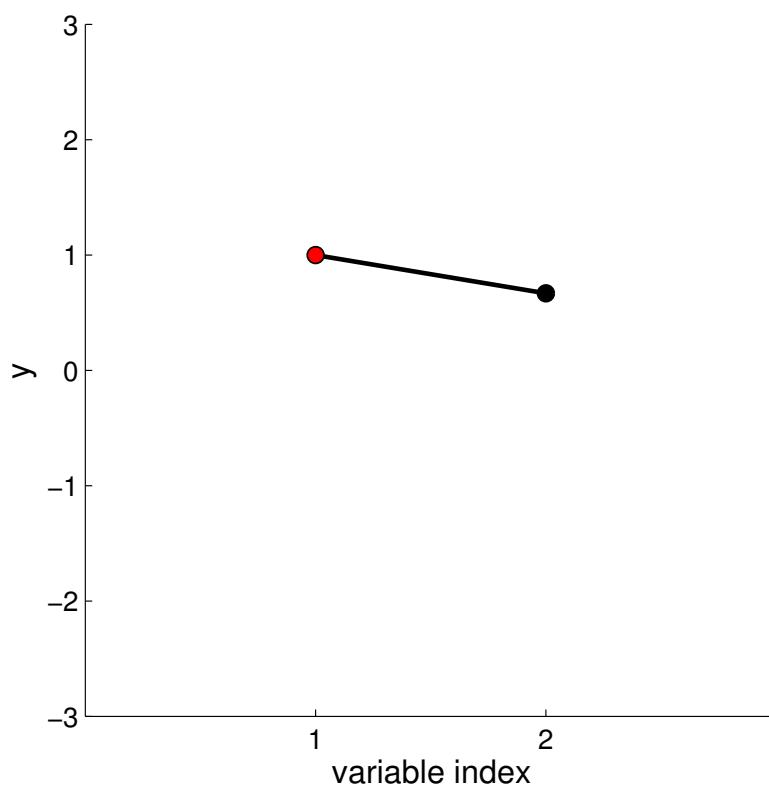
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



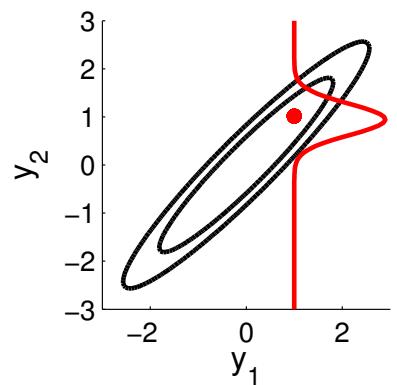
New visualisation



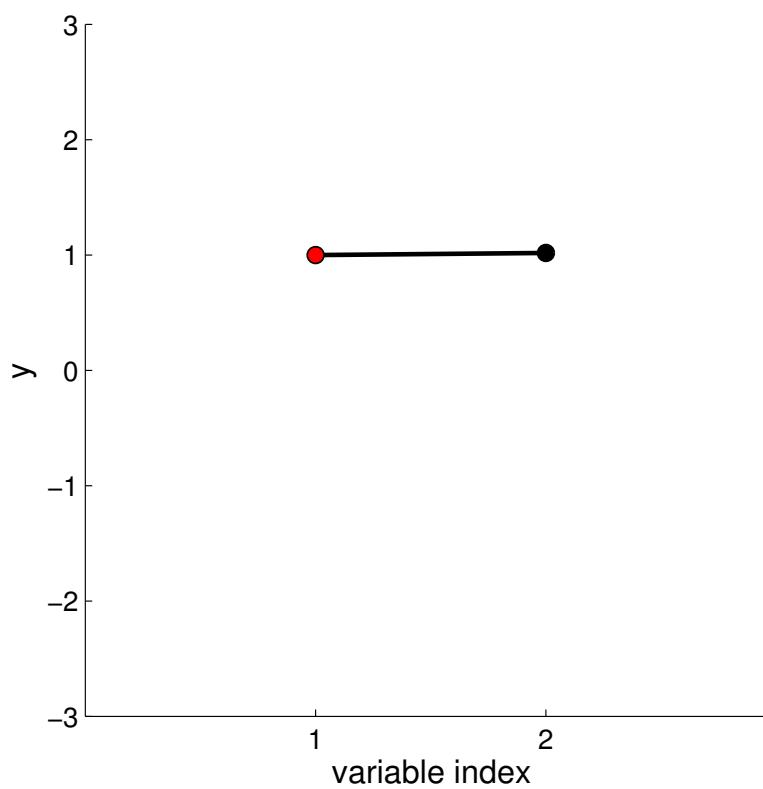
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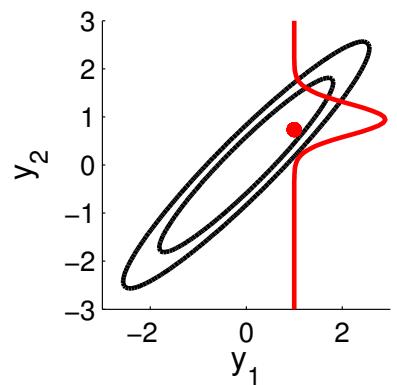
New visualisation



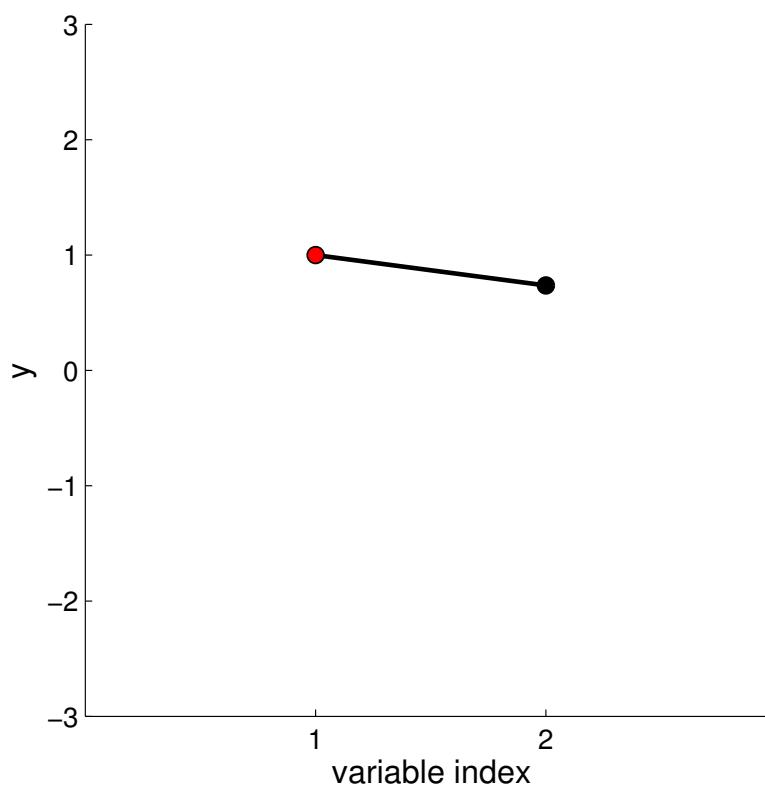
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



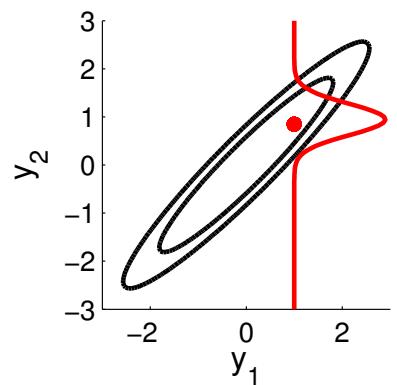
New visualisation



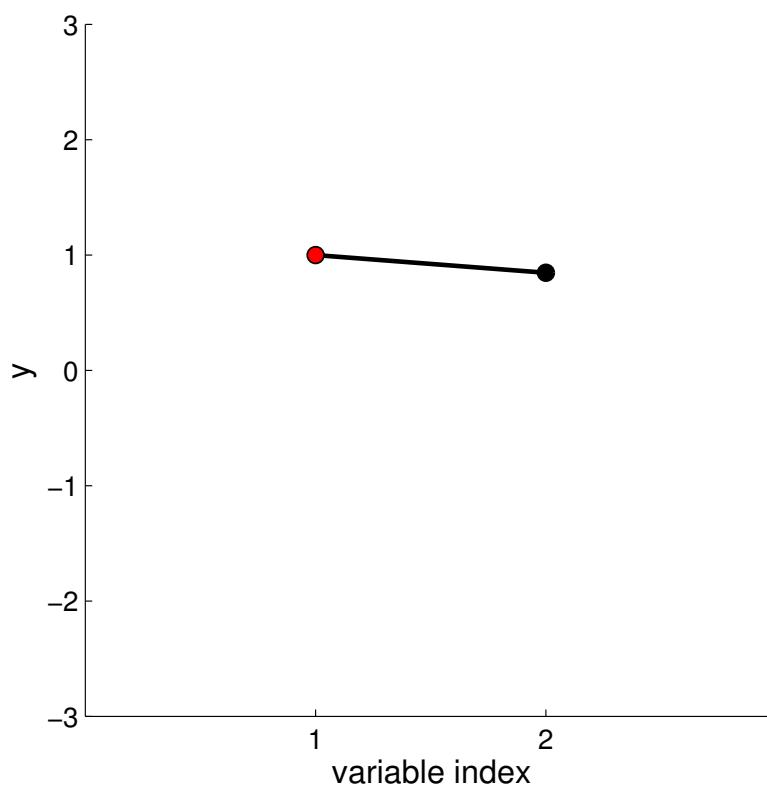
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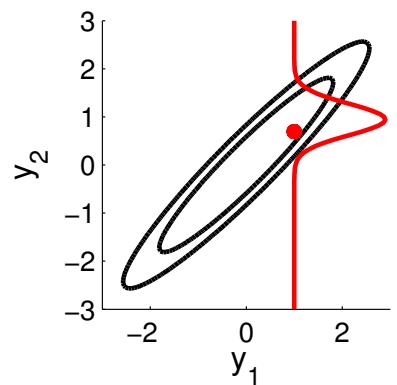
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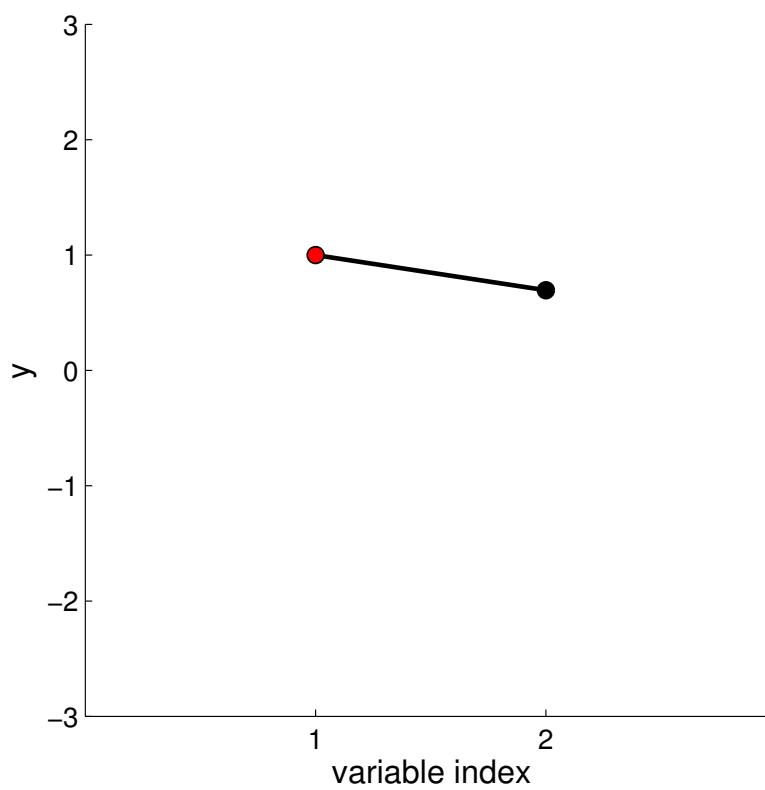
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



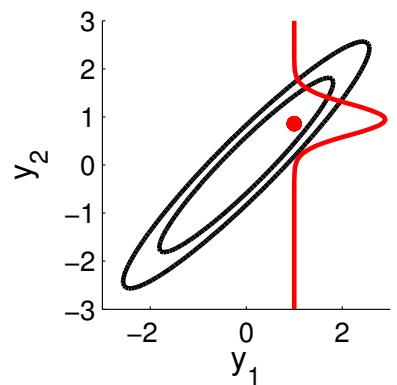
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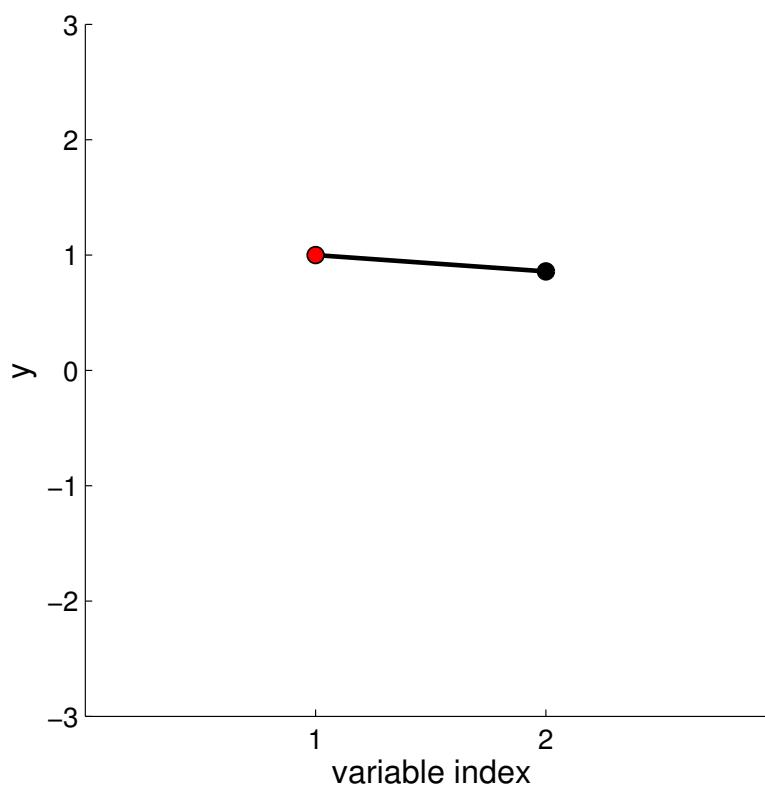
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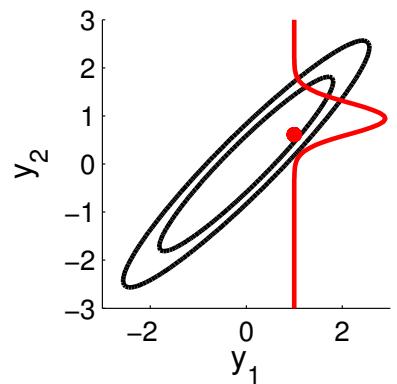
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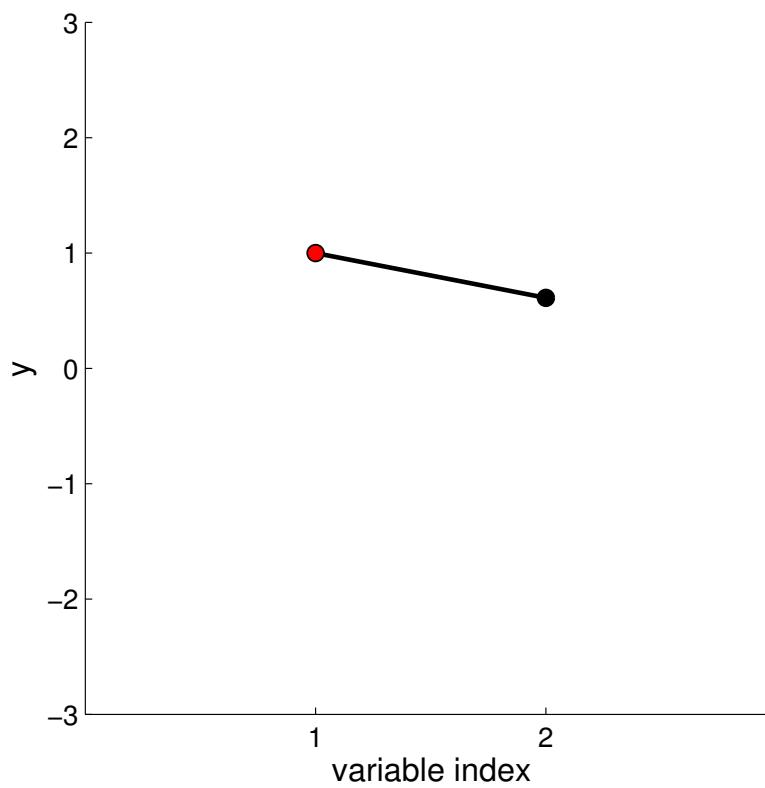
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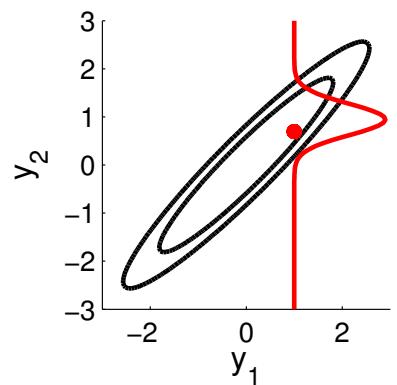
New visualisation



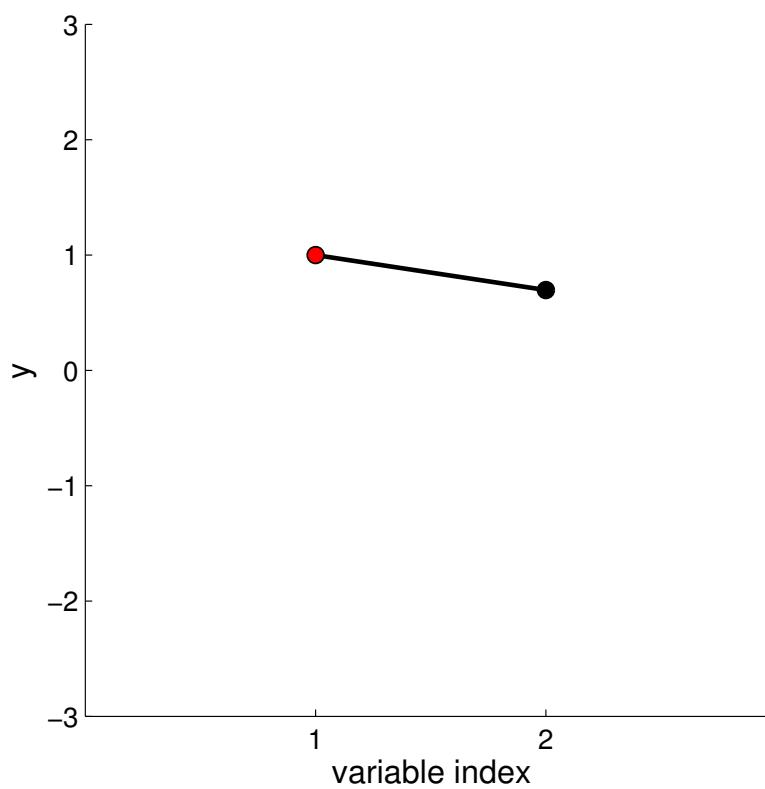
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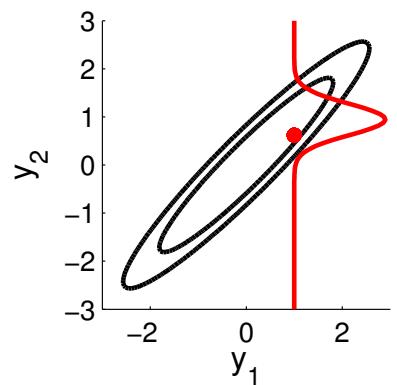
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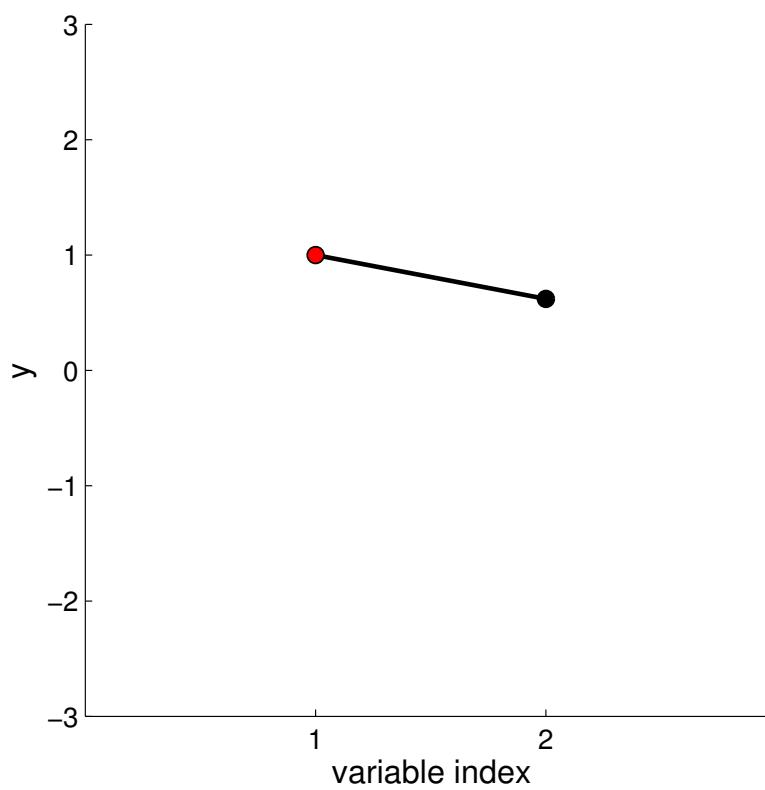
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



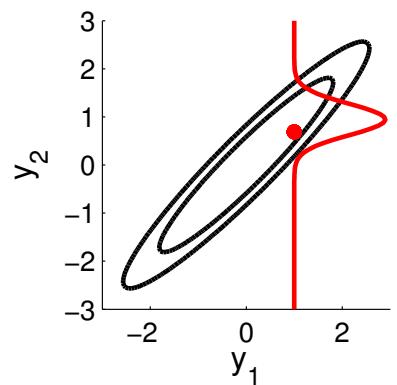
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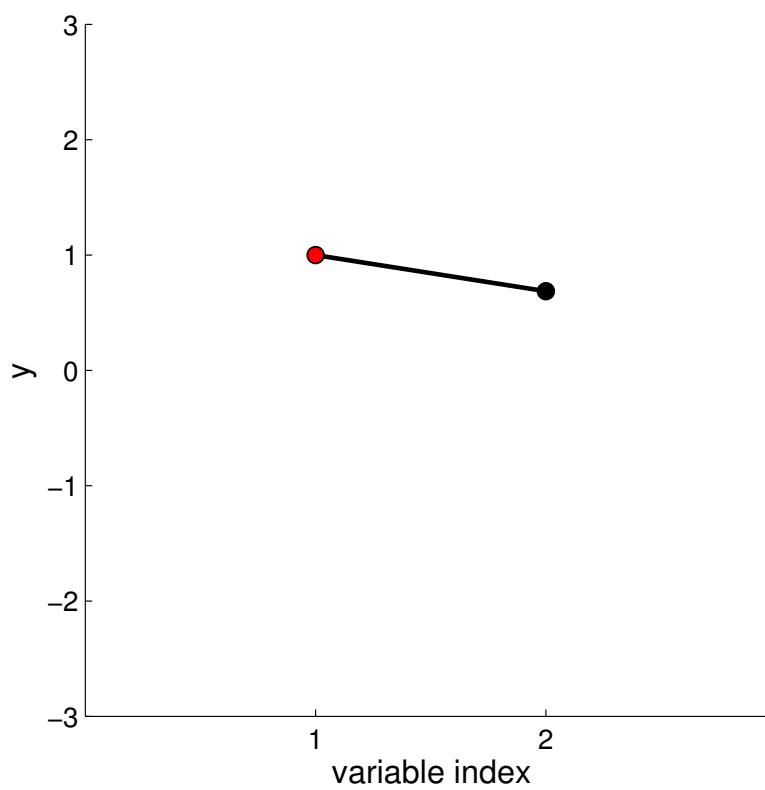
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



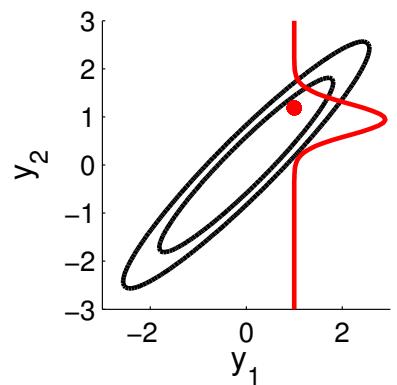
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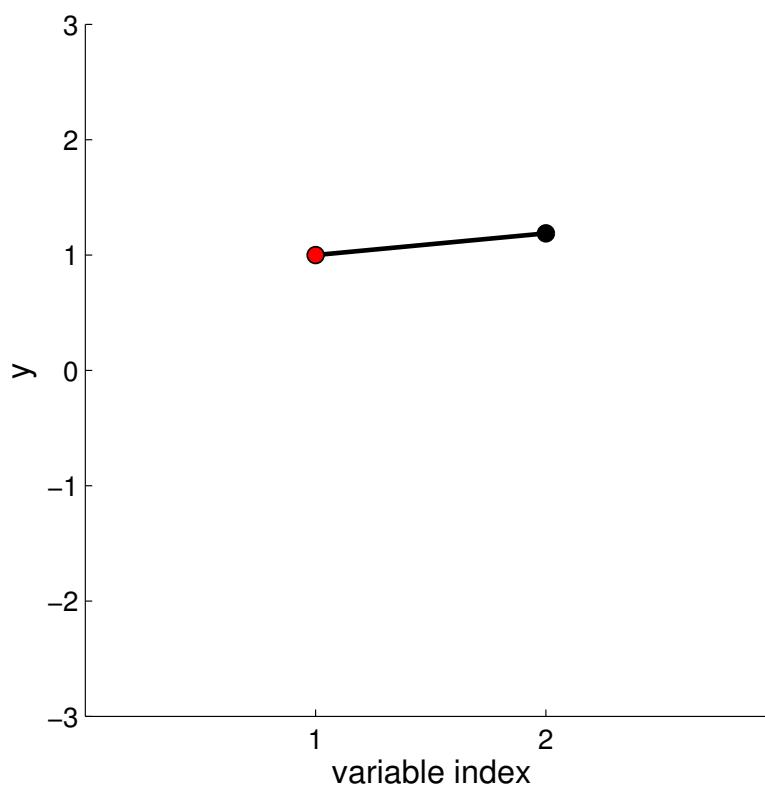
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



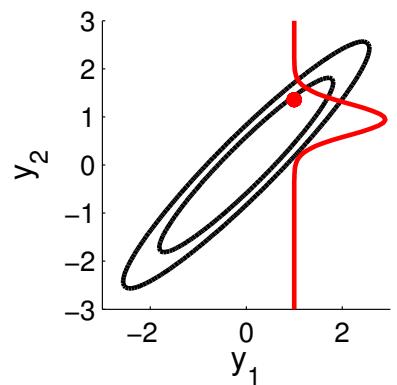
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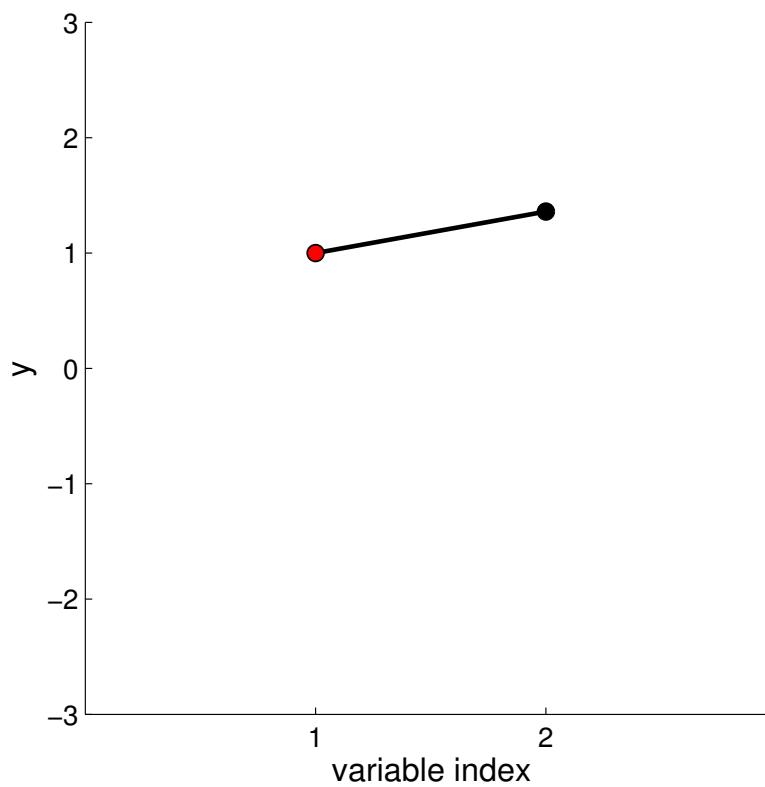
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



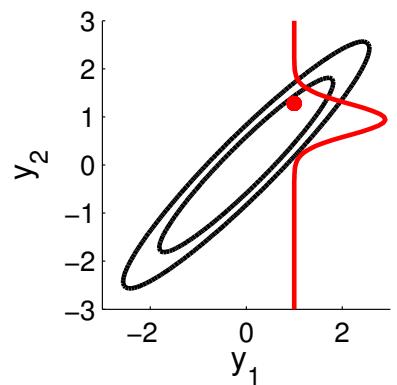
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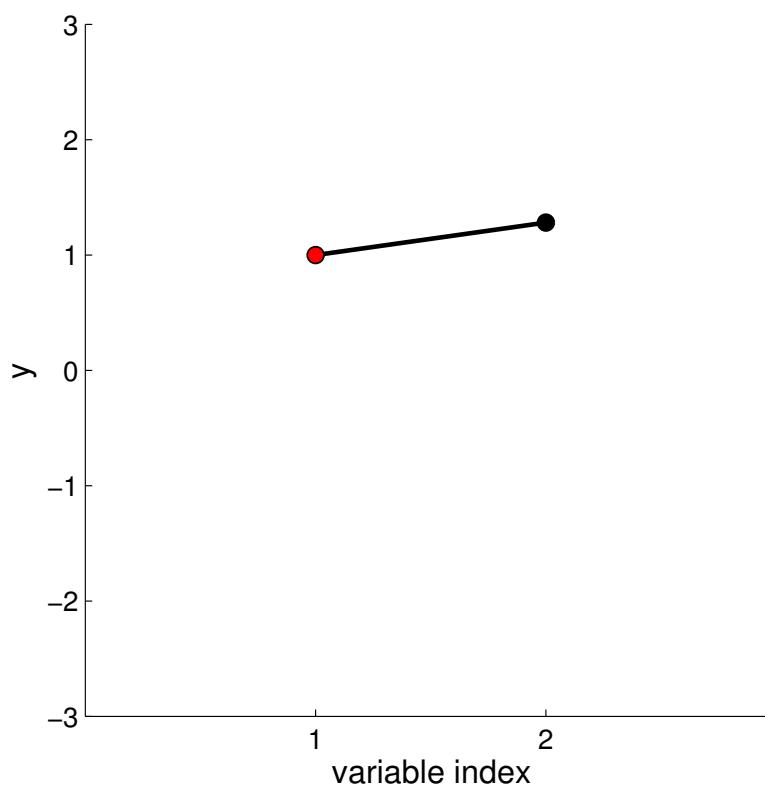
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



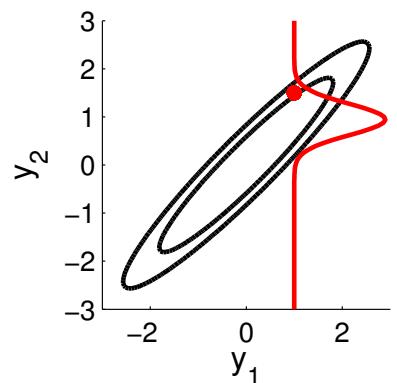
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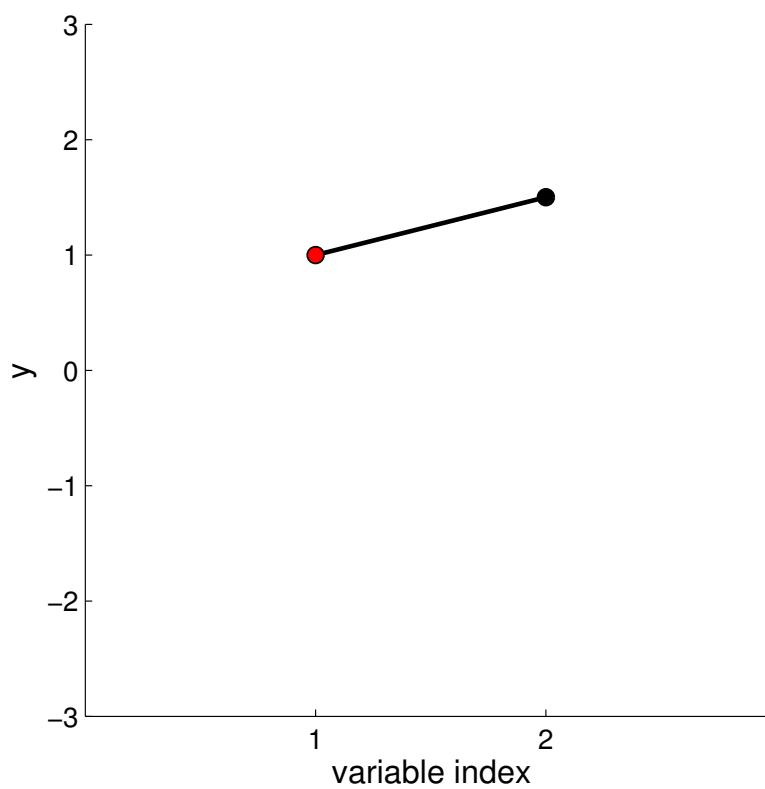
$$\Sigma = \begin{bmatrix} 1 & .9 \\ .9 & 1 \end{bmatrix}$$



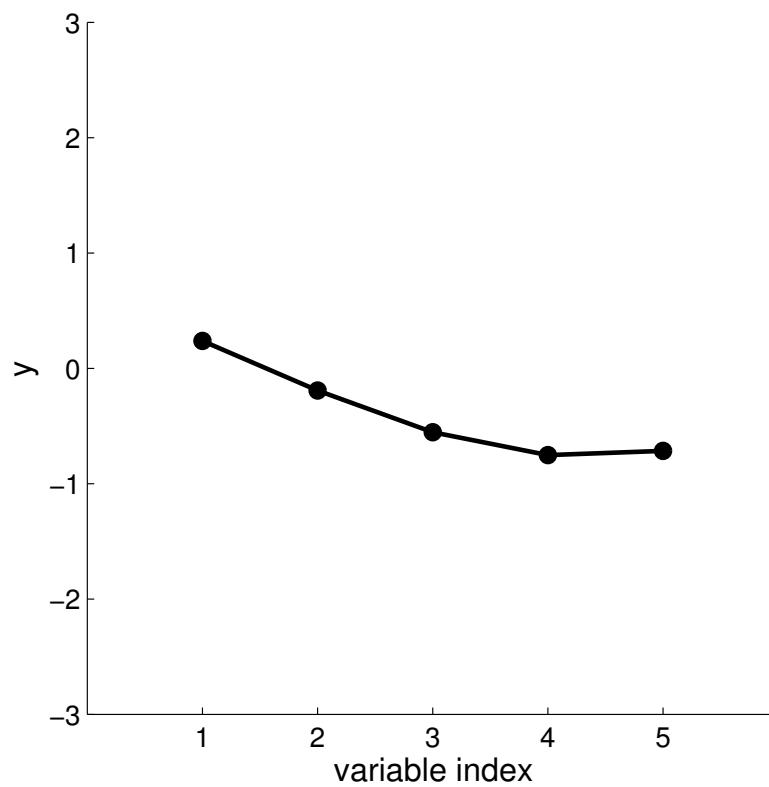
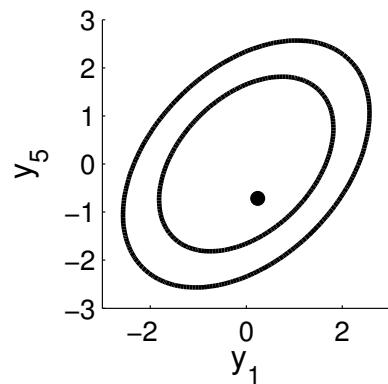
New visualisation



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

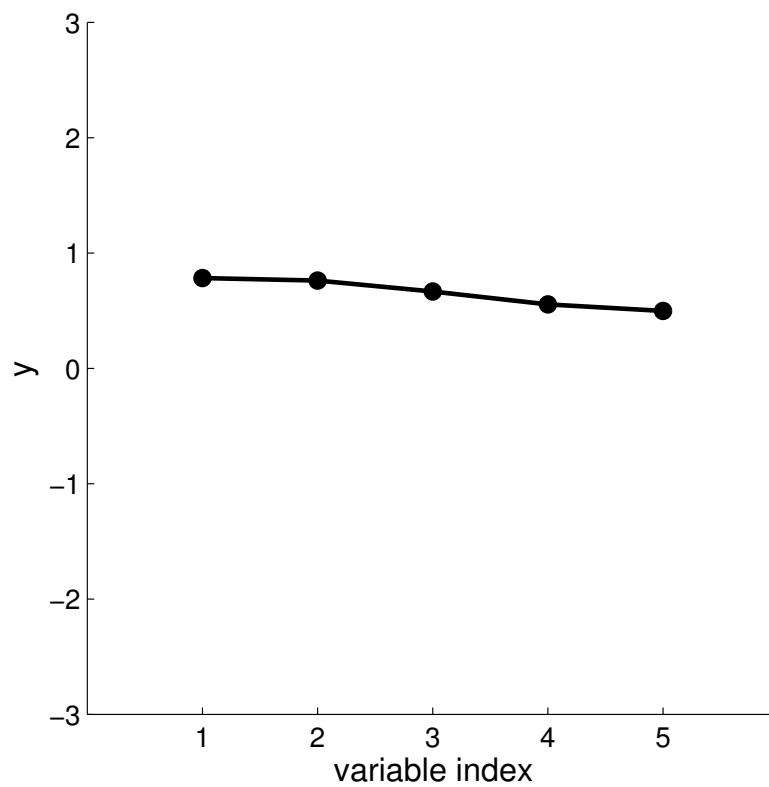
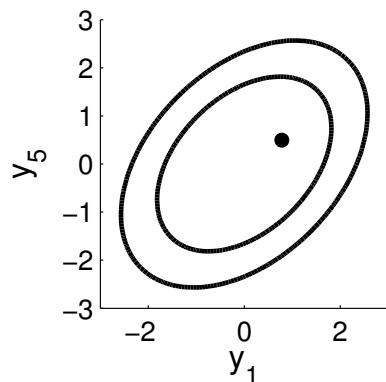


New visualisation



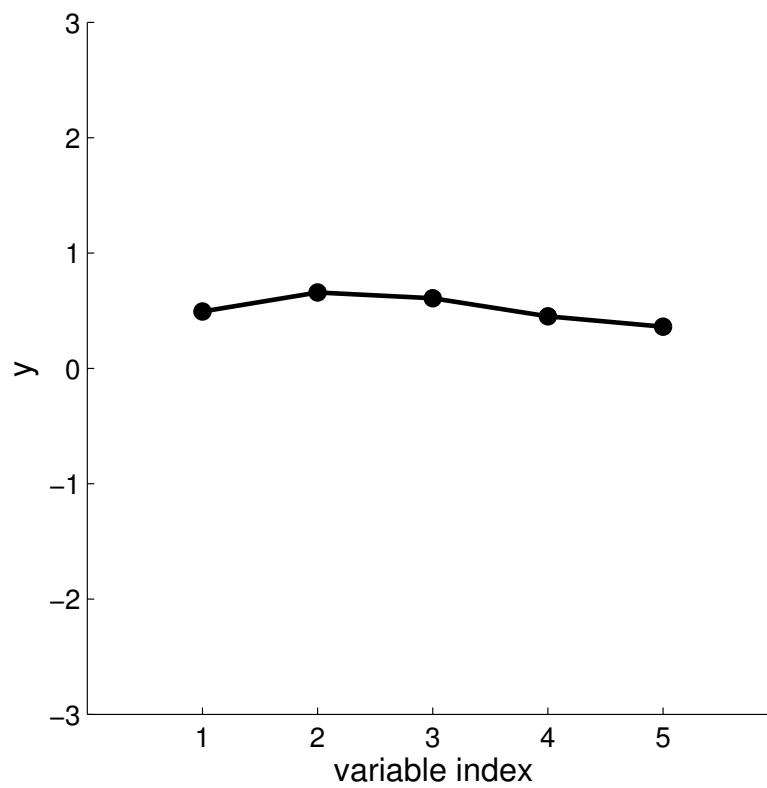
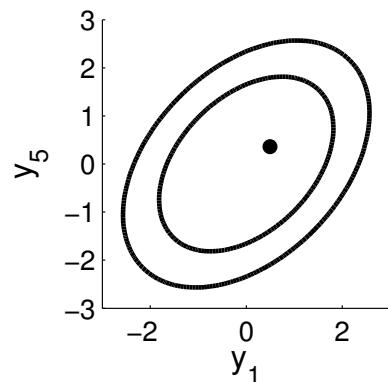
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



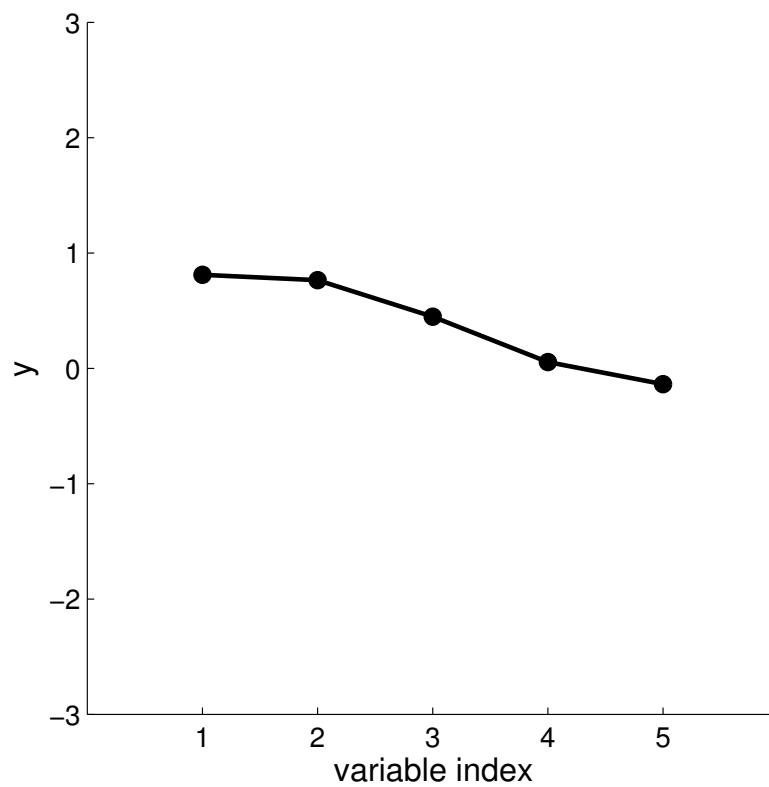
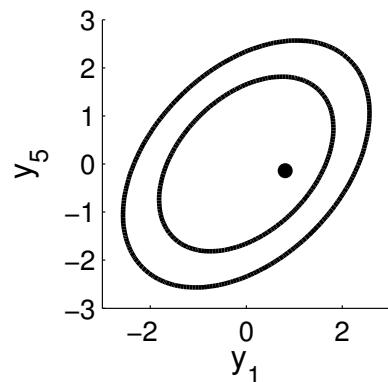
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



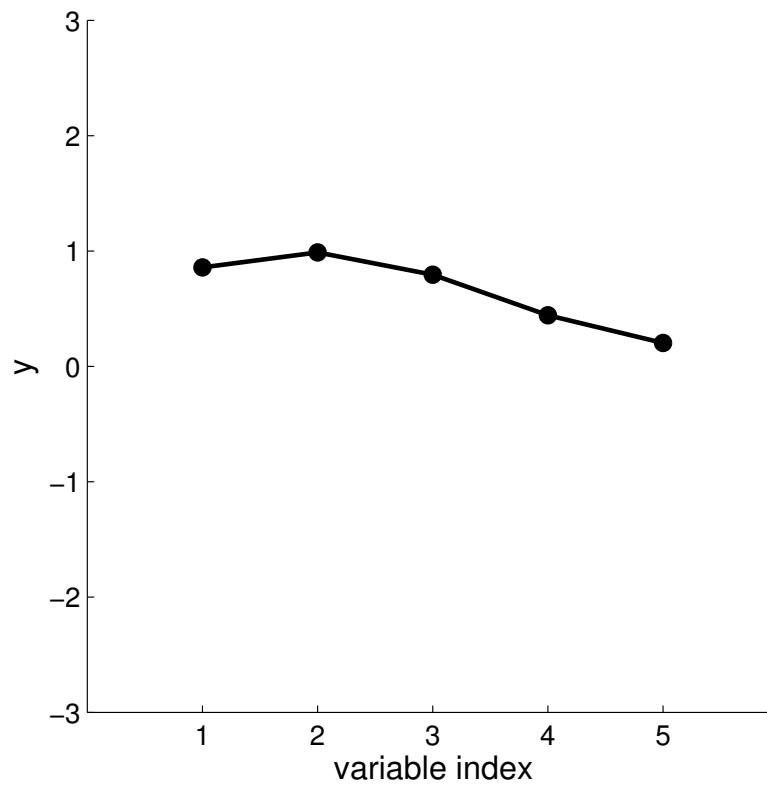
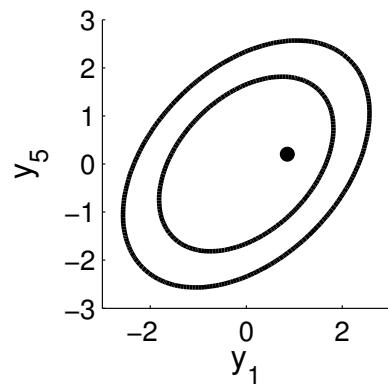
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



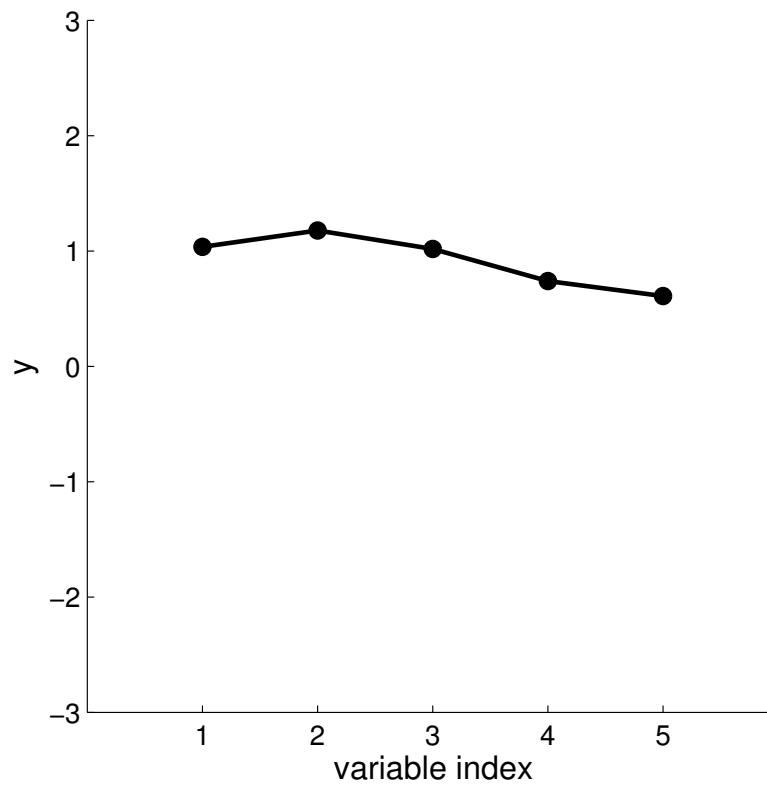
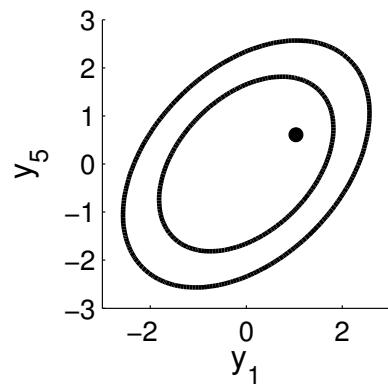
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New visualisation



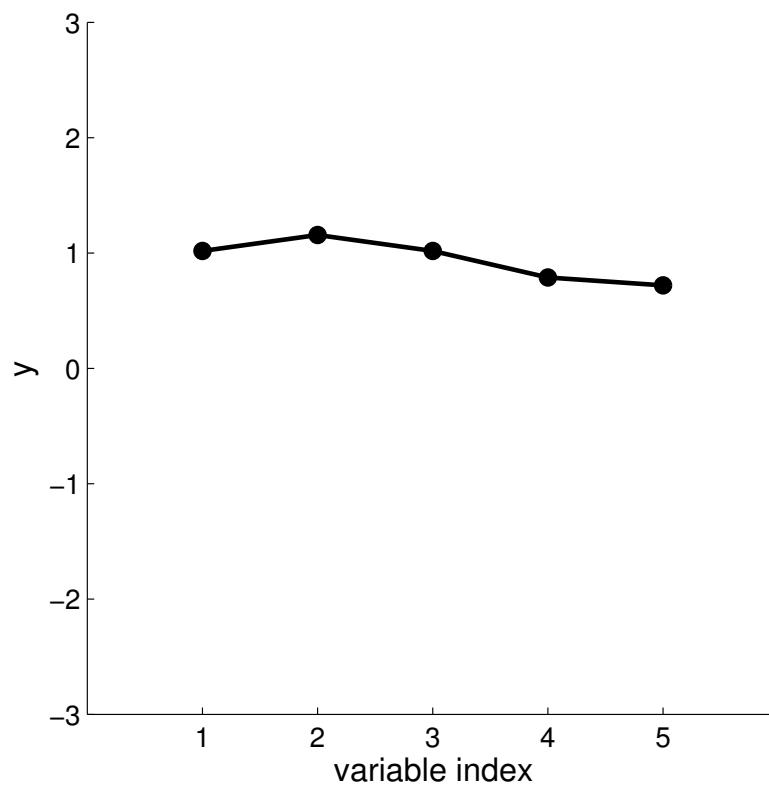
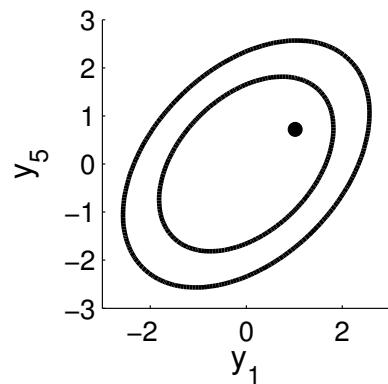
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New visualisation



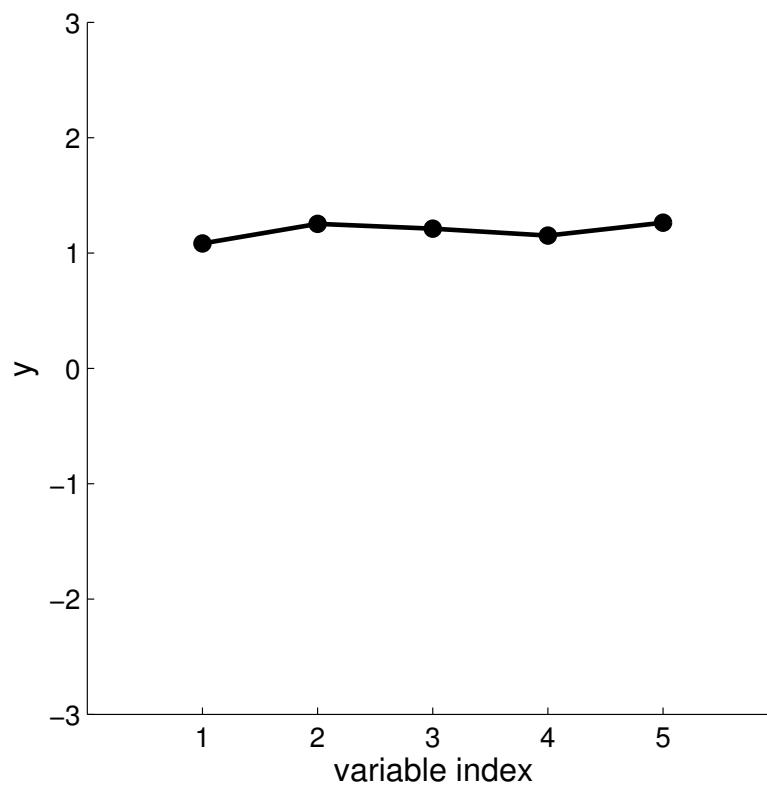
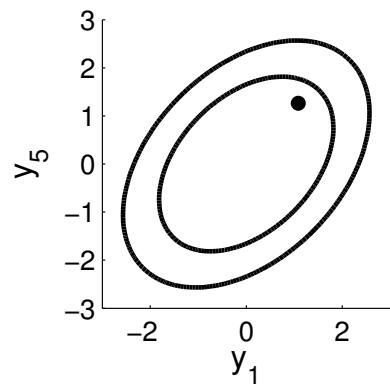
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



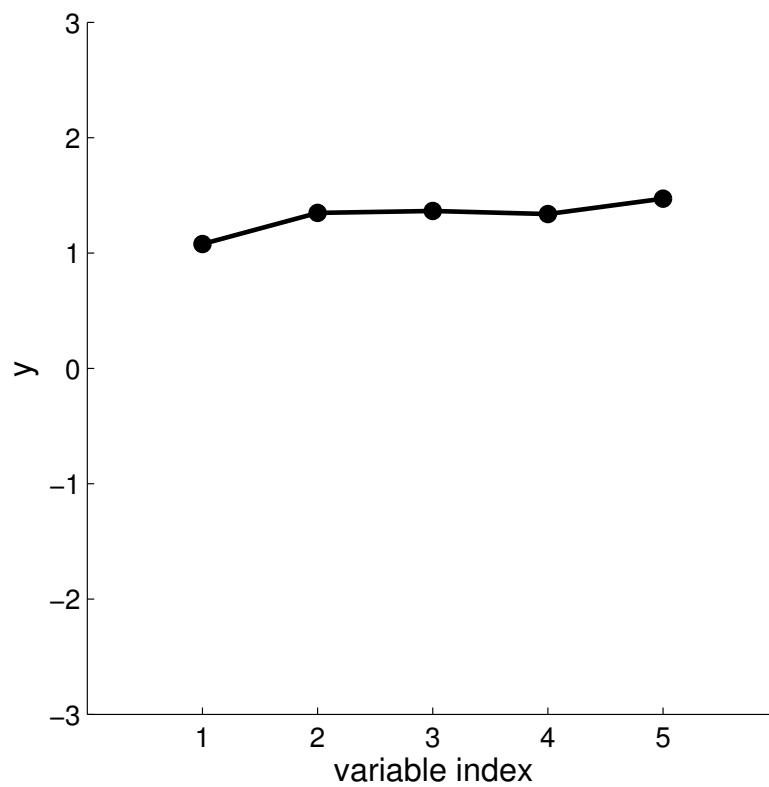
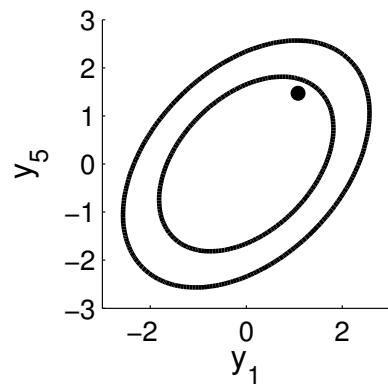
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New visualisation



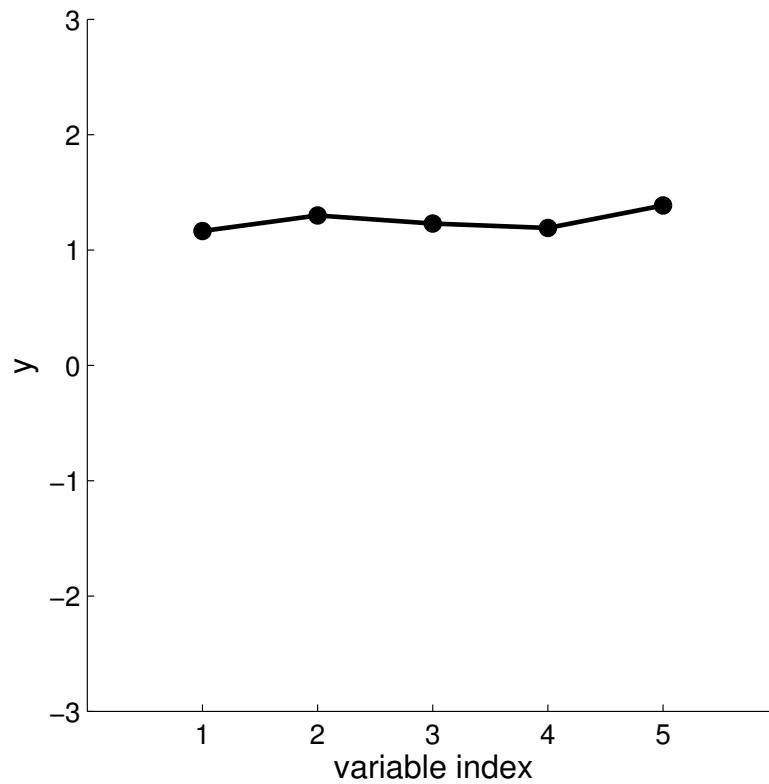
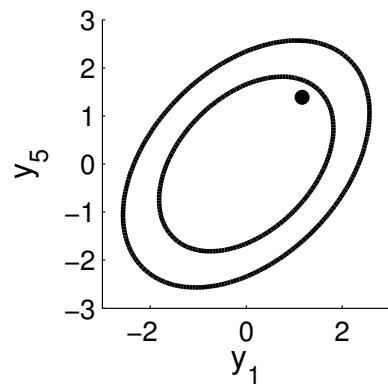
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



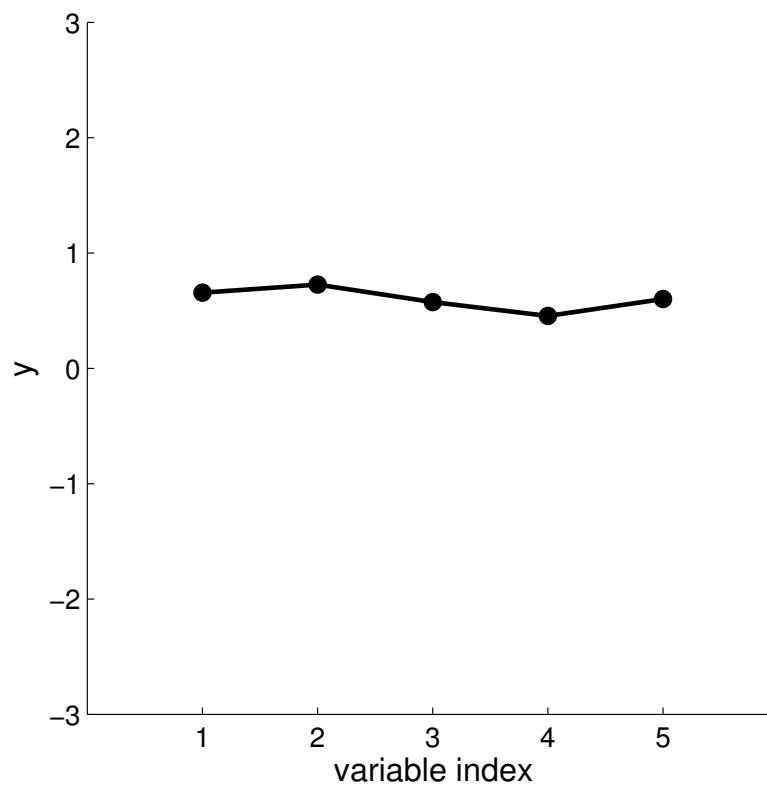
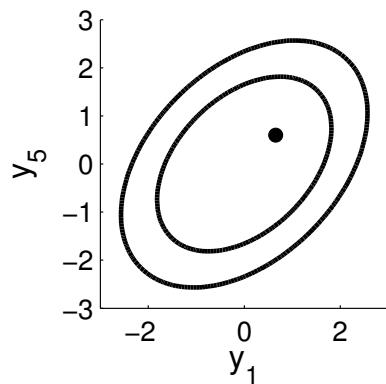
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



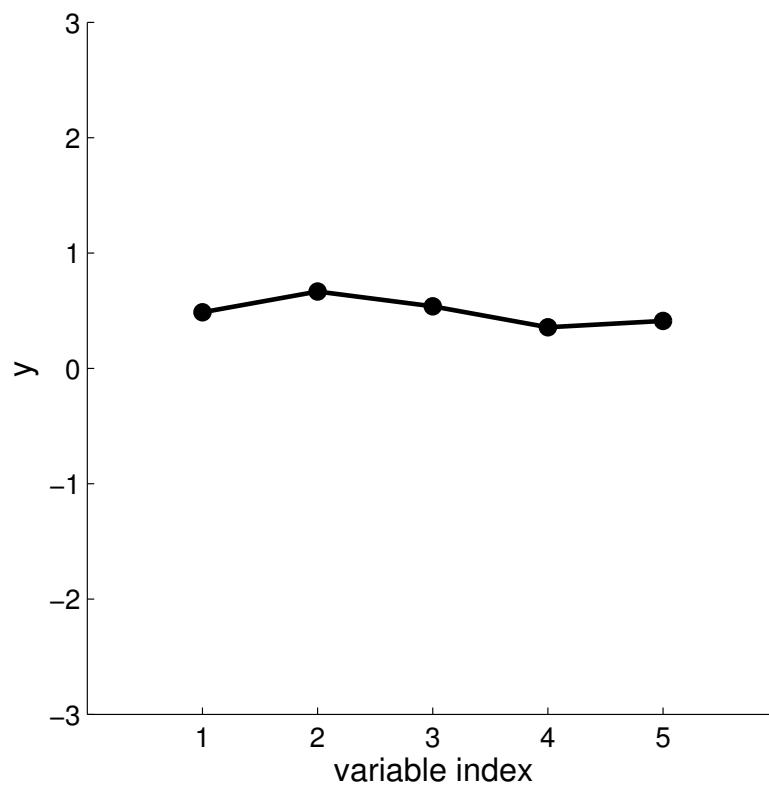
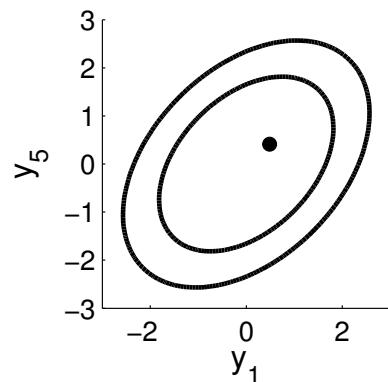
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New visualisation



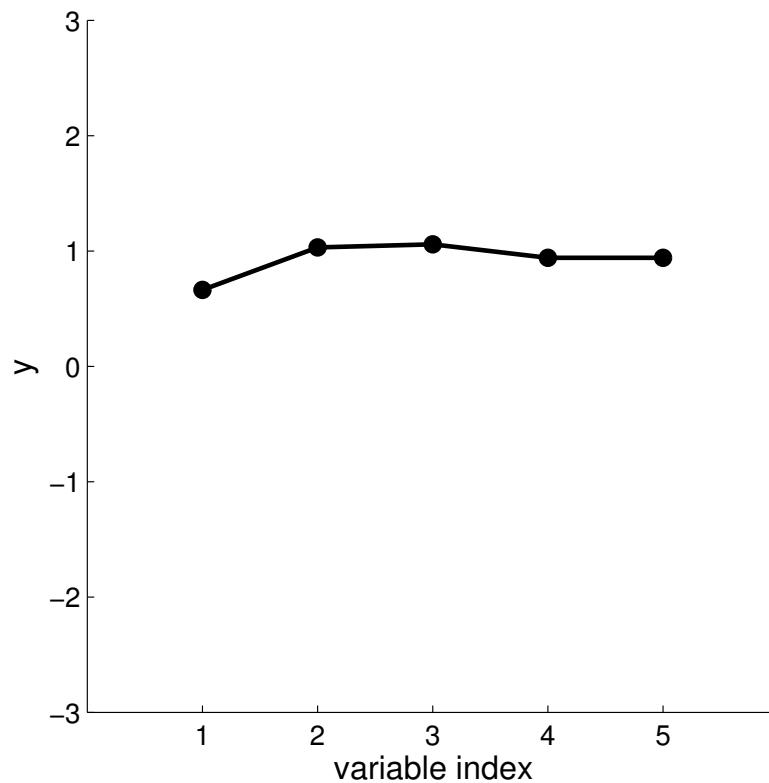
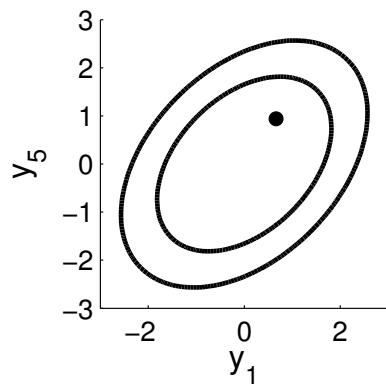
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



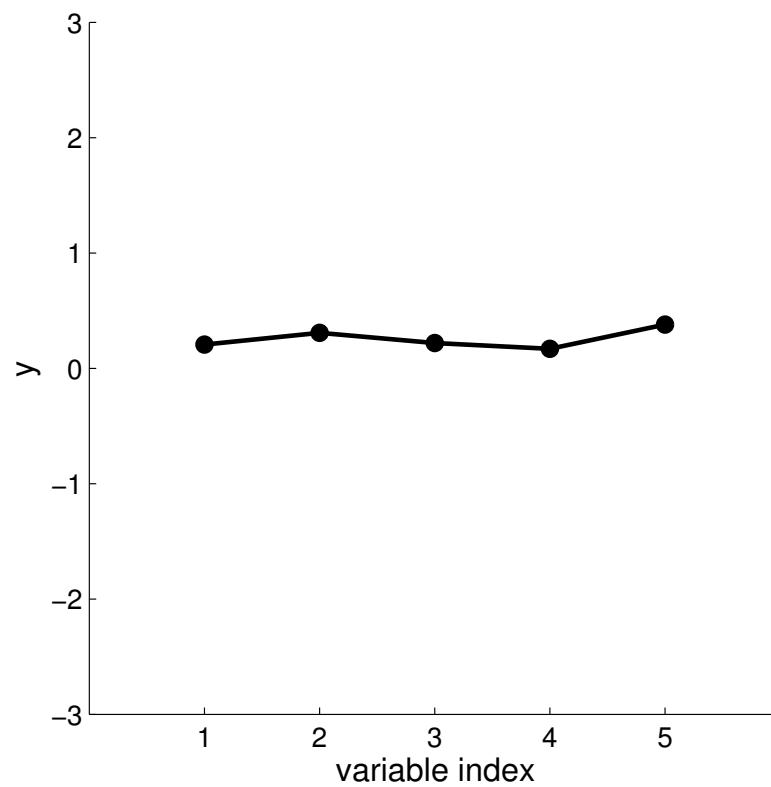
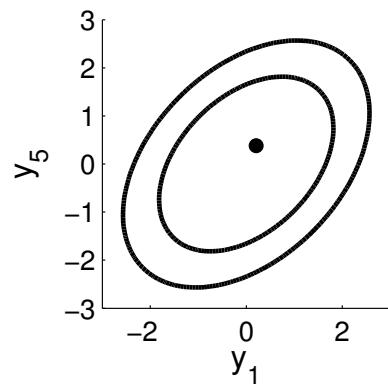
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



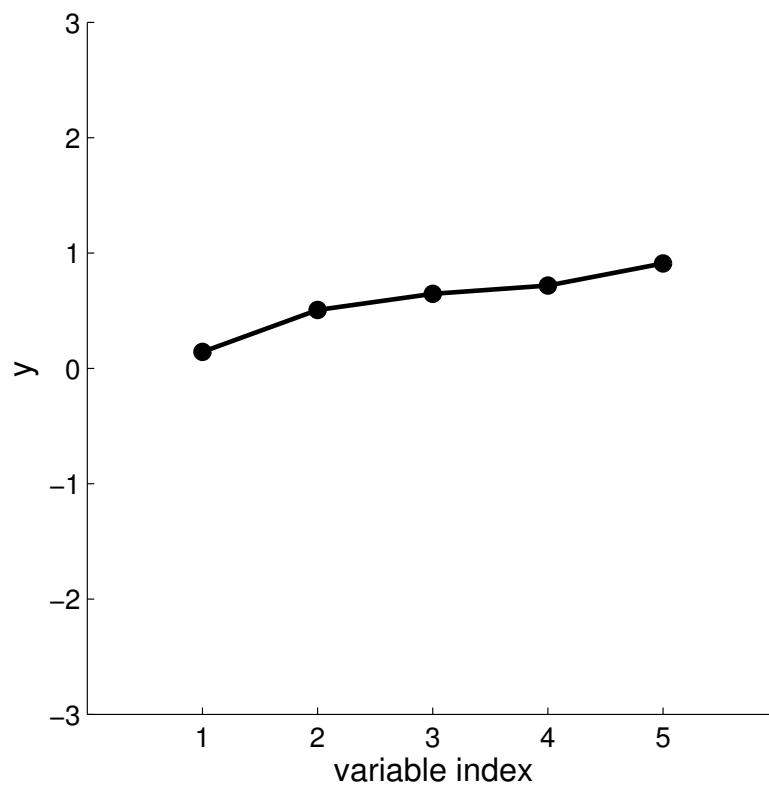
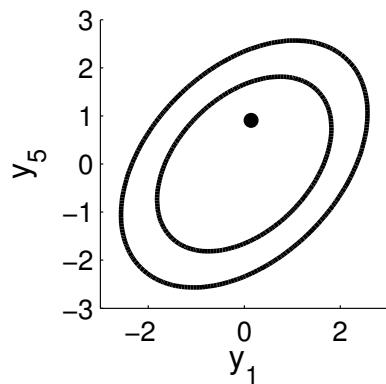
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New visualisation



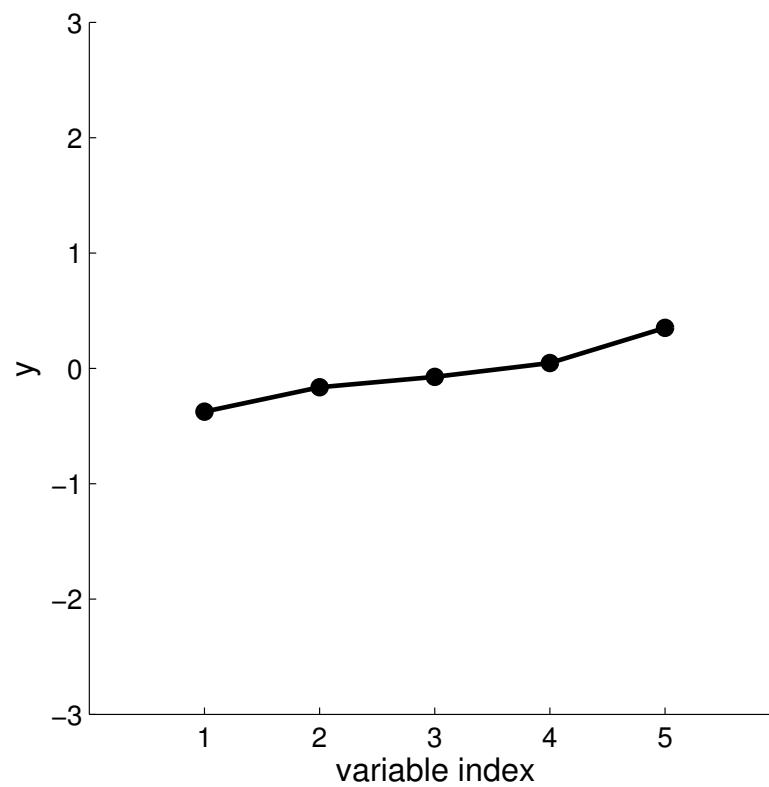
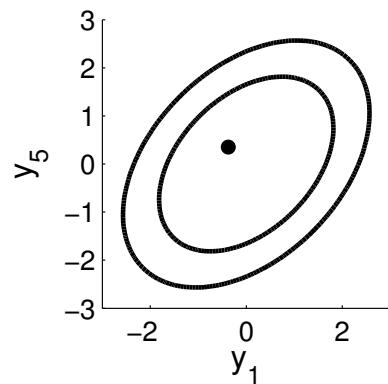
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New visualisation



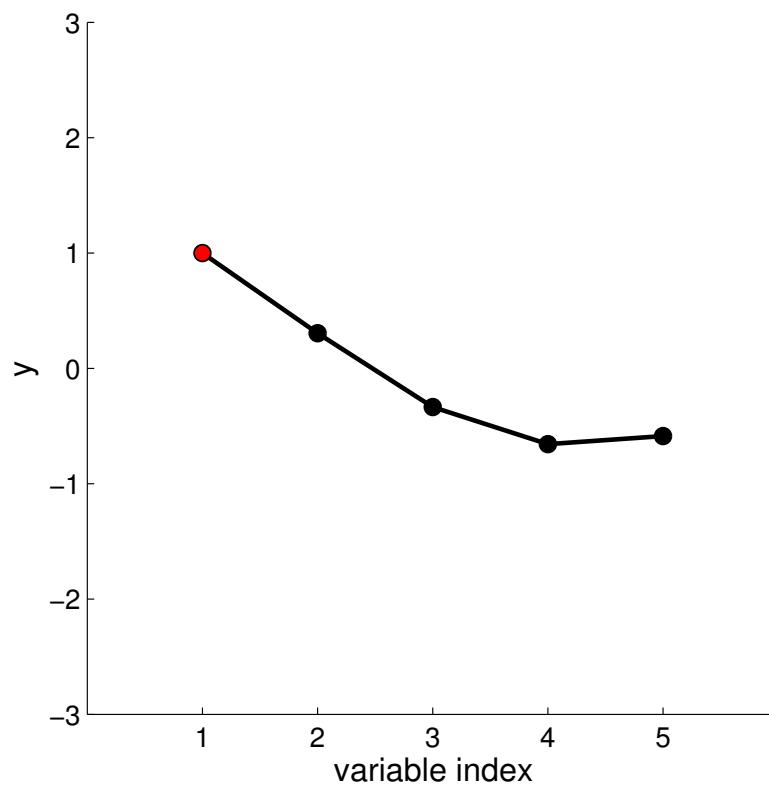
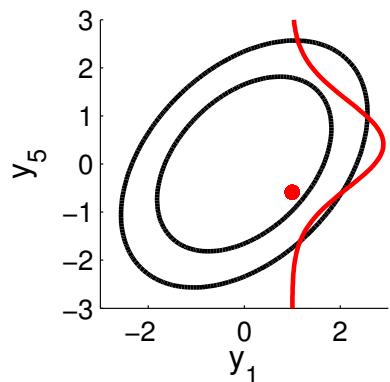
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



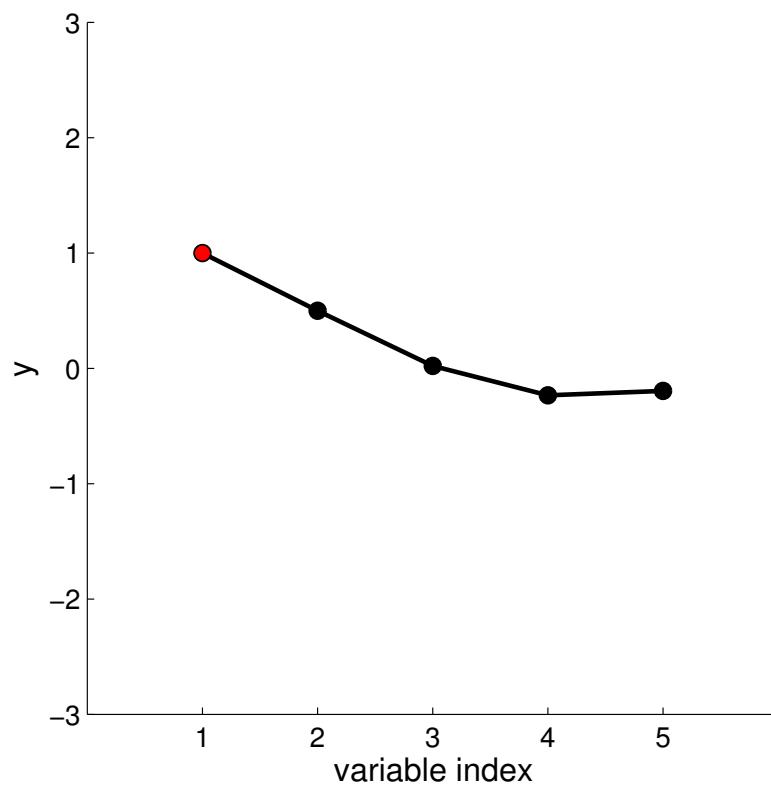
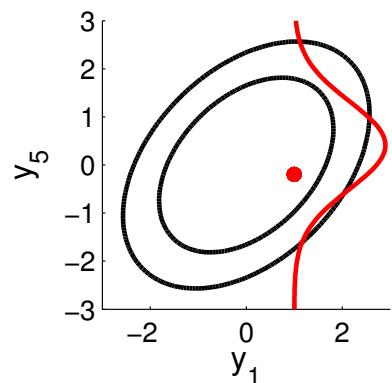
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New visualisation



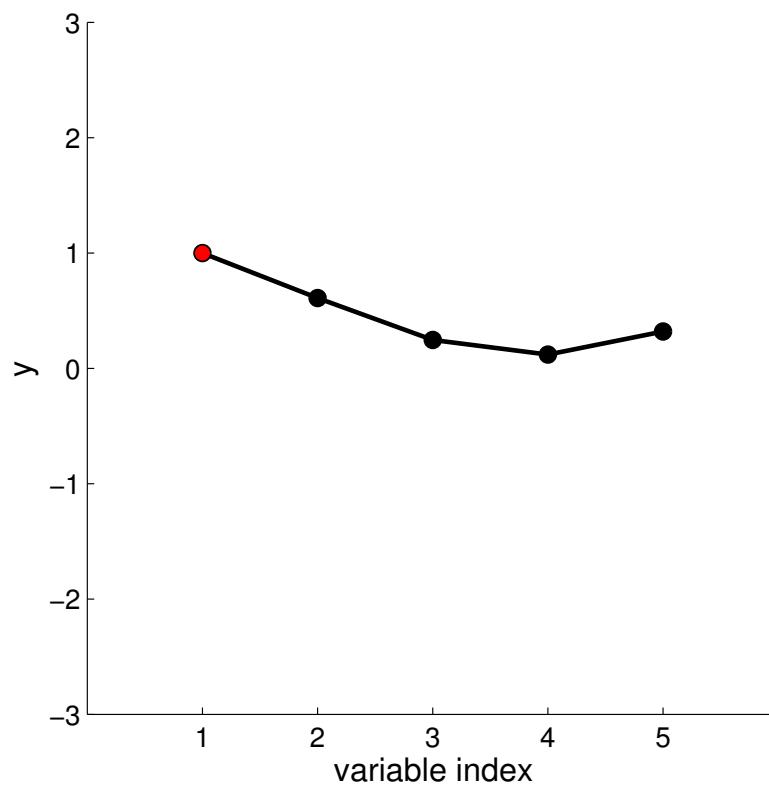
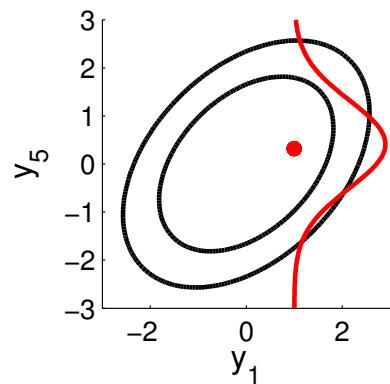
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New visualisation



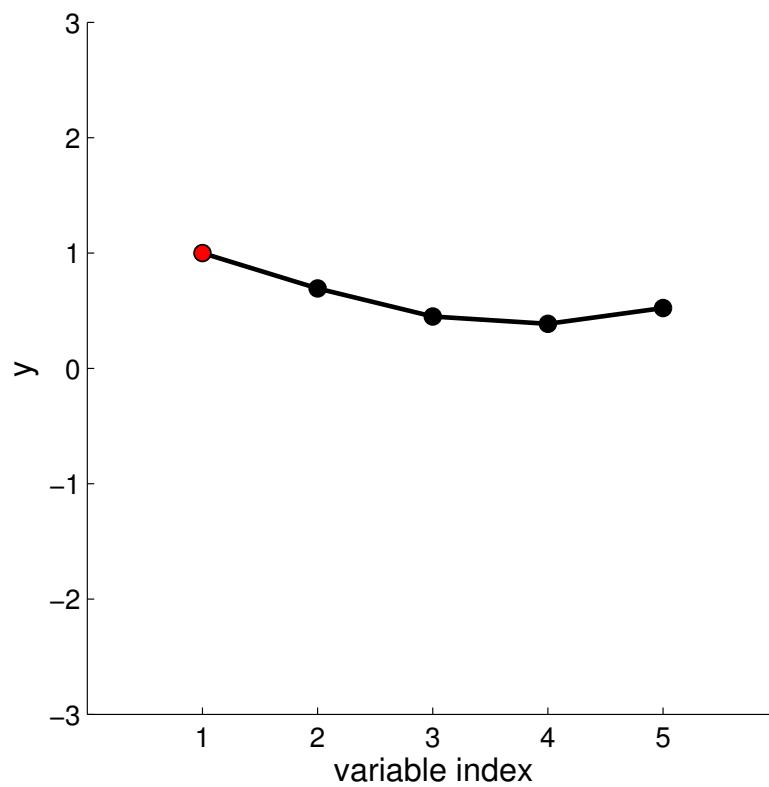
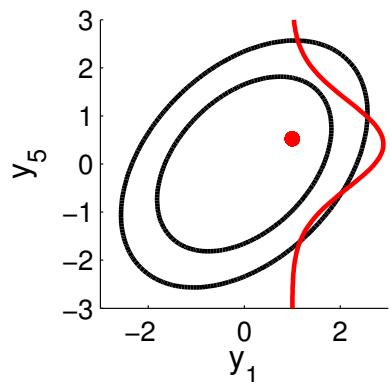
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New visualisation



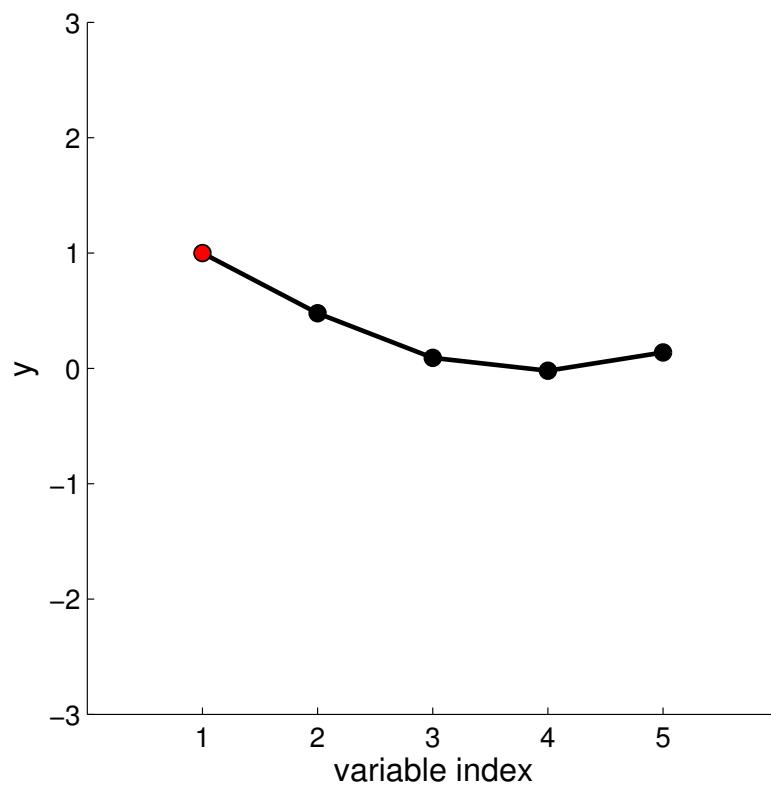
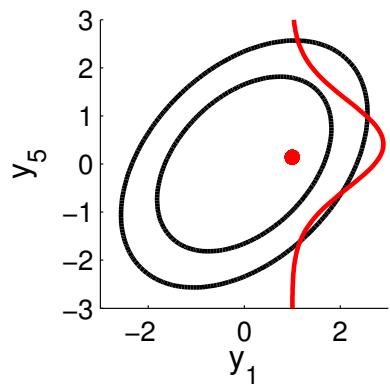
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New visualisation



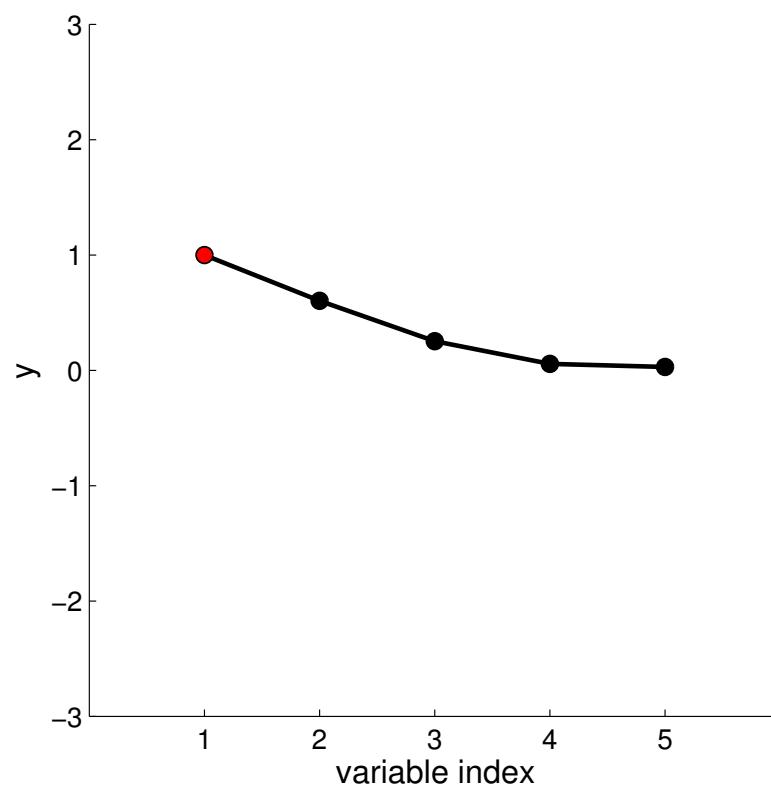
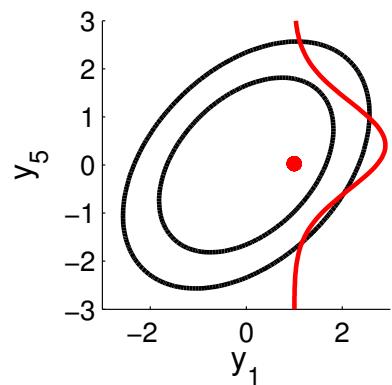
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



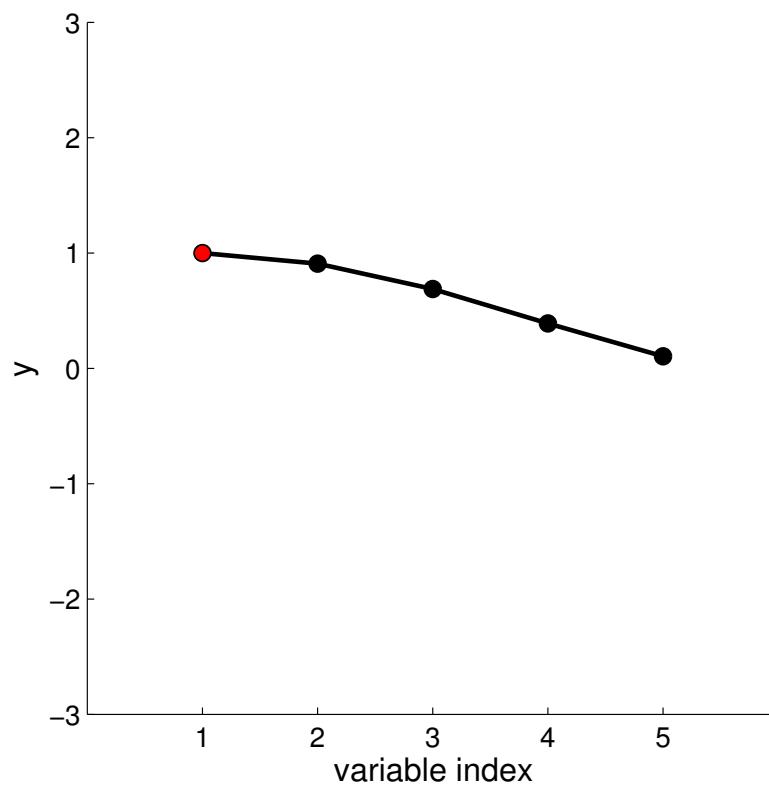
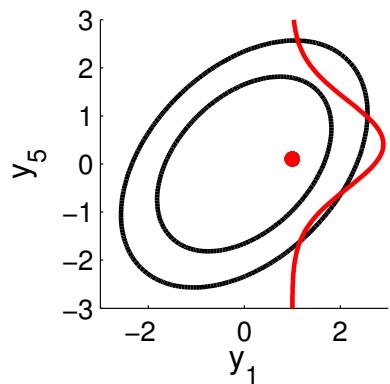
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



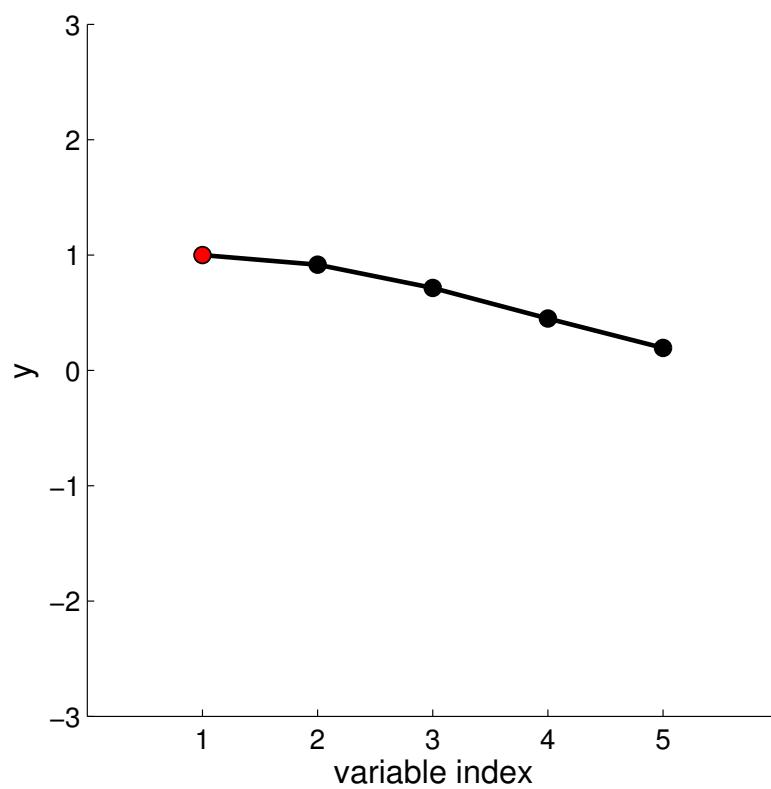
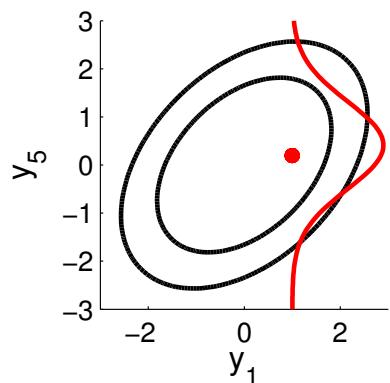
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



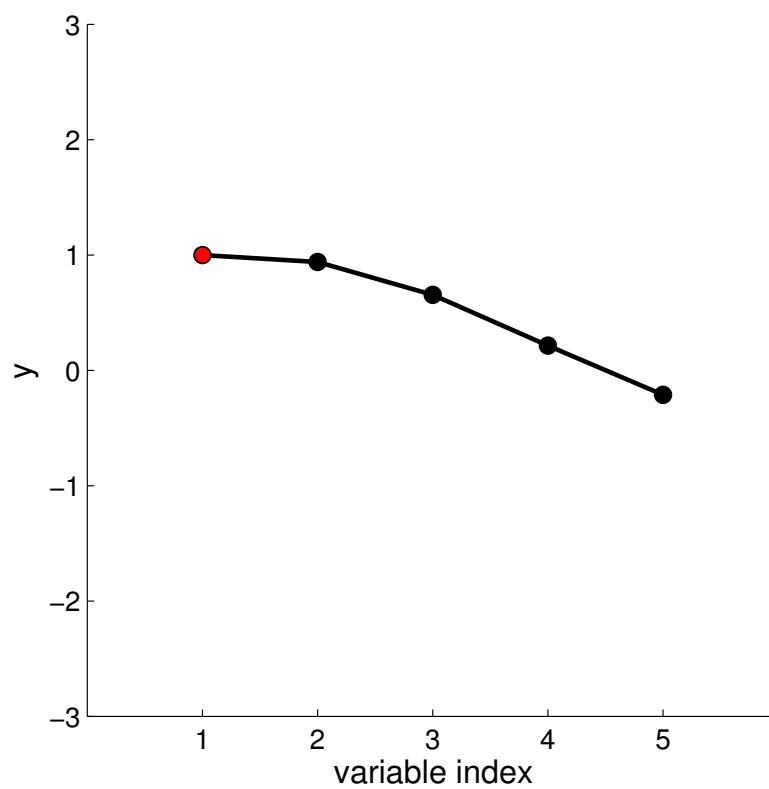
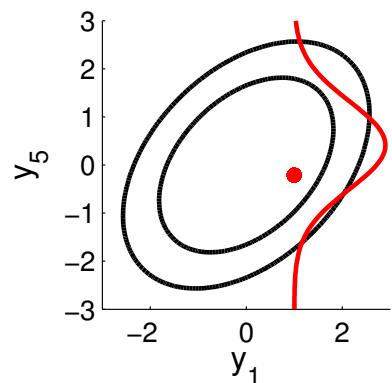
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



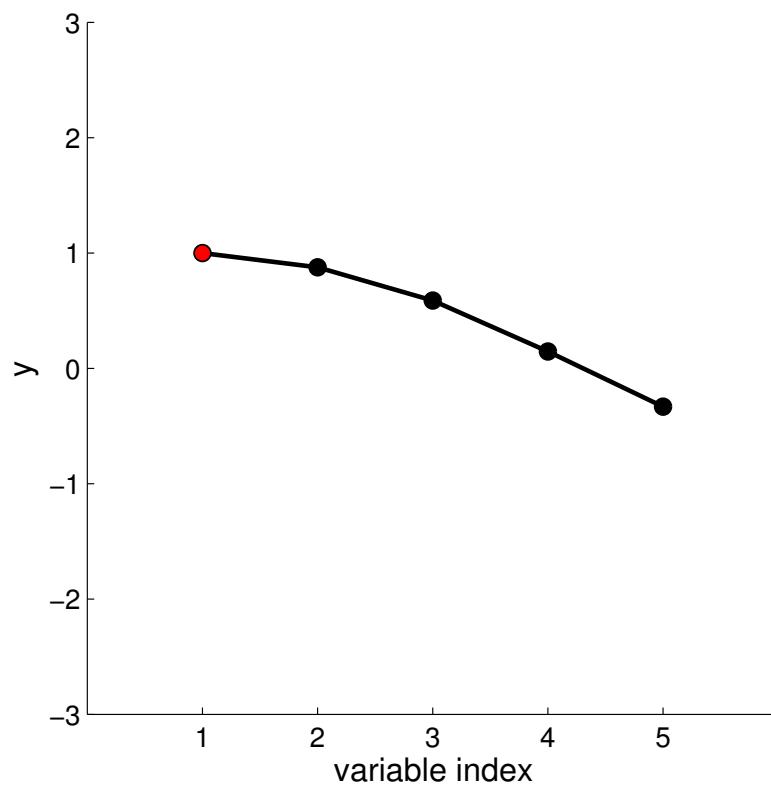
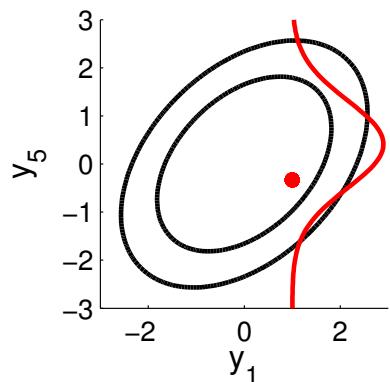
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



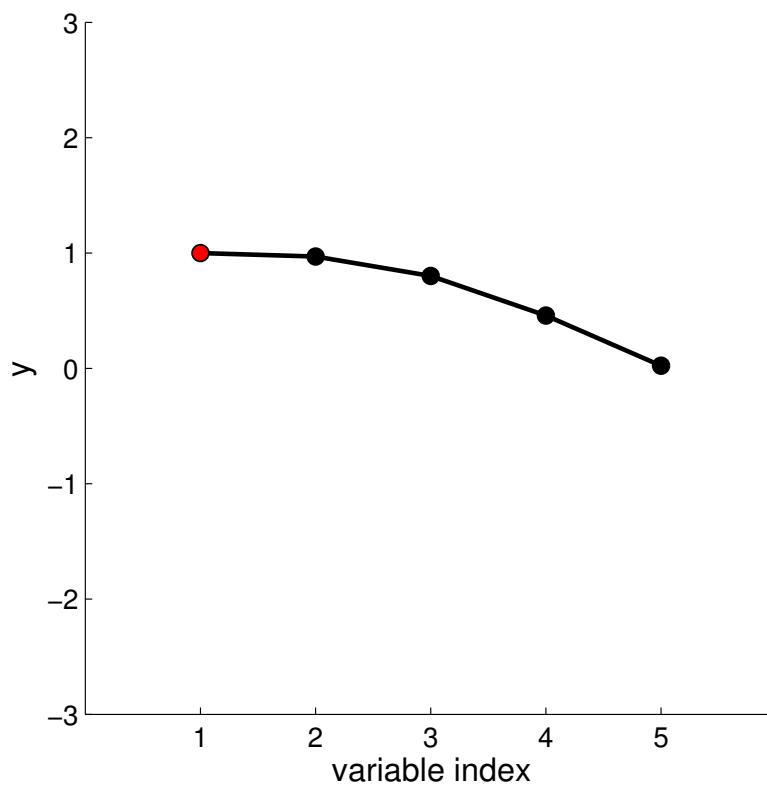
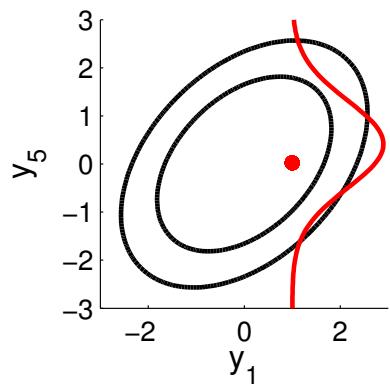
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



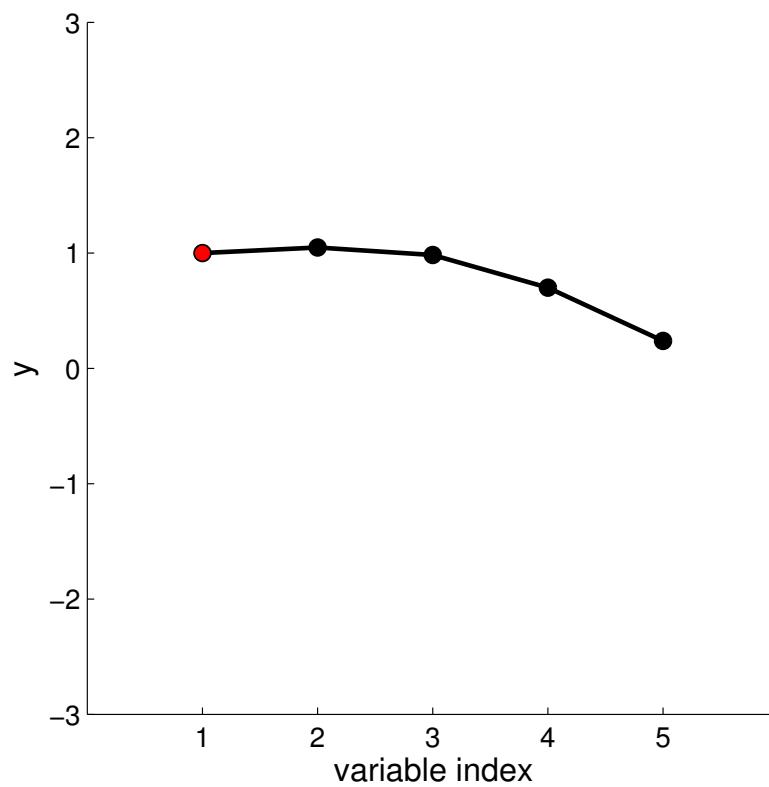
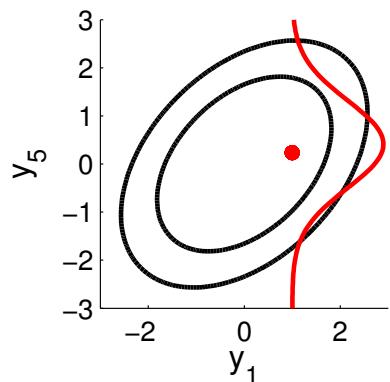
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



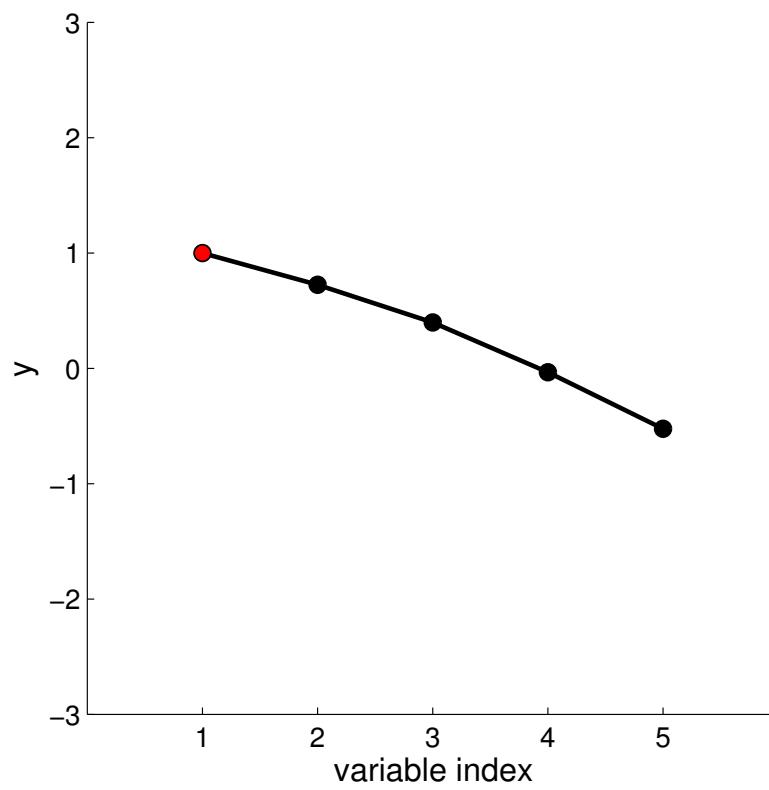
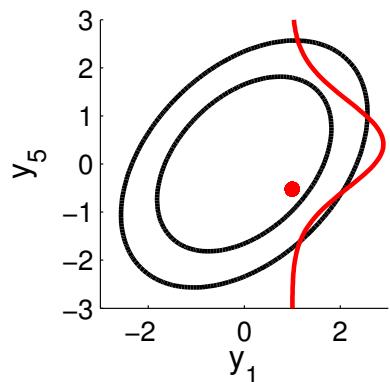
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New visualisation



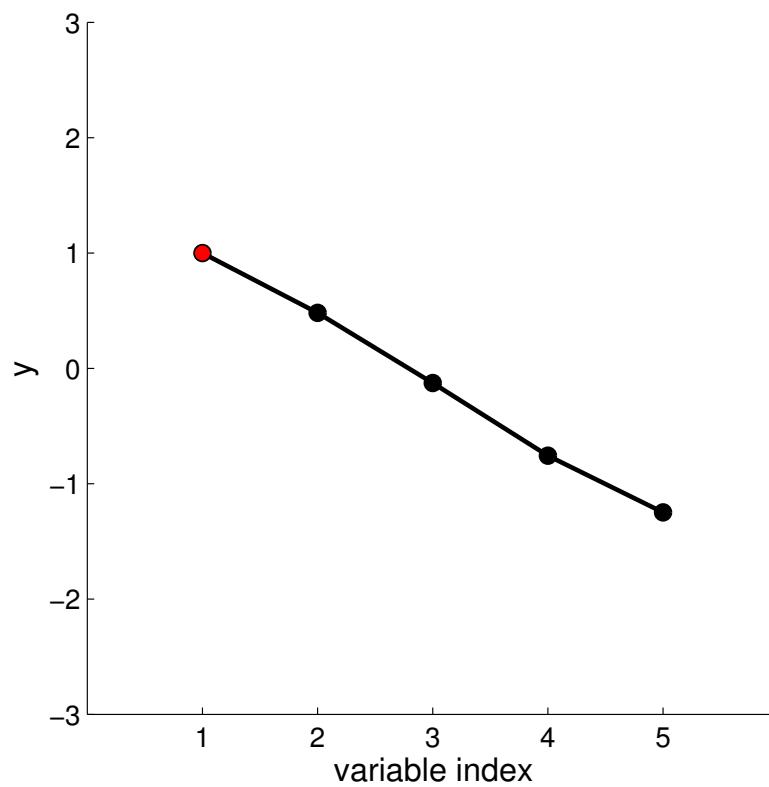
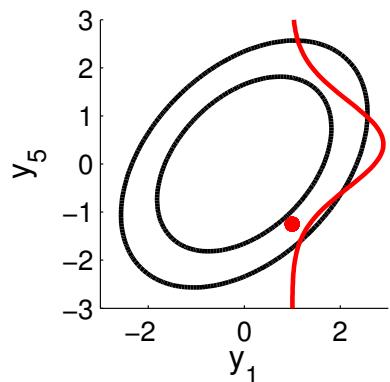
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New visualisation



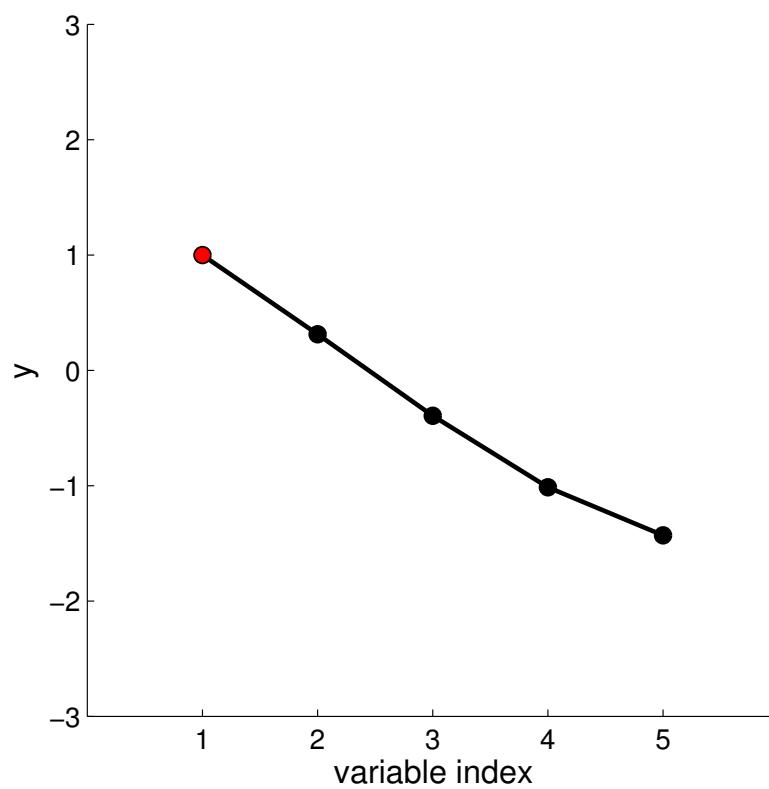
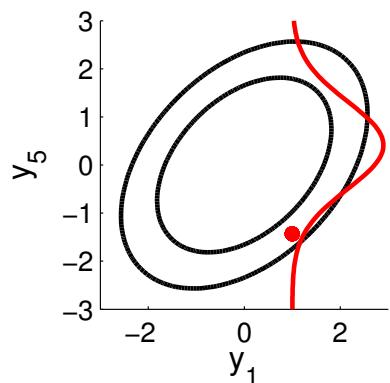
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



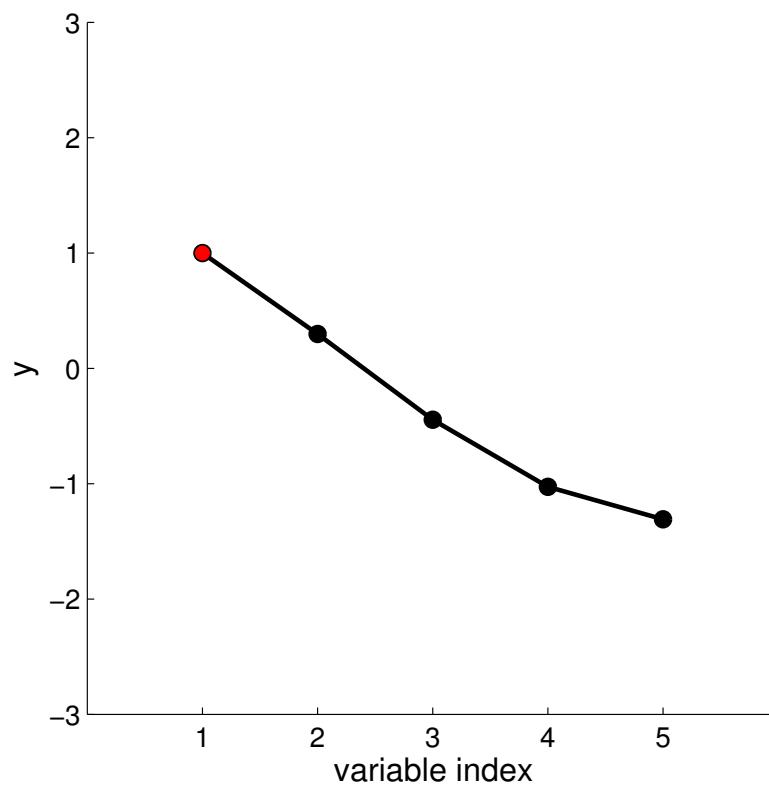
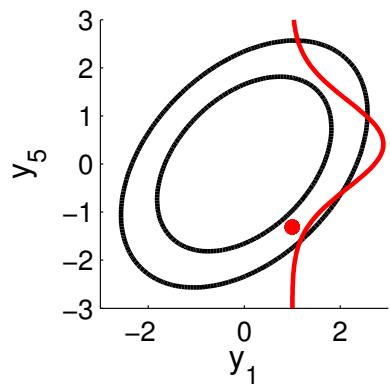
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



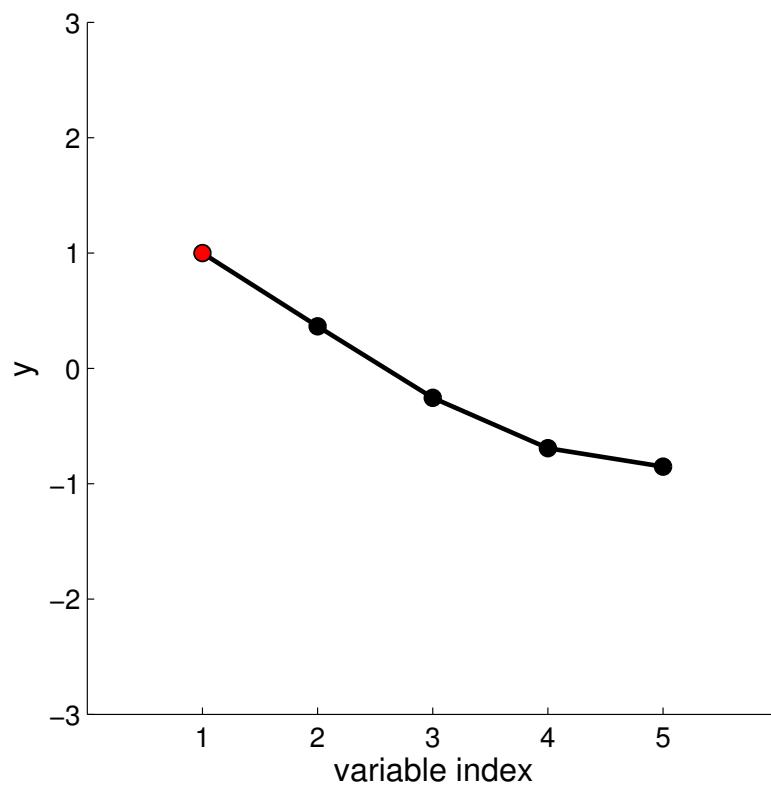
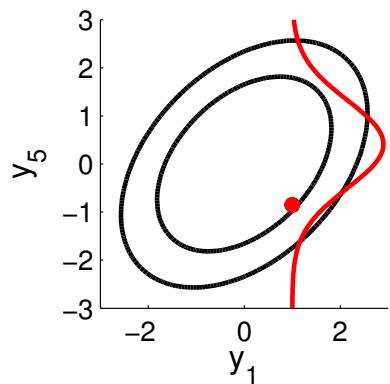
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



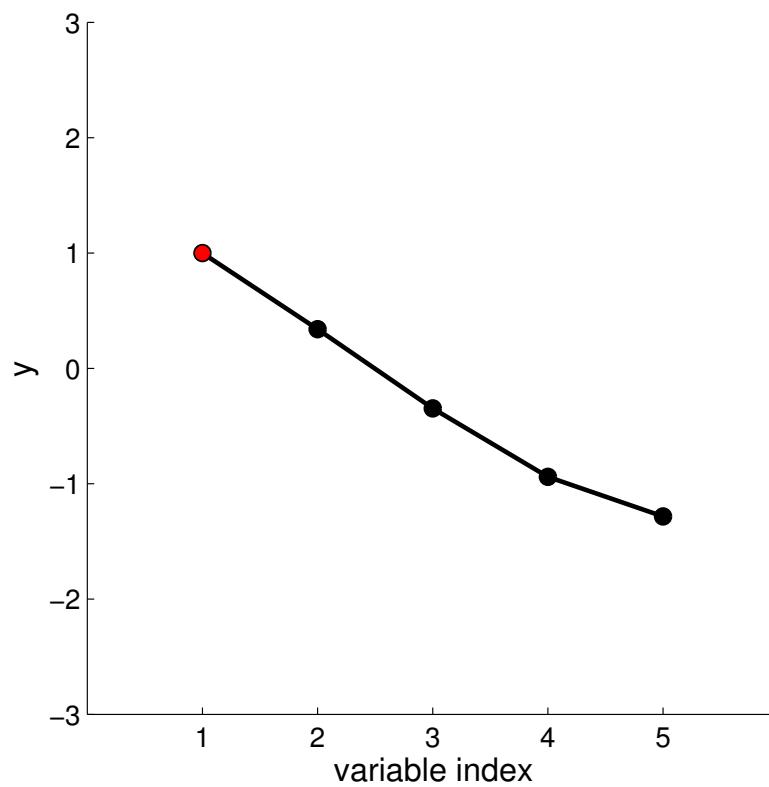
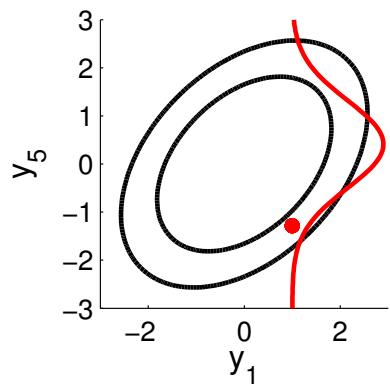
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



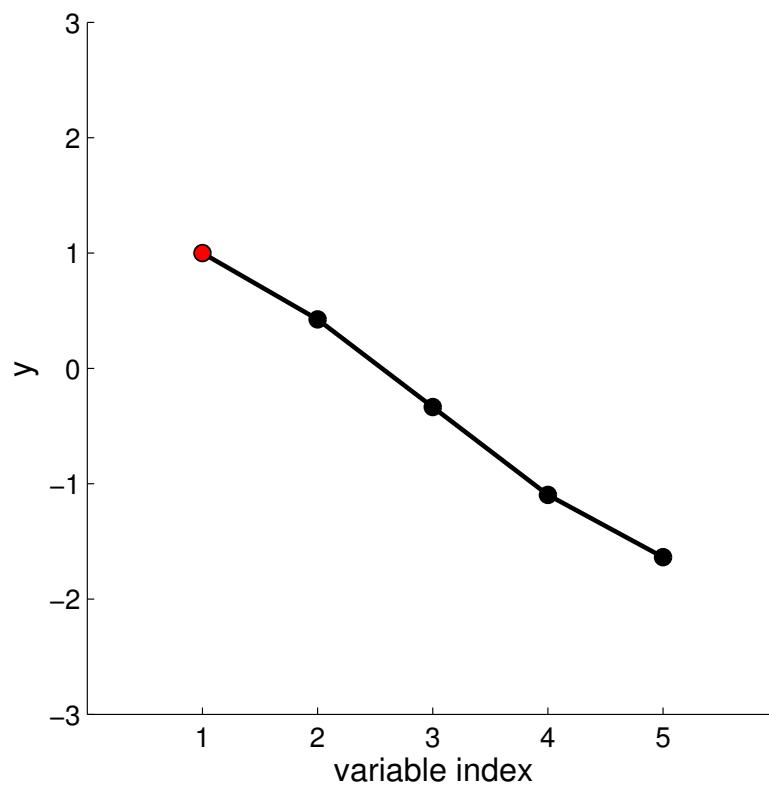
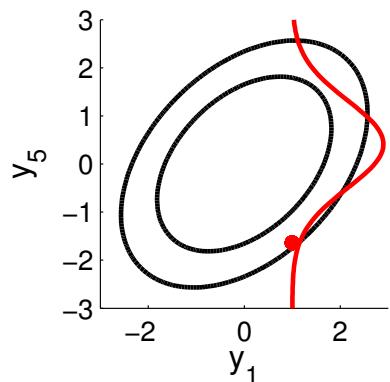
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



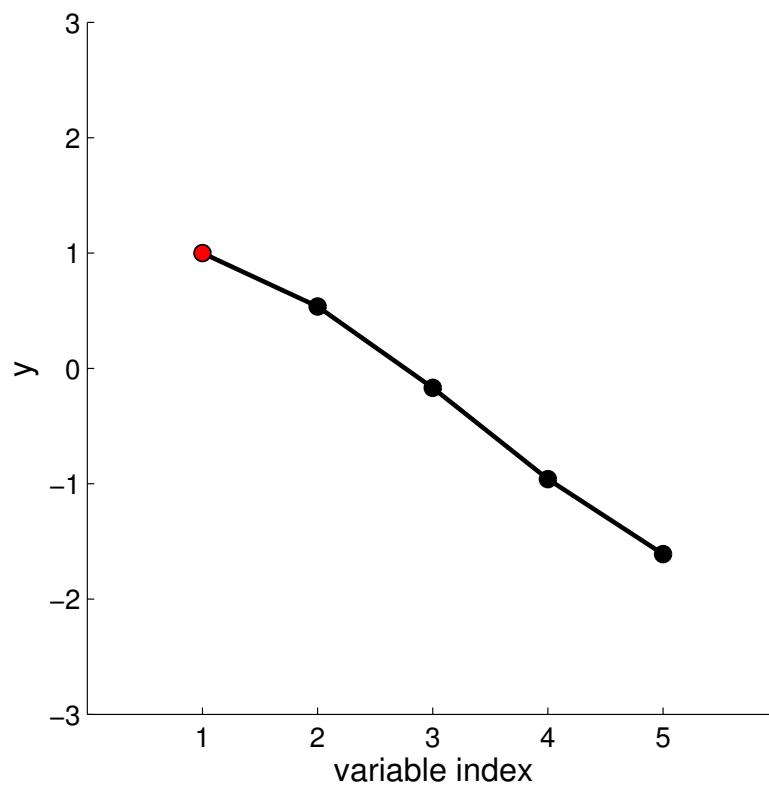
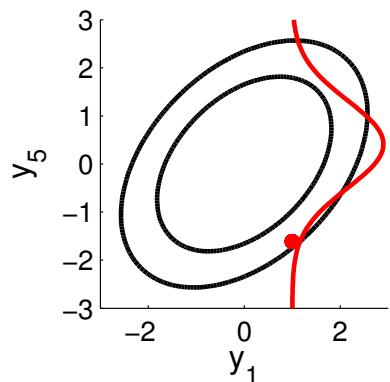
$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

New visualisation



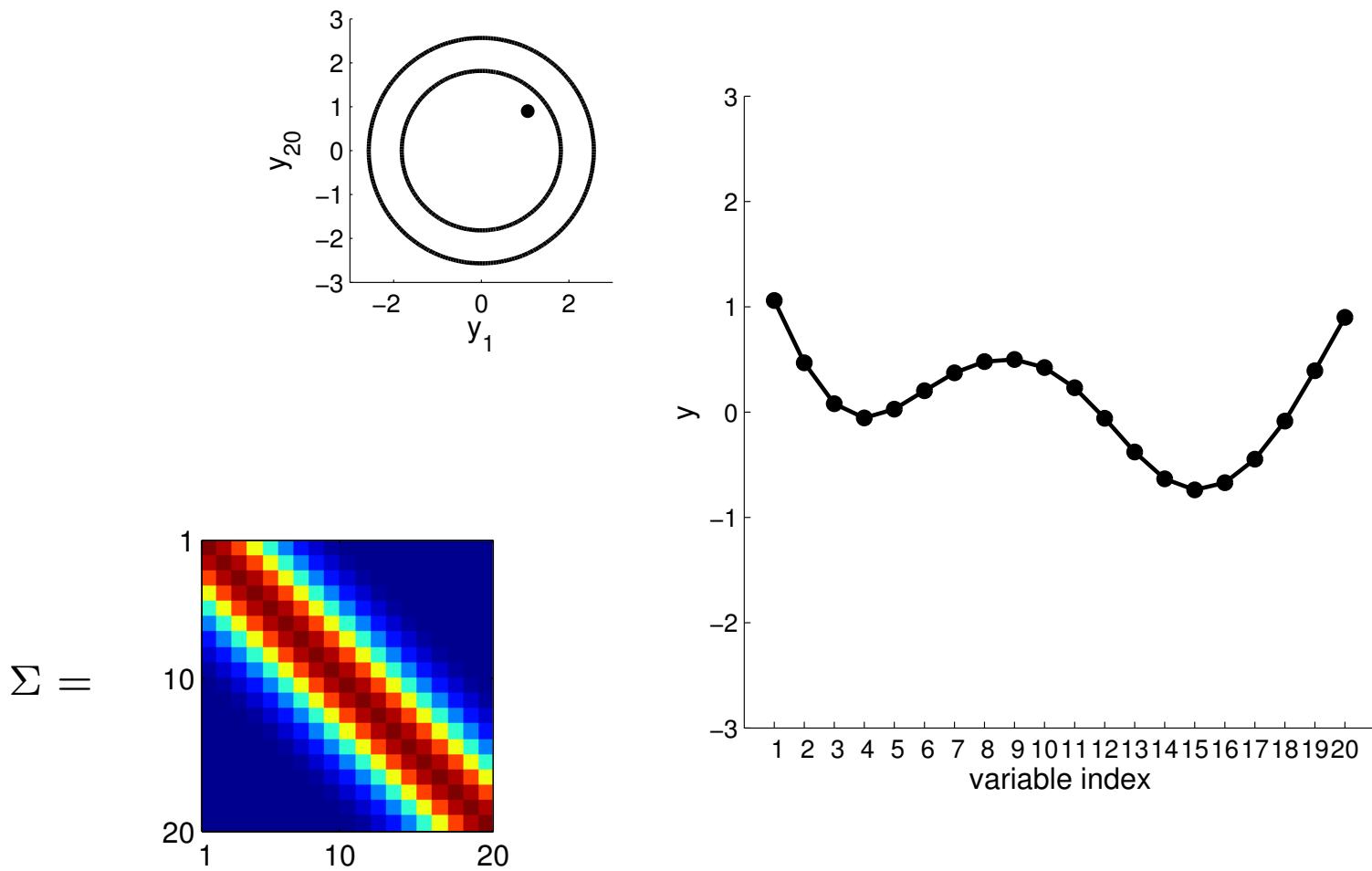
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New visualisation

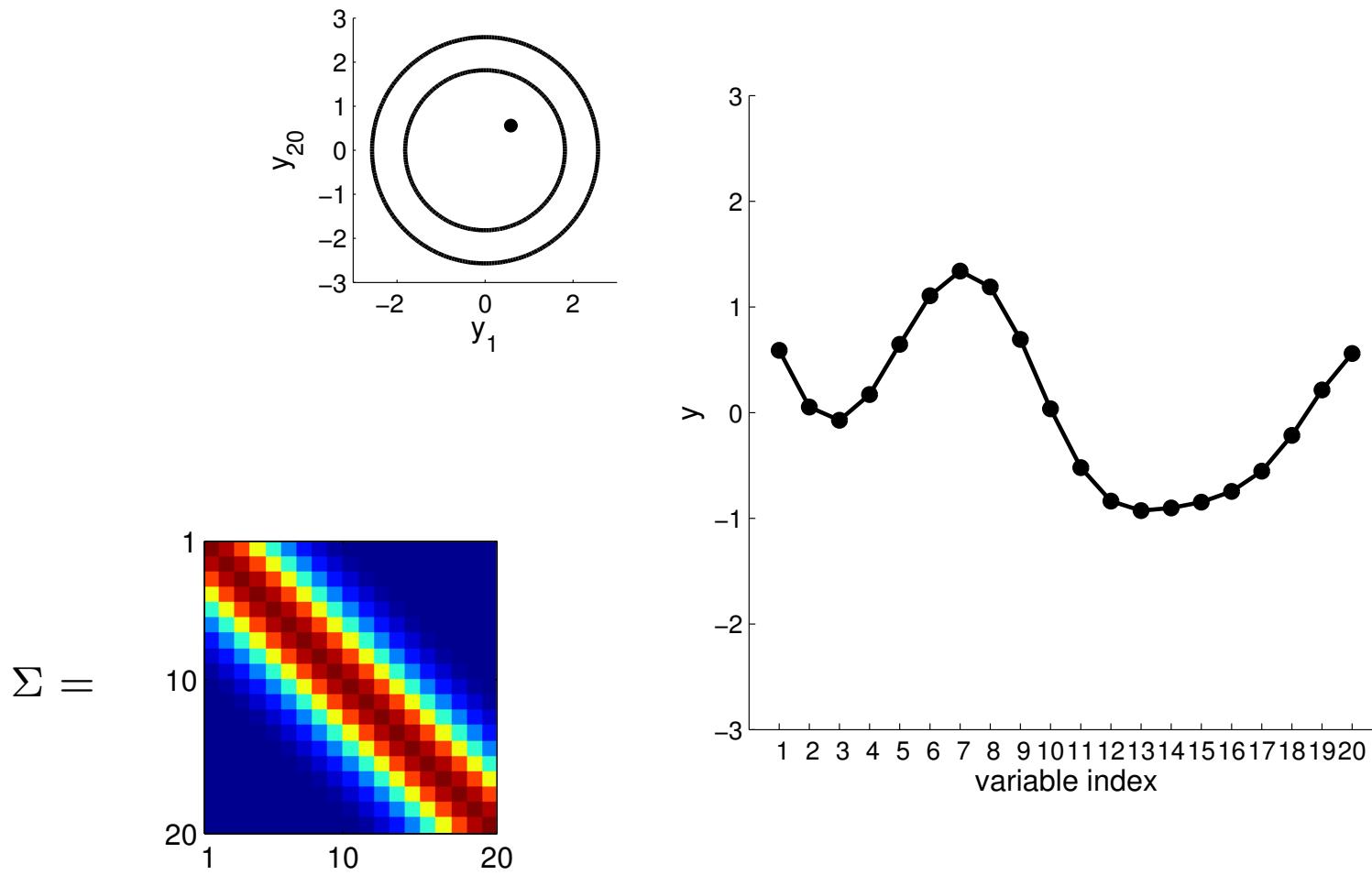


$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$

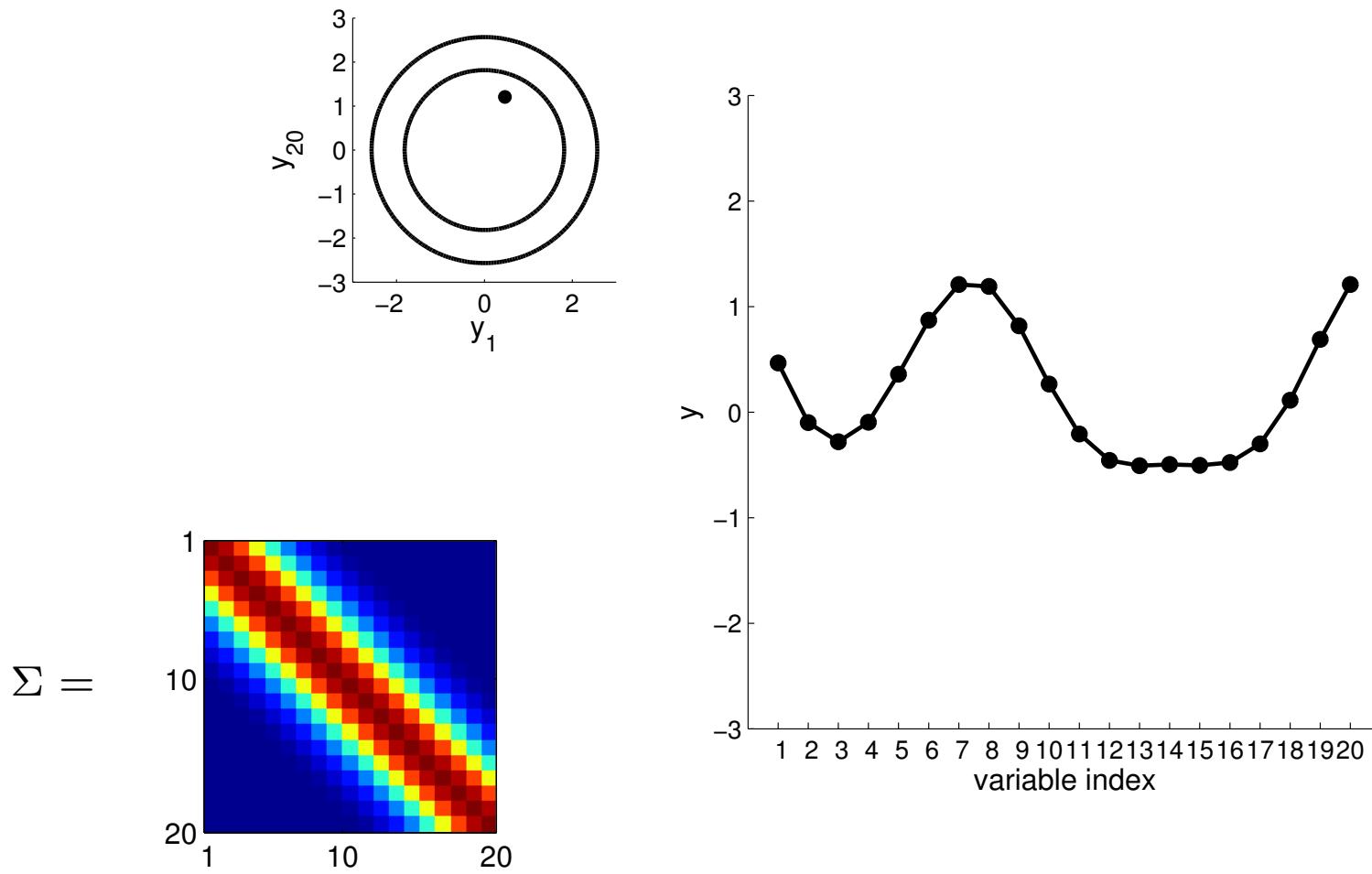
New visualisation



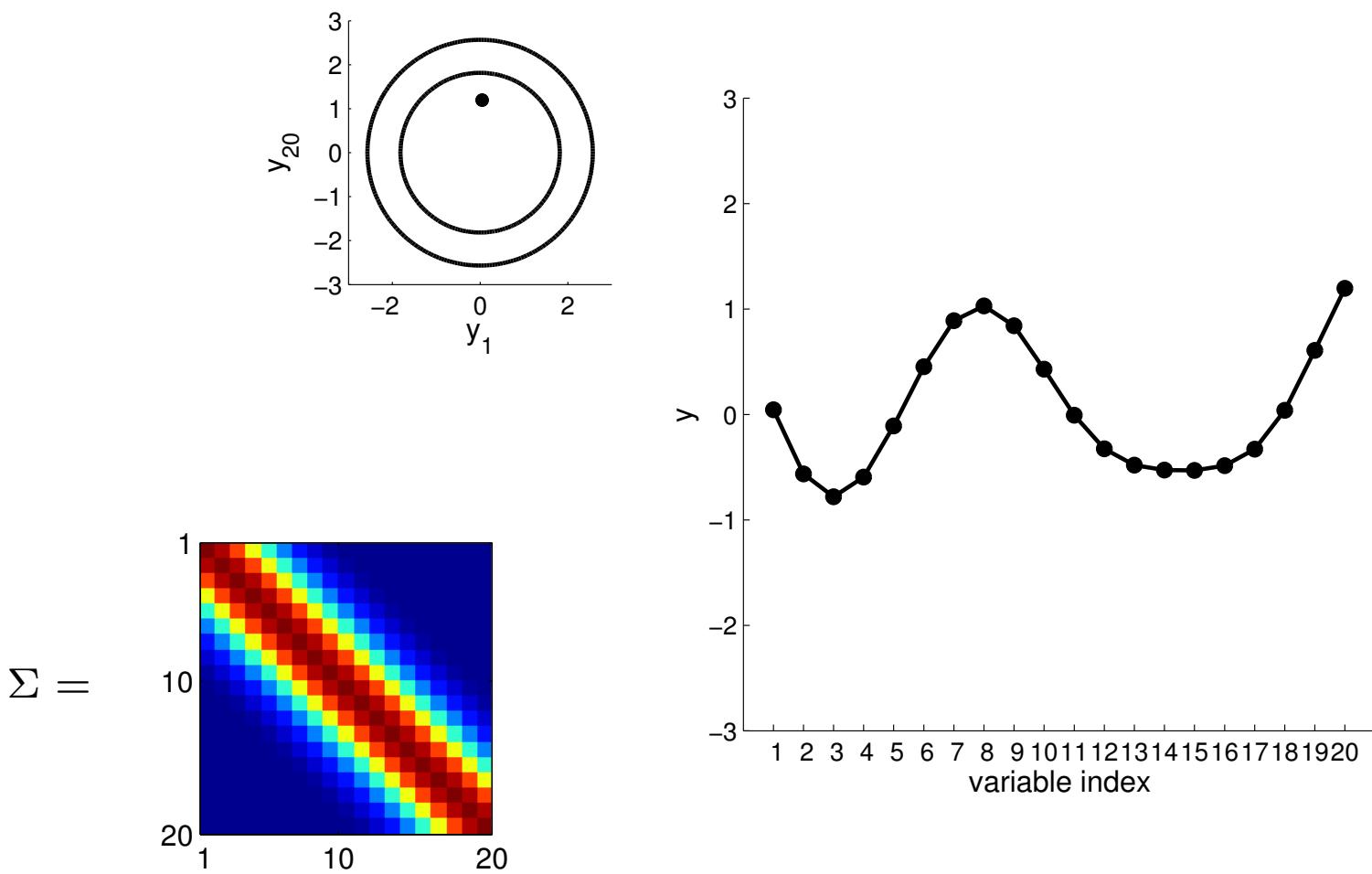
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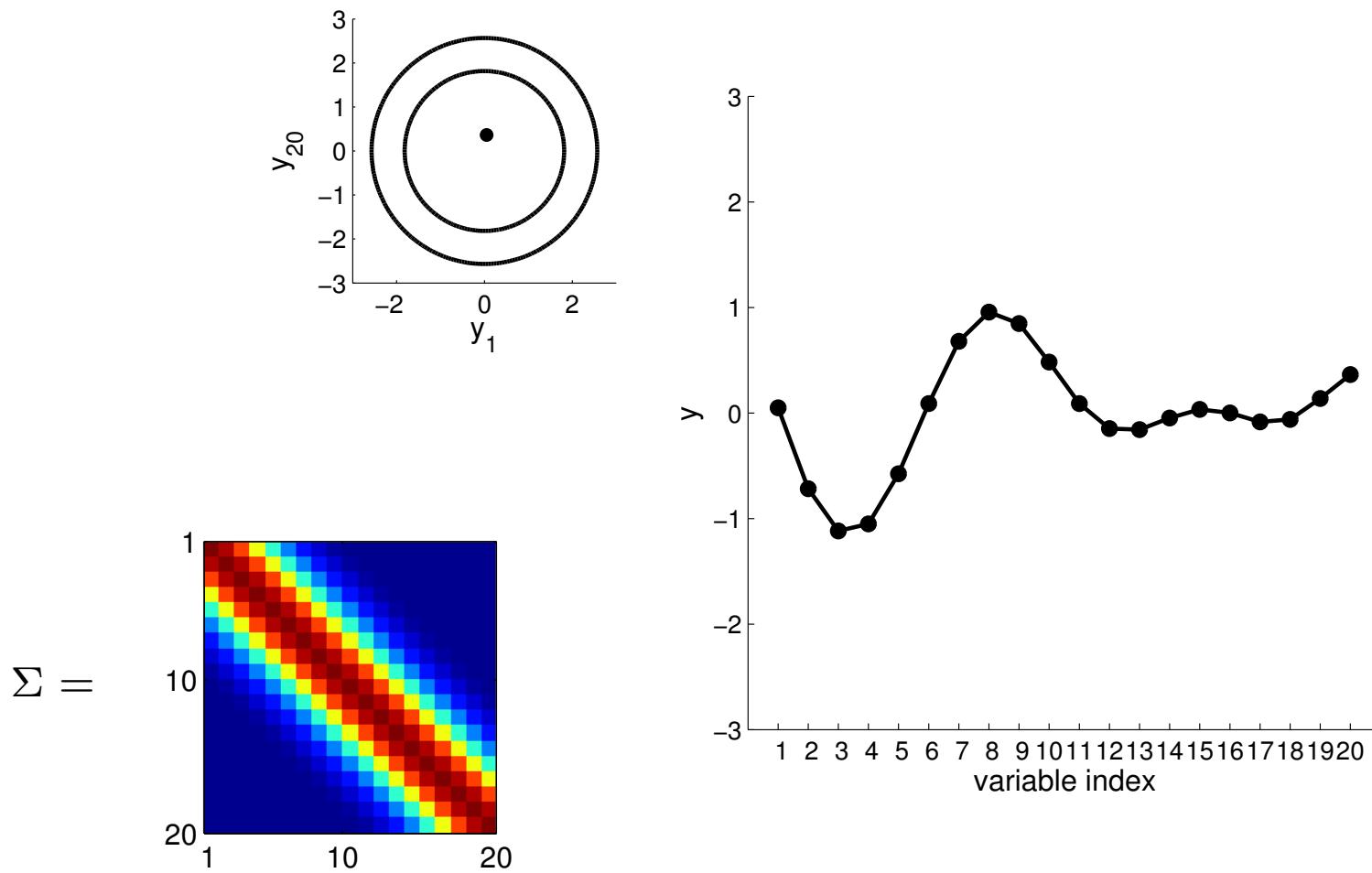
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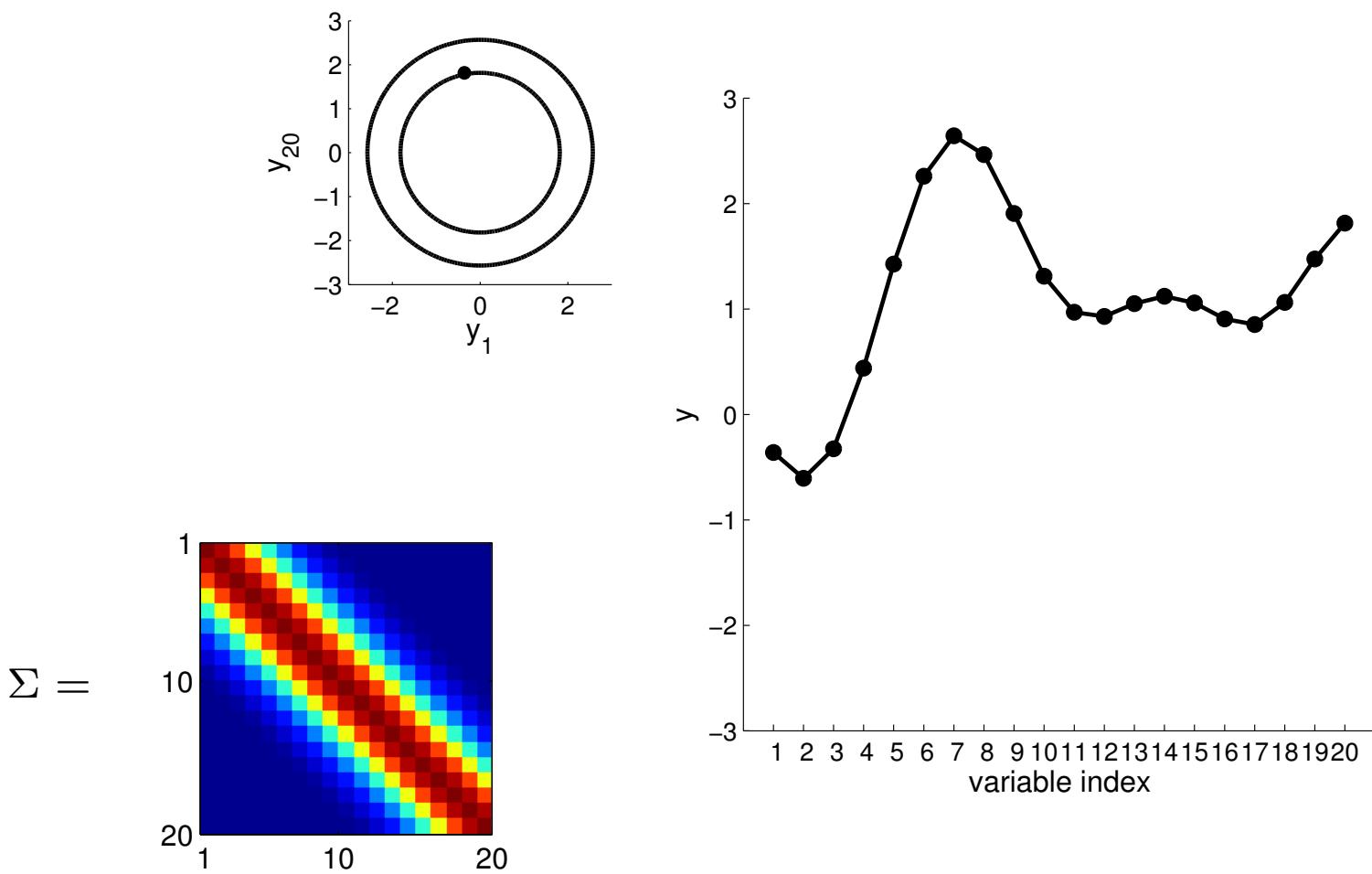
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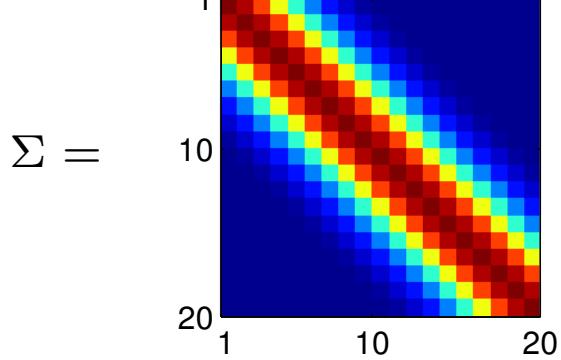
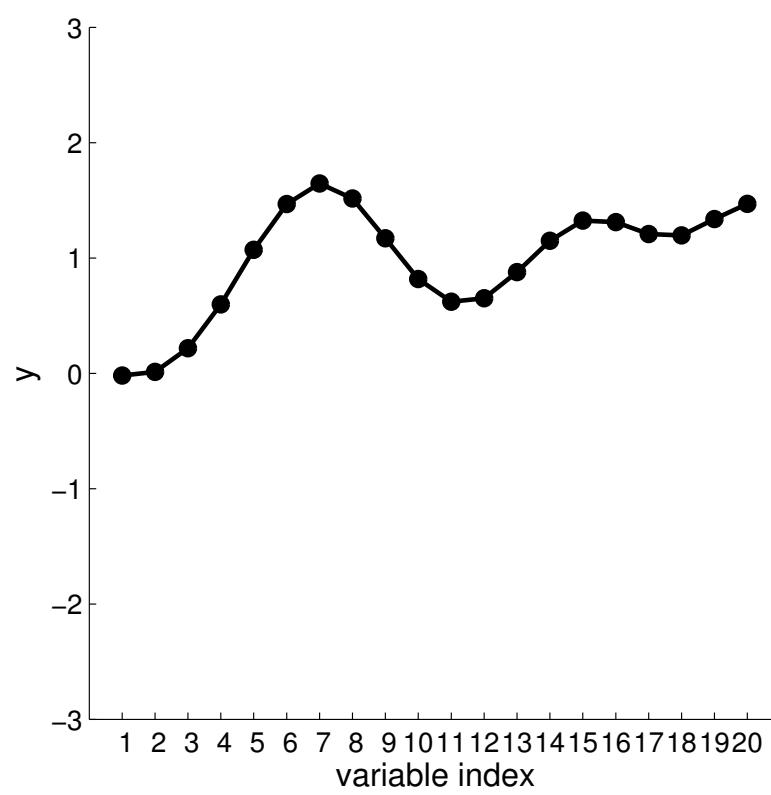
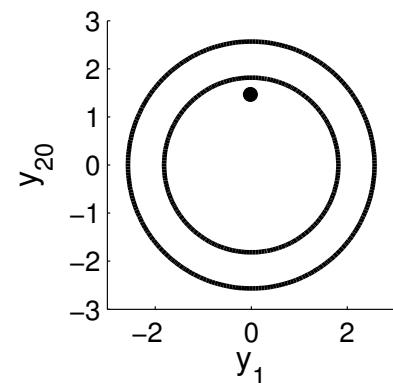
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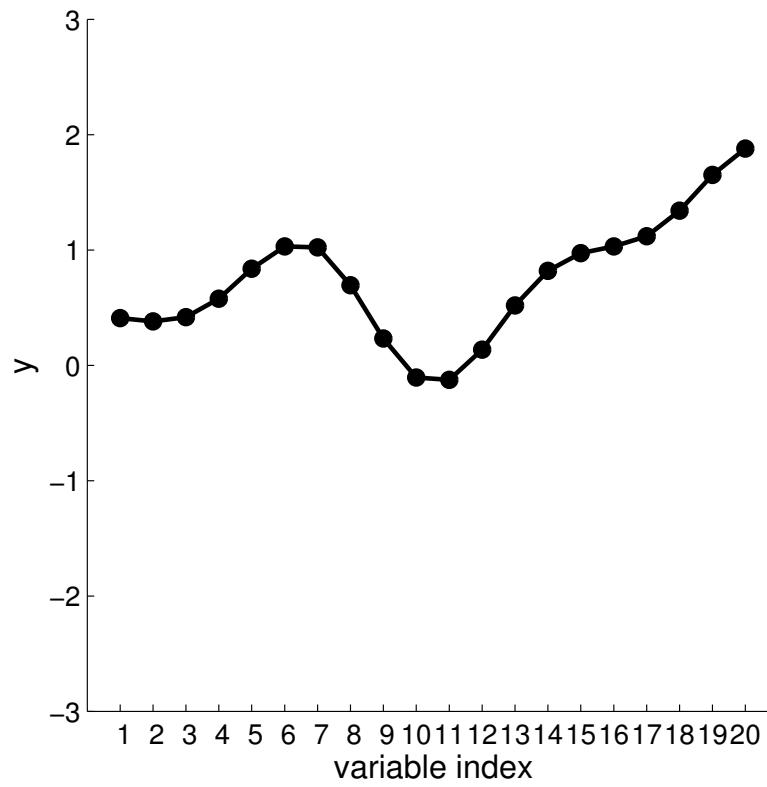
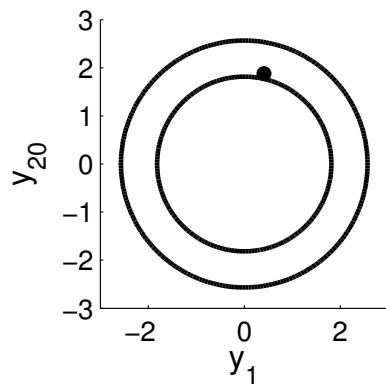
New visualisation



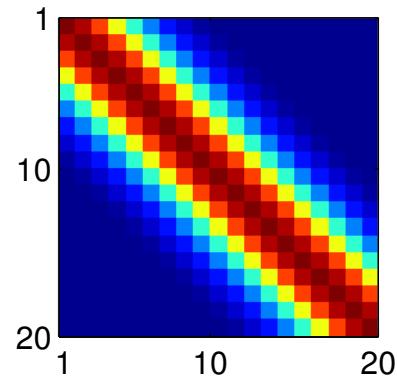
New visualisation



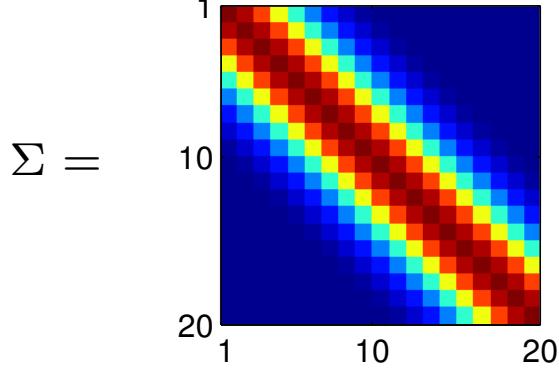
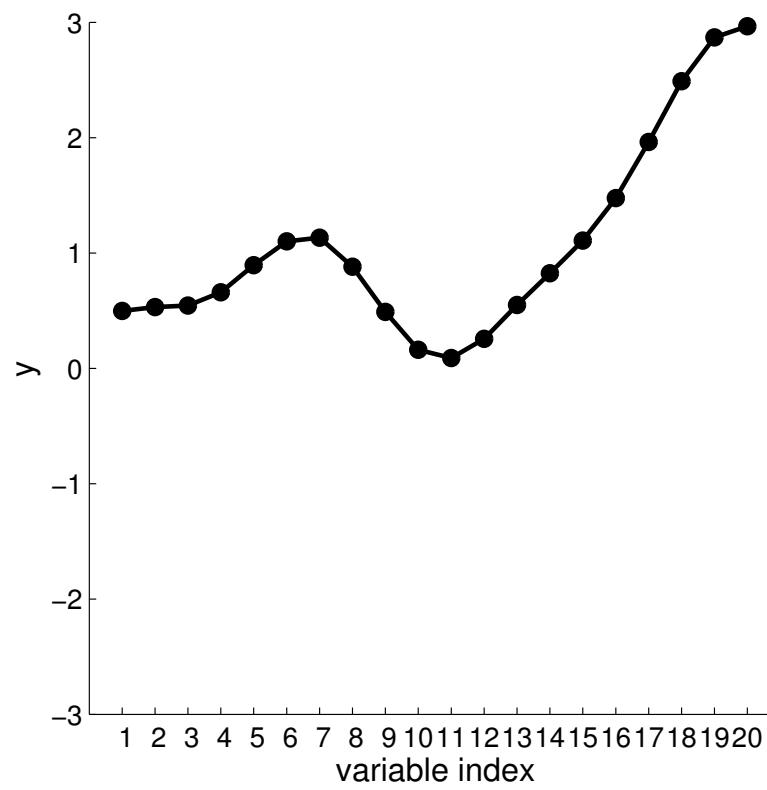
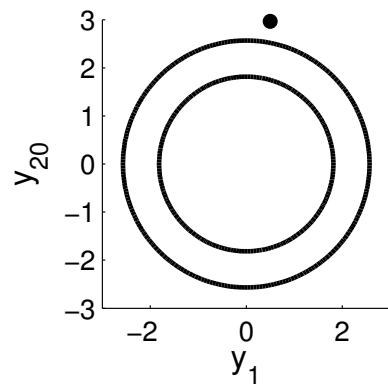
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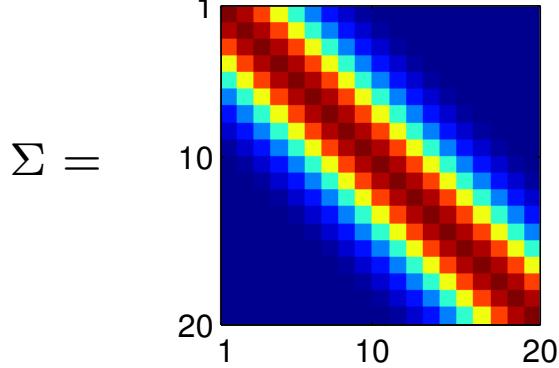
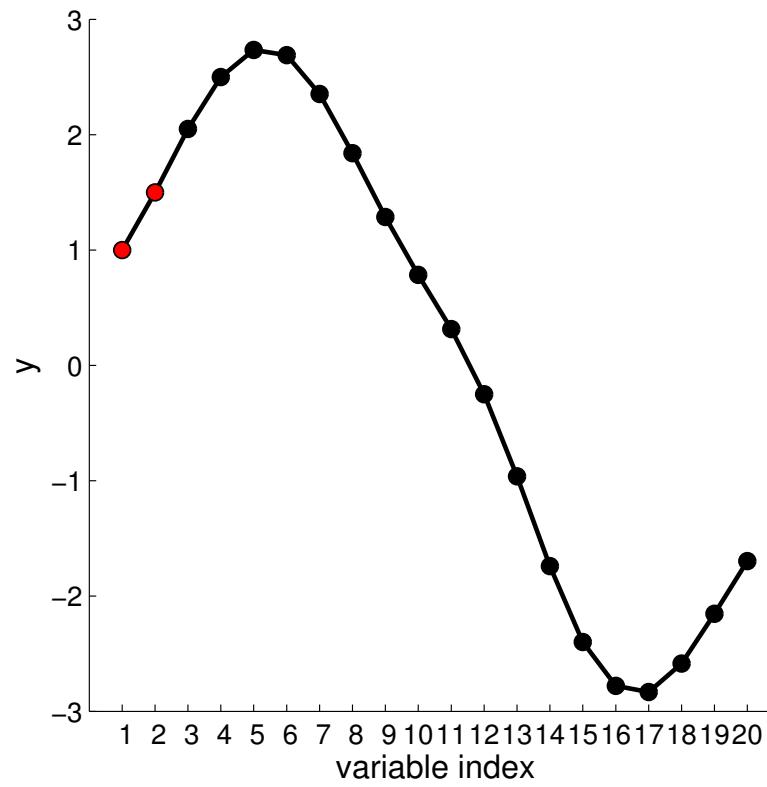
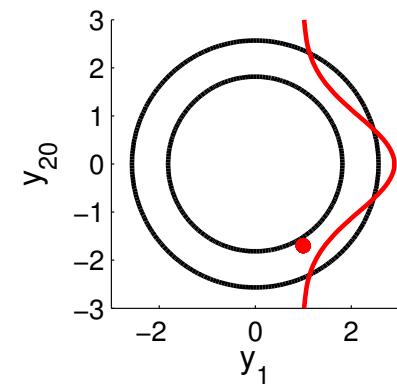
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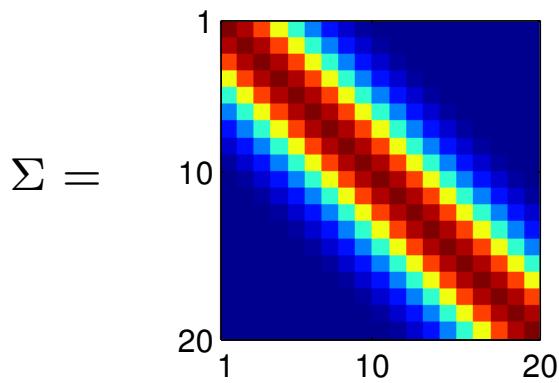
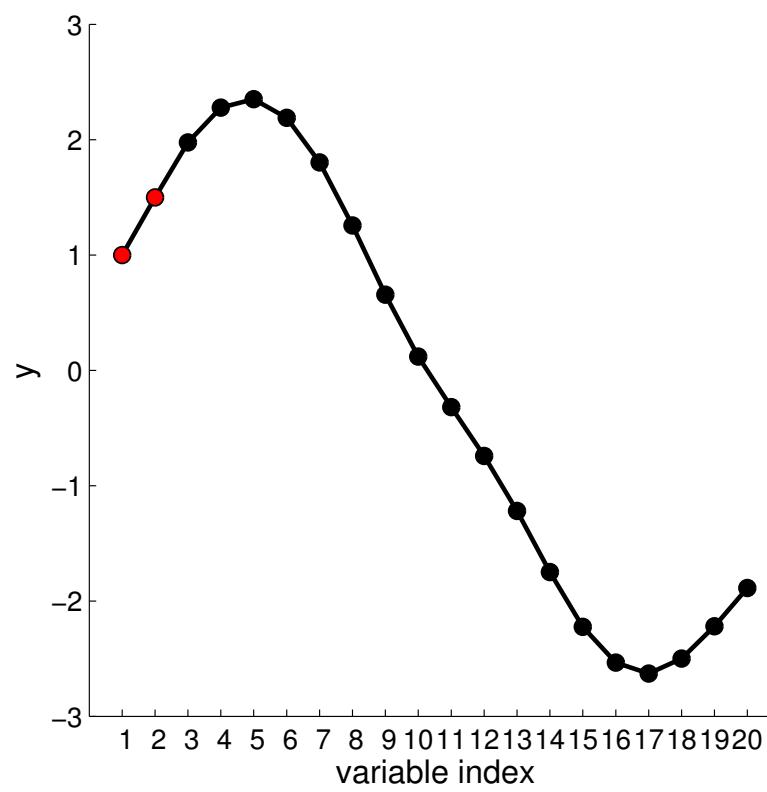
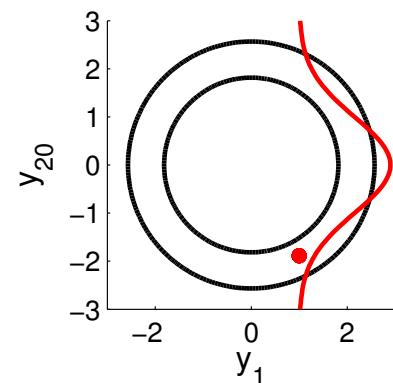
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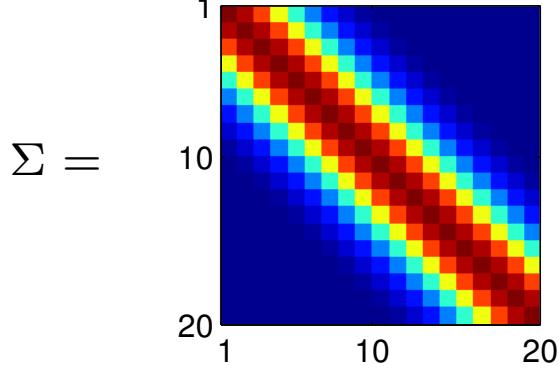
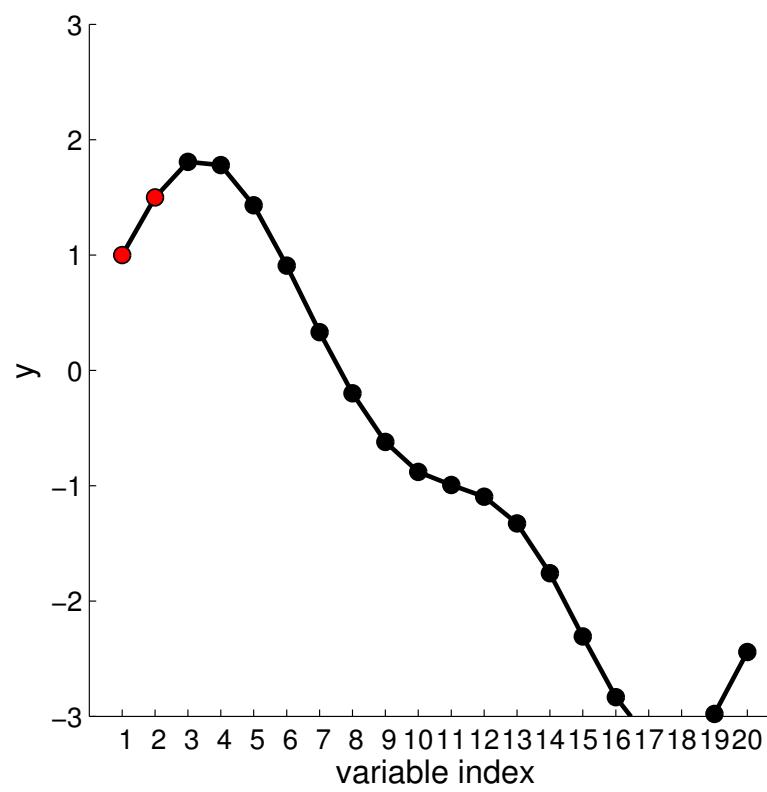
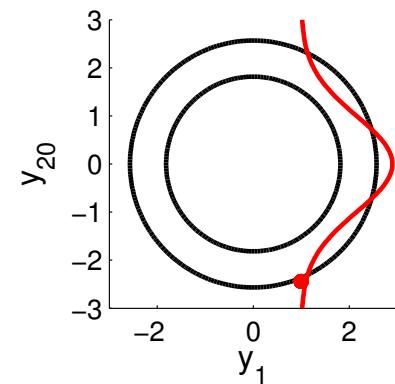
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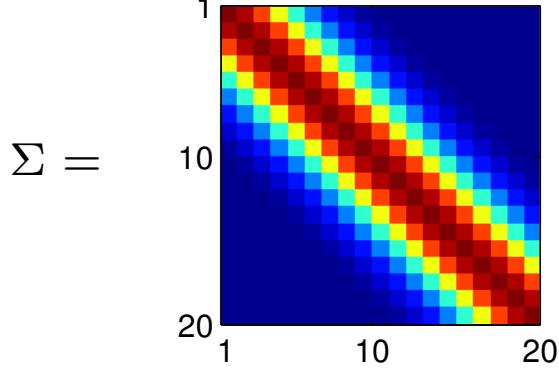
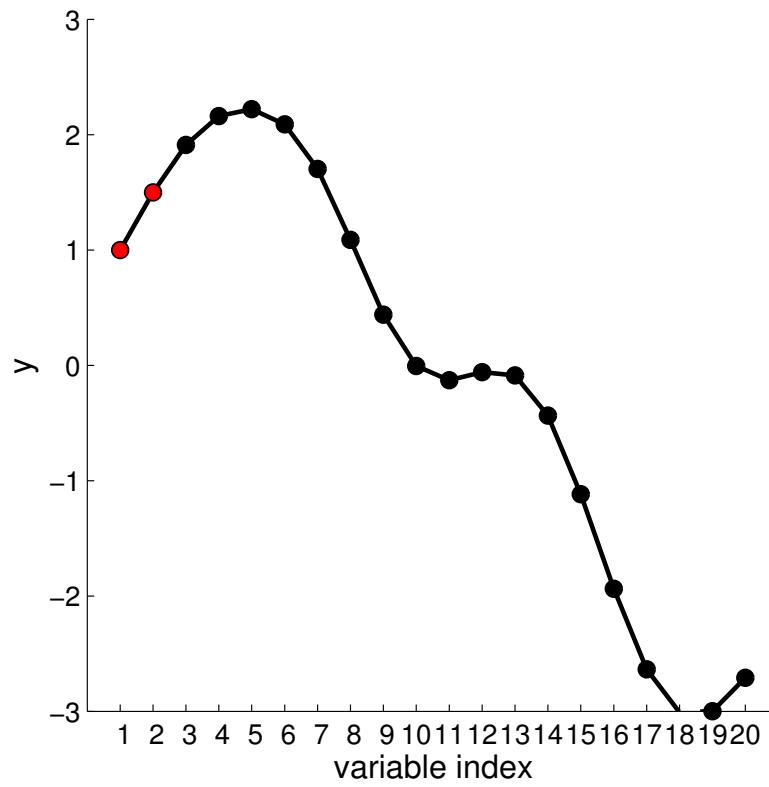
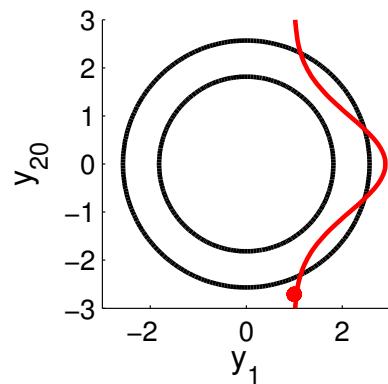
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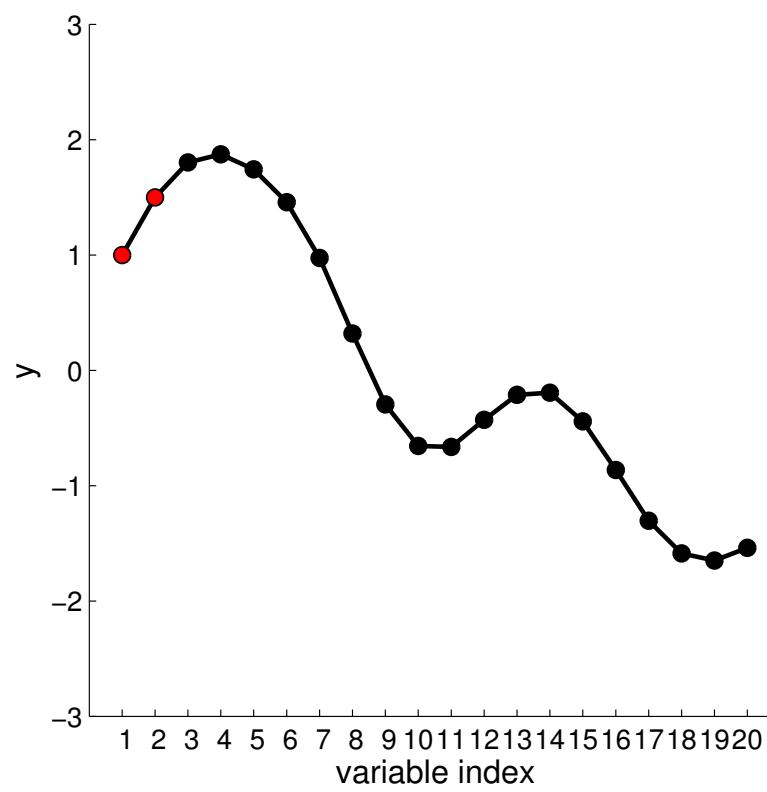
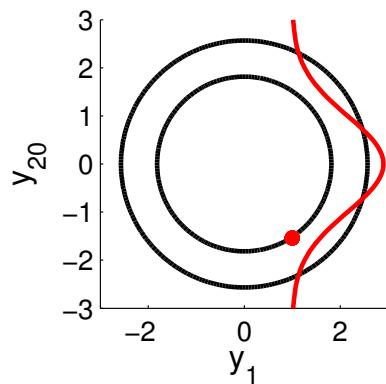
New visualisation



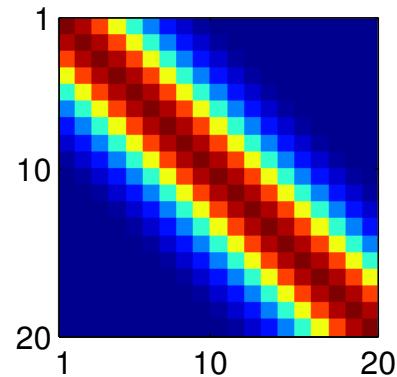
New visualisation



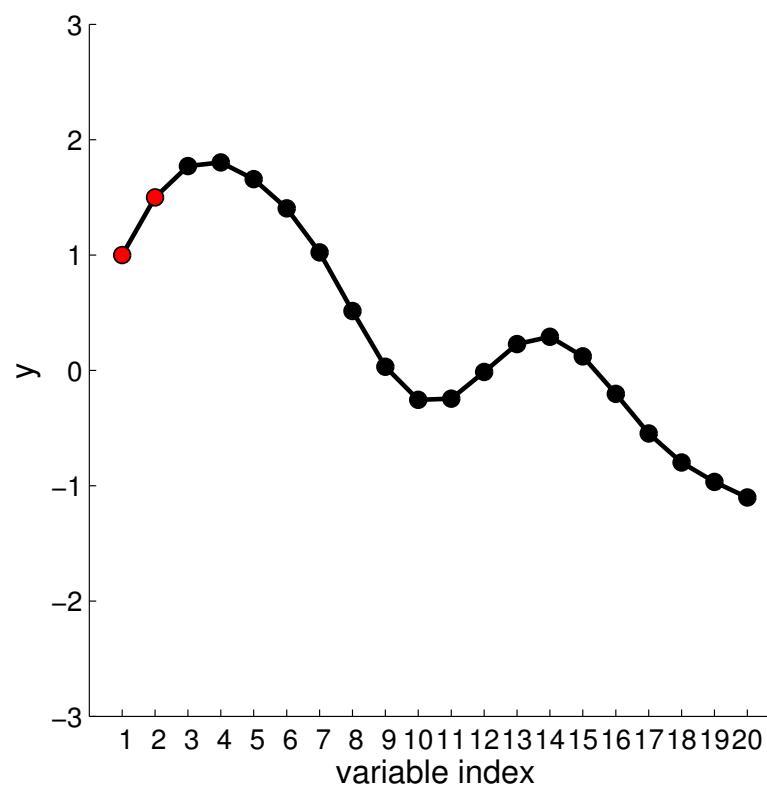
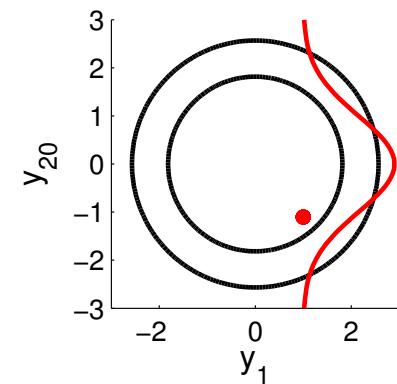
New visualisation



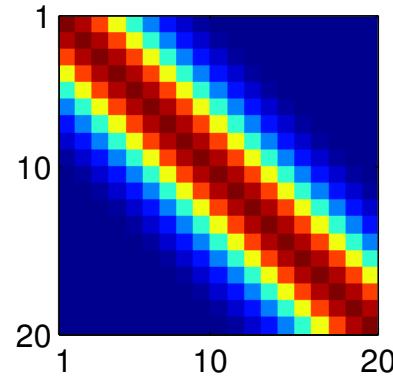
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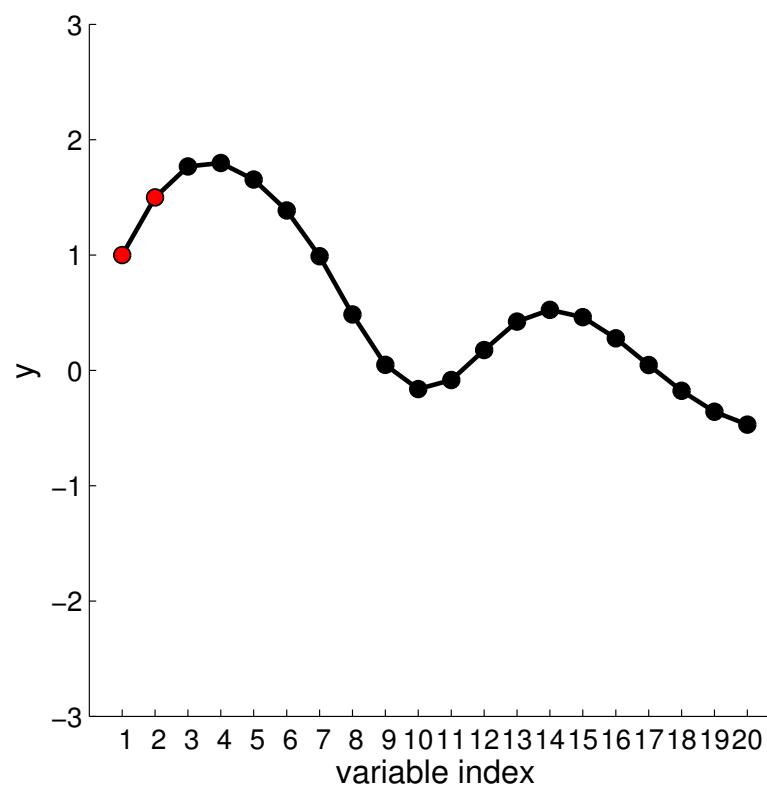
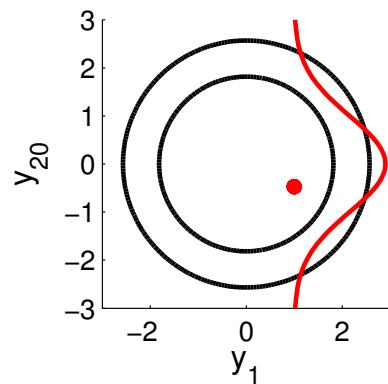
New visualisation



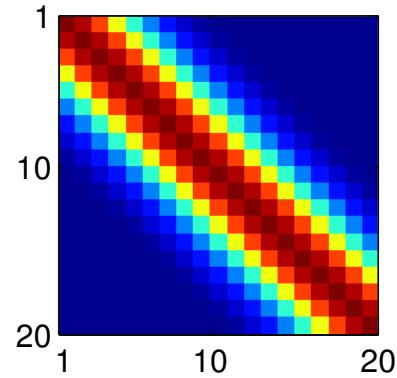
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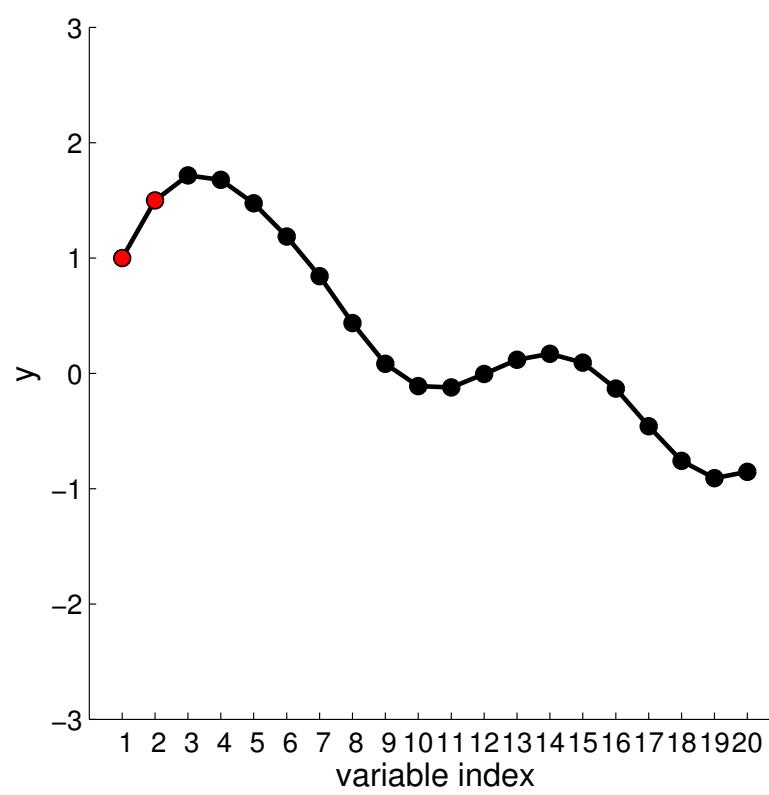
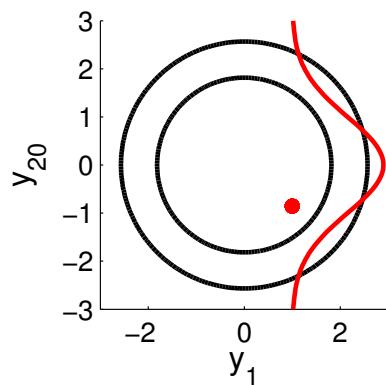
New visualisation



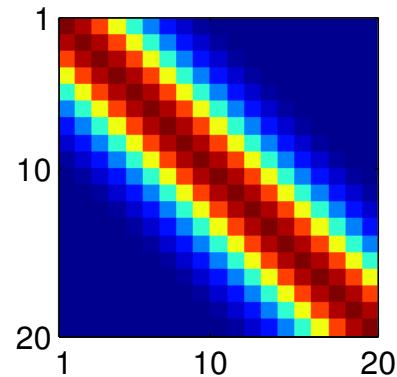
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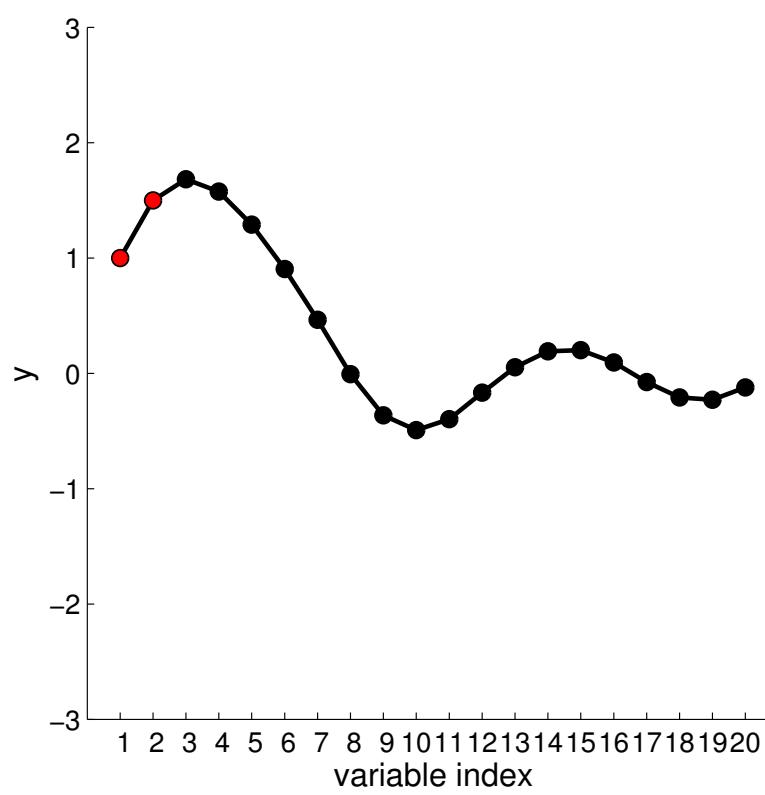
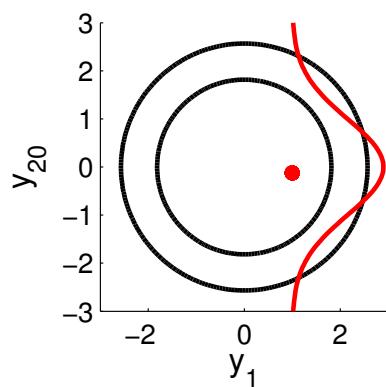
New visualisation



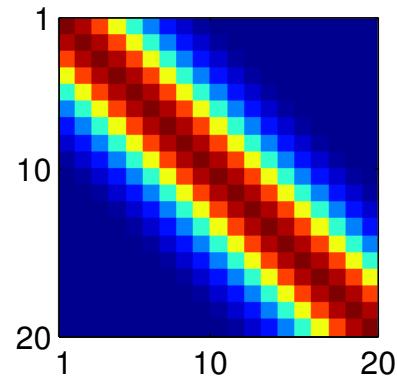
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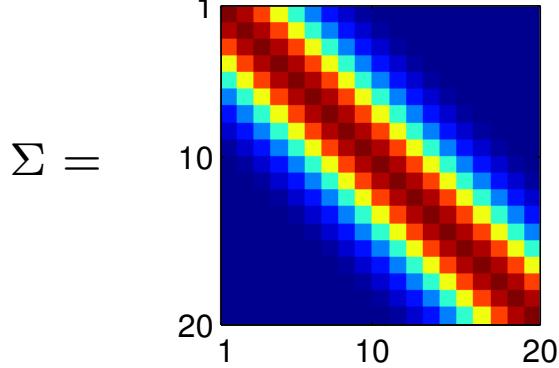
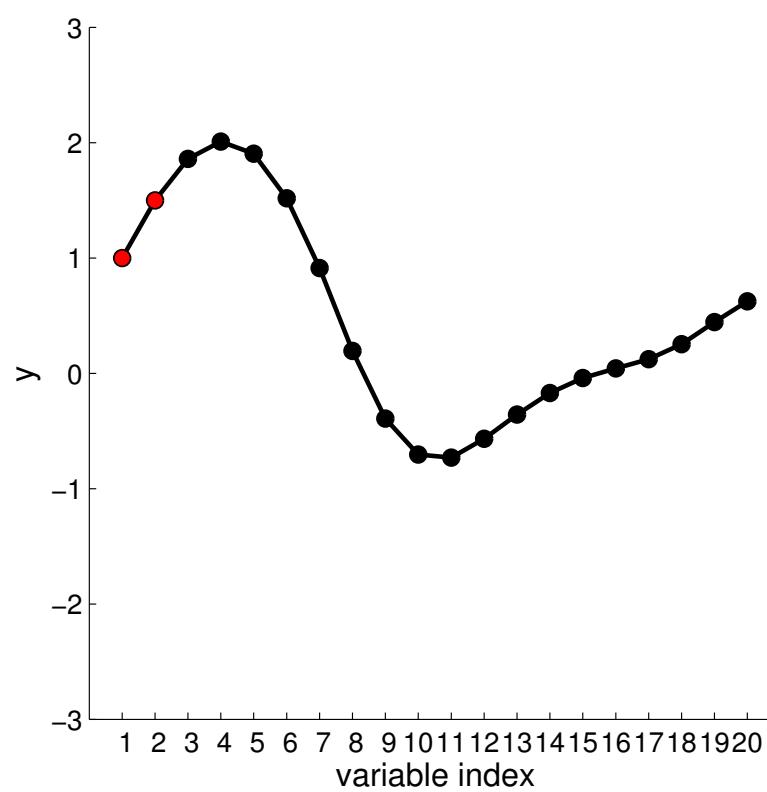
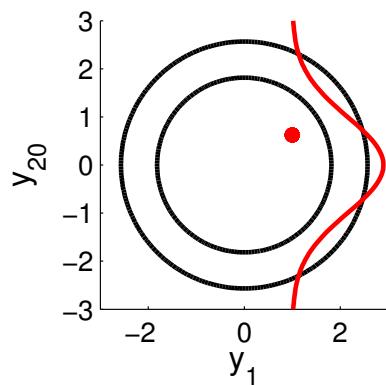
New visualisation



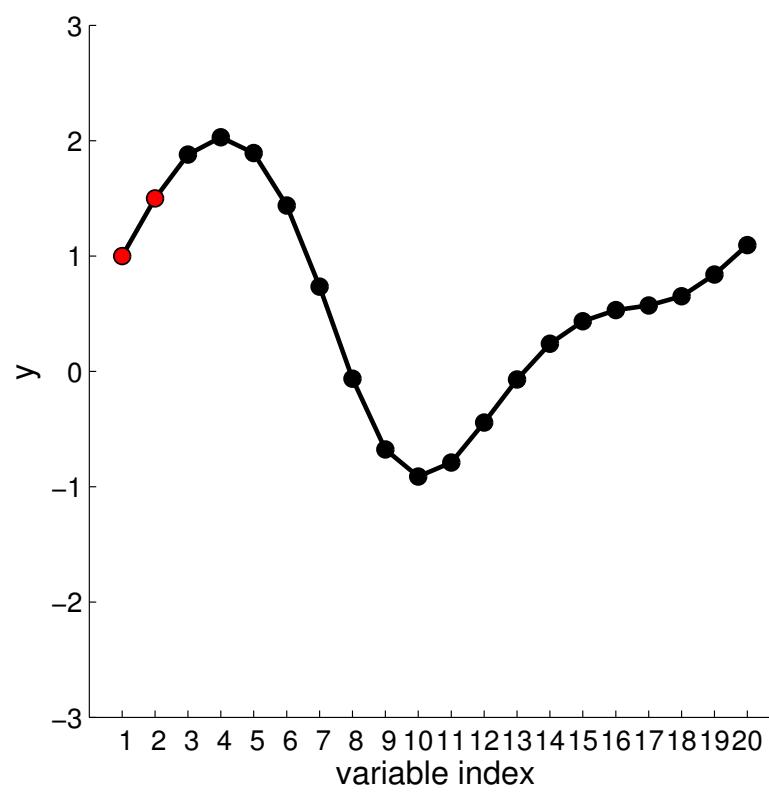
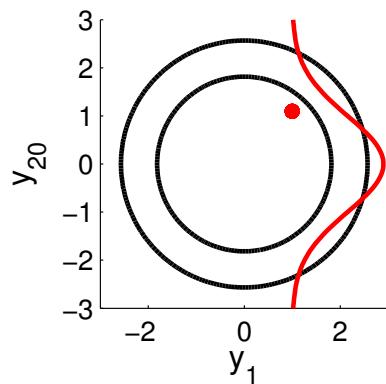
$\Sigma =$



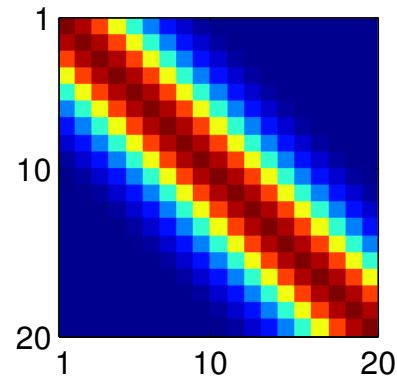
New visualisation



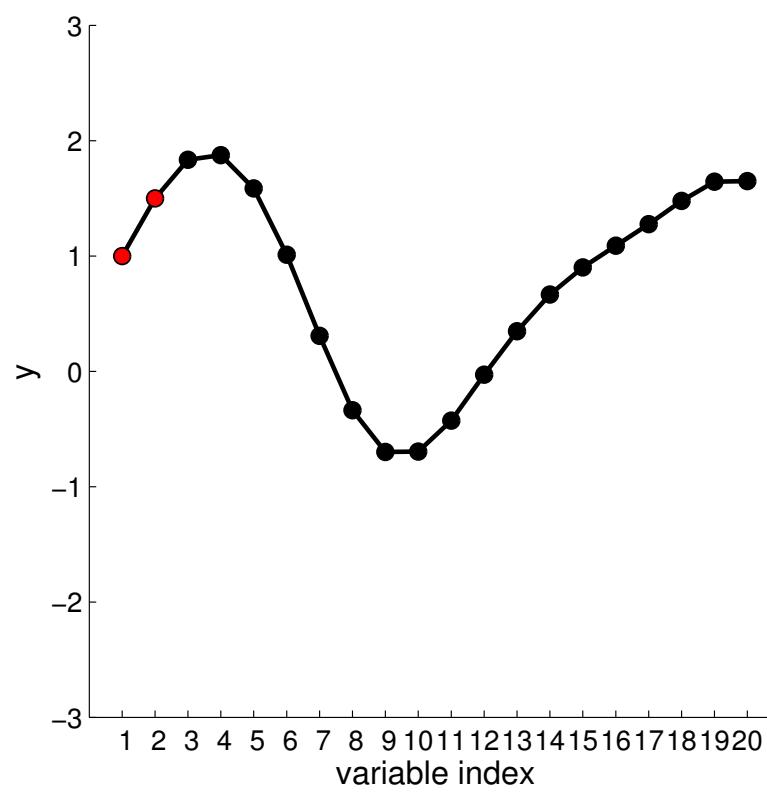
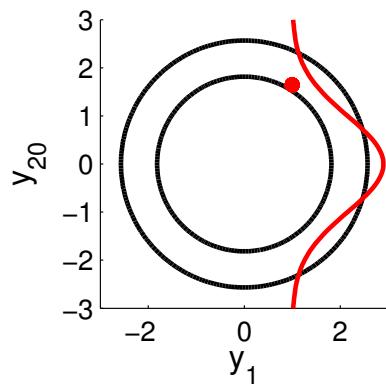
New visualisation



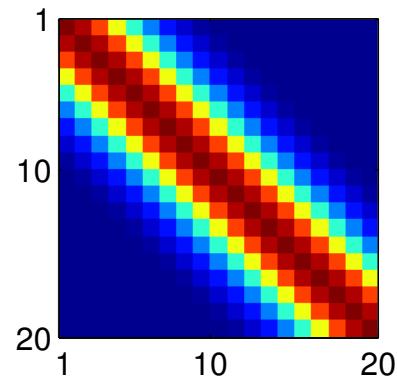
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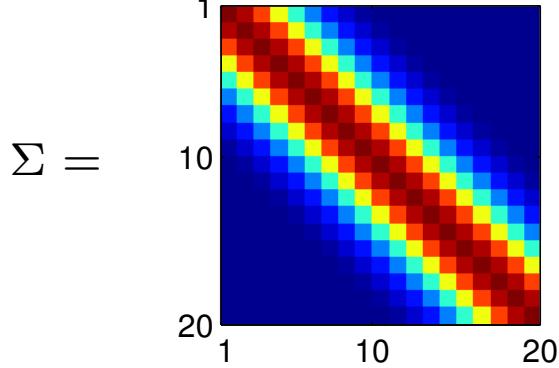
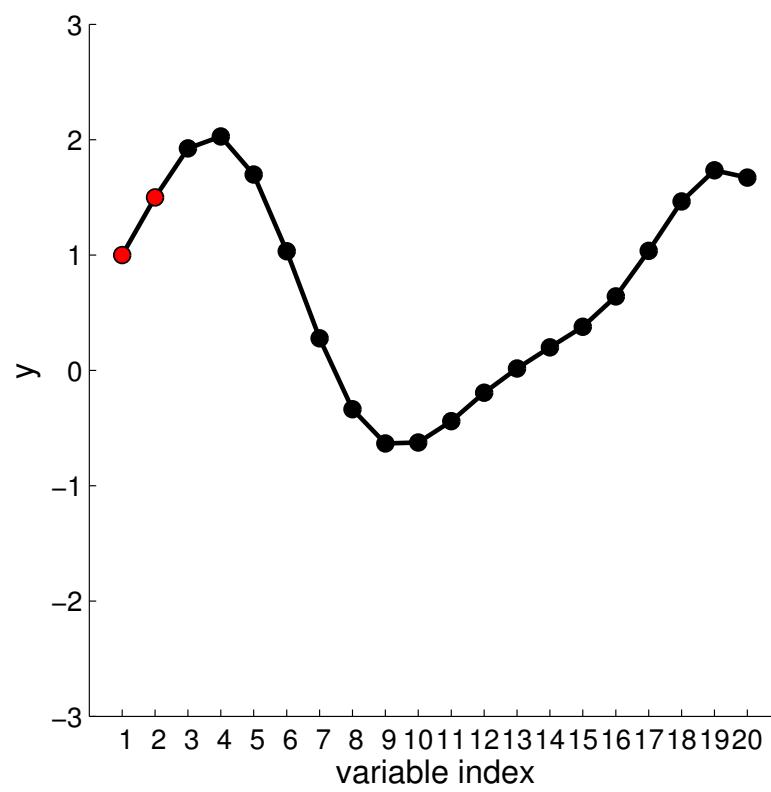
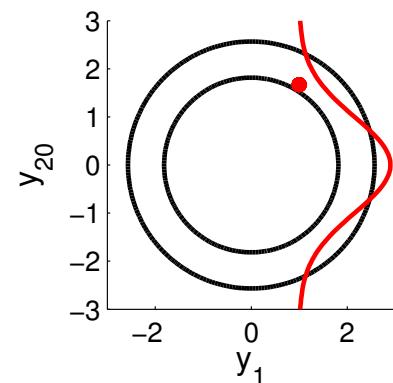
New visualisation



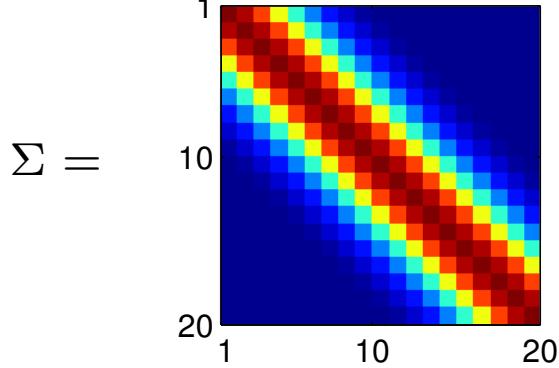
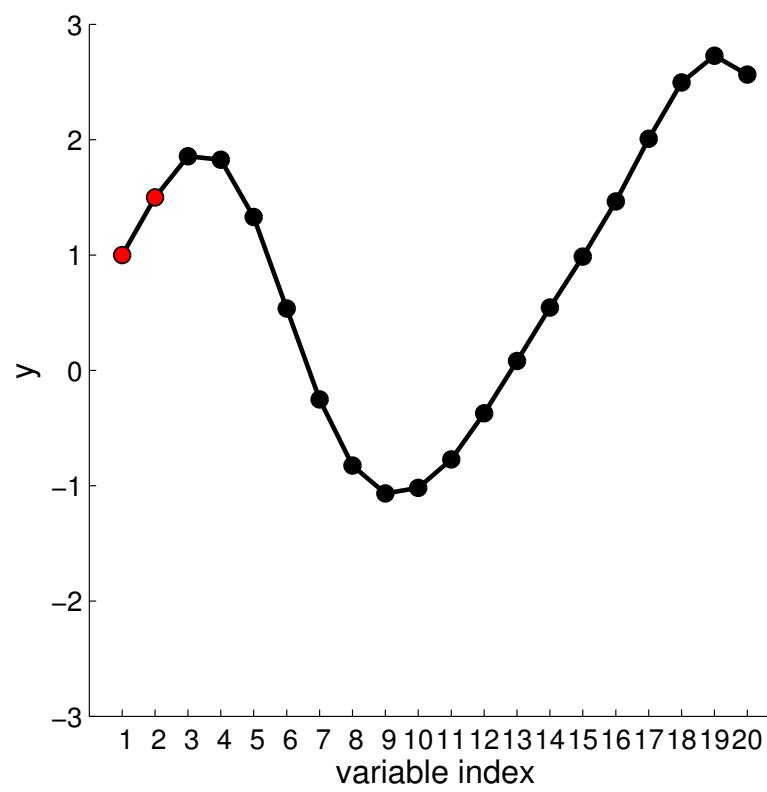
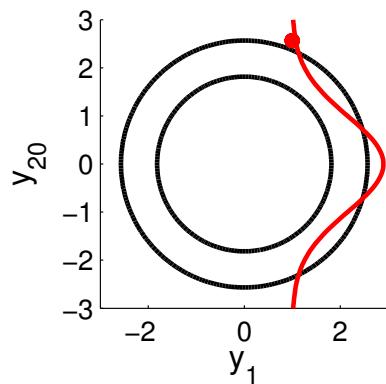
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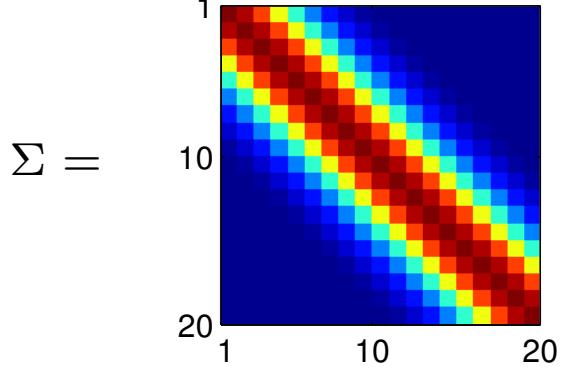
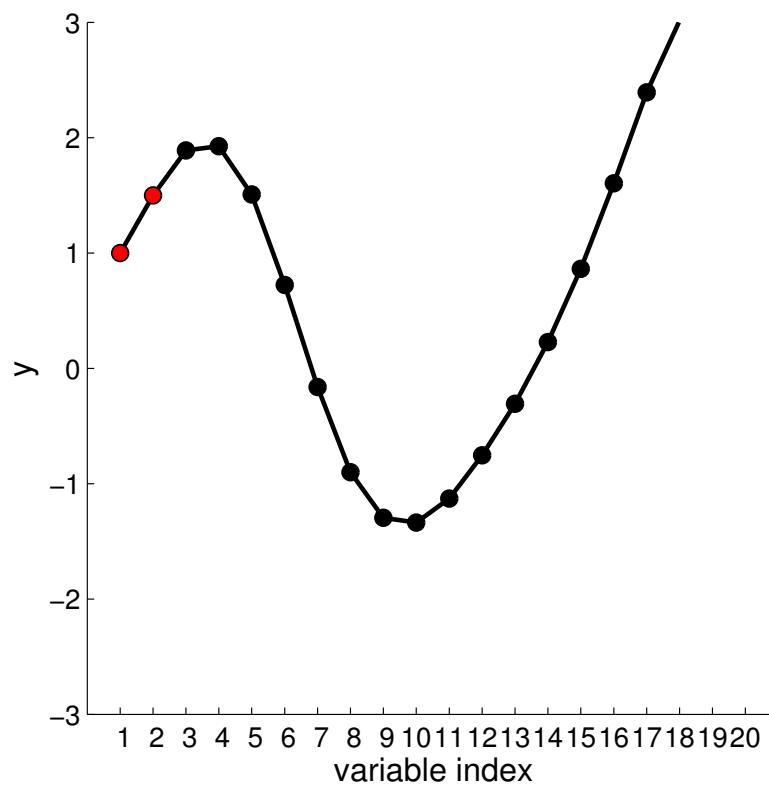
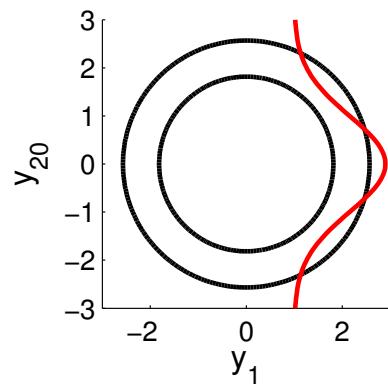
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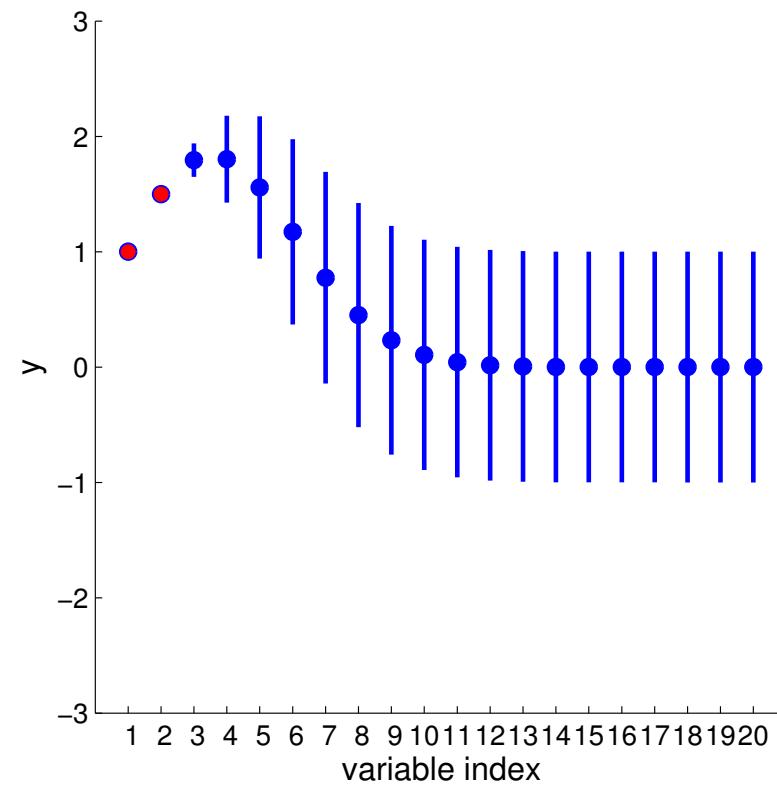
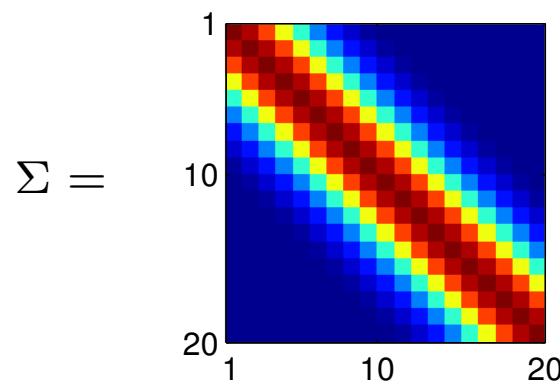
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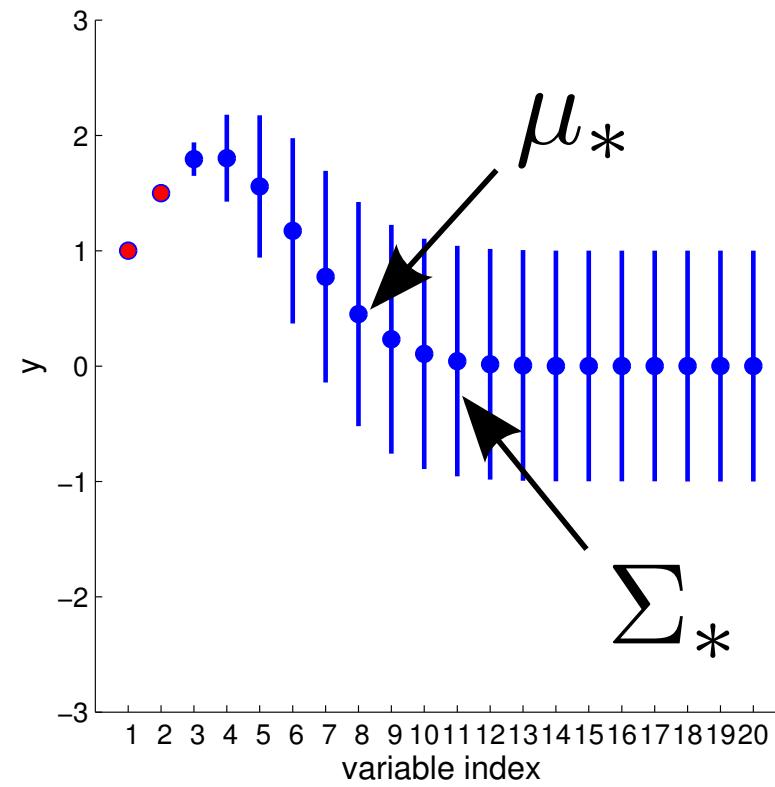
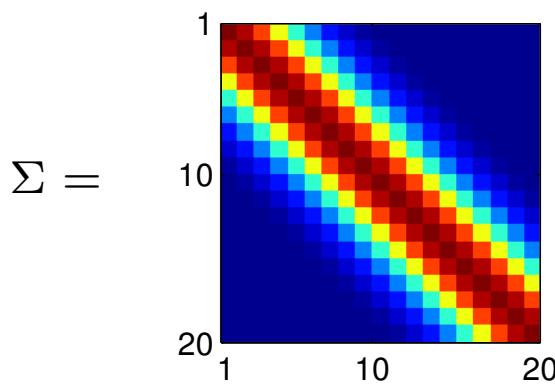
New visualisation



Regression using Gaussians

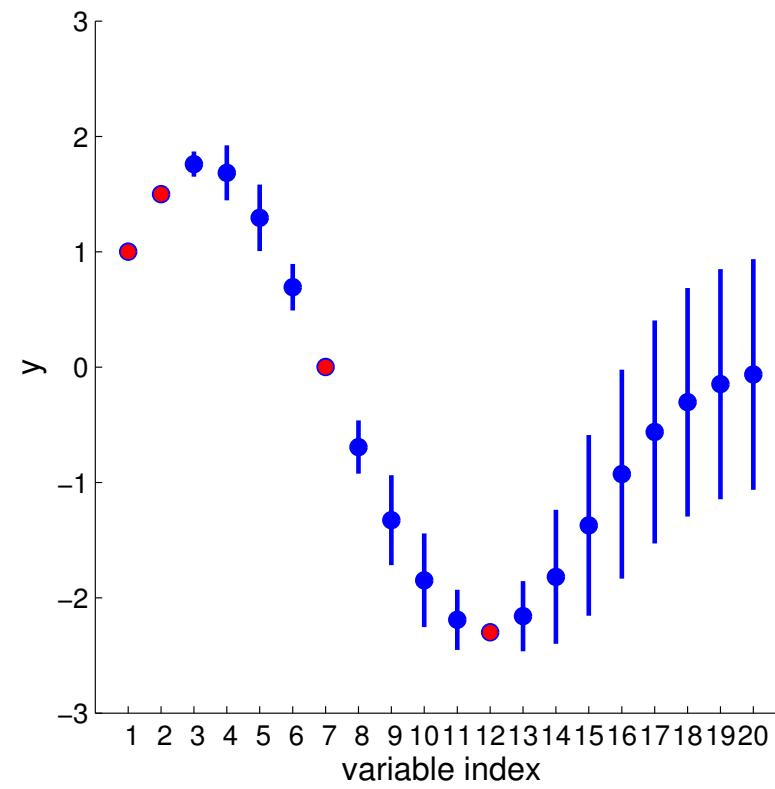
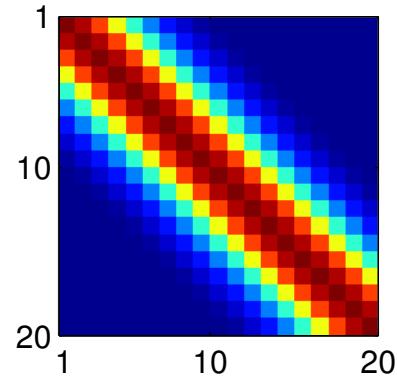


Regression using Gaussians



Regression using Gaussians

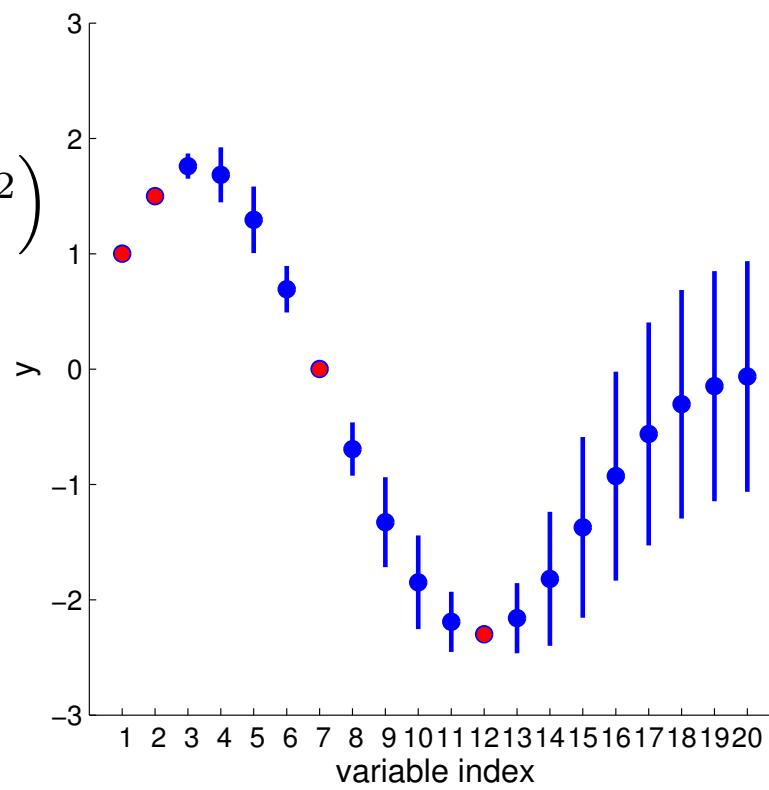
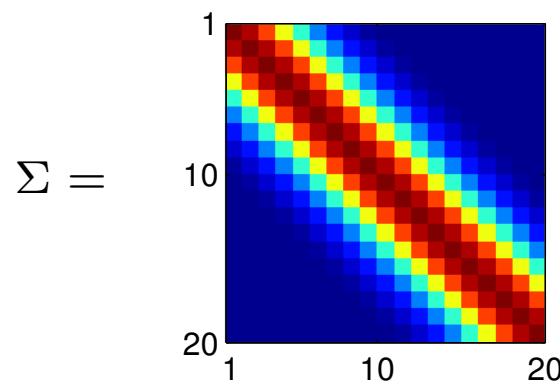
$$\Sigma =$$



Regression using Gaussians

$$\Sigma(\mathbf{x}_1, \mathbf{x}_2) = K(\mathbf{x}_1, \mathbf{x}_2) + I\sigma_y^2$$

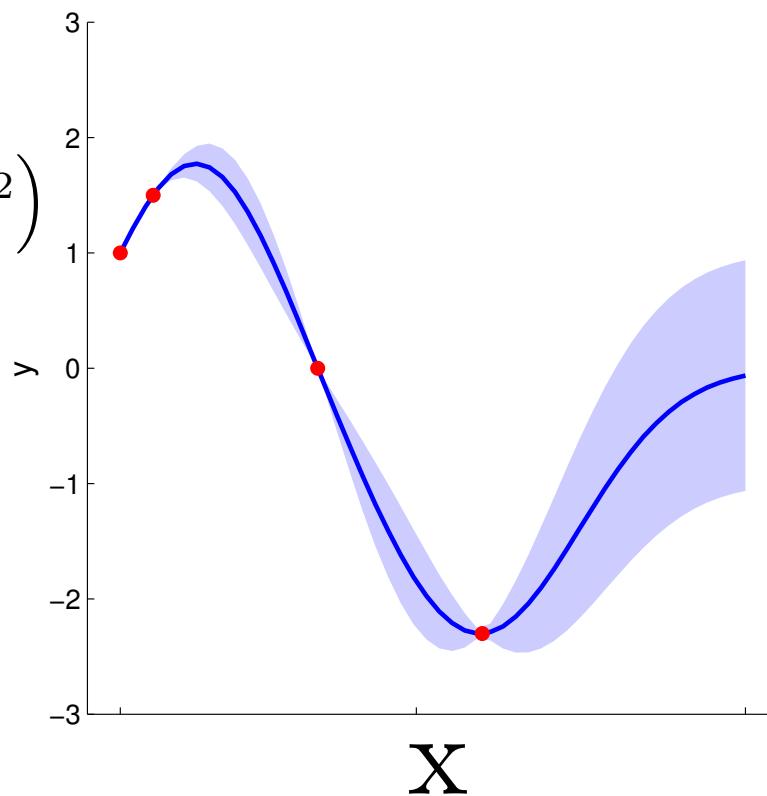
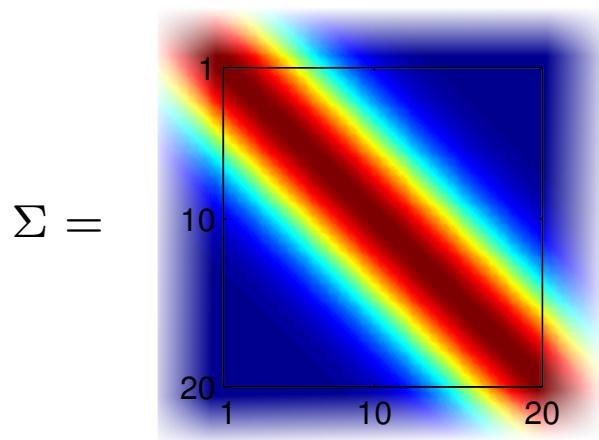
$$K(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 \exp\left(-\frac{1}{2l^2}(\mathbf{x}_1 - \mathbf{x}_2)^2\right)$$



Regression: probabilistic inference in function space

$$\Sigma(\mathbf{x}_1, \mathbf{x}_2) = K(\mathbf{x}_1, \mathbf{x}_2) + I\sigma_y^2$$

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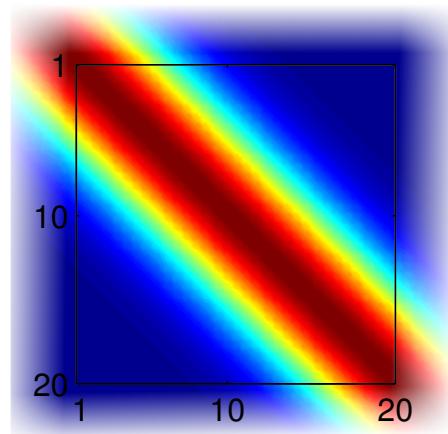
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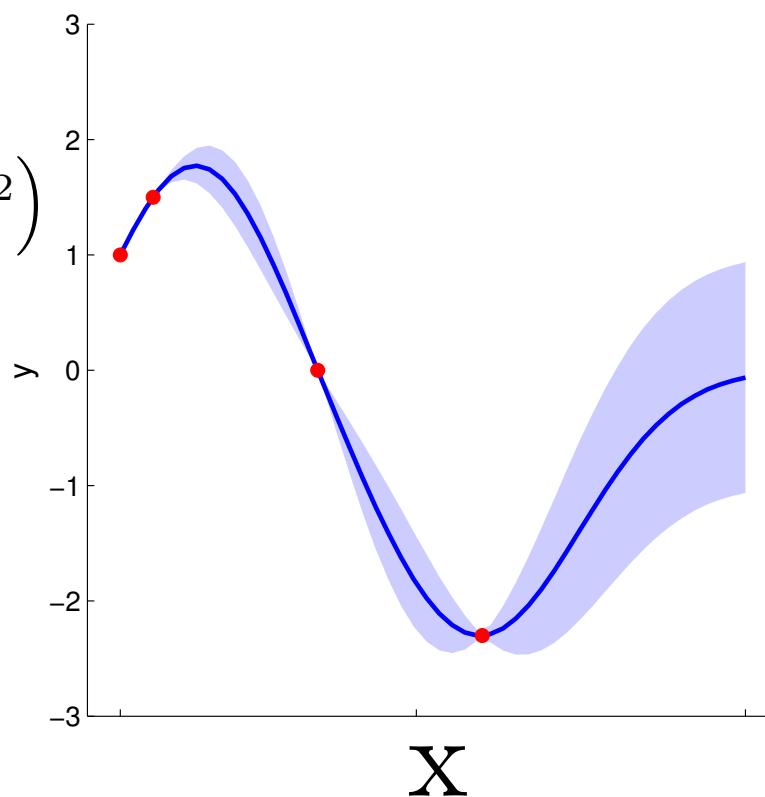
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Parametric model

$$\mathbf{y}(\mathbf{x}) = f(\mathbf{x}; \theta) + \sigma_y \epsilon$$

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



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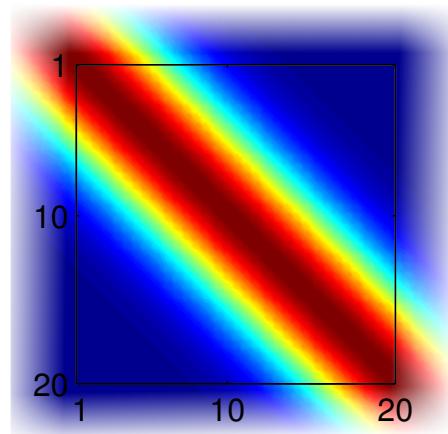
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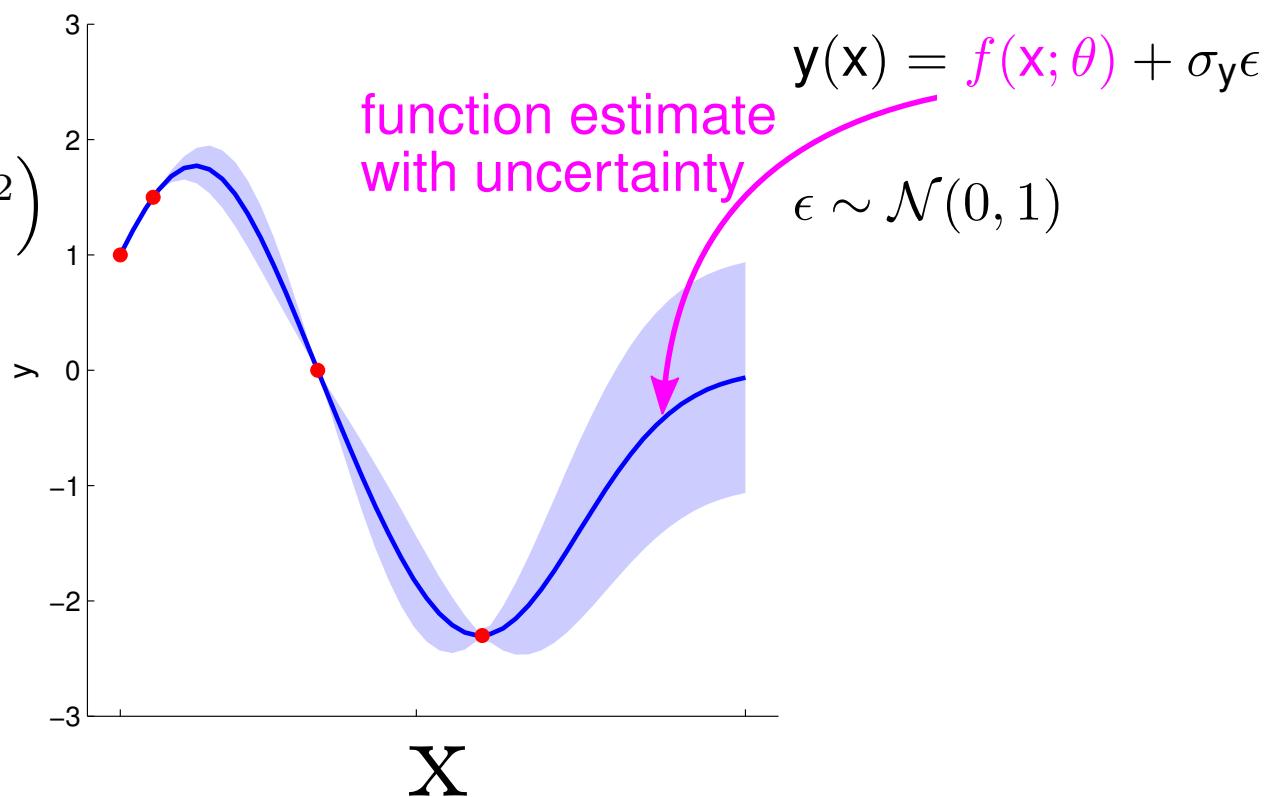
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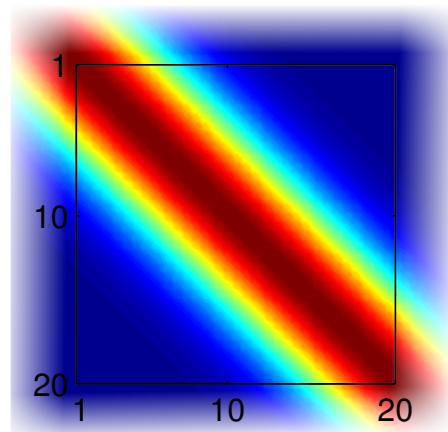
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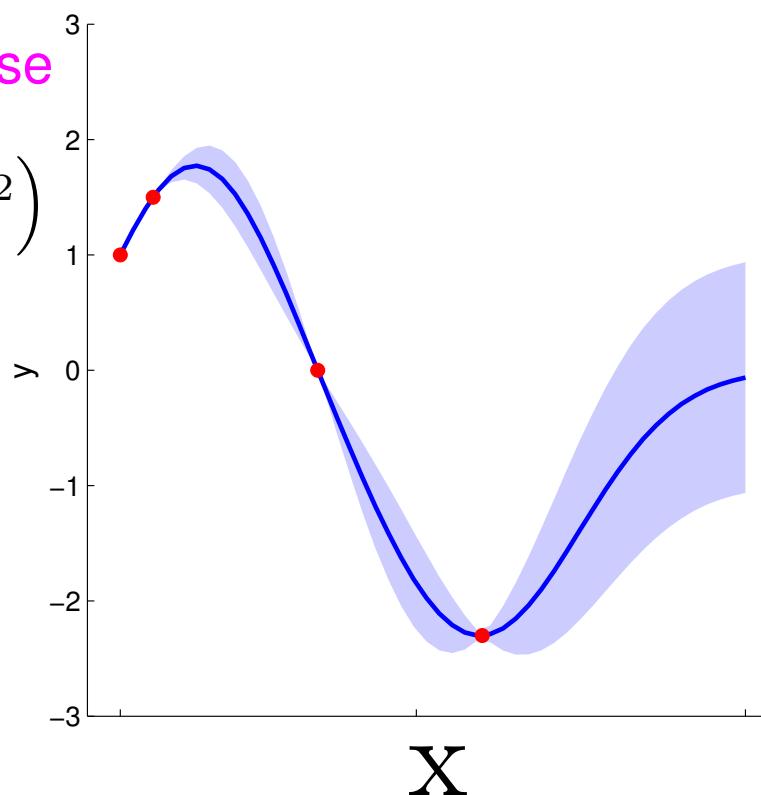
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Regression: probabilistic inference in function space

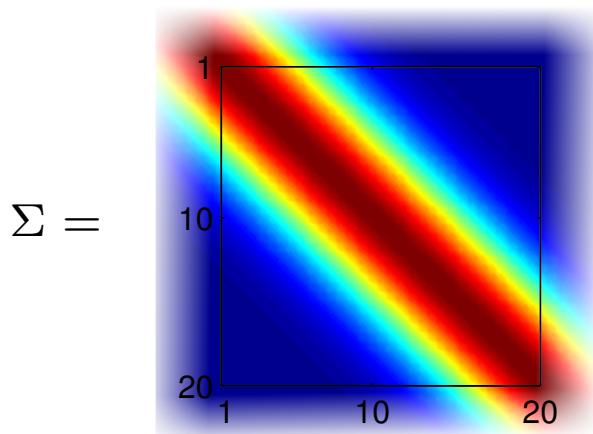
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↑
horizontal-scale

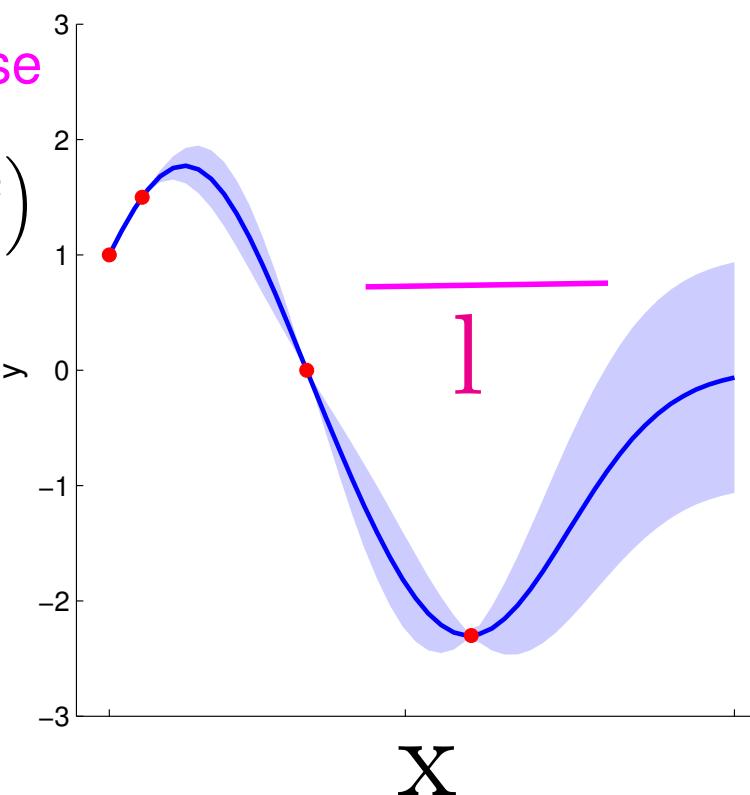


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Regression: probabilistic inference in function space

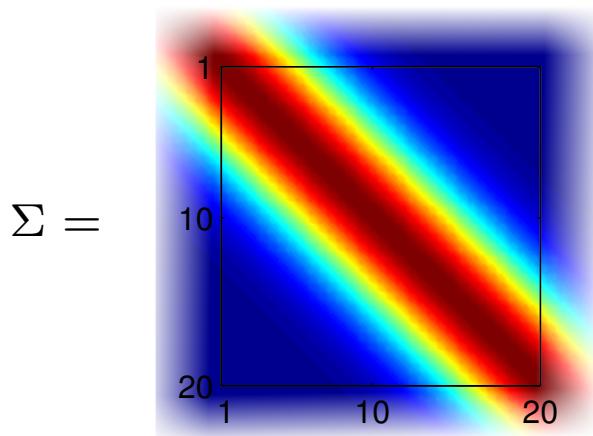
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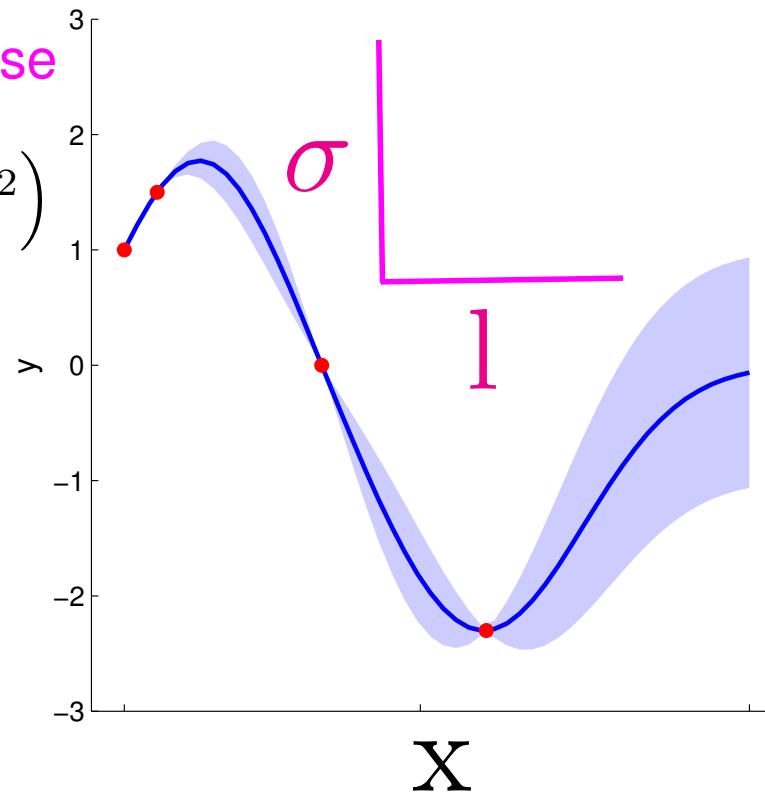
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vertical-scale horizontal-scale



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Mathematical Foundations: Definition

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

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

A Gaussian distribution is fully specified by a mean vector, μ , and covariance matrix Σ :

$$\mathbf{f} = (f_1, \dots, f_n) \sim \mathcal{N}(\mu, \Sigma), \text{ indices } i = 1, \dots, n$$

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

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

Mathematical Foundations: Marginalisation

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

Mathematical Foundations: Marginalisation

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We are saved by the marginalisation property:

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

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

⇒ Only need to represent finite dimensional projections of GPs on computer.

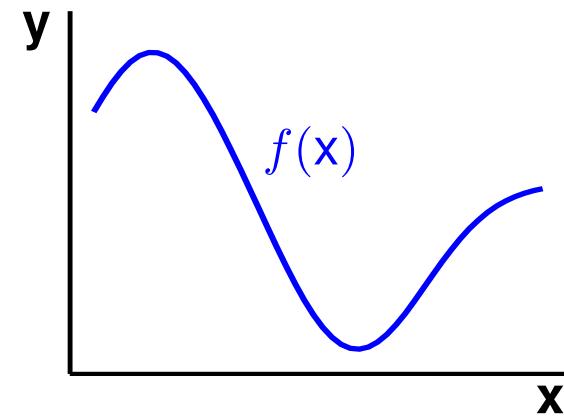
nonparametric model: complexity increases with size of the data

Mathematical Foundations: Regression

Q3. What's the formal justification for how we were using GPs for regression?

Generative model (like non-linear regression)

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



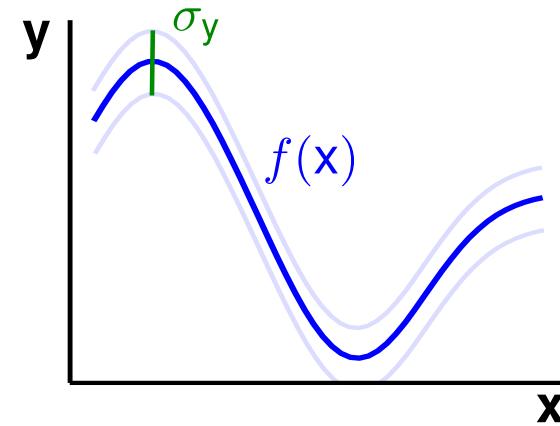
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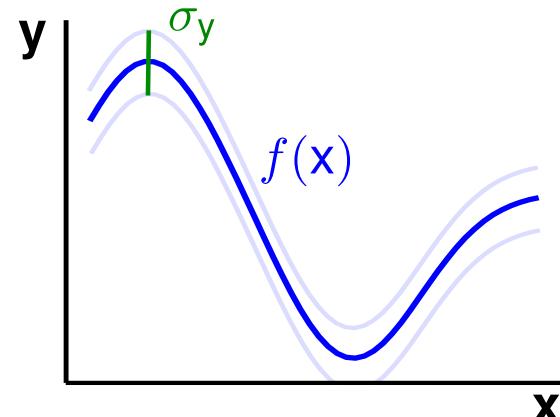
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$$p(\epsilon) = \mathcal{N}(0, 1)$$

place GP prior over the non-linear function

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

$$K(x, x') = \sigma^2 \exp\left(-\frac{1}{2l^2}(x - x')^2\right) \quad (\text{smoothly wiggling functions expected})$$



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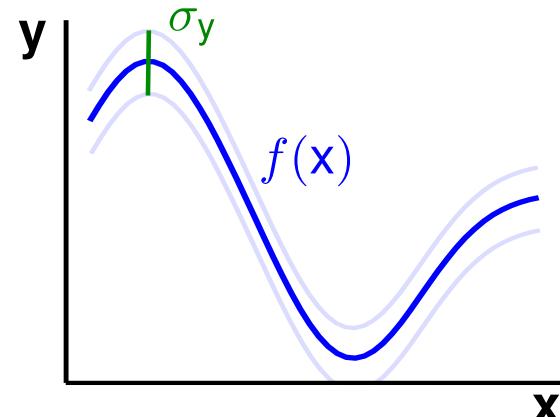
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since the sum of two Gaussians is a Gaussian, the model induces a GP over $y(x)$

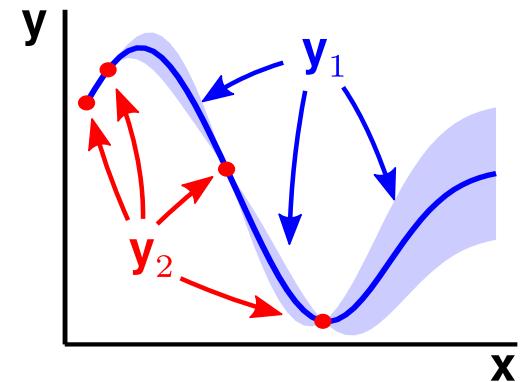
$$p(y(x)|\theta) = \mathcal{GP}(0, K(x, x') + I\sigma_y^2)$$



Mathematical foundations: Prediction

Q4. How do we make predictions?

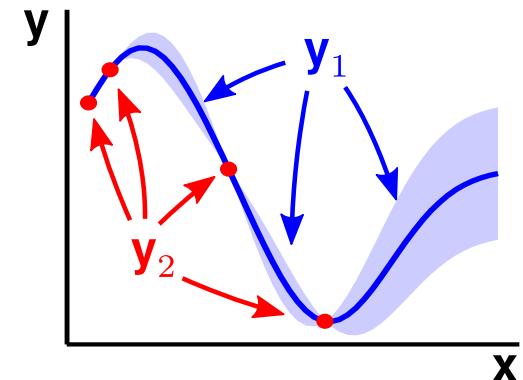
$$p(\mathbf{y}_1|\mathbf{y}_2) = \frac{p(\mathbf{y}_1, \mathbf{y}_2)}{p(\mathbf{y}_2)}$$



Mathematical foundations: Prediction

Q4. How do we make predictions?

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

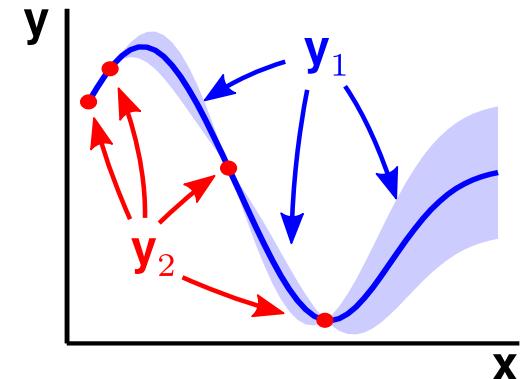


$$\implies p(\mathbf{y}_1 | \mathbf{y}_2) = \mathcal{N}(\mathbf{a} + \mathbf{B}\mathbf{C}^{-1}(\mathbf{y}_2 - \mathbf{b}), \mathbf{A} - \mathbf{B}\mathbf{C}^{-1}\mathbf{B}^\top)$$

Mathematical foundations: Prediction

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predictive mean

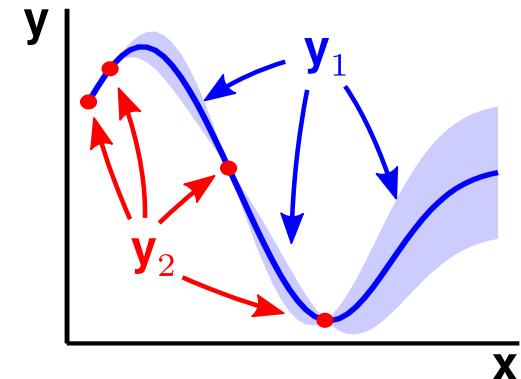
$$\begin{aligned} \mu_{\mathbf{y}_1 | \mathbf{y}_2} &= \mathbf{a} + \mathbf{B}\mathbf{C}^{-1}(\mathbf{y}_2 - \mathbf{b}) \\ &= \mathbf{B}\mathbf{C}^{-1}\mathbf{y}_2 \\ &= \mathbf{W}\mathbf{y}_2 \end{aligned}$$

linear in the data

Mathematical foundations: Prediction

Q4. How do we make predictions?

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linear in the data

predictive covariance

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

predictive uncertainty = prior uncertainty - reduction in uncertainty

predictions more confident than prior

What effect do the hyper-parameters have?

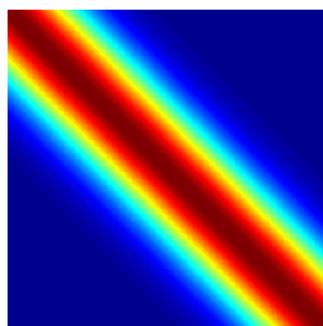
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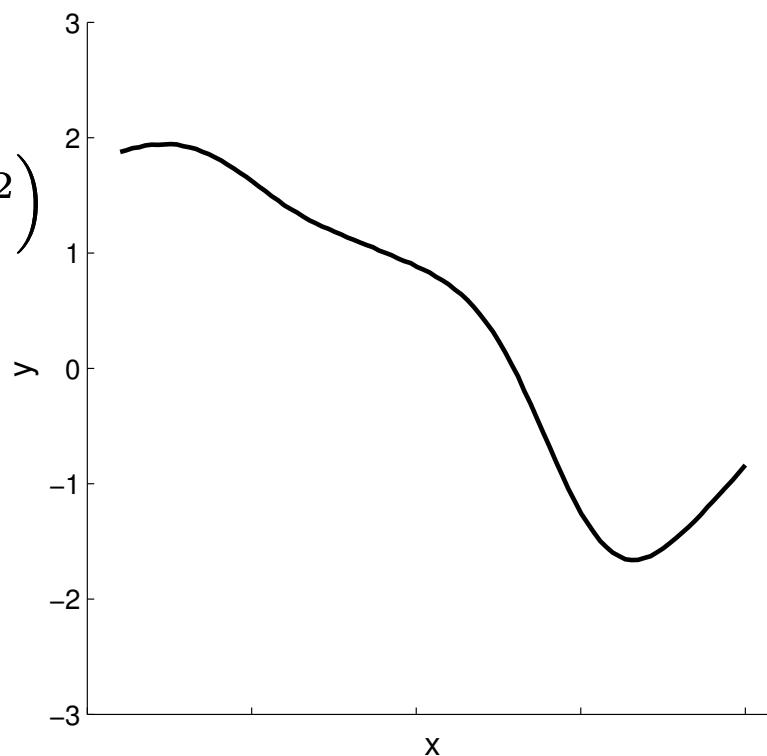
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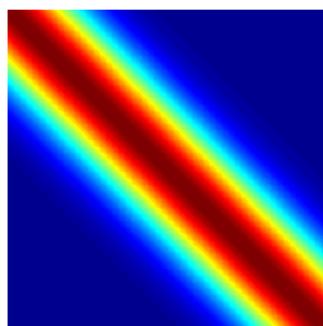
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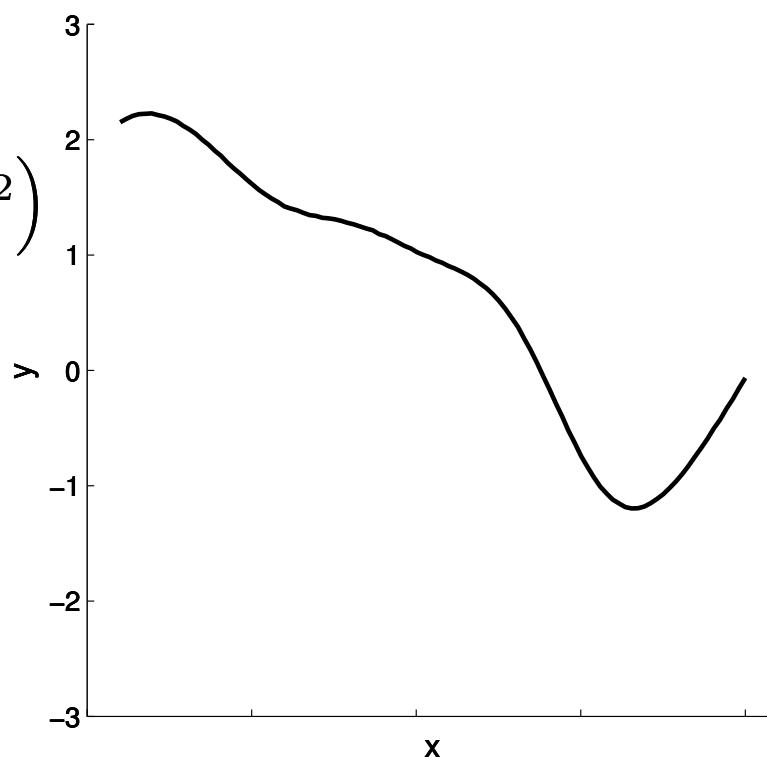
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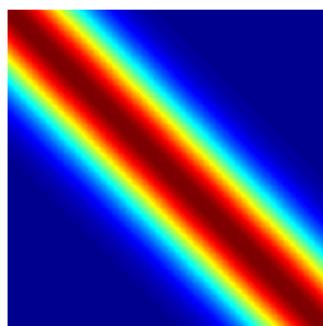
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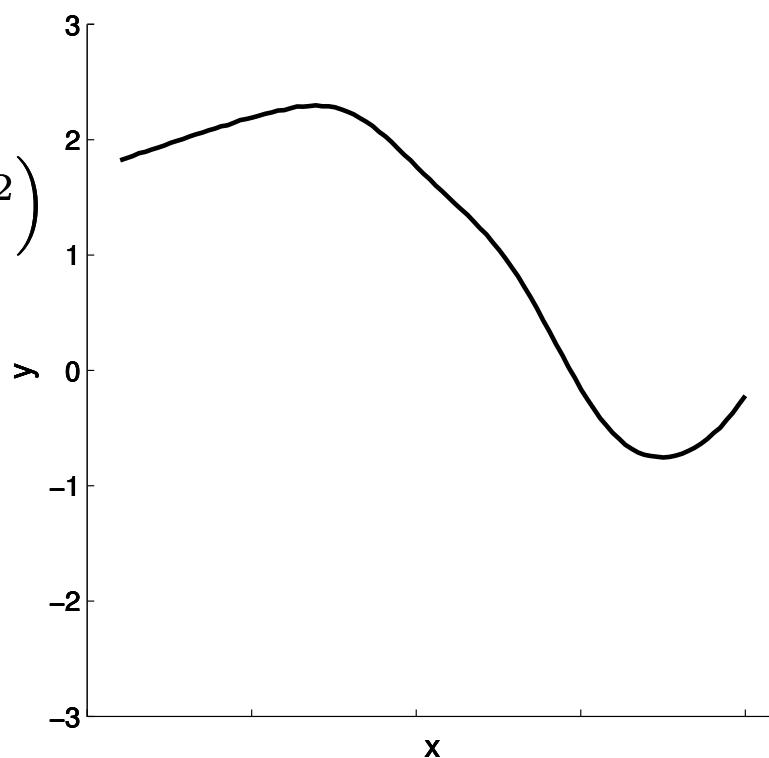
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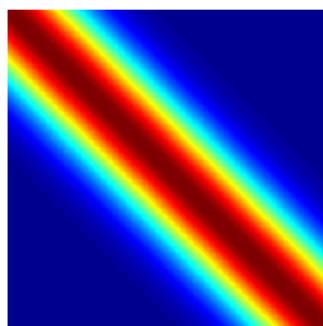
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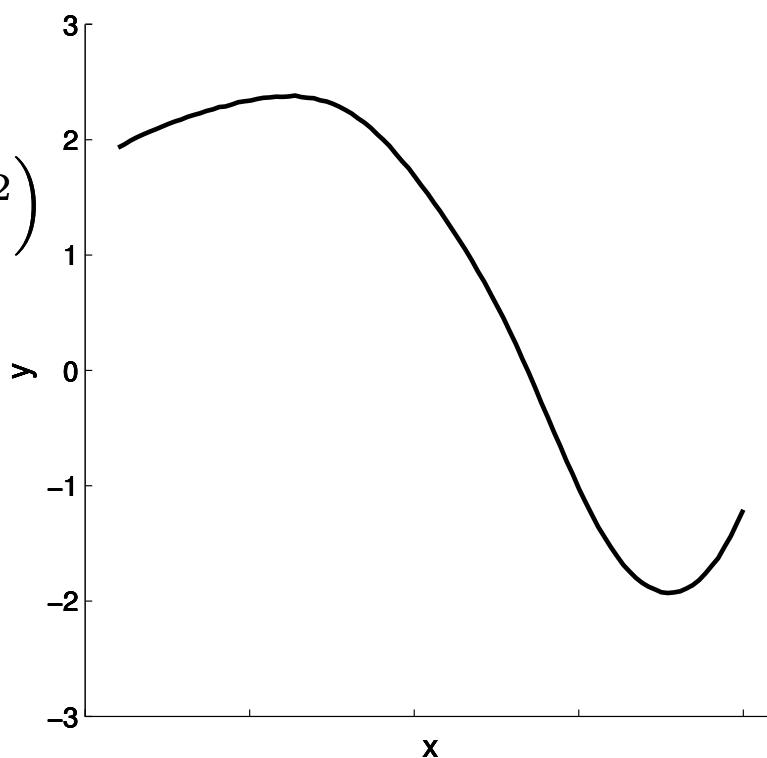
$$\Sigma =$$



Parametric model

$$\mathbf{y}(\mathbf{x}) = f(\mathbf{x}; \theta) + \sigma_y \epsilon$$

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



What effect do the hyper-parameters have?

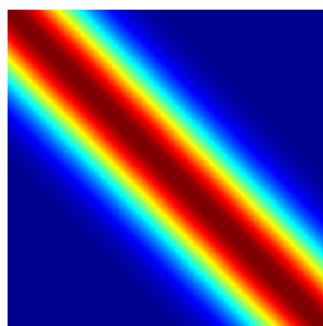
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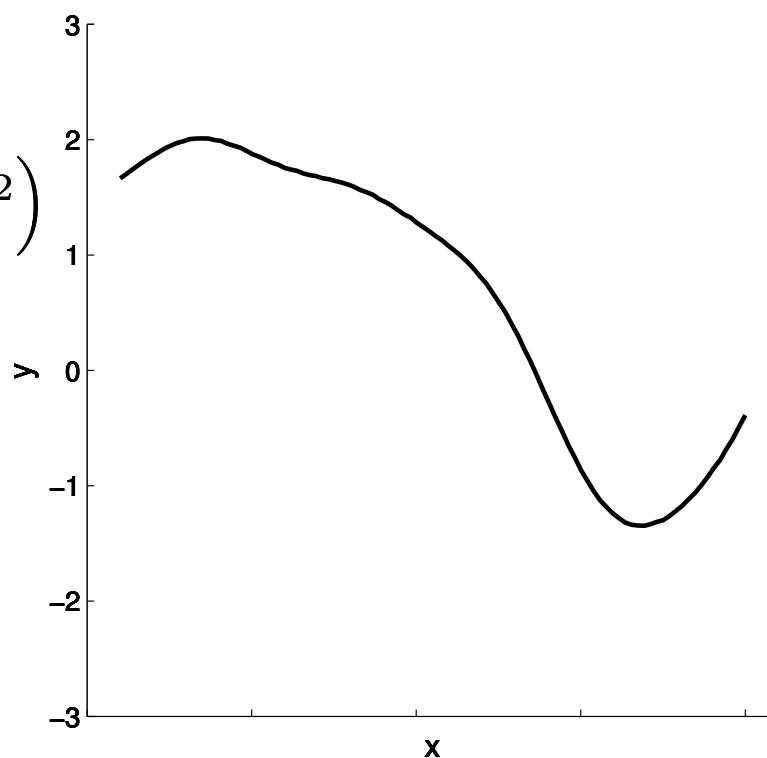
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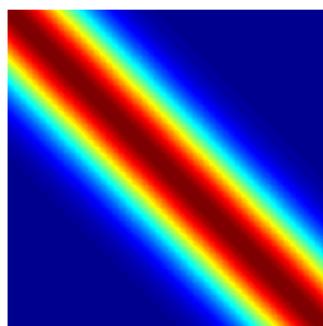
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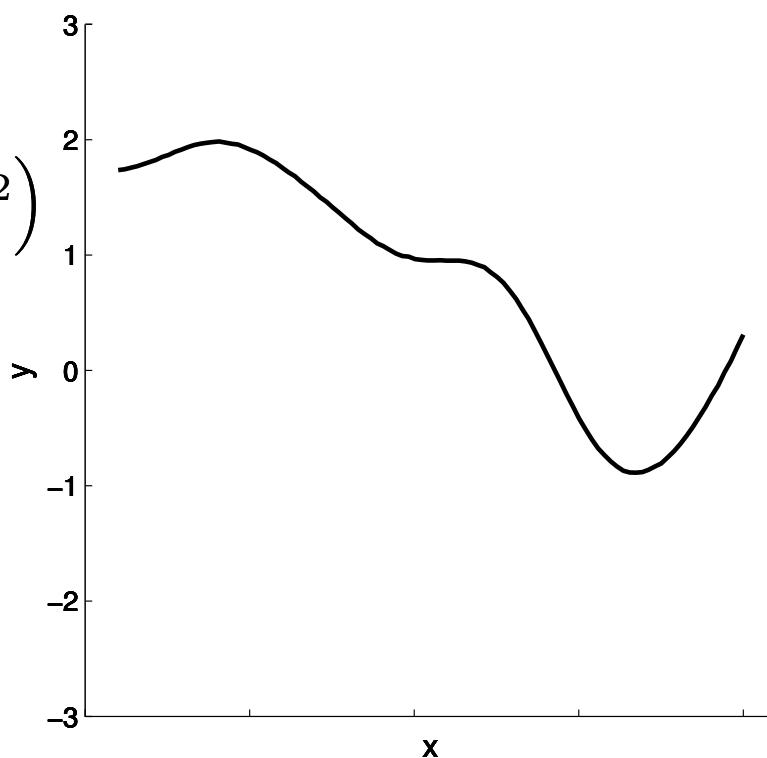
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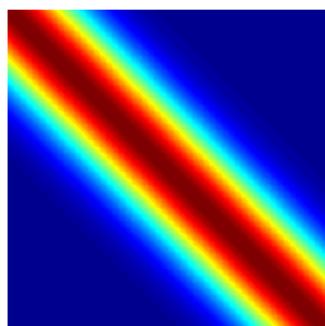
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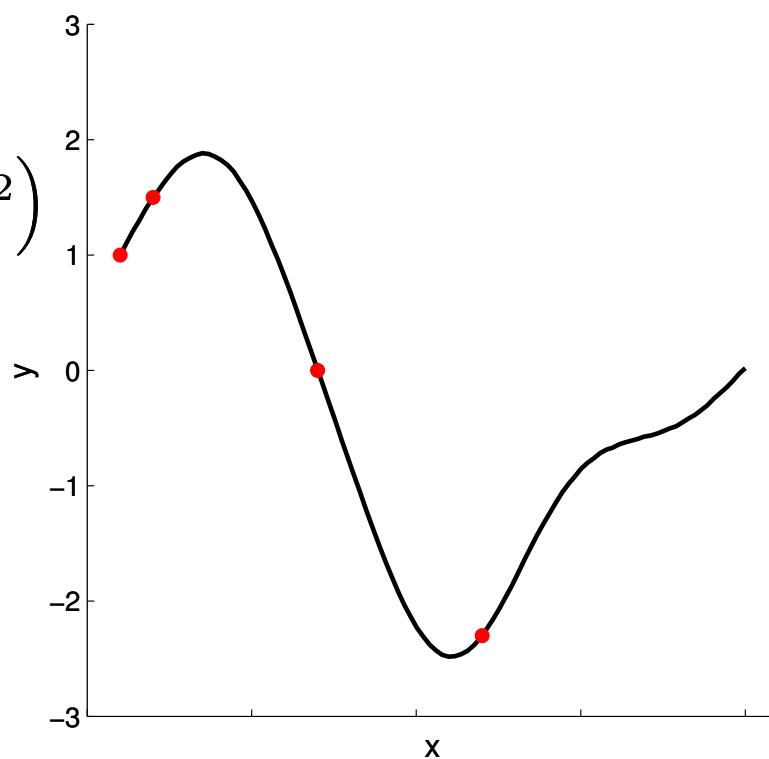
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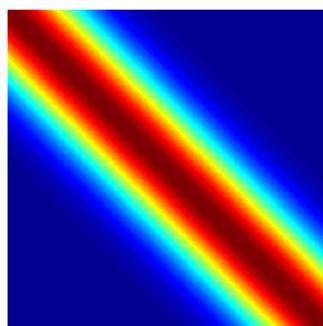
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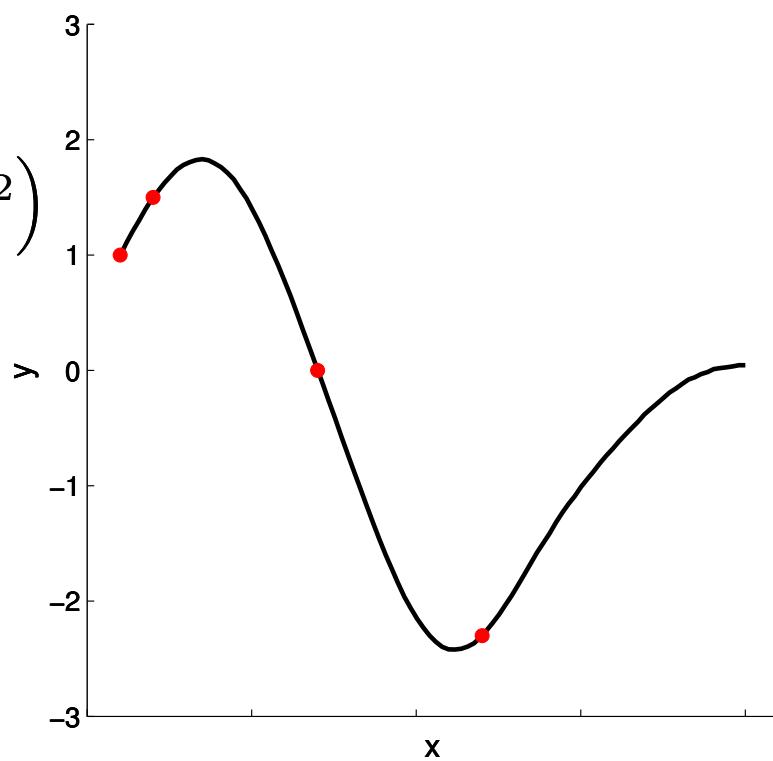
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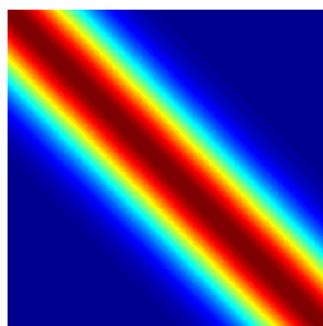
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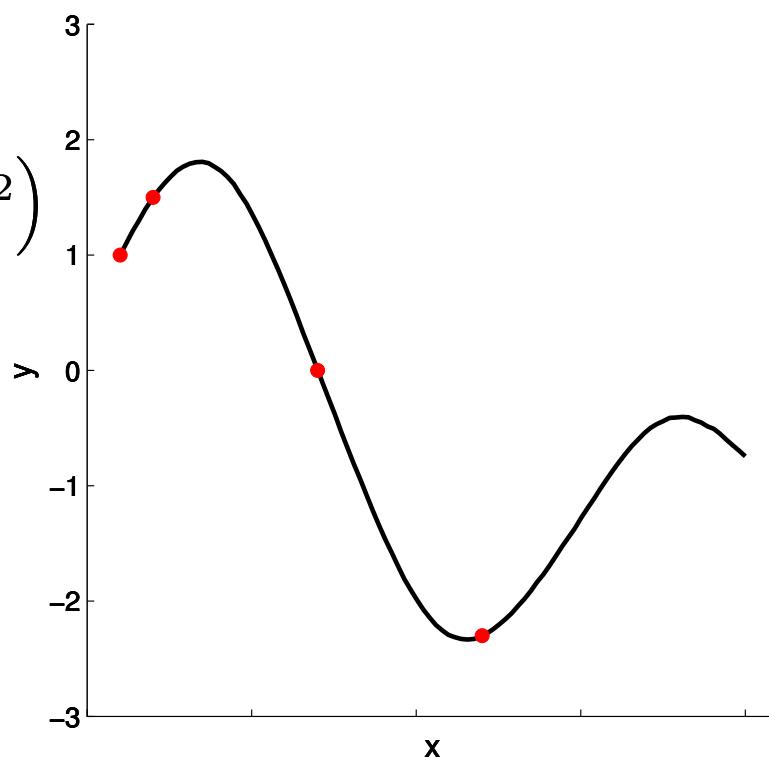
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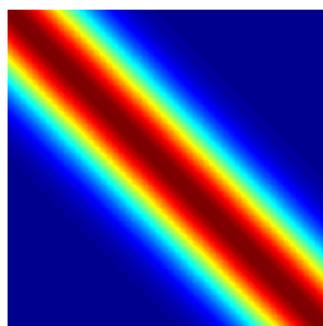
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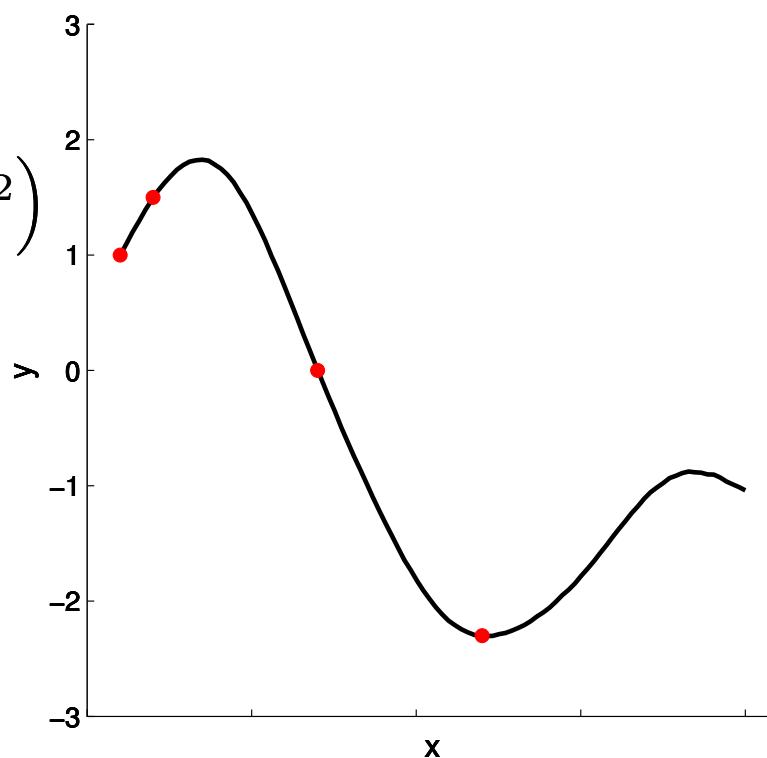
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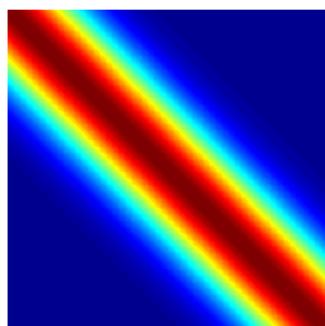
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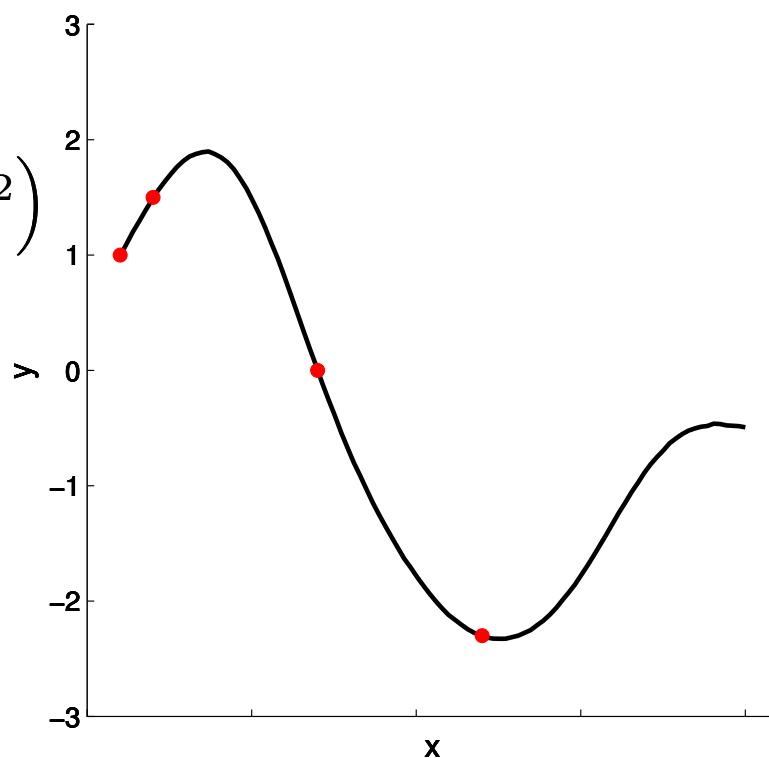
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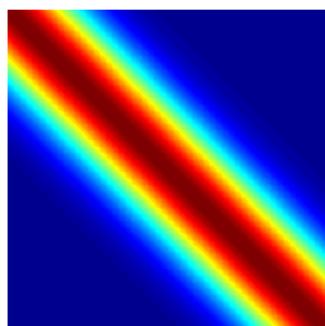
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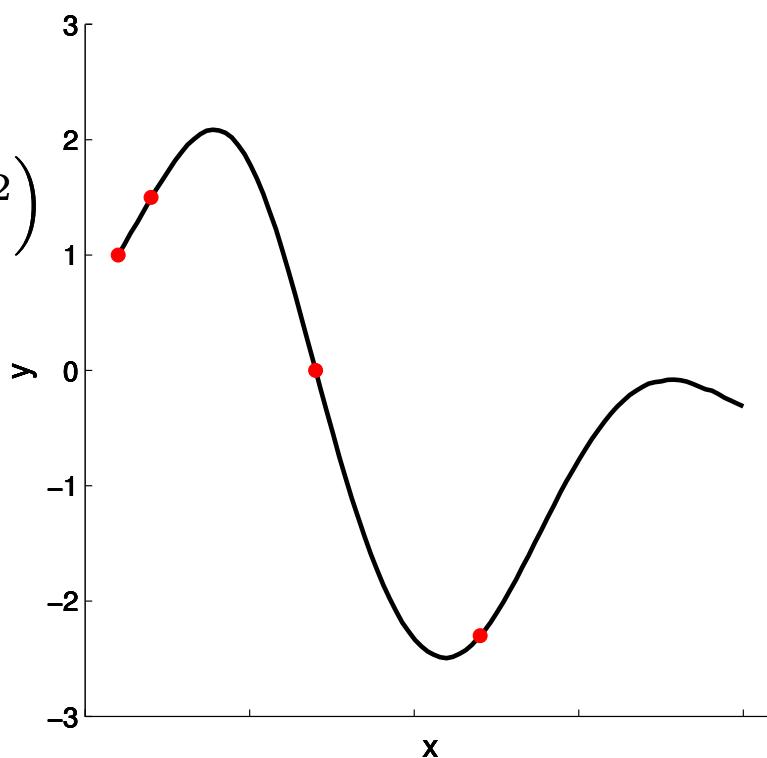
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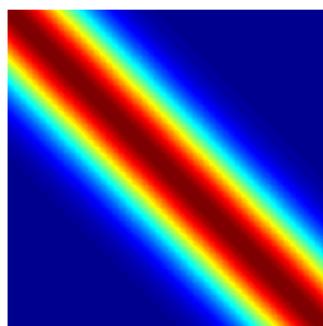
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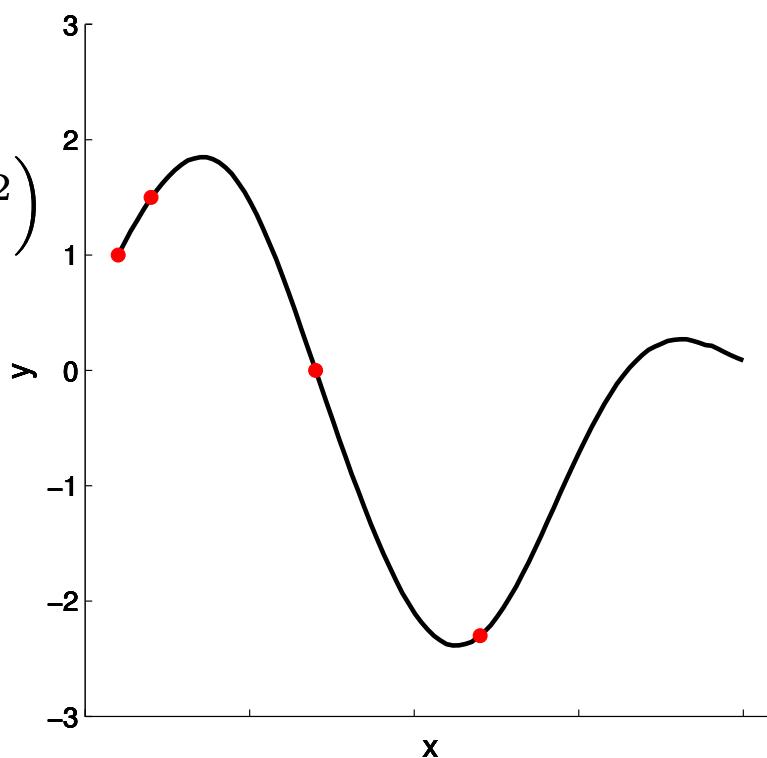
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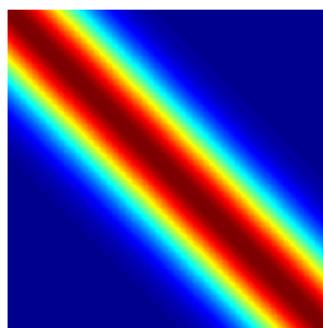
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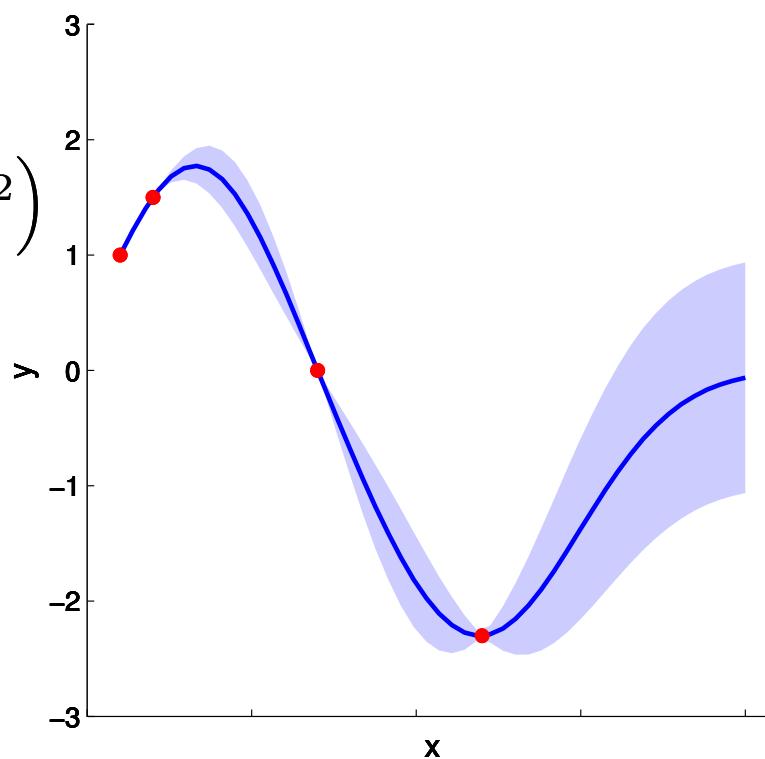
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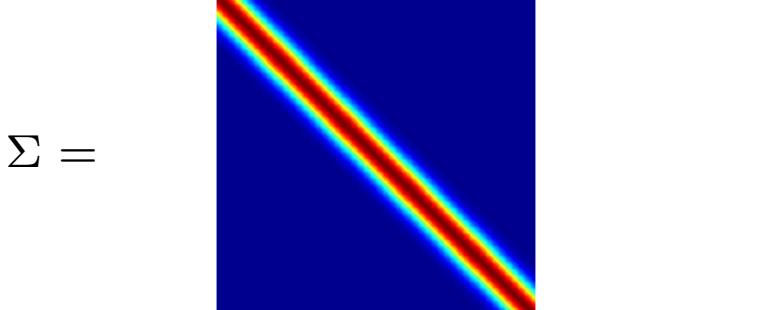
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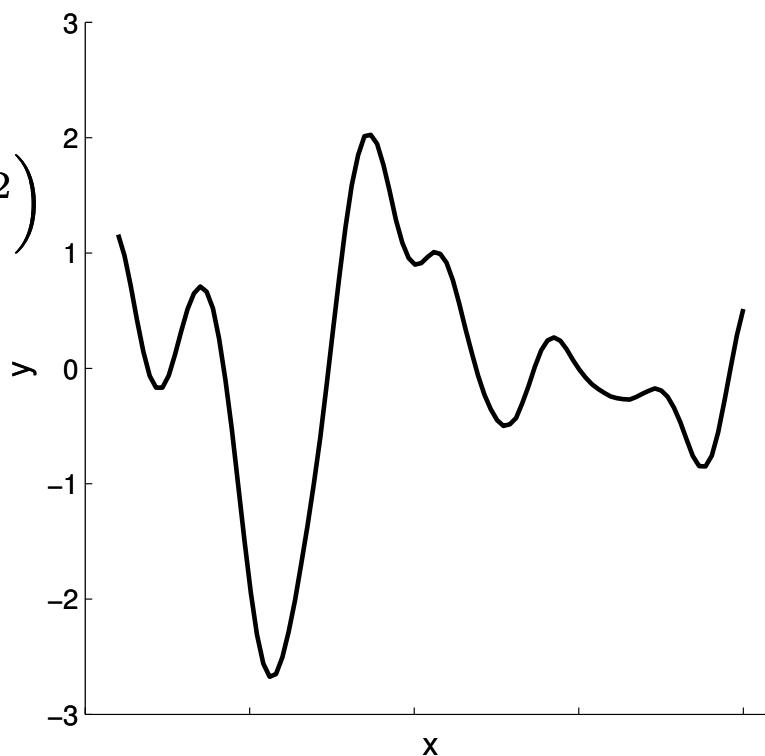


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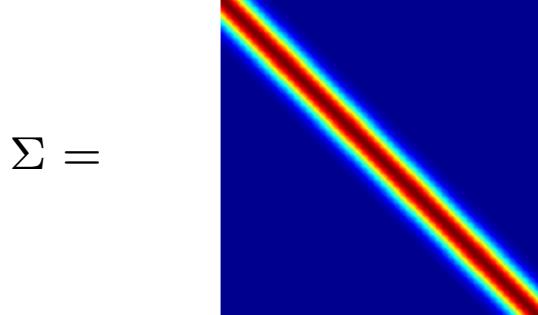
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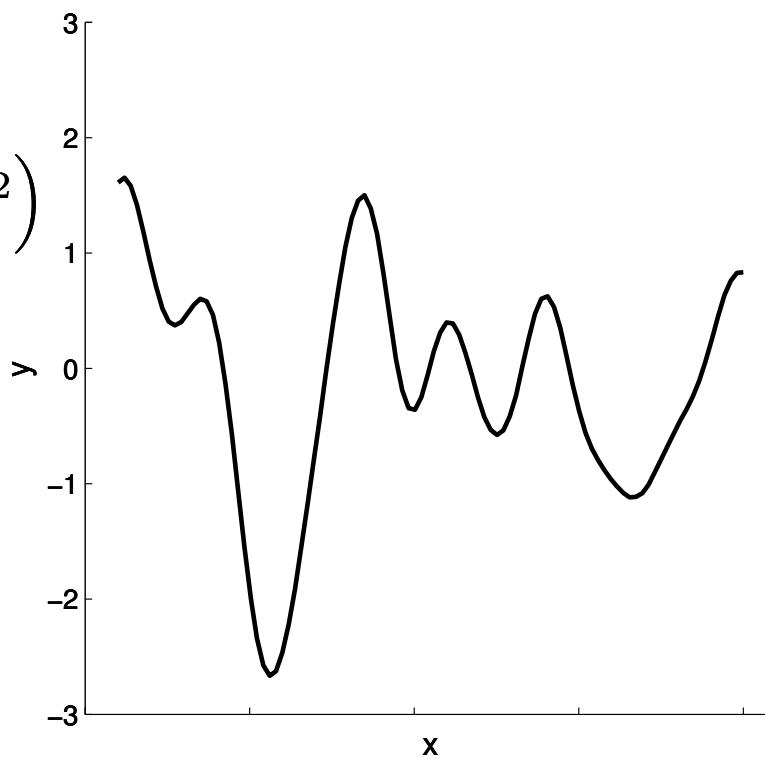


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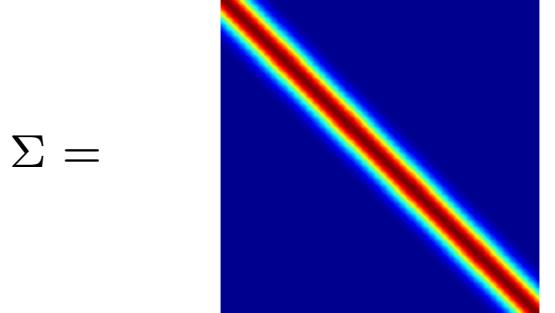
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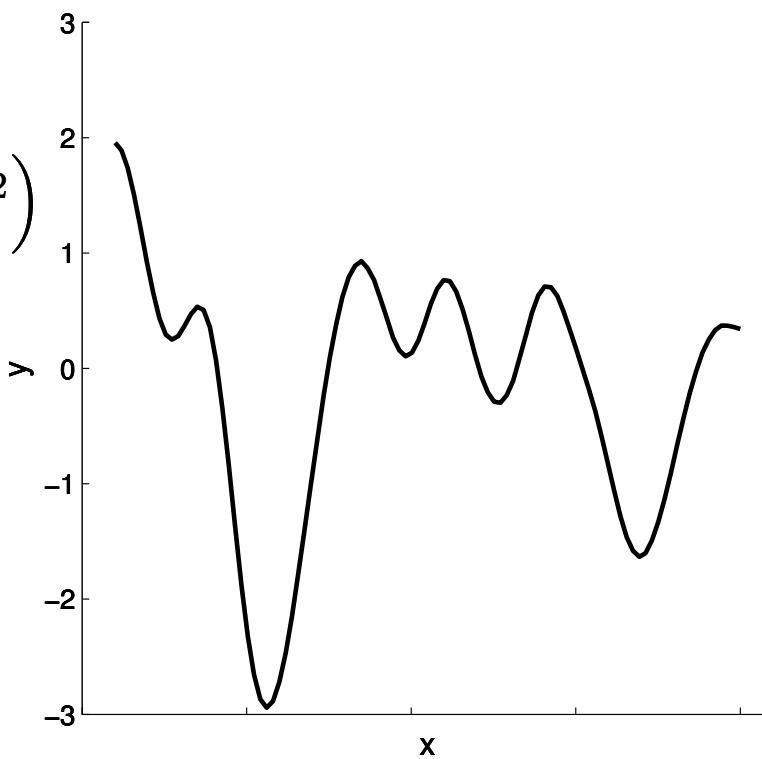


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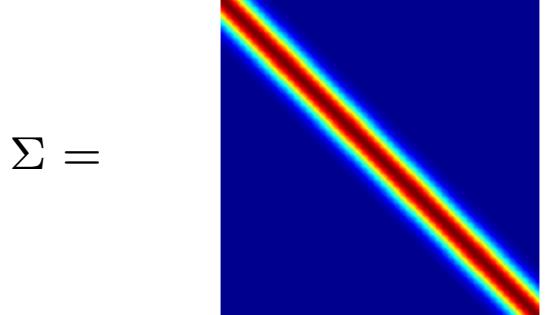
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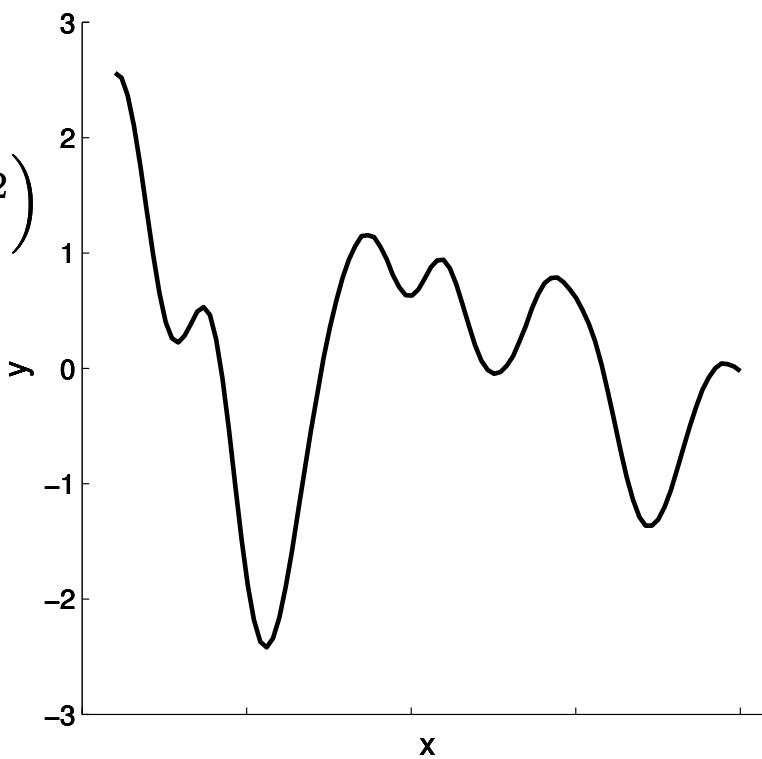


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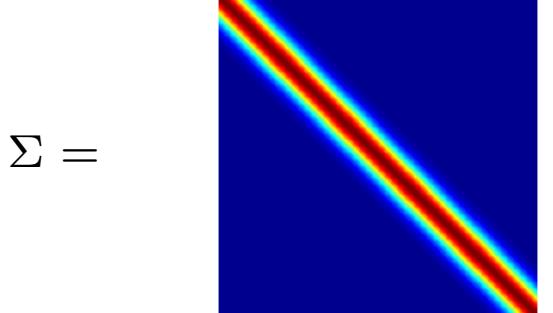
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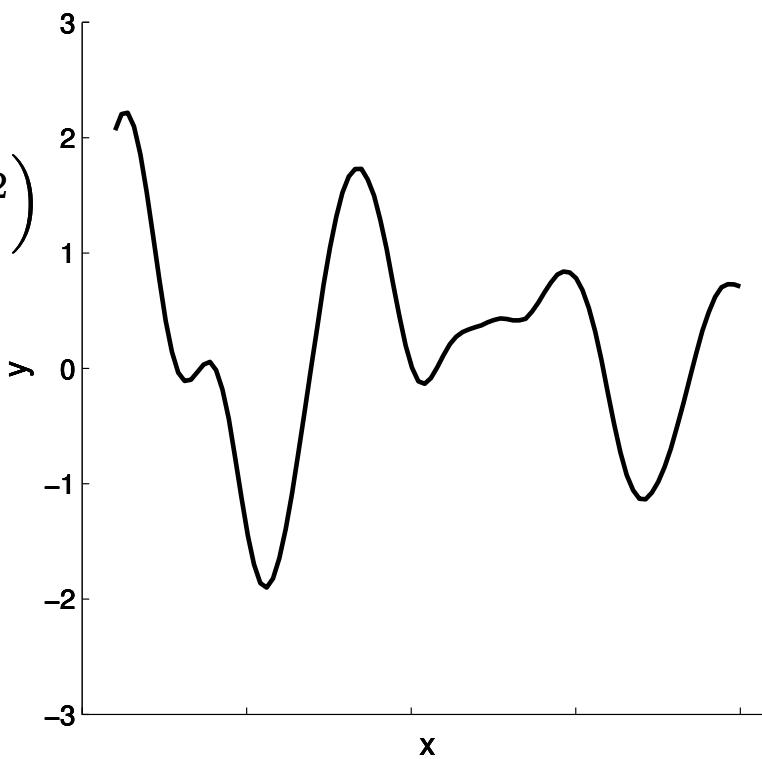


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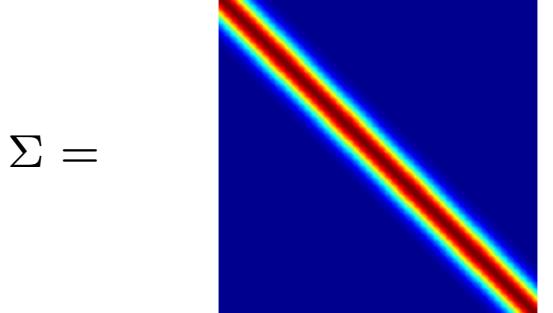
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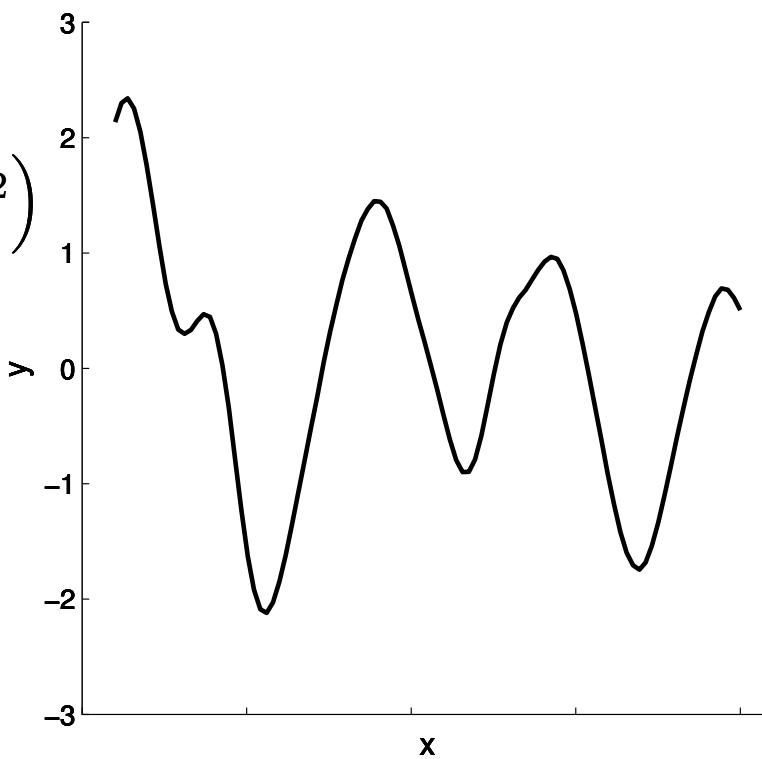


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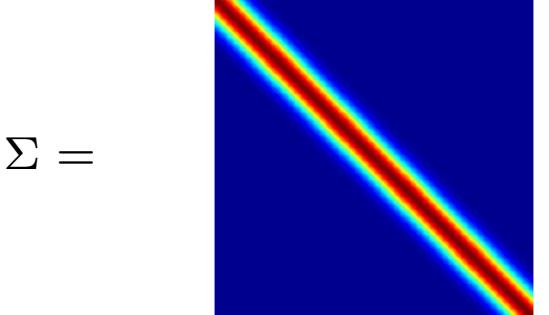
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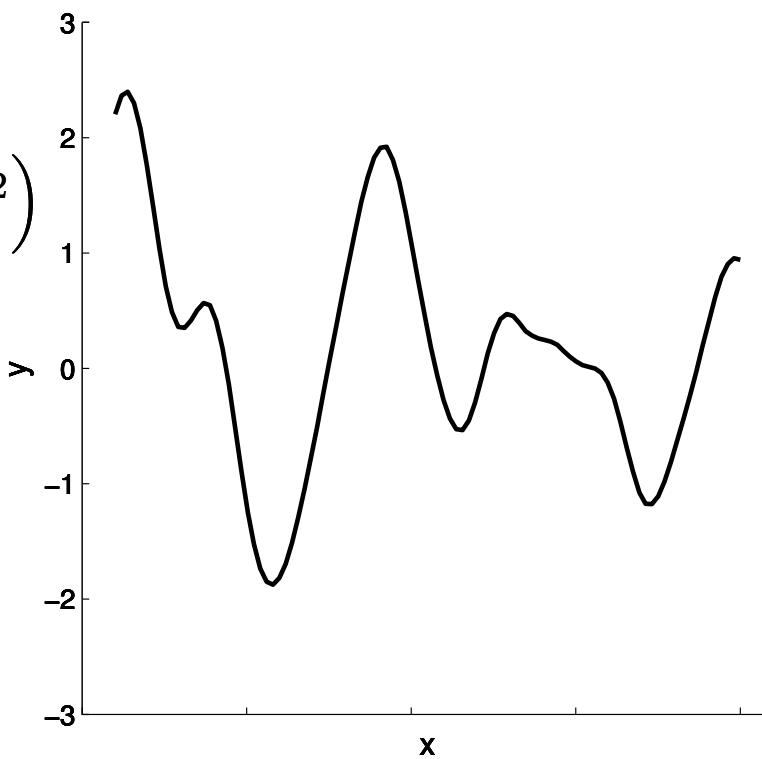


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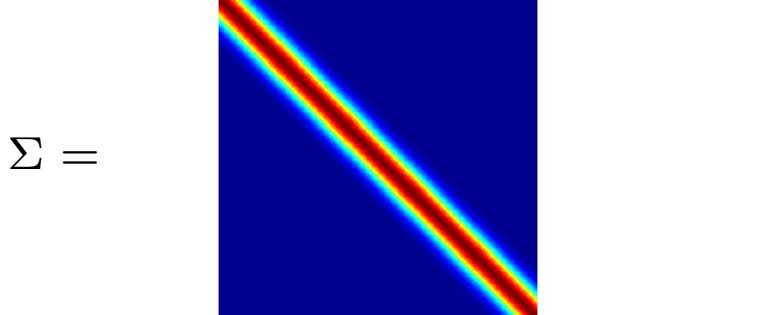
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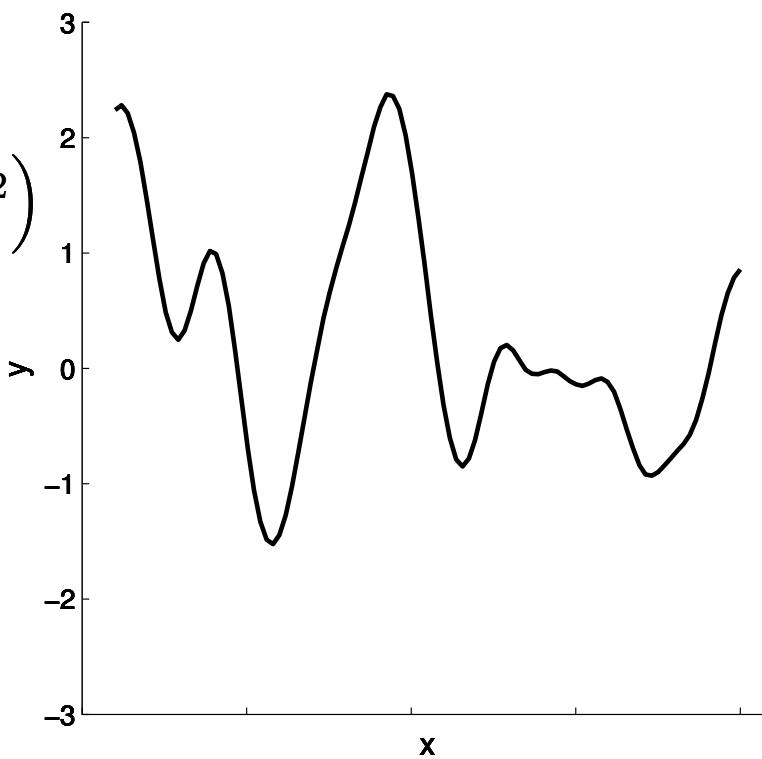


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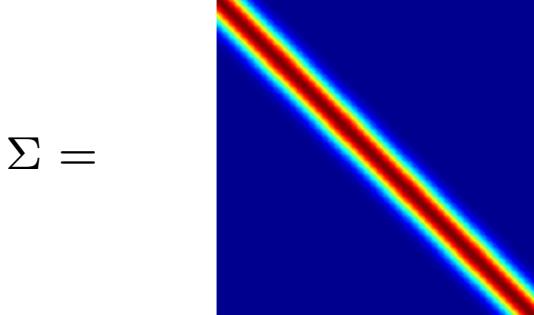
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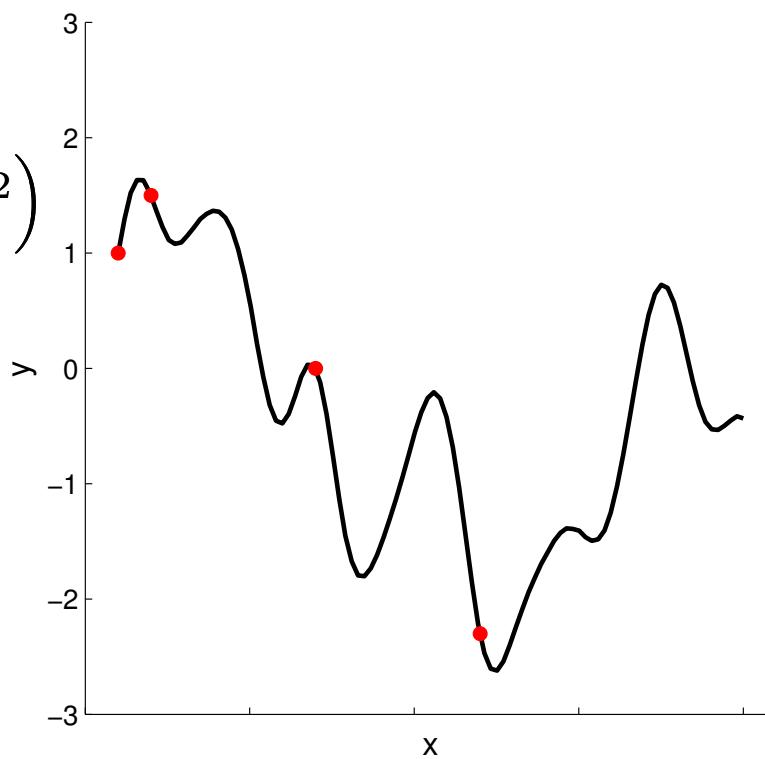


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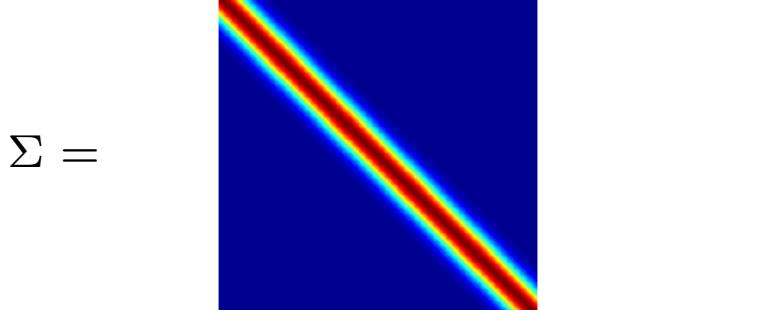
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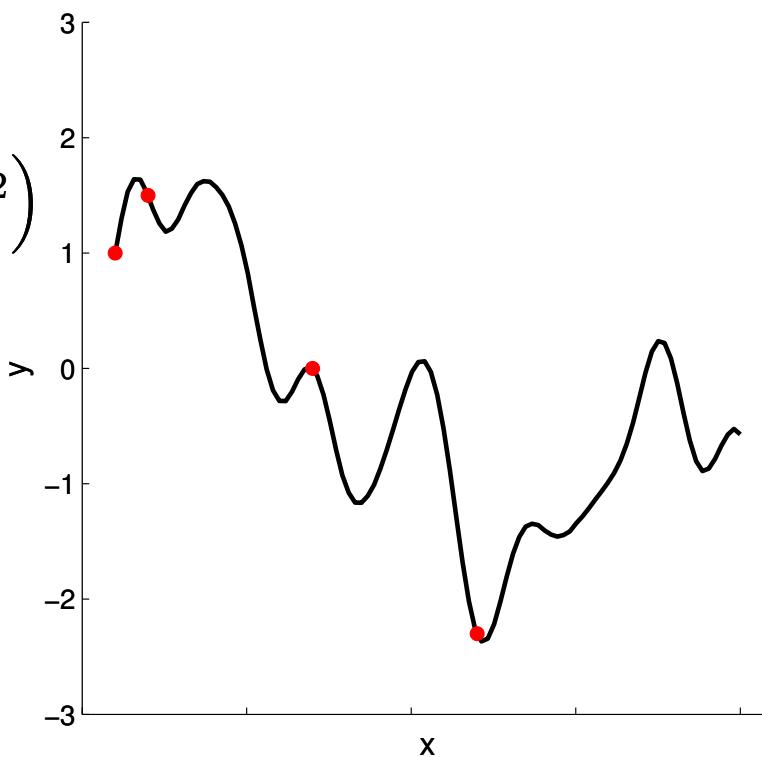


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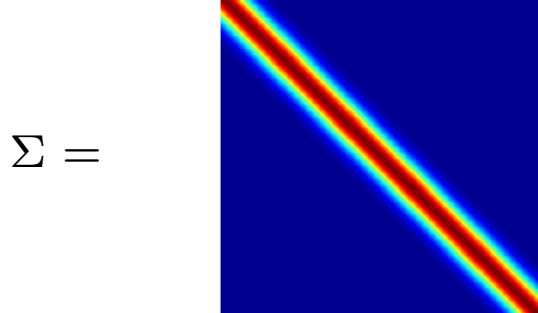
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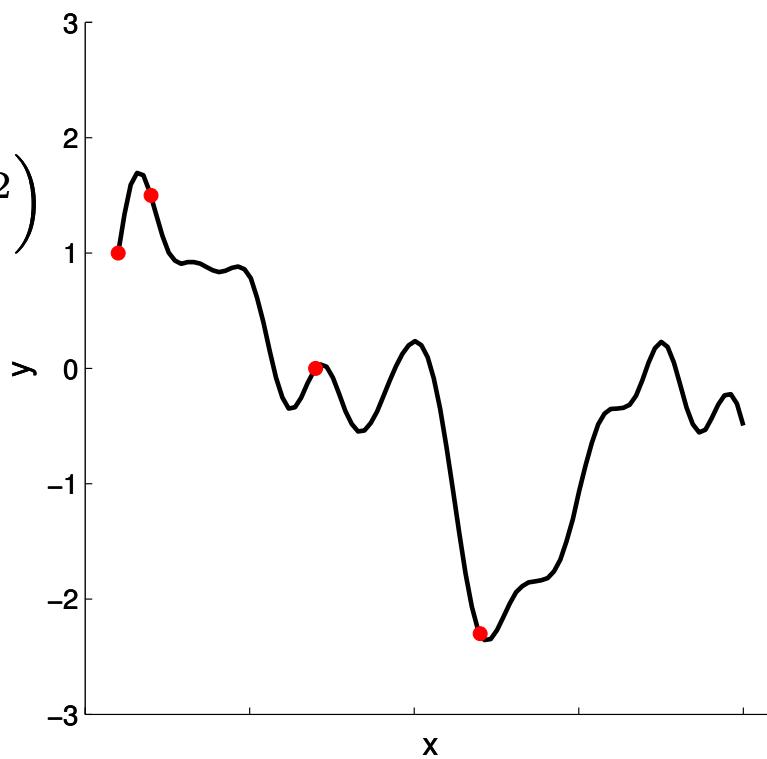


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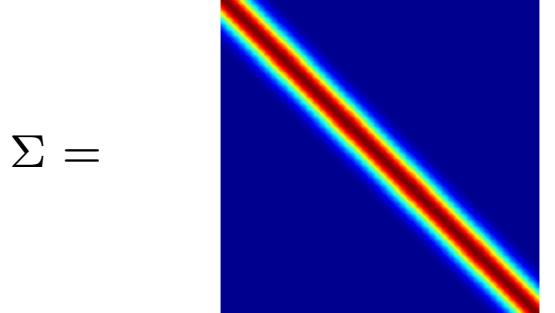
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$$K(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 \exp\left(-\frac{1}{2l^2}(\mathbf{x}_1 - \mathbf{x}_2)^2\right)$$

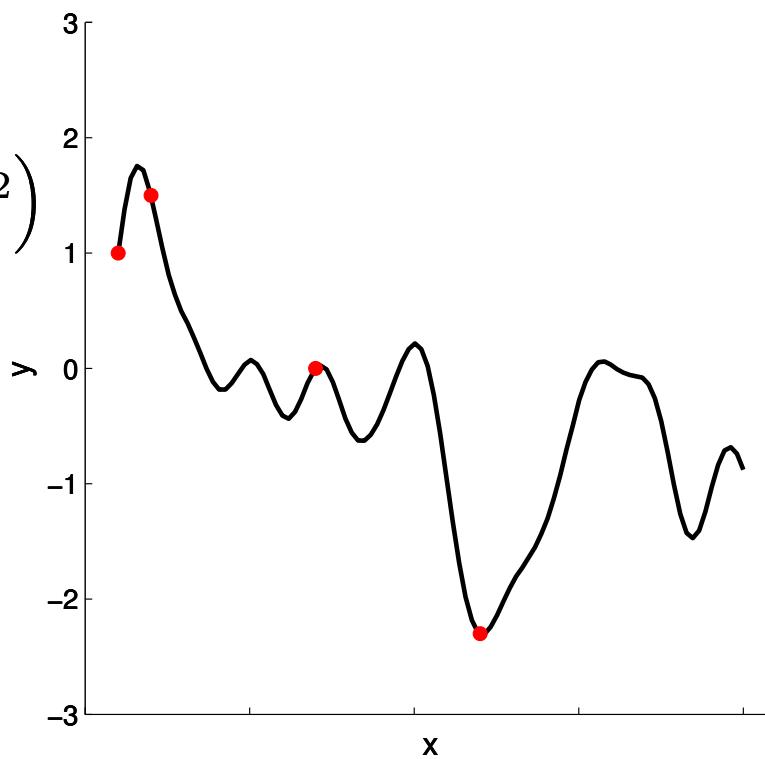


$$\Sigma =$$

Parametric model

$$y(\mathbf{x}) = f(\mathbf{x}; \theta) + \sigma_y \epsilon$$

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



What effect do the hyper-parameters have?

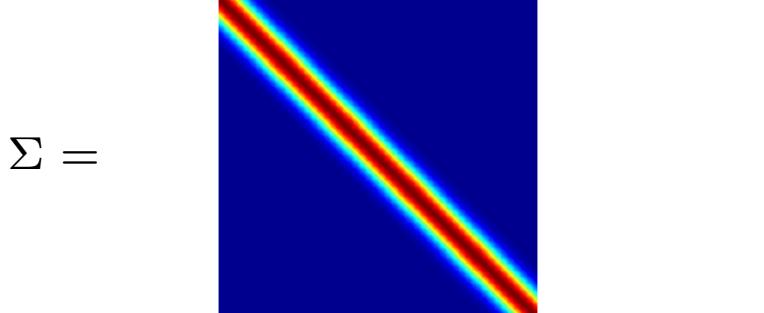
short horizontal length-scale

Non-parametric (∞ -parametric)

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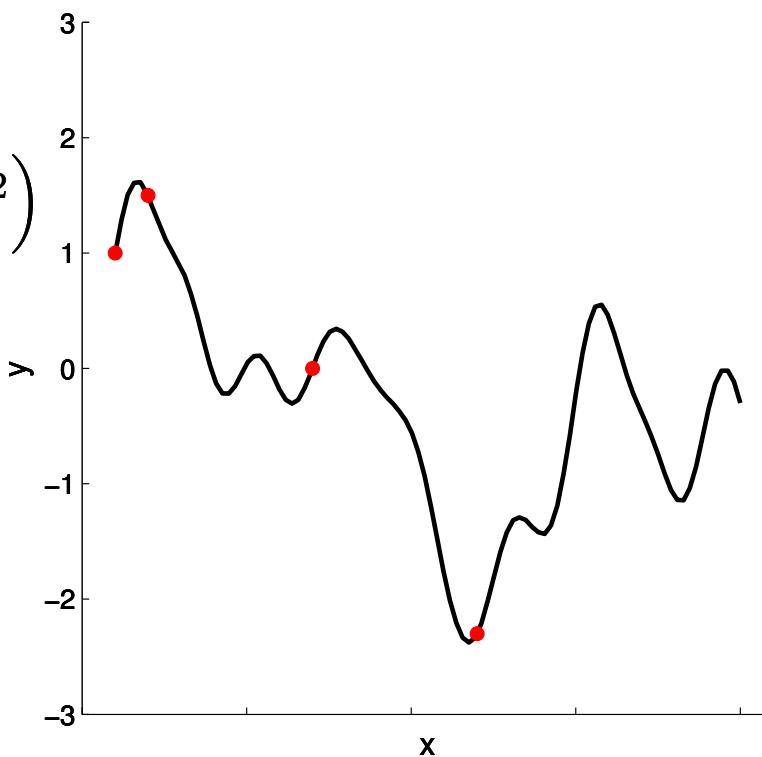


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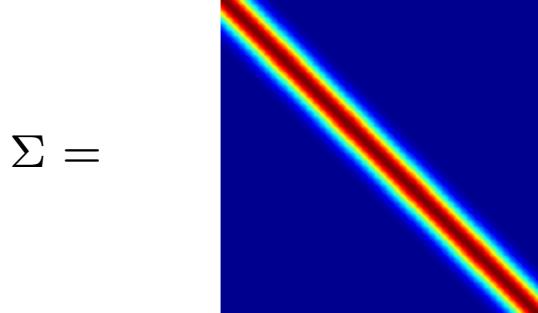
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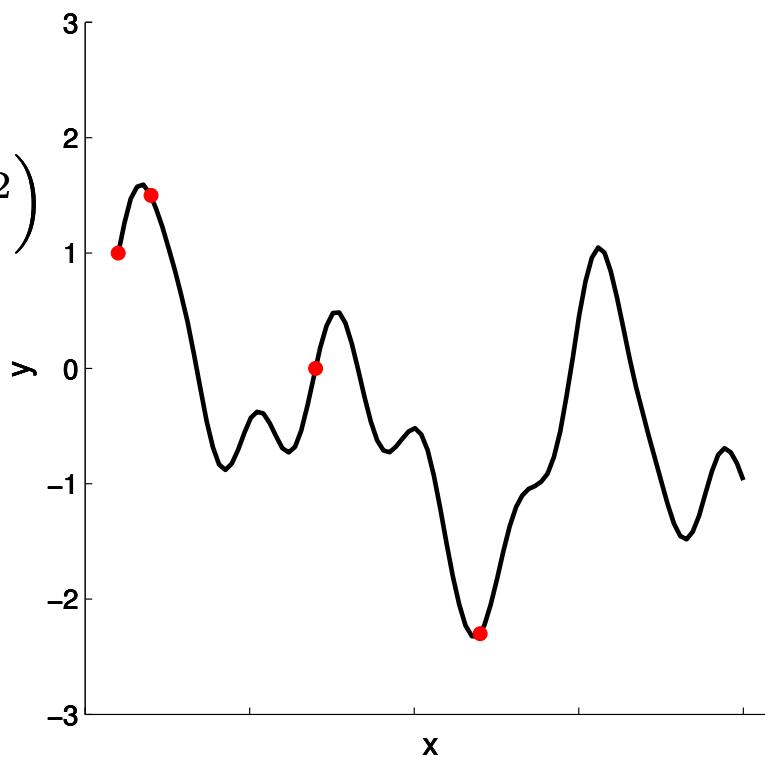


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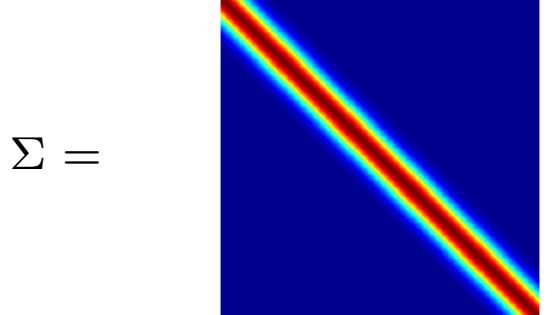
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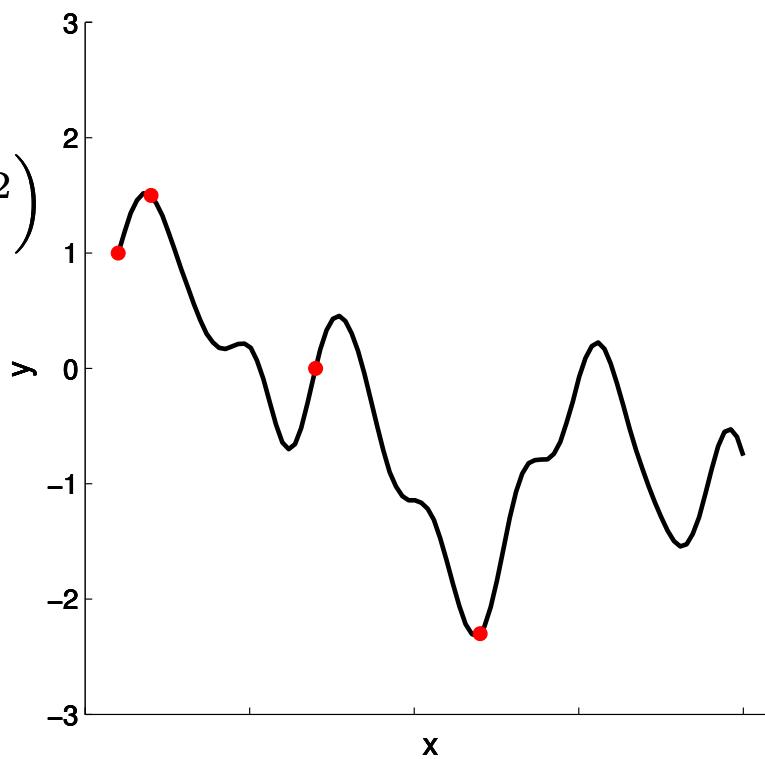


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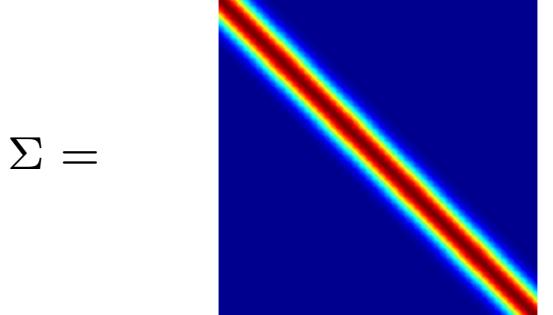
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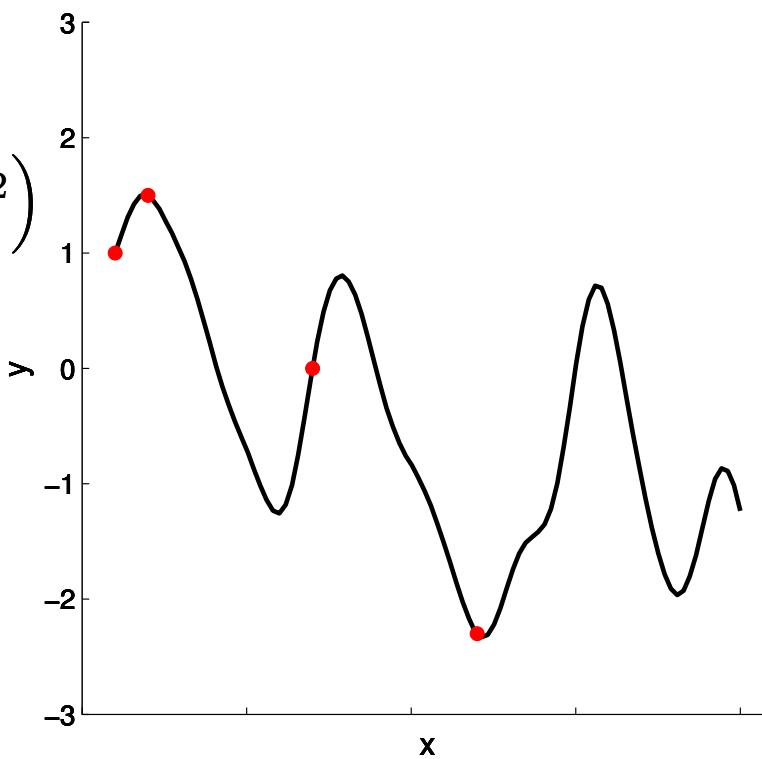


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What effect do the hyper-parameters have?

short horizontal length-scale

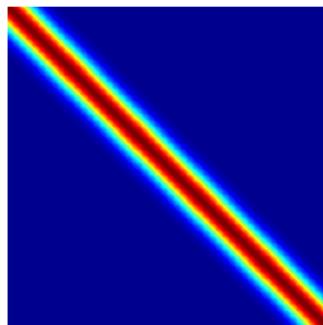
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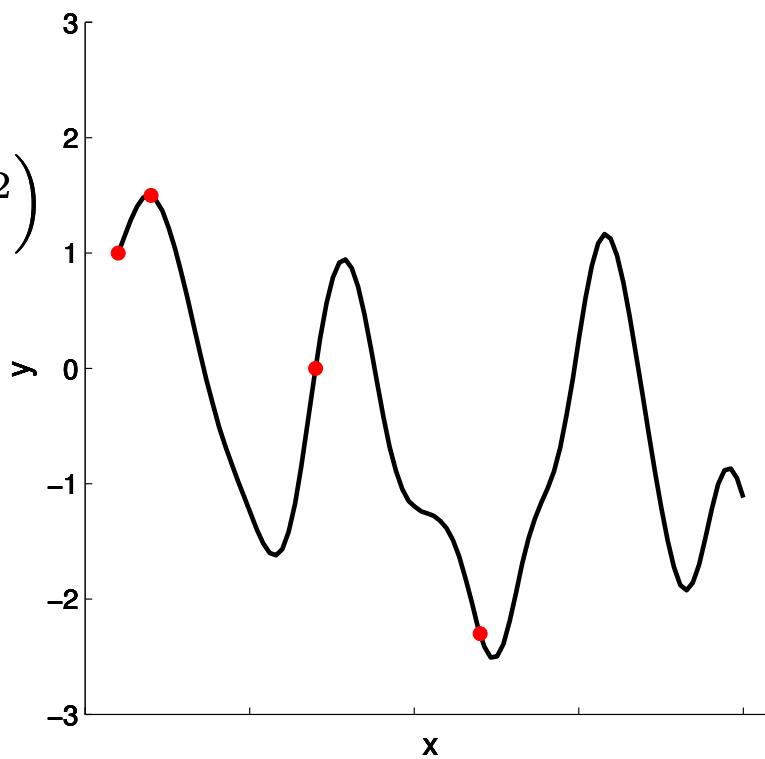
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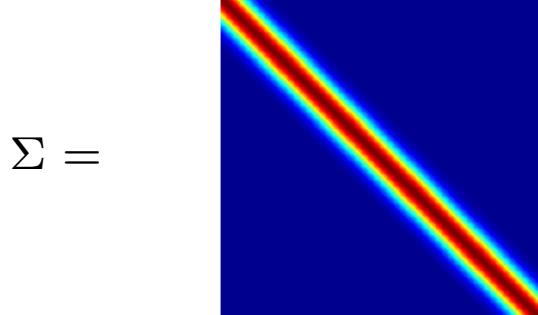
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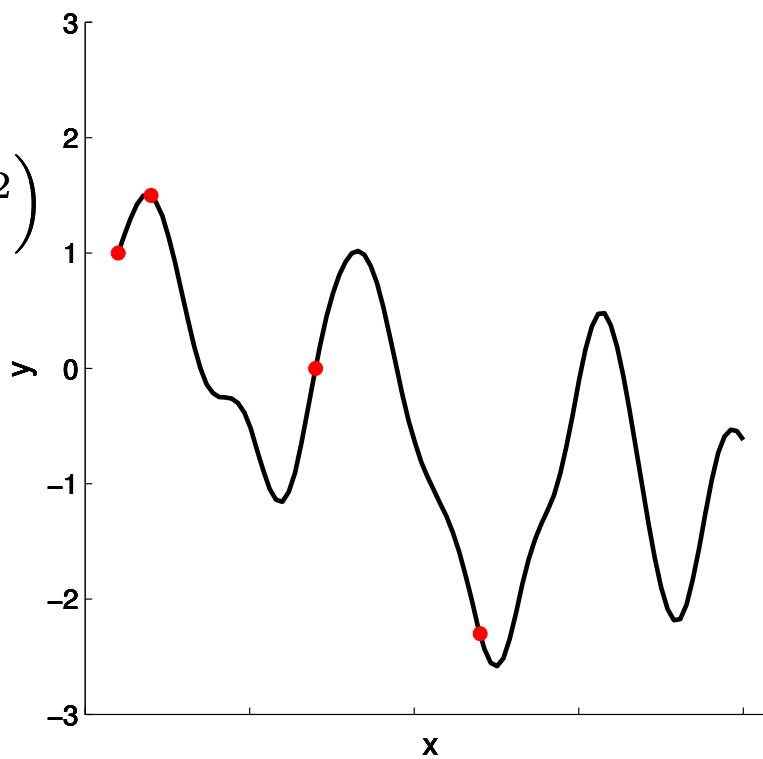


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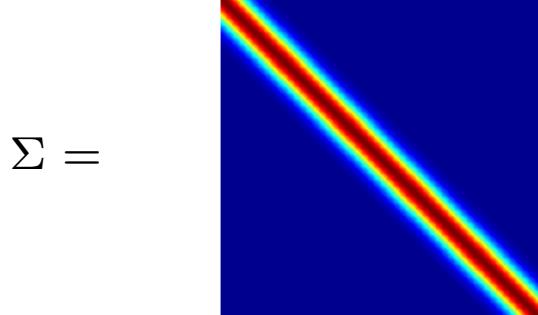
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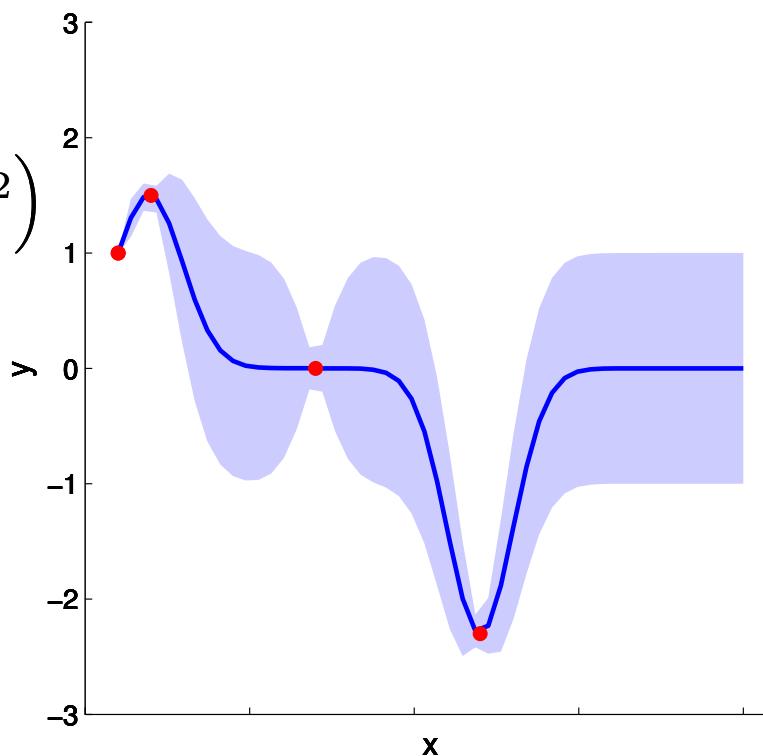


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What effect do the hyper-parameters have?

long horizontal length-scale

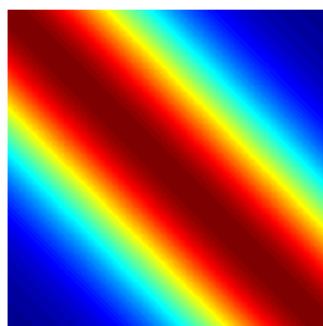
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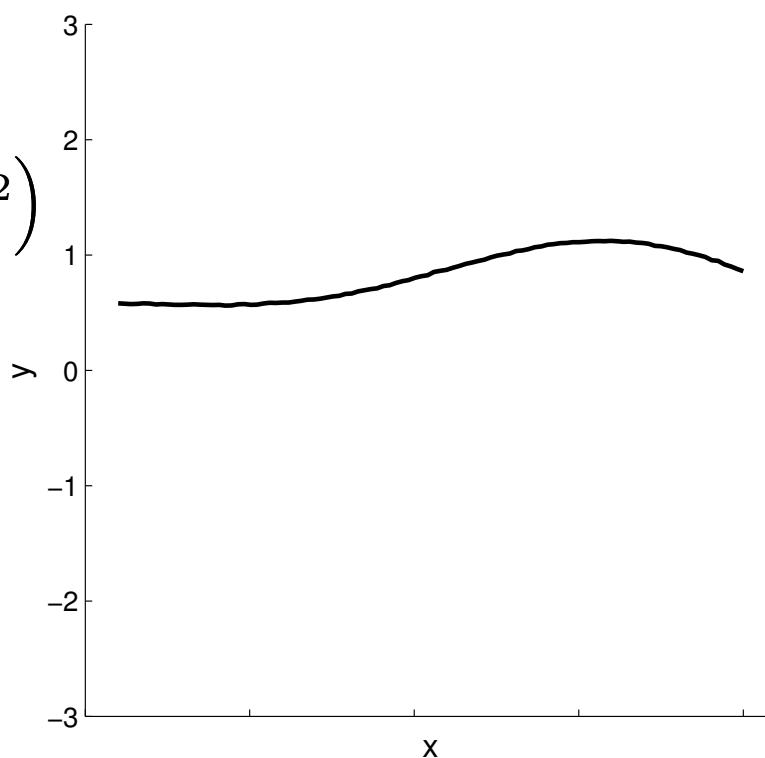
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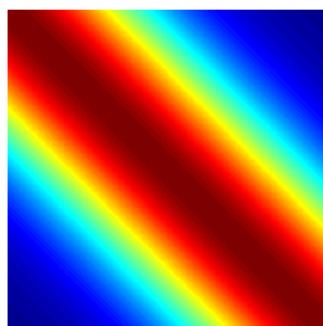
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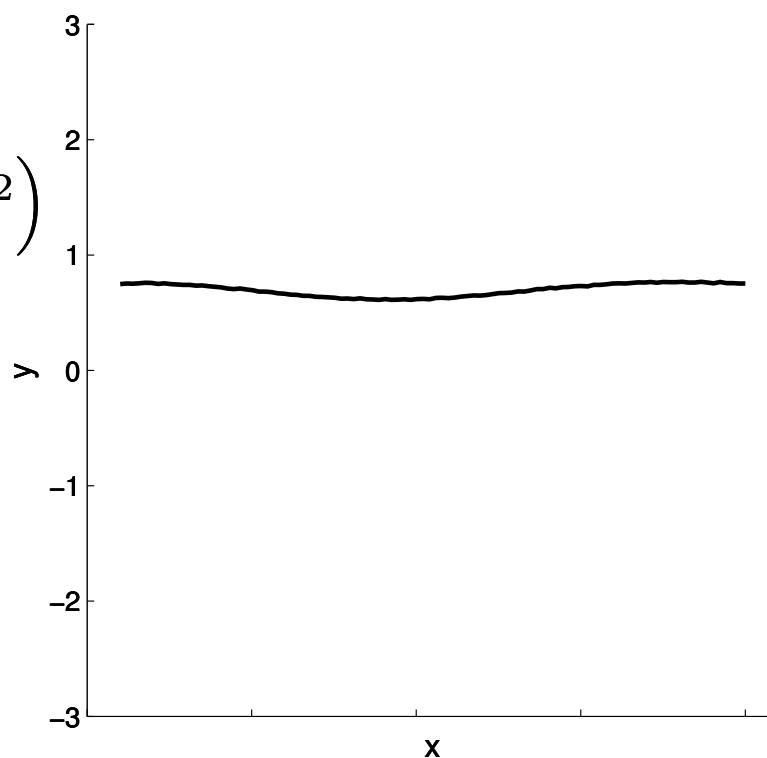
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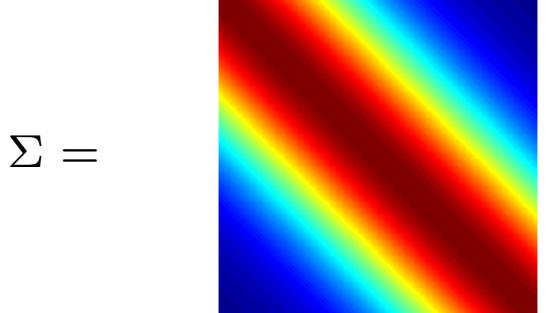
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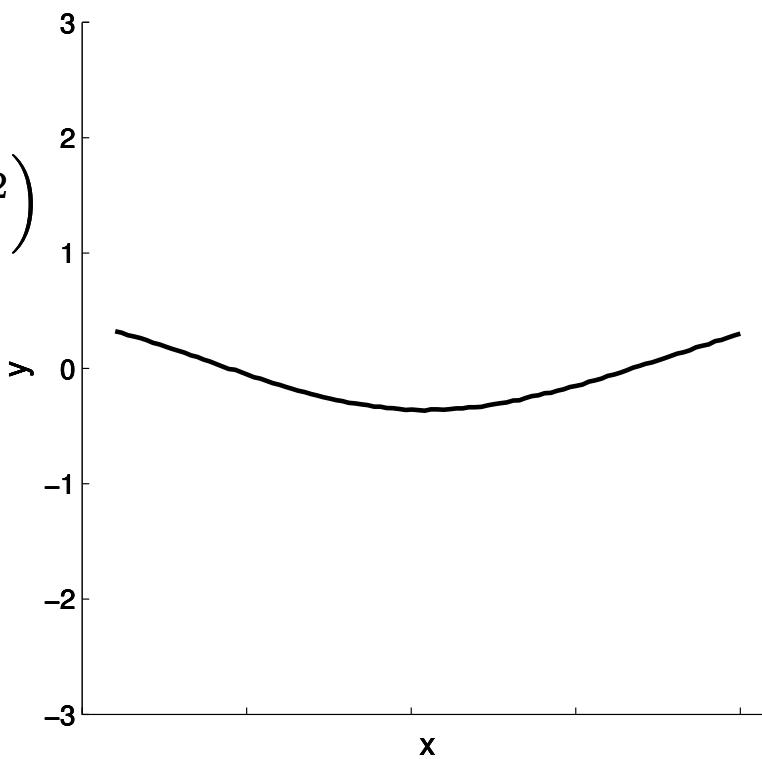


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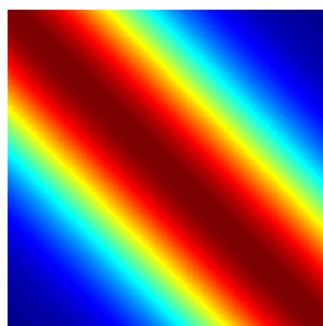
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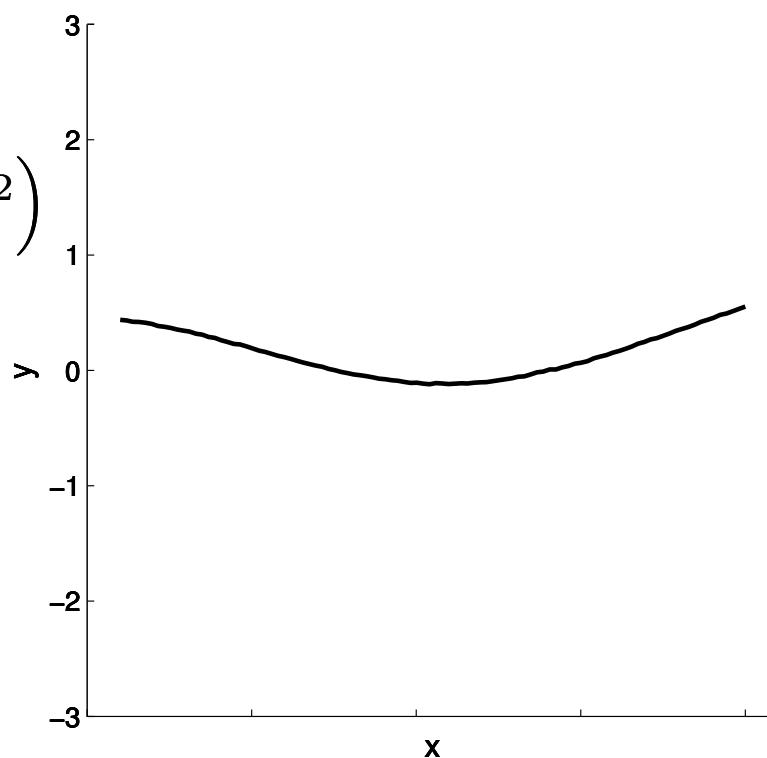
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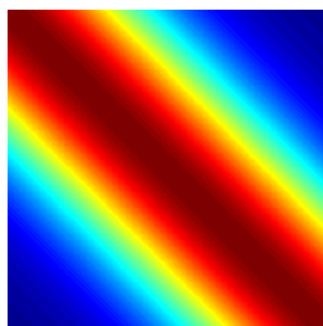
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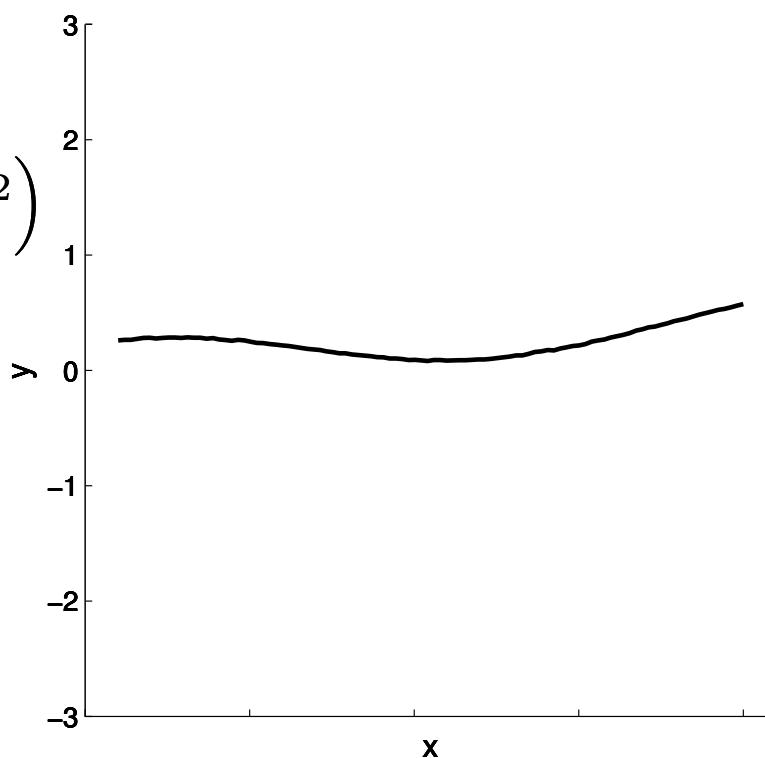
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What effect do the hyper-parameters have?

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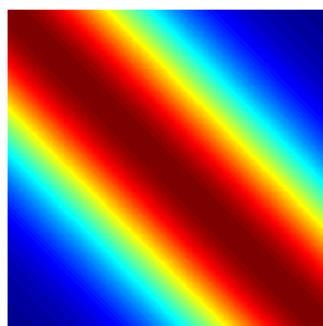
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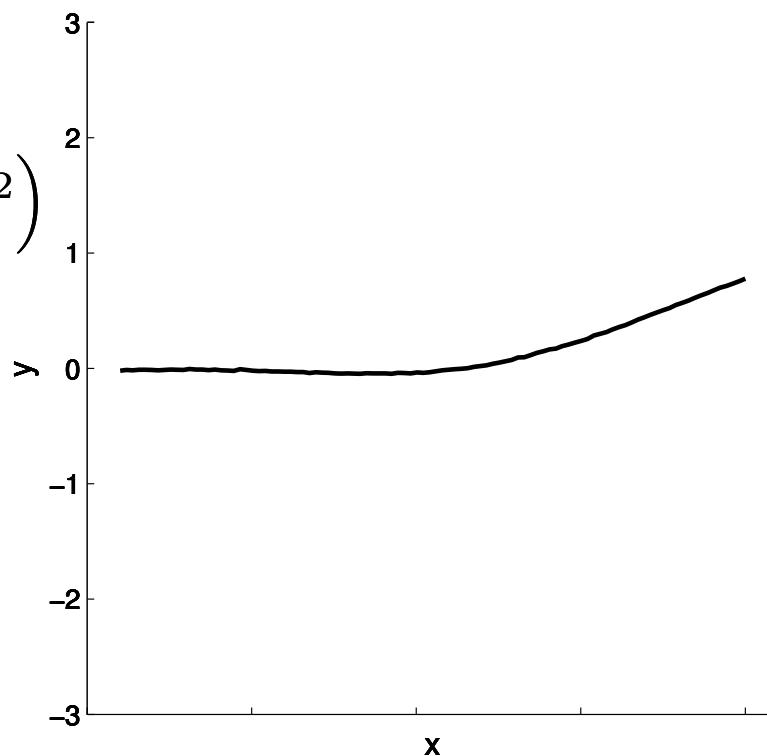
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What effect do the hyper-parameters have?

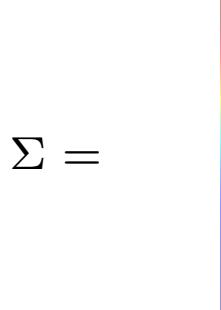
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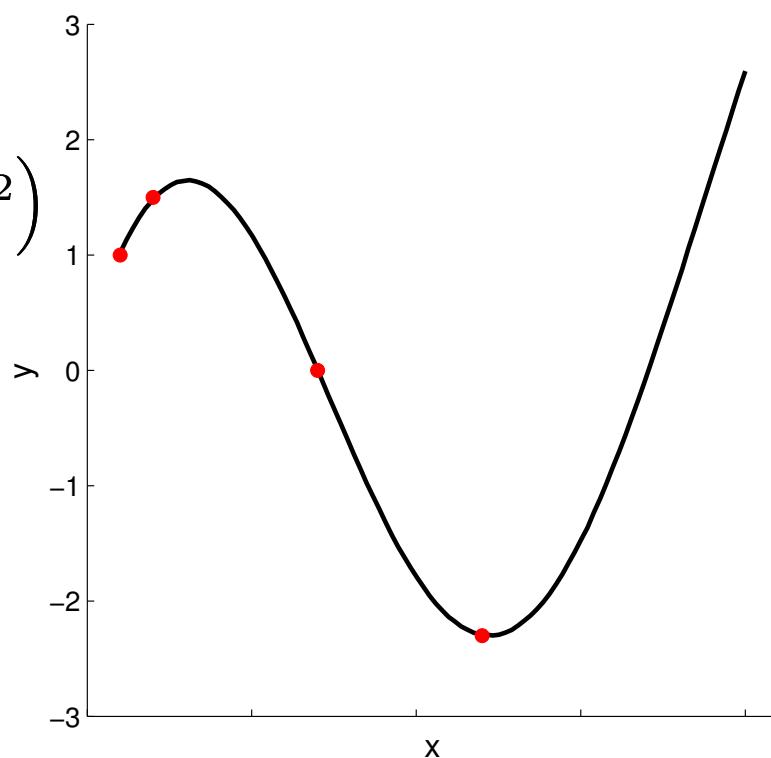
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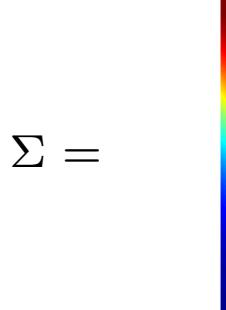
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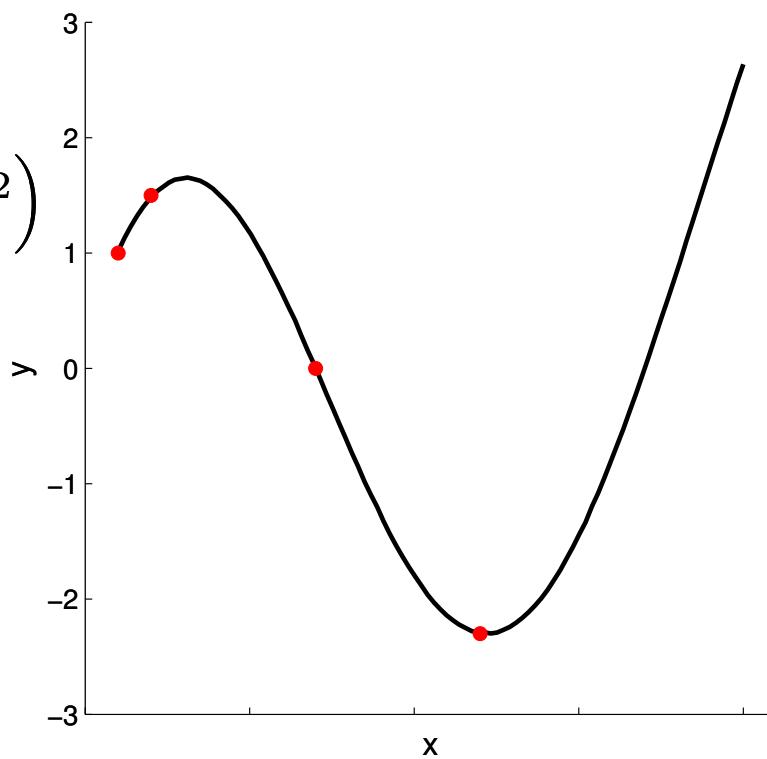
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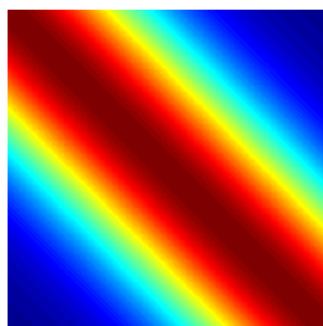
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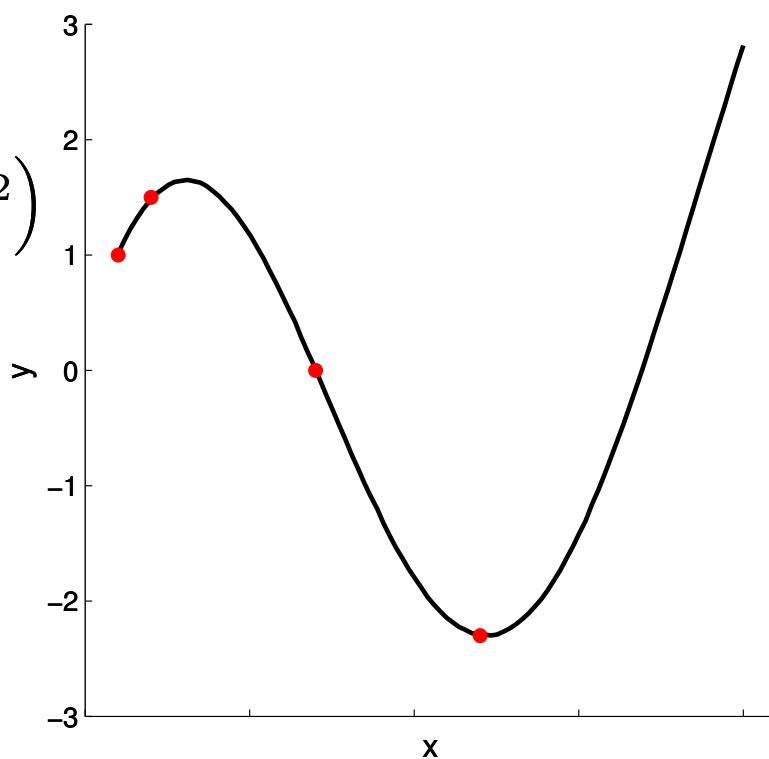
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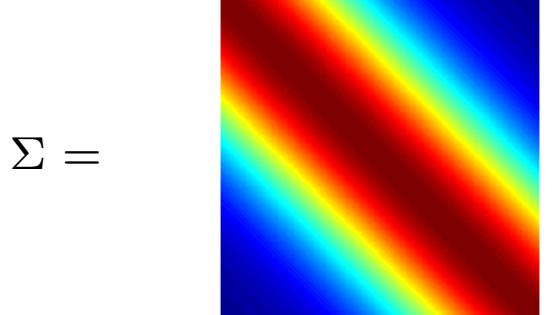
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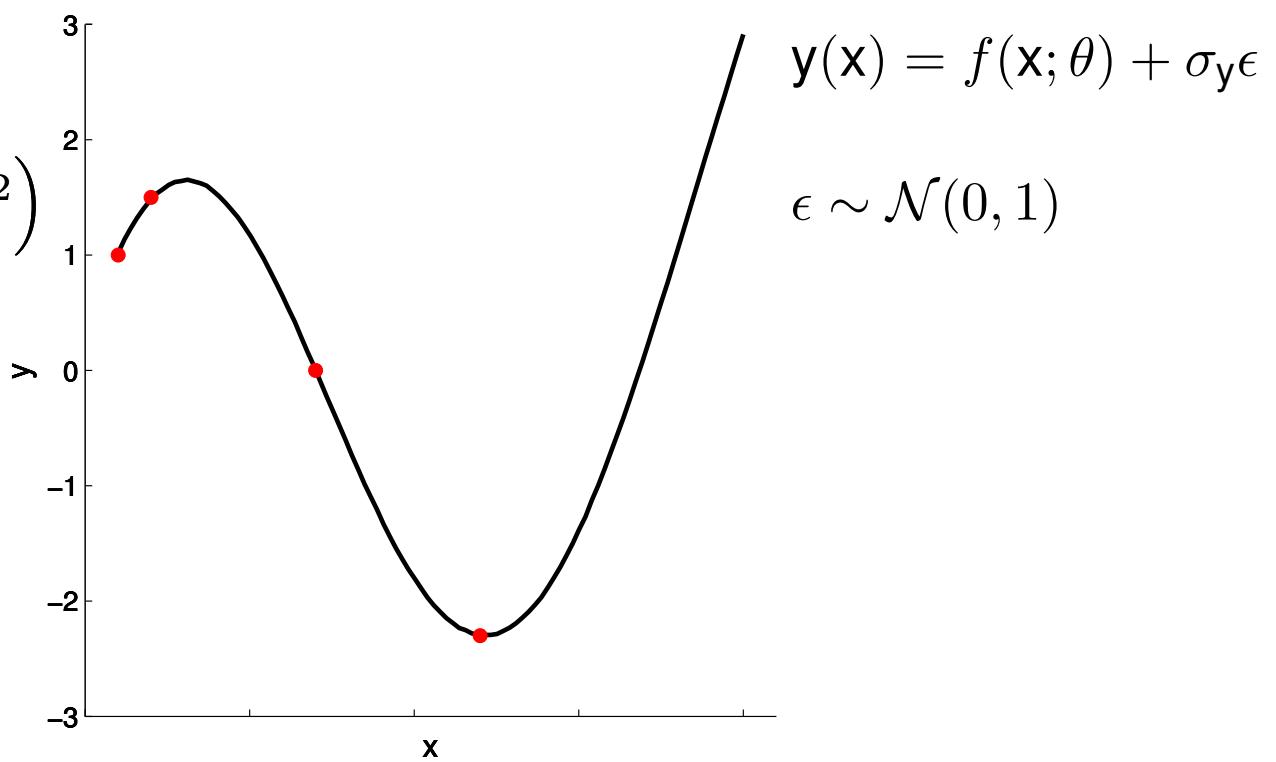
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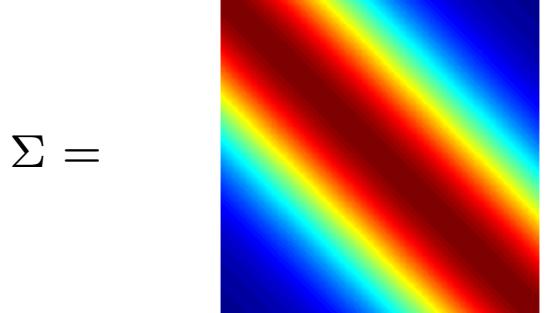
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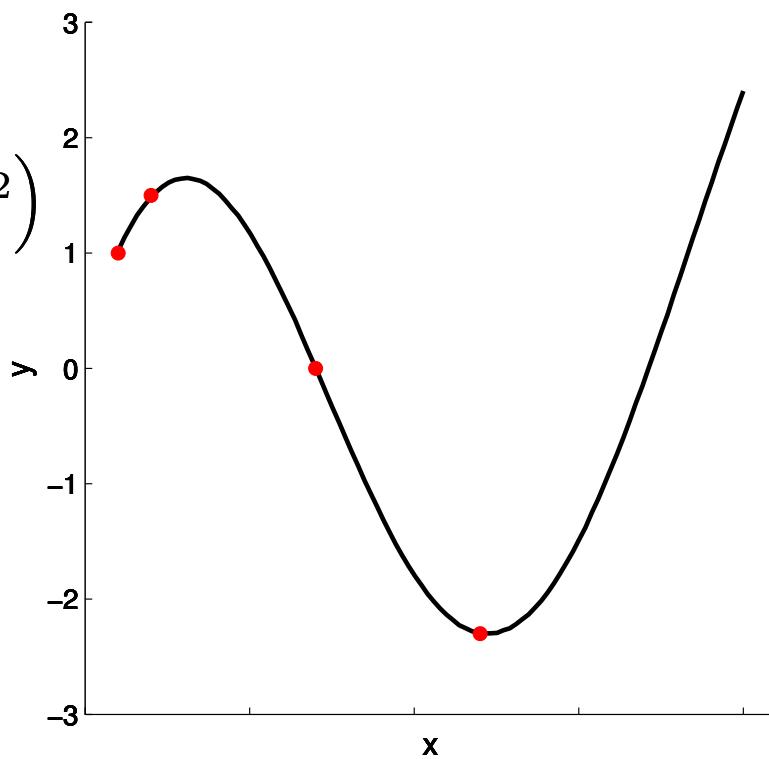


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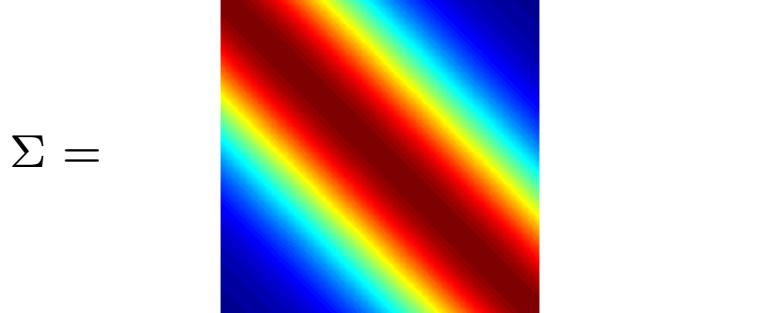
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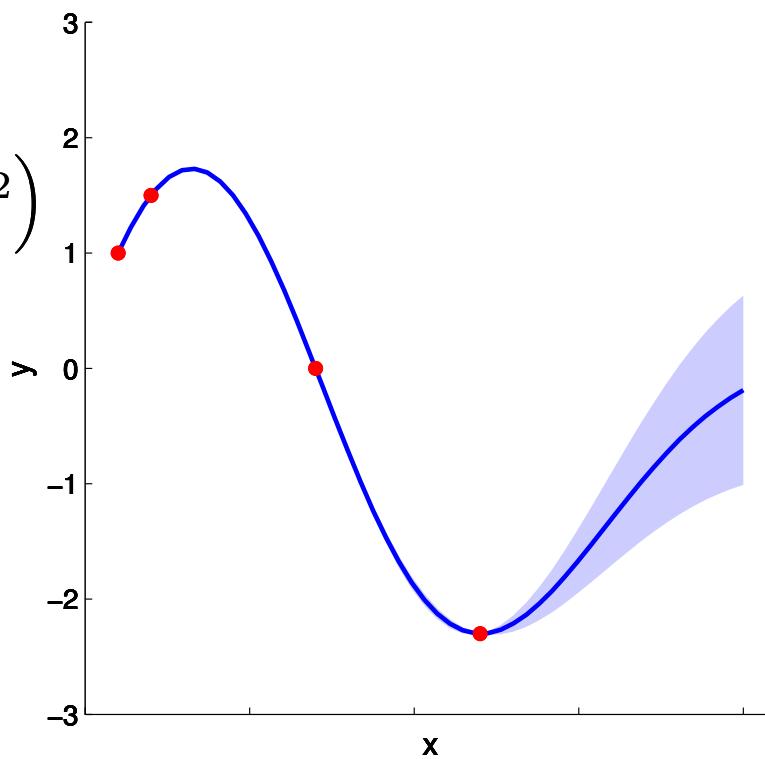


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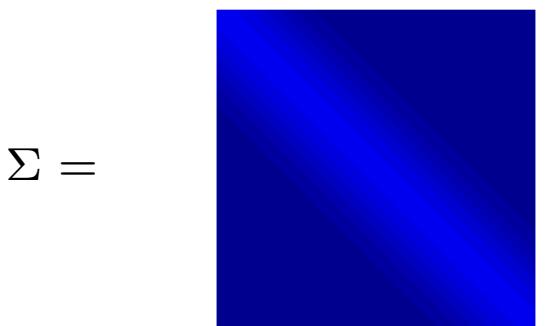
small vertical scale

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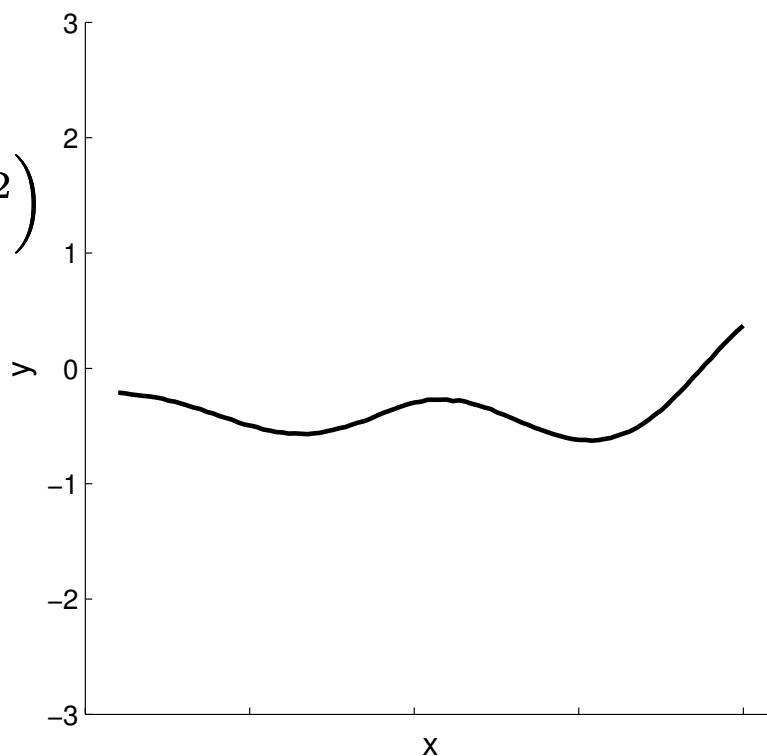


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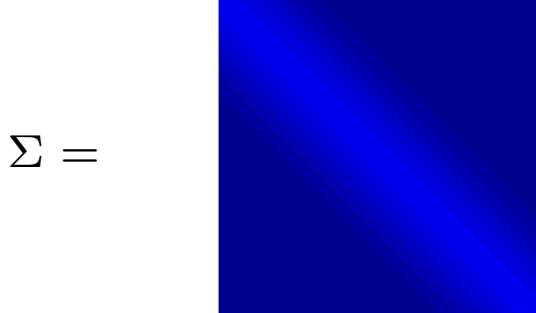
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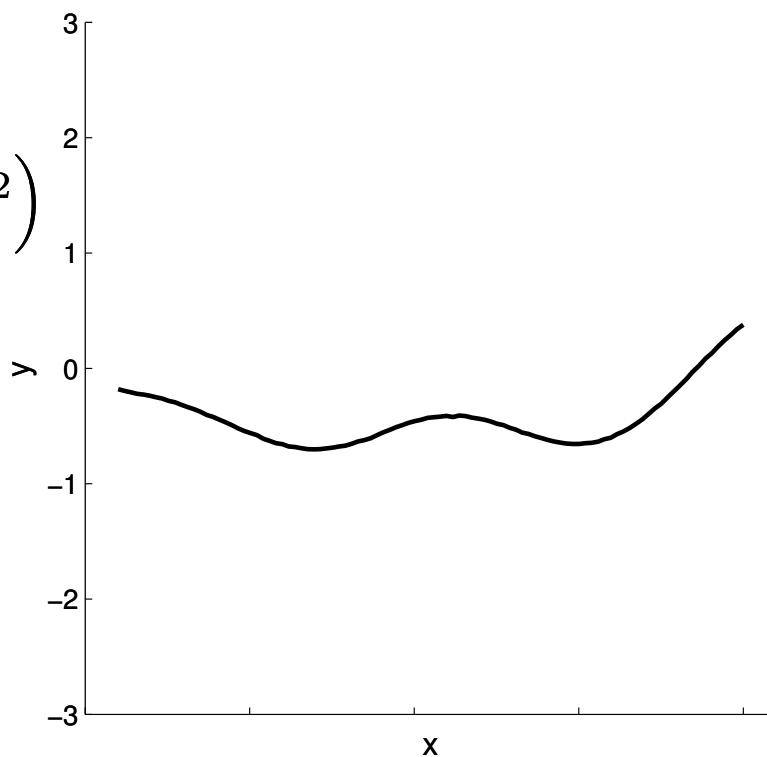


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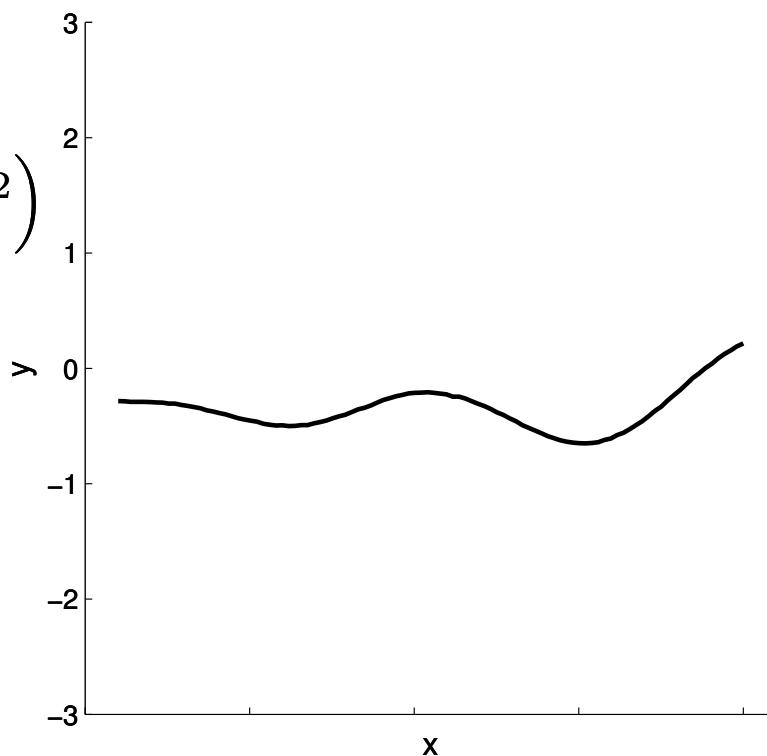


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What effect do the hyper-parameters have?

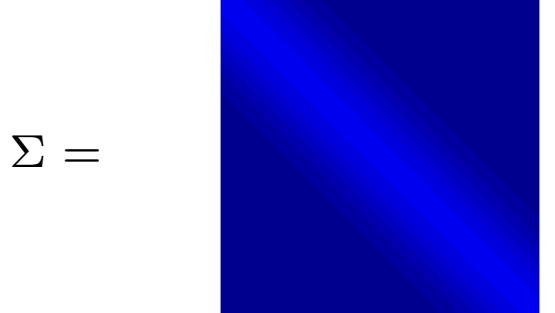
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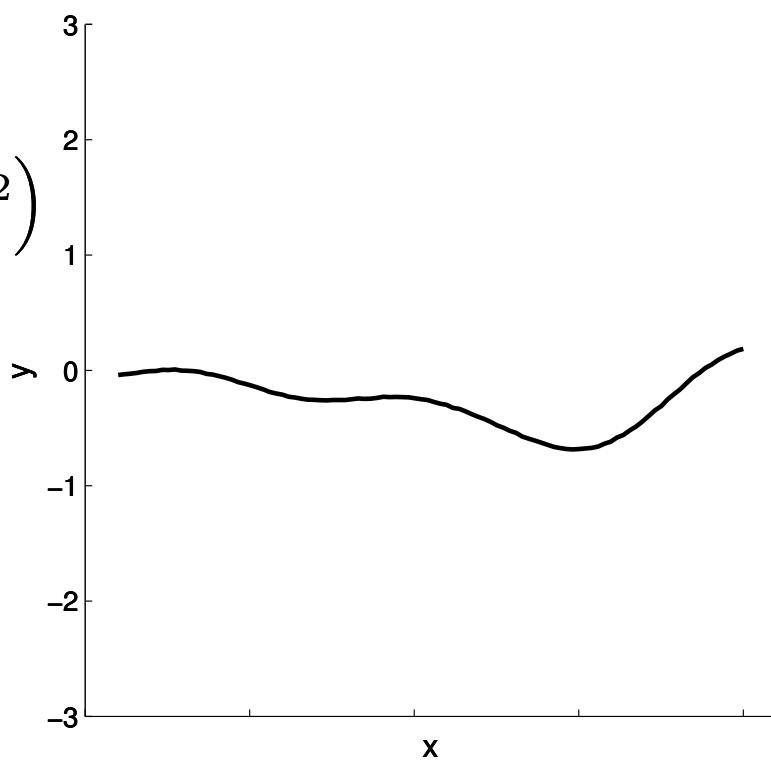


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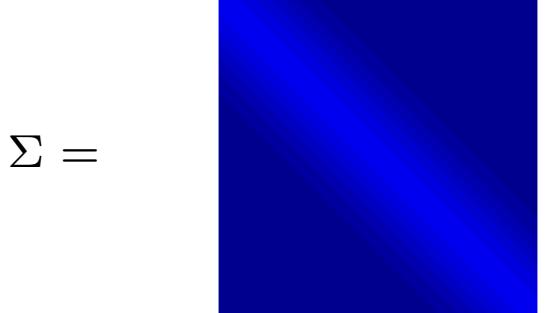
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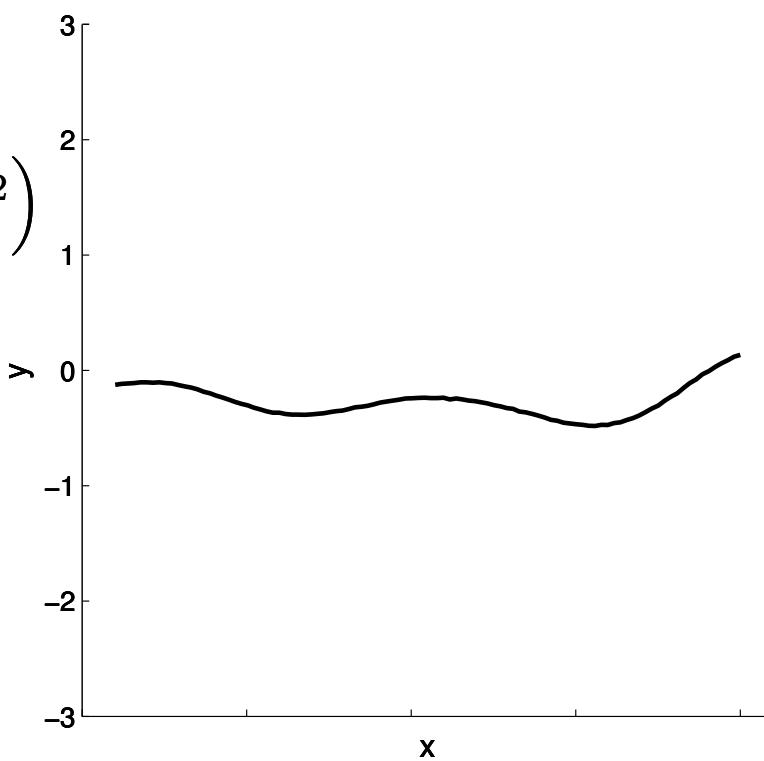


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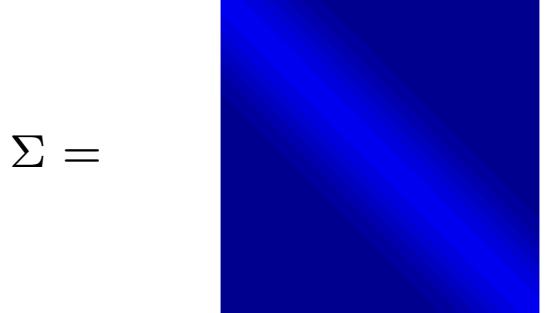
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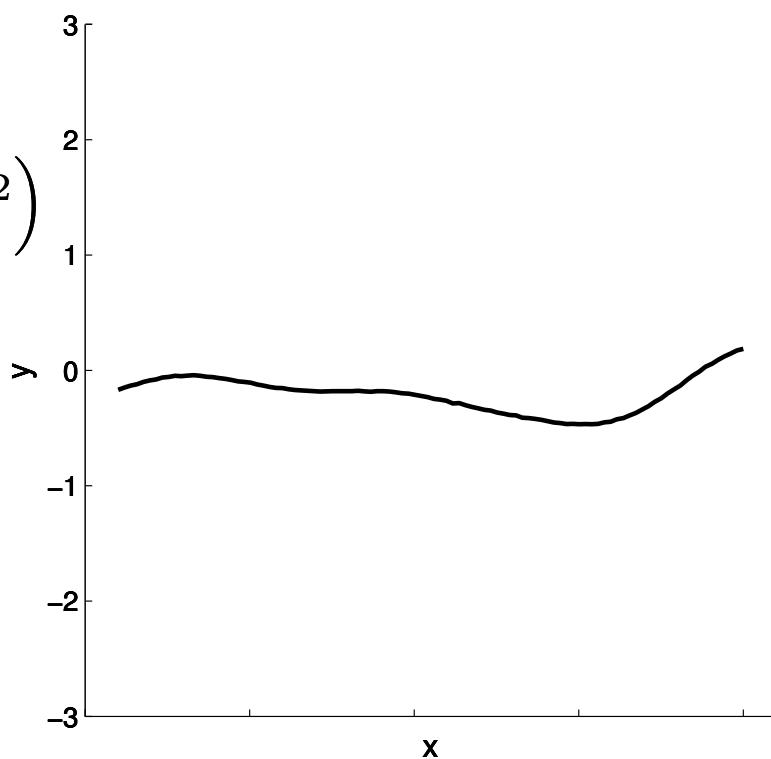


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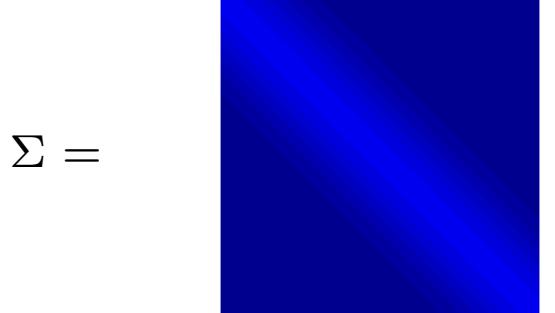
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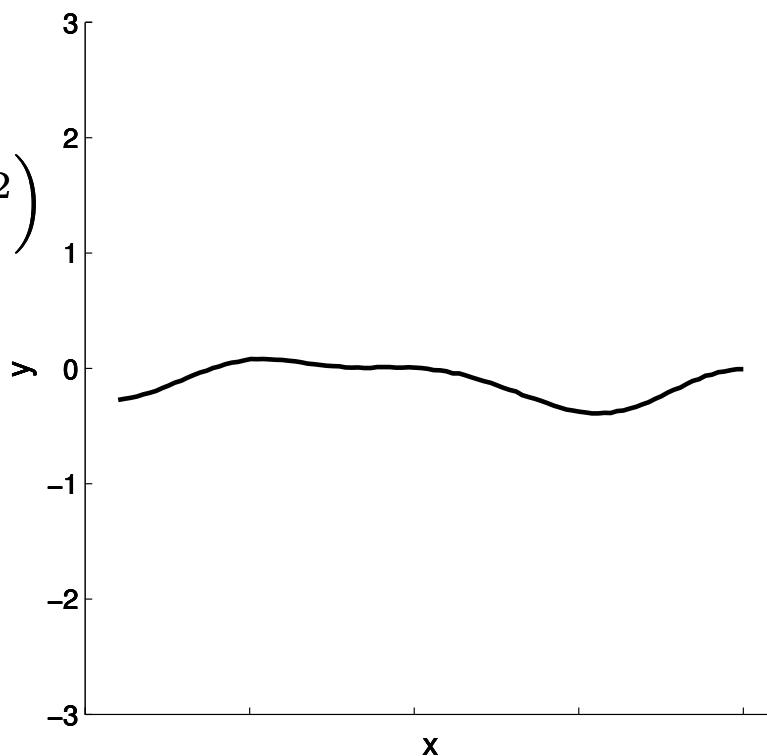


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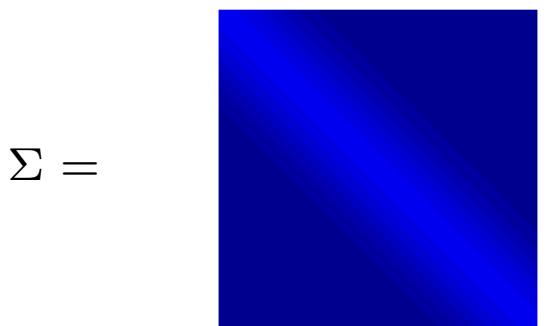
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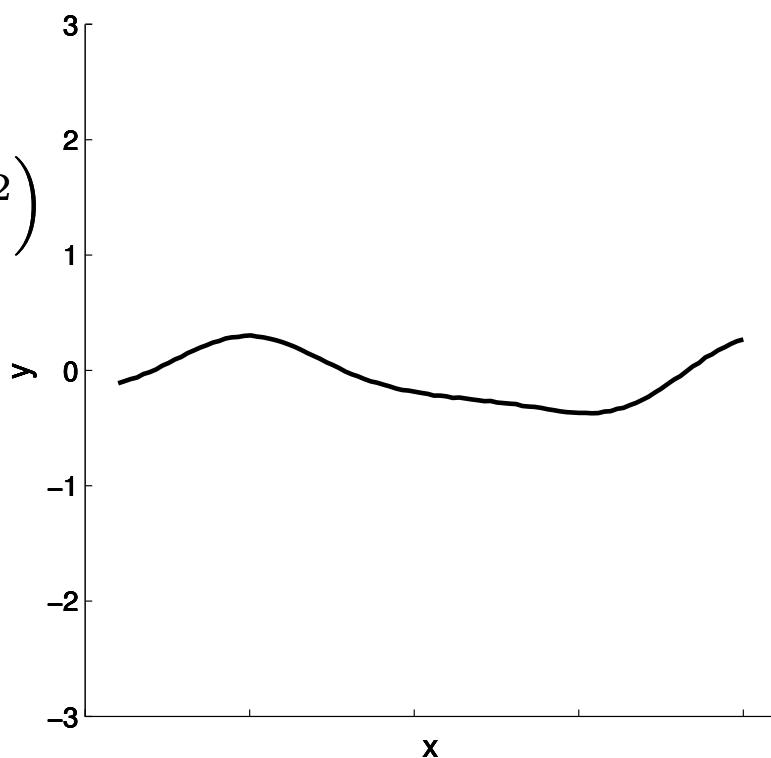


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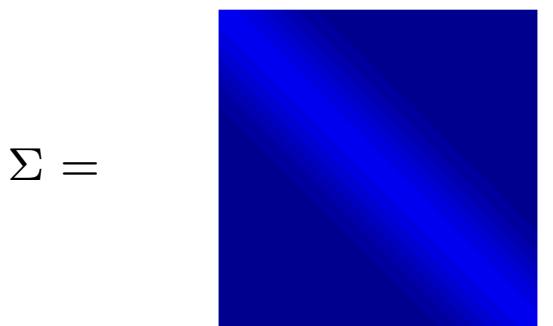
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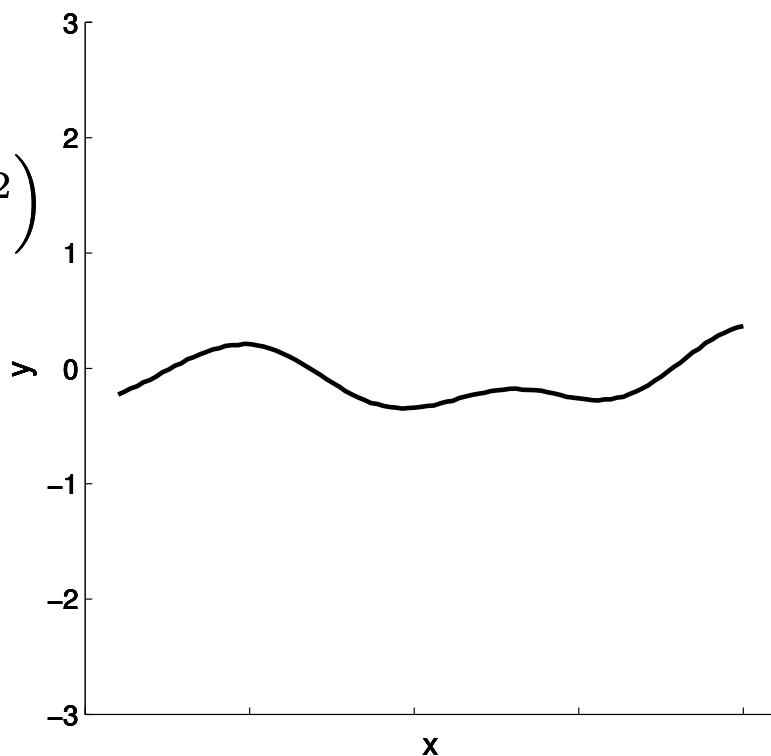


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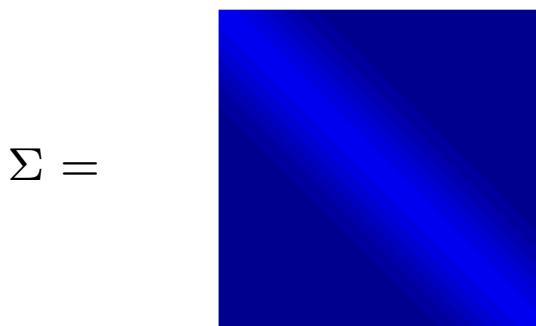
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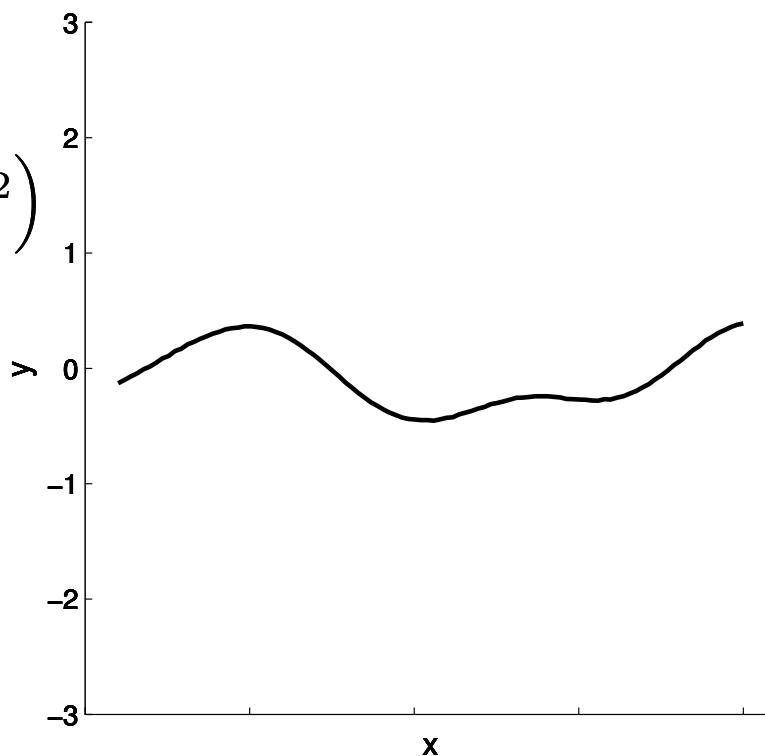


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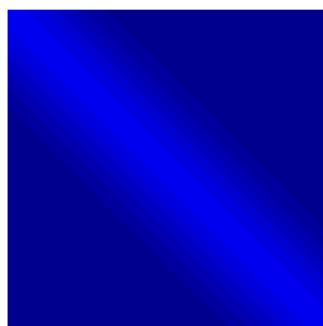
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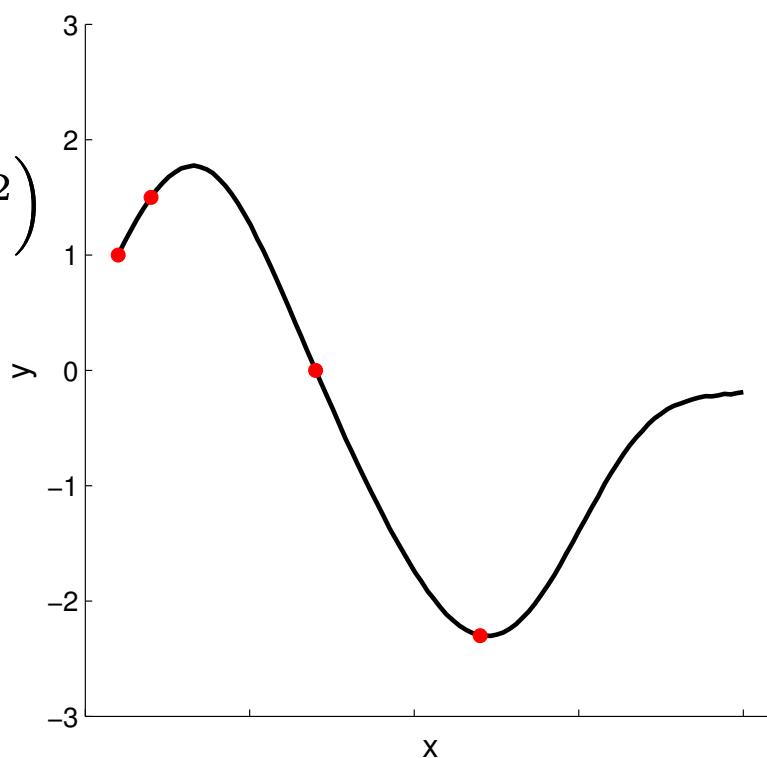
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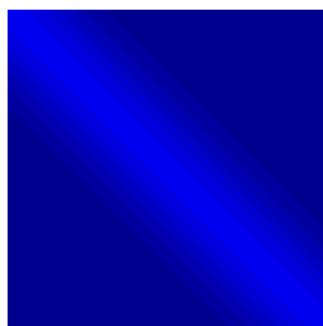
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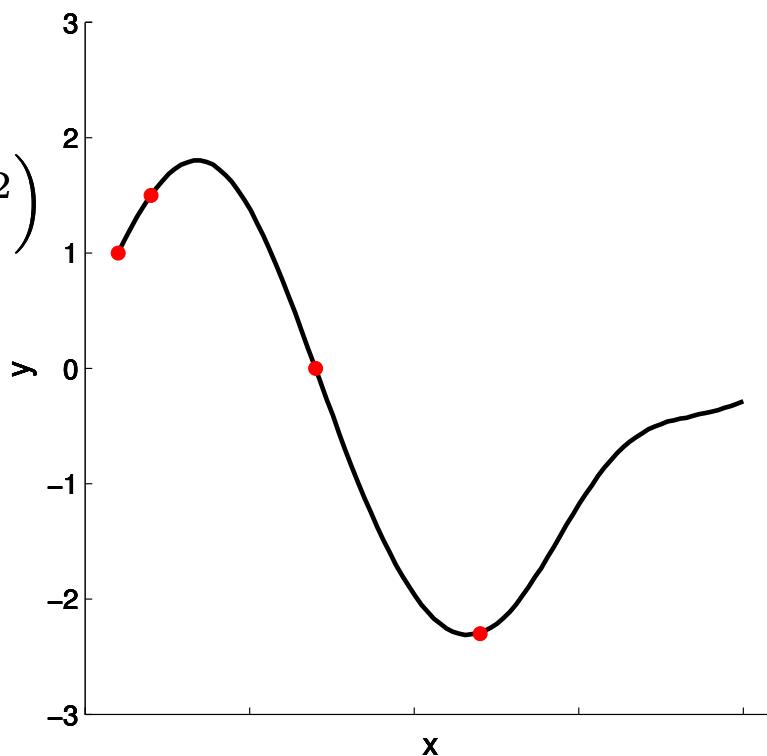
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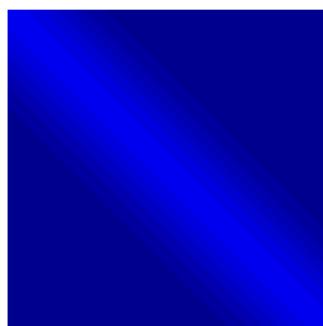
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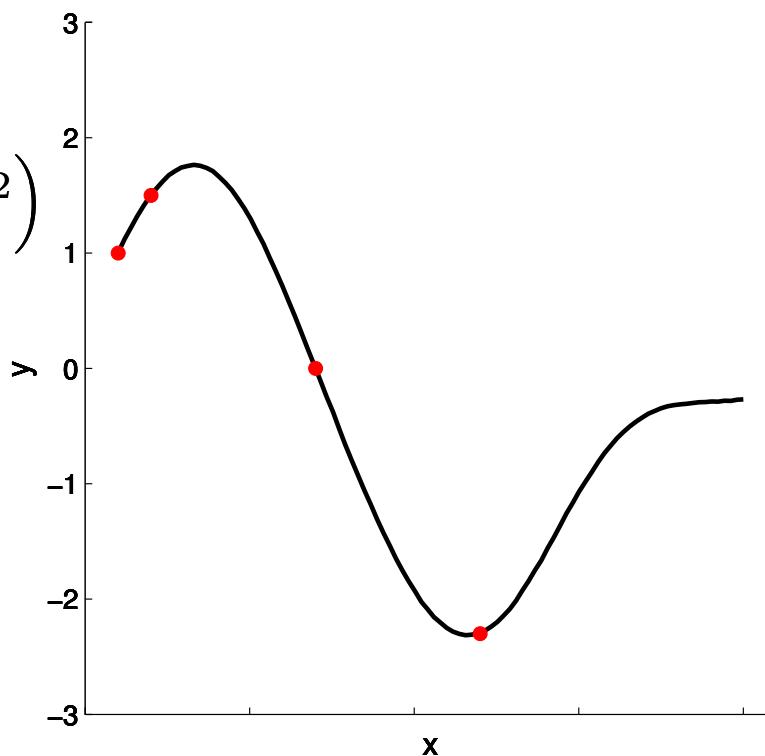
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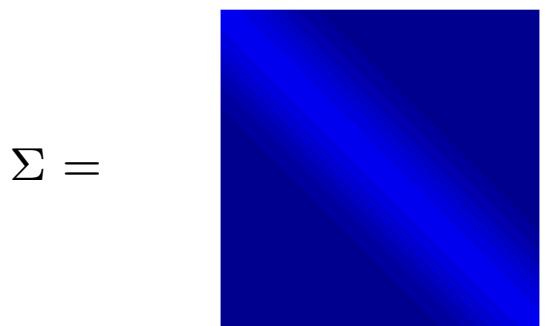
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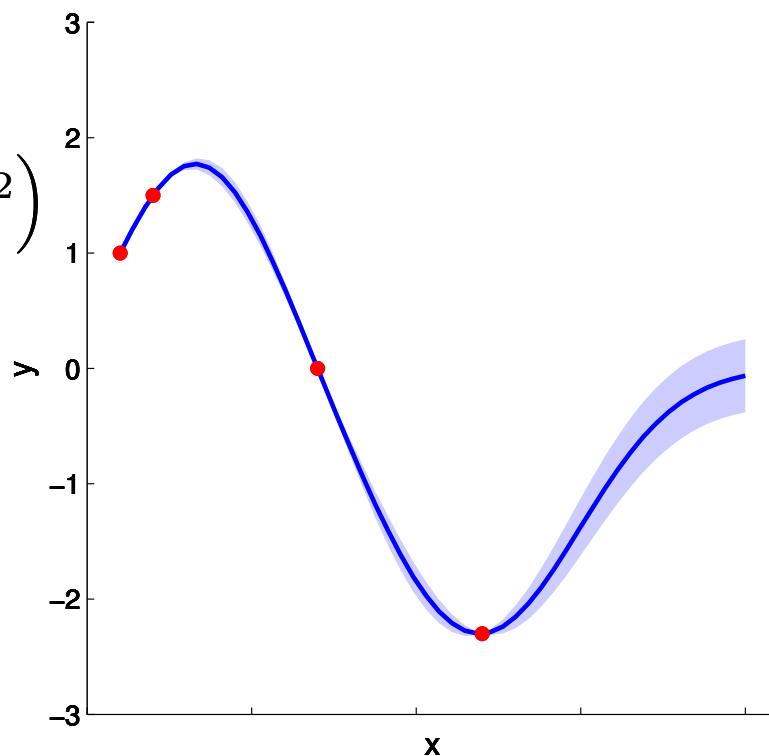
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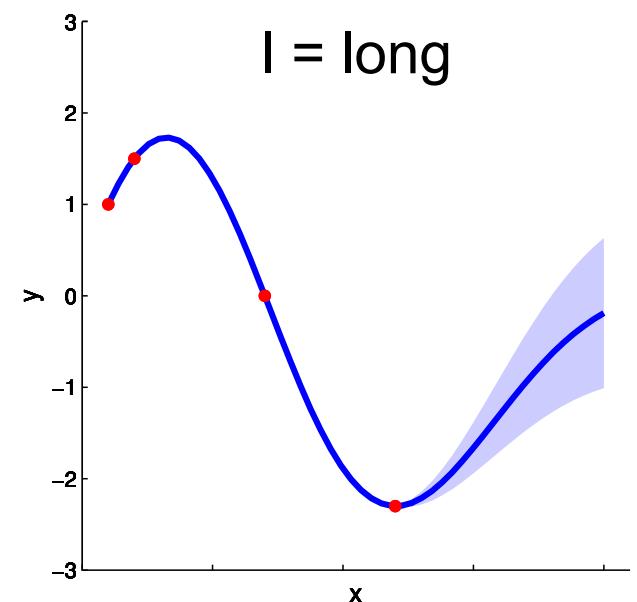
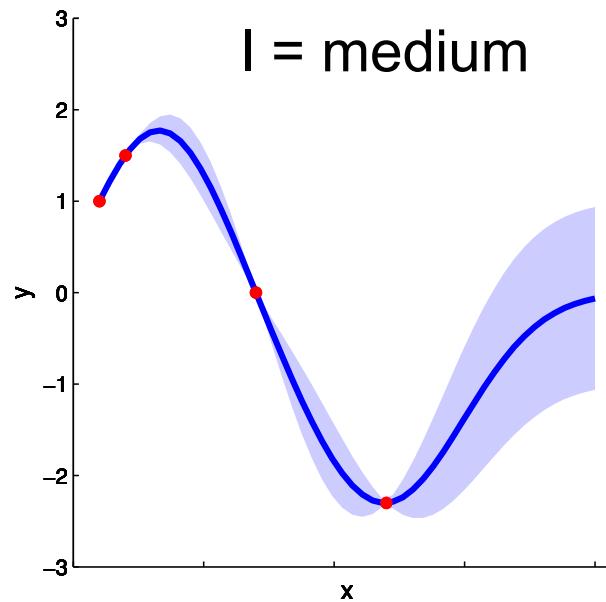
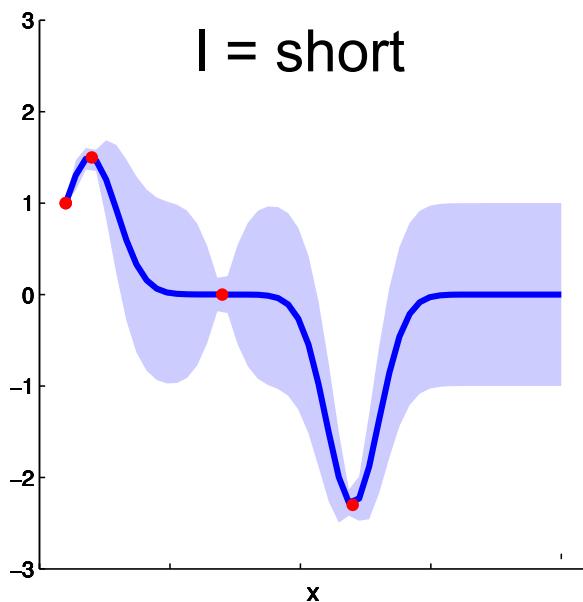
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What effect do the hyper-parameters have?

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

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



What effect does the form of the covariance function have?

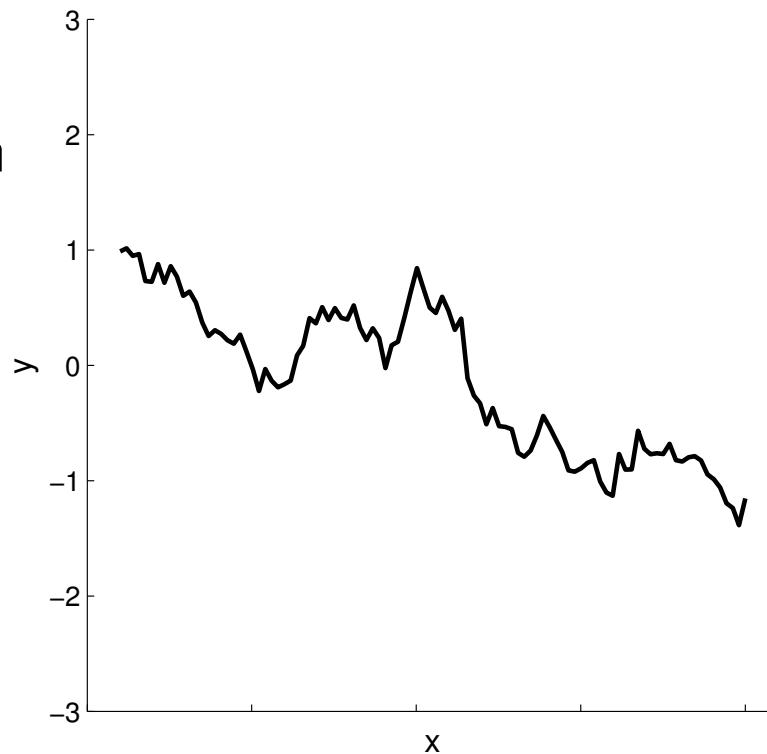
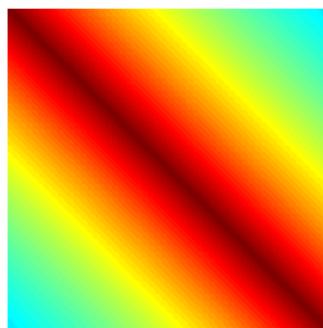
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Laplacian covariance function

Browninan motion

Ornstein-Uhlenbeck

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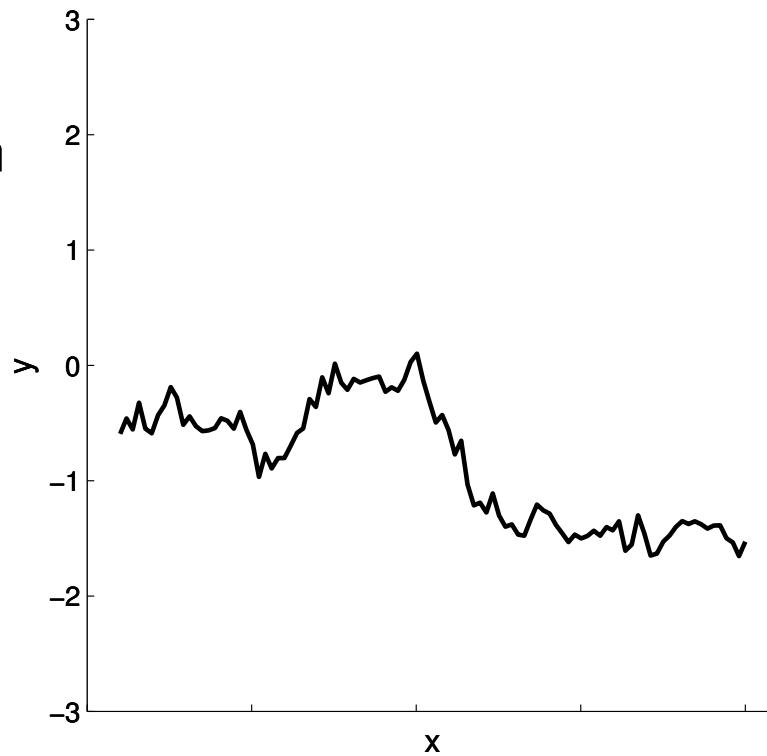
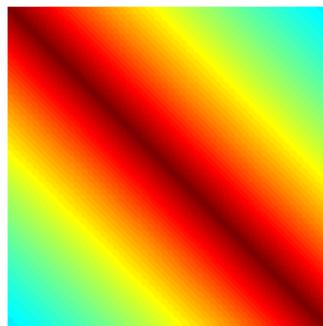
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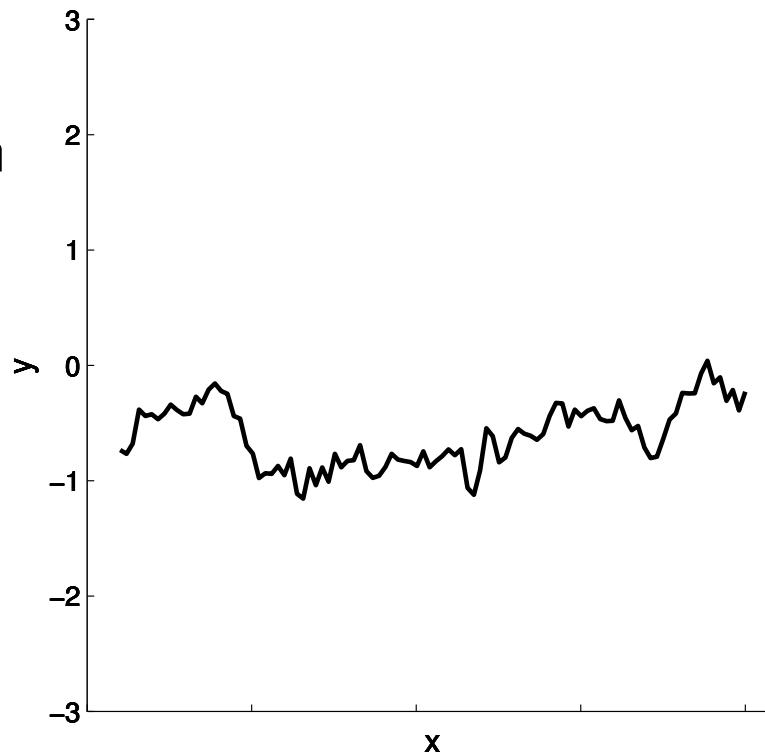
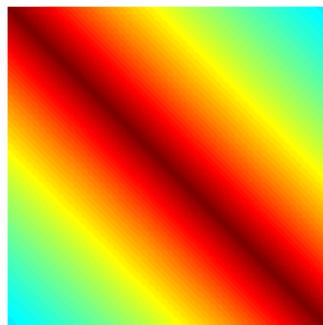
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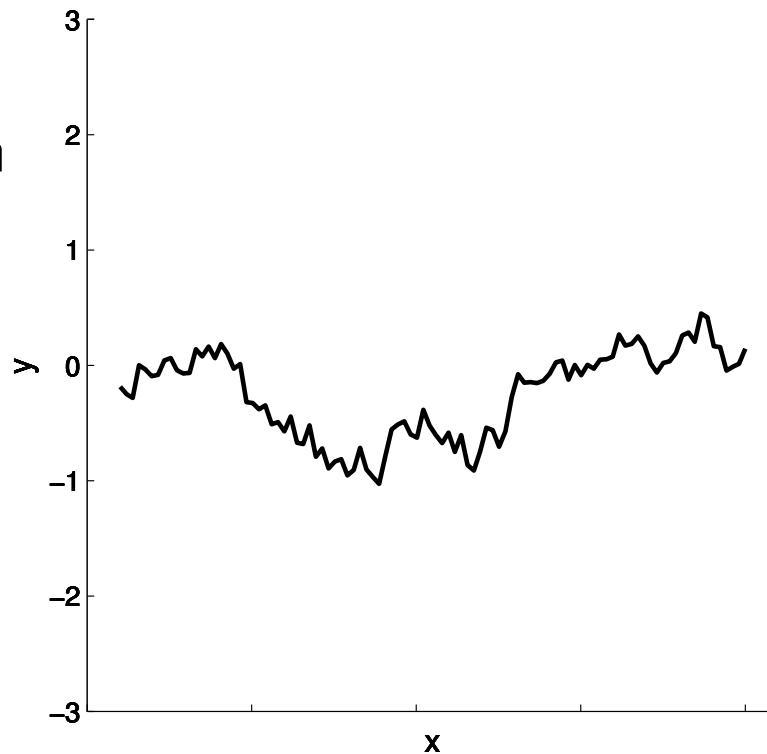
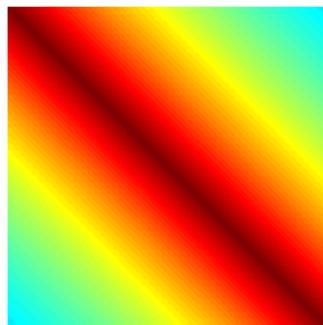
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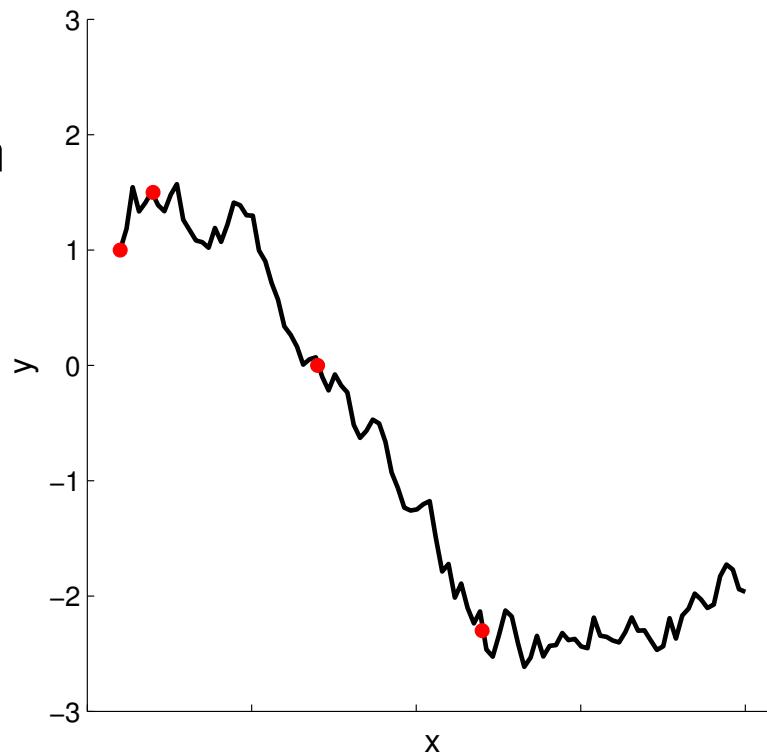
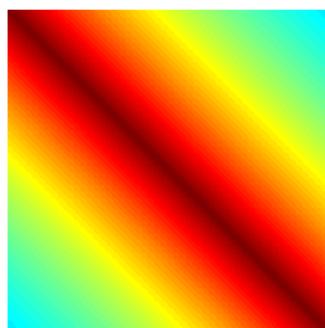
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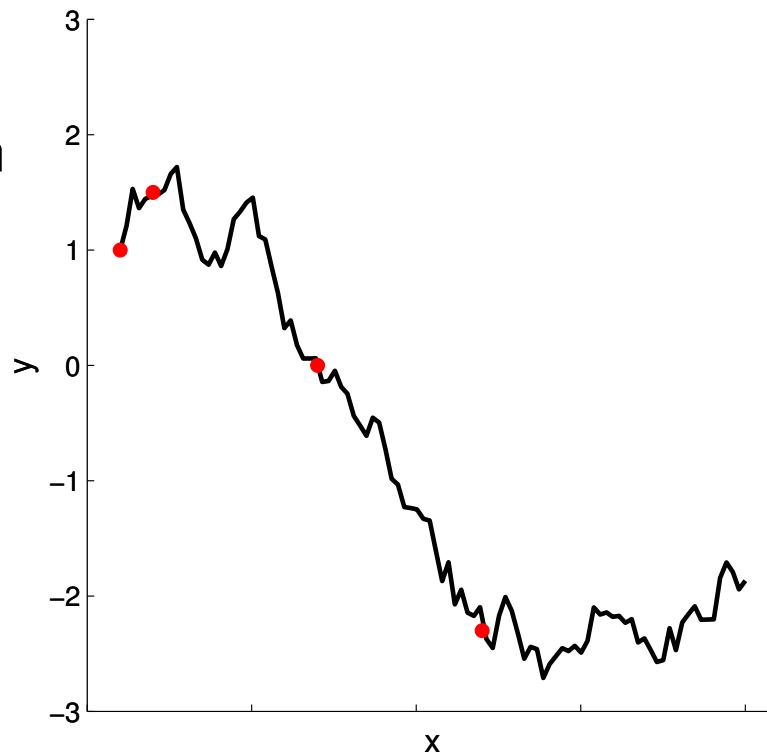
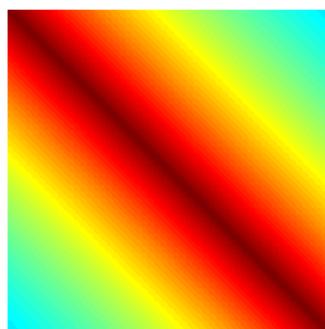
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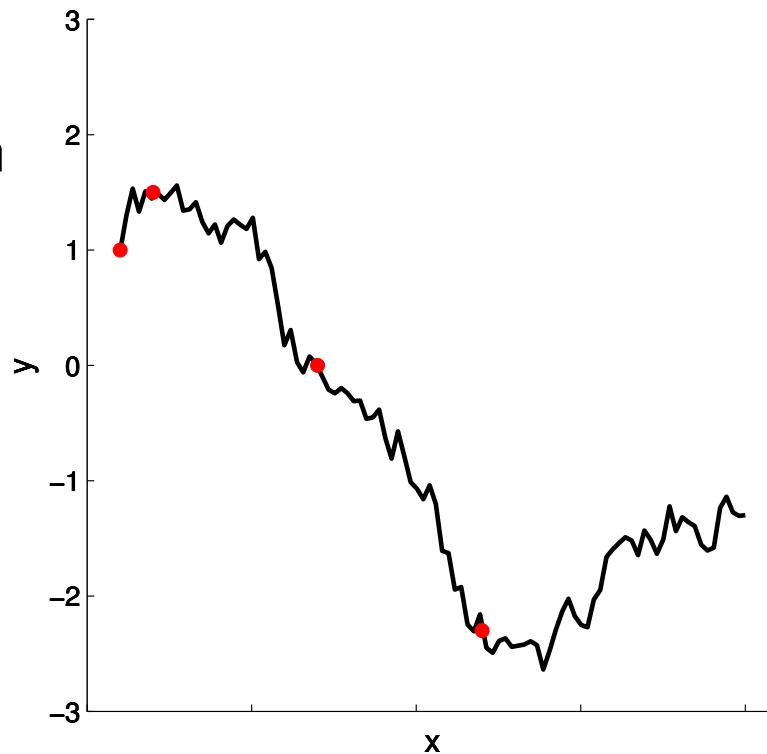
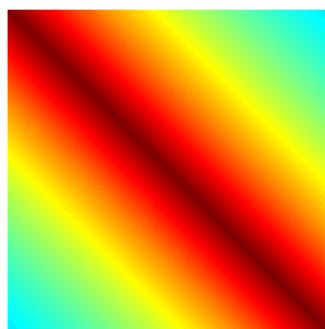
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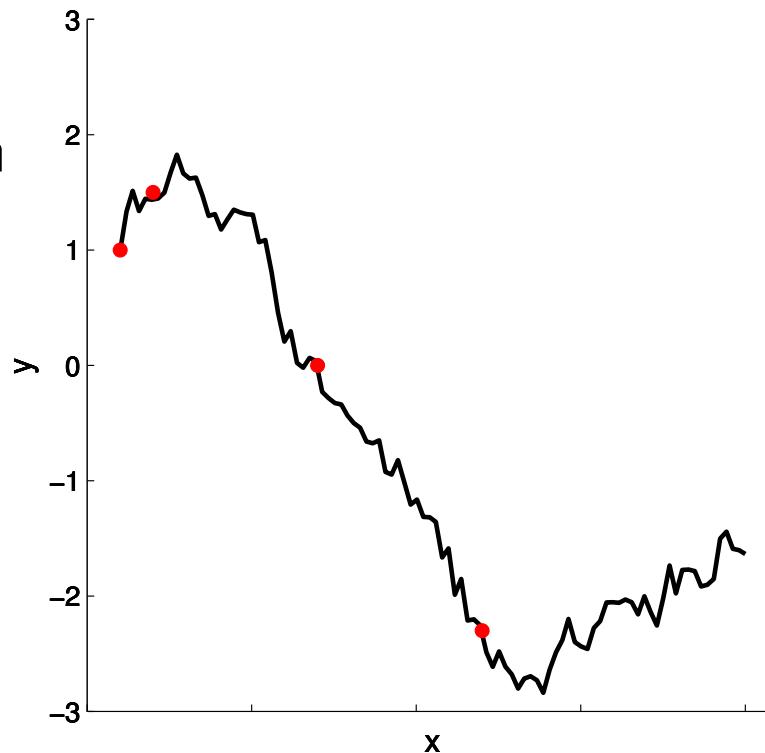
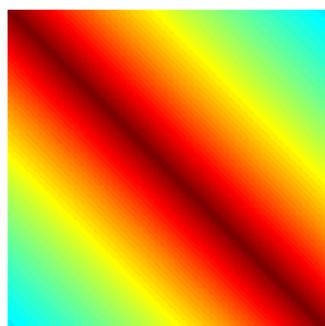
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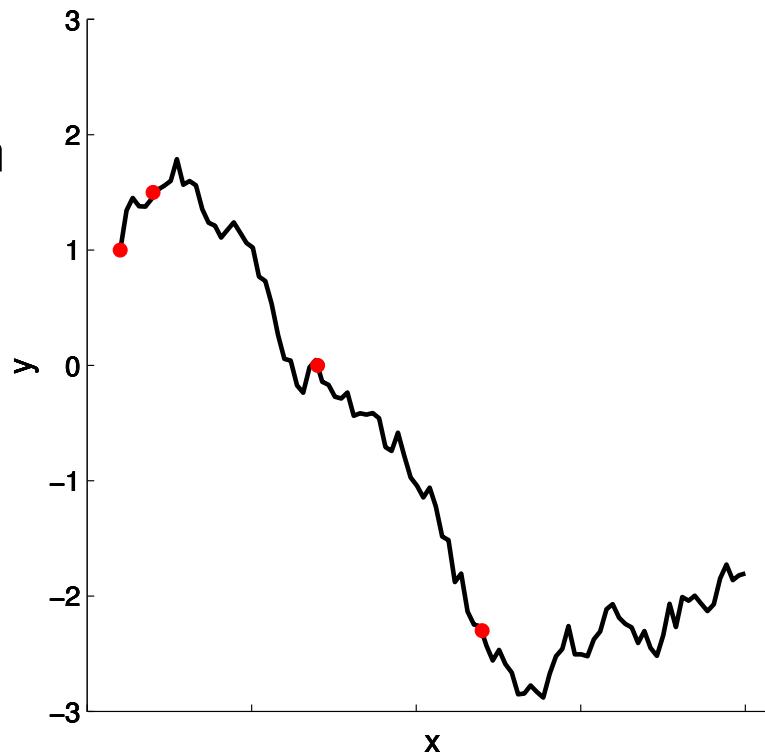
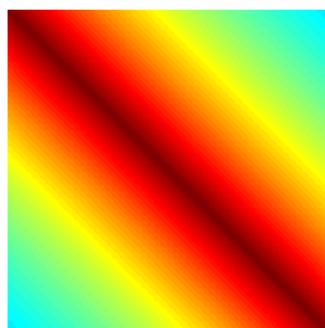
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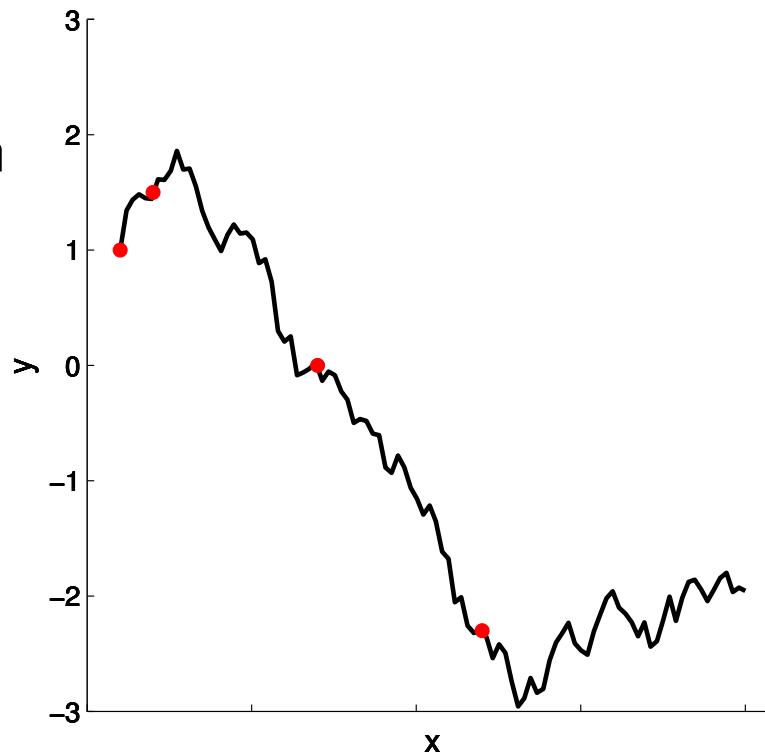
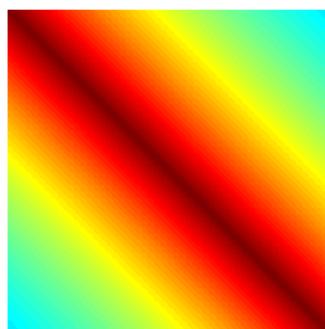
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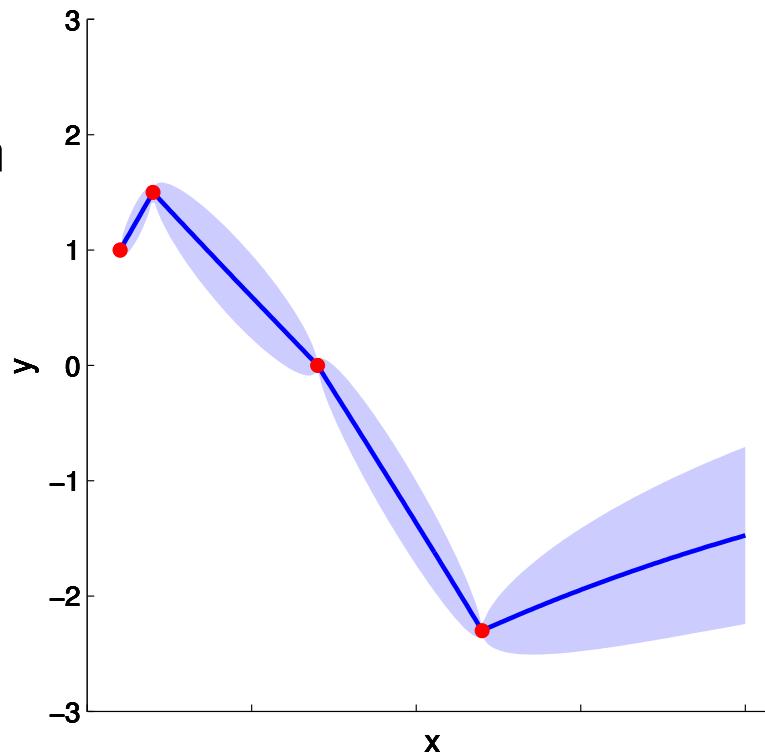
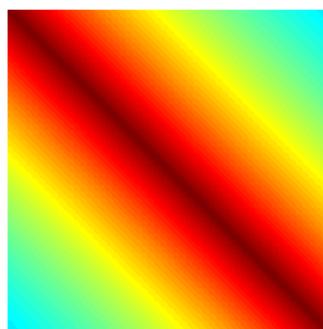
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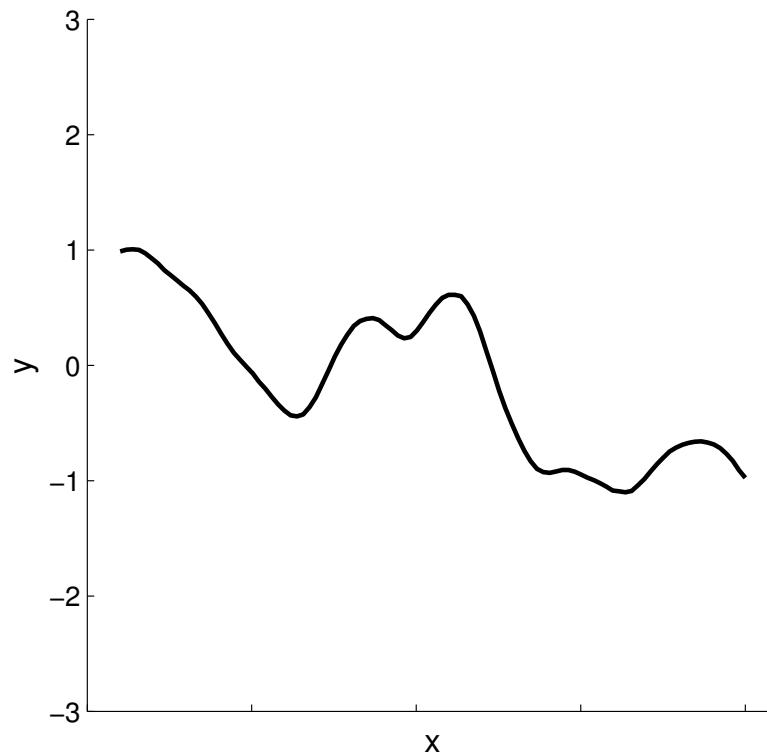
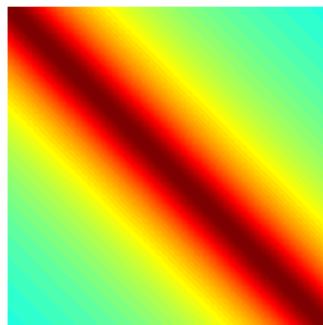


What effect does the form of the covariance function have?

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

Rational Quadratic

$\Sigma =$

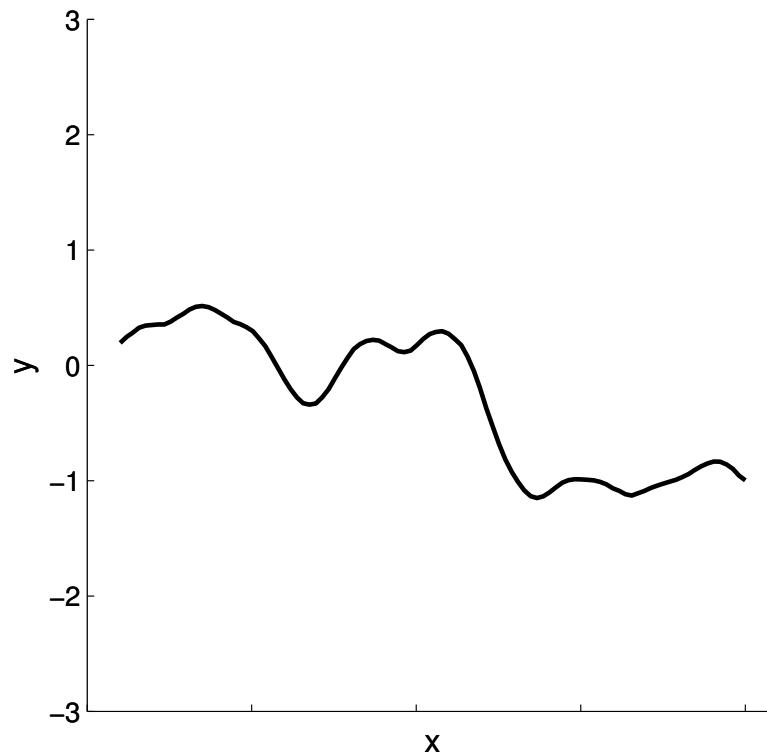
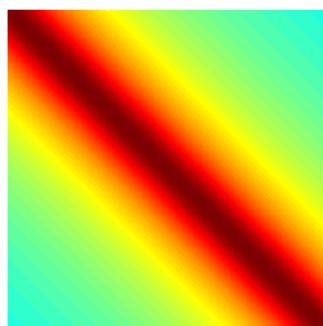


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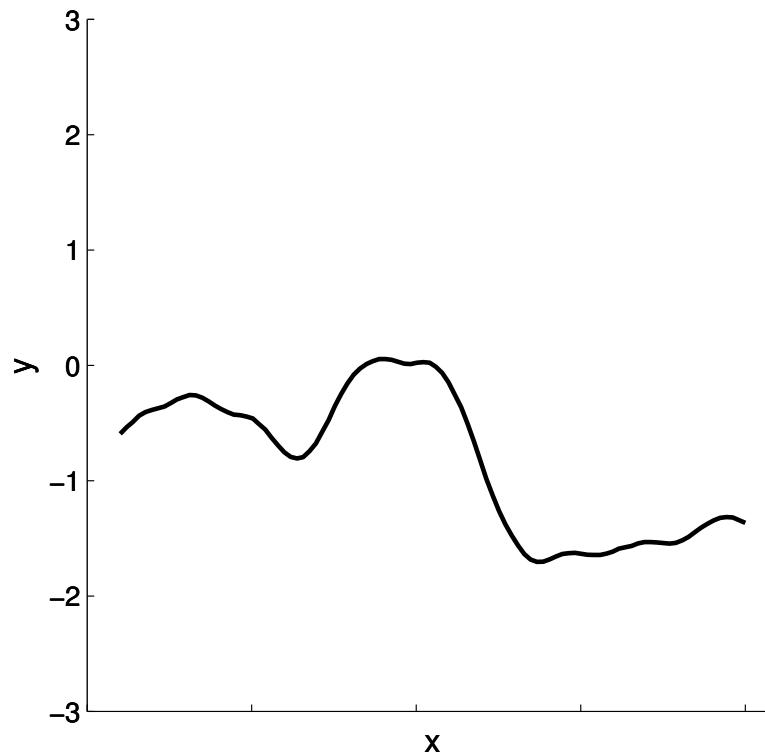
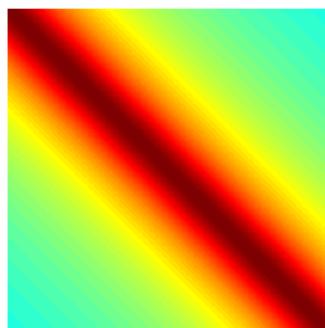


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Rational Quadratic

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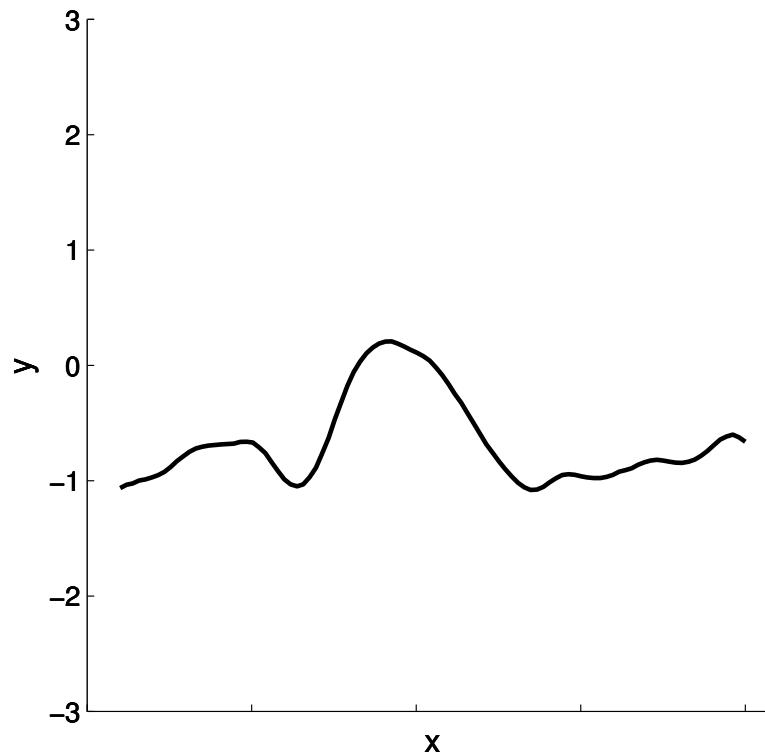
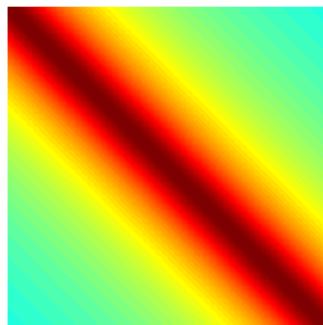


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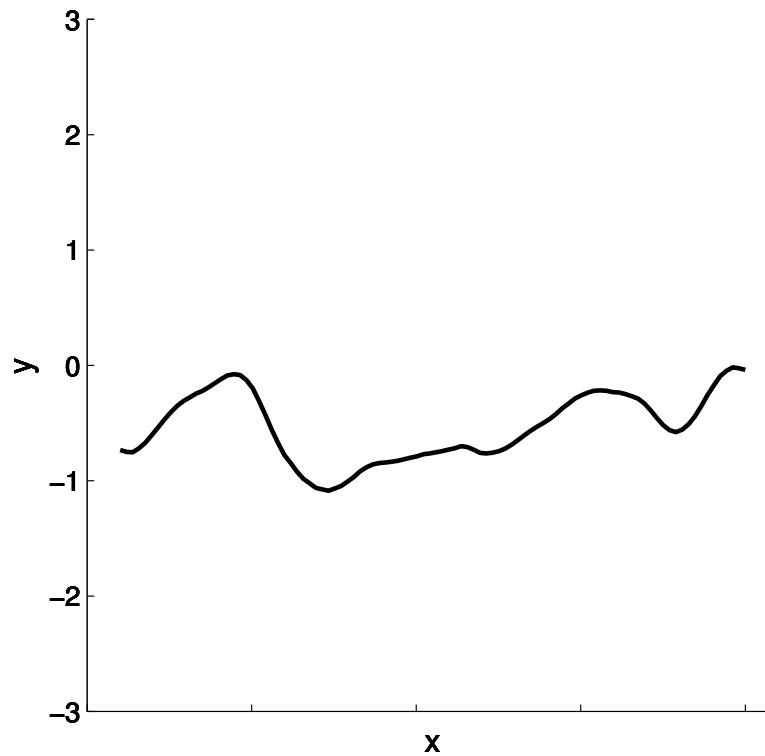
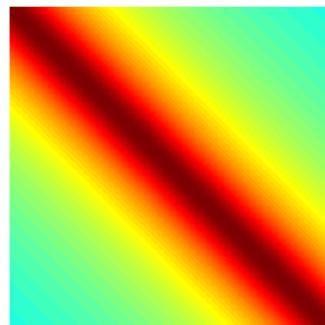


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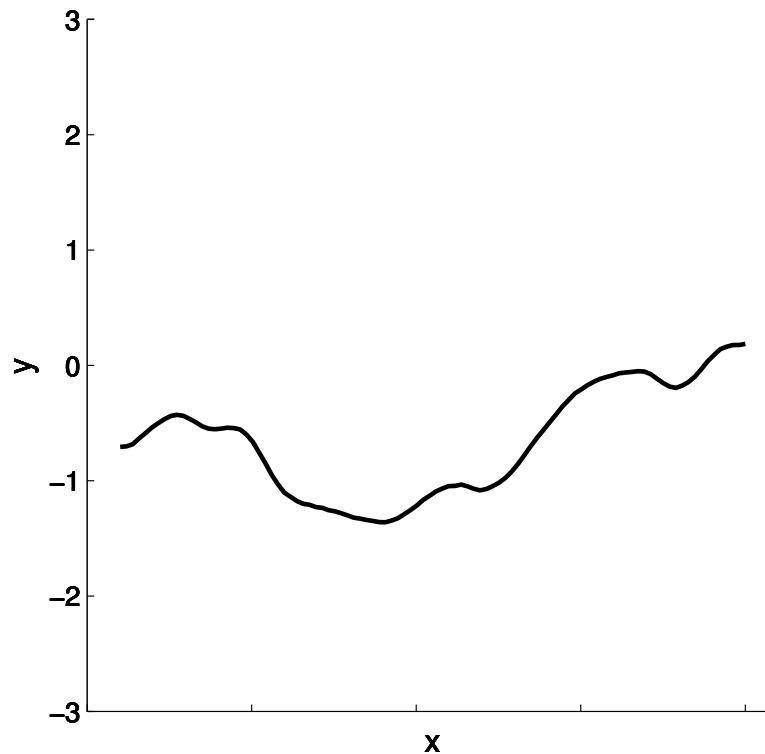
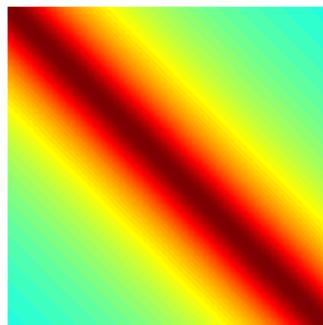


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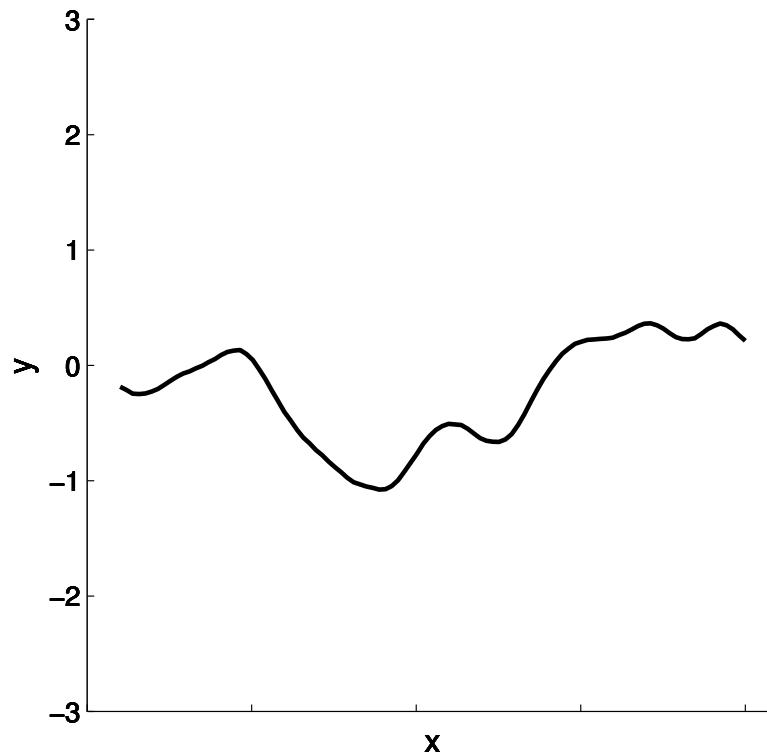
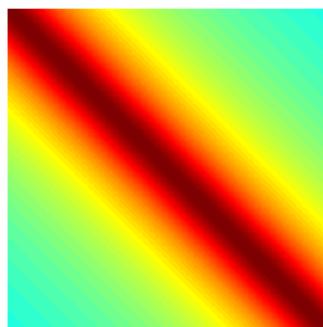


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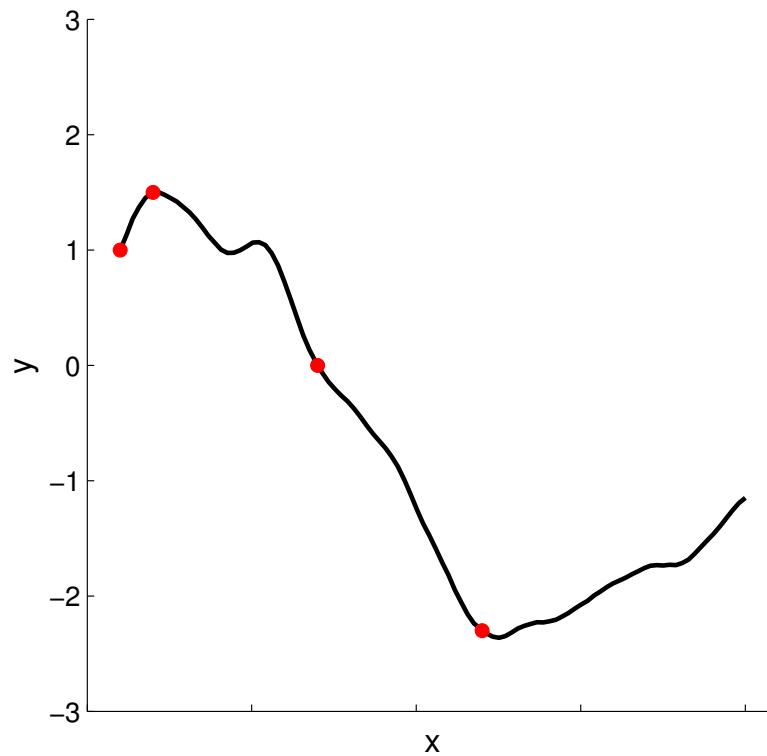
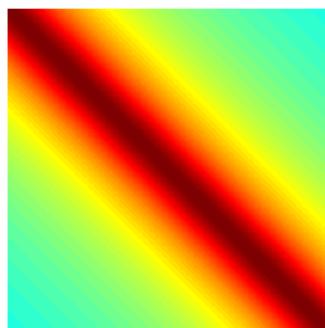


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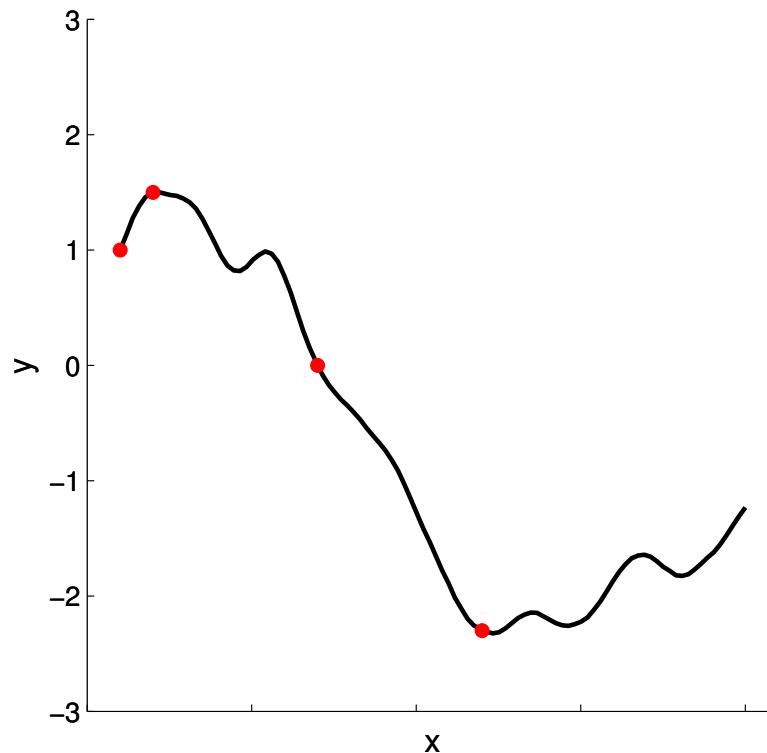
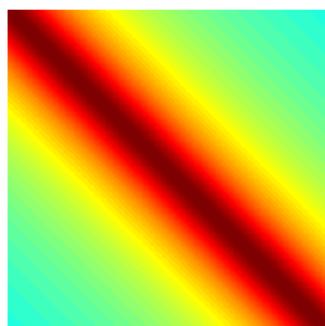


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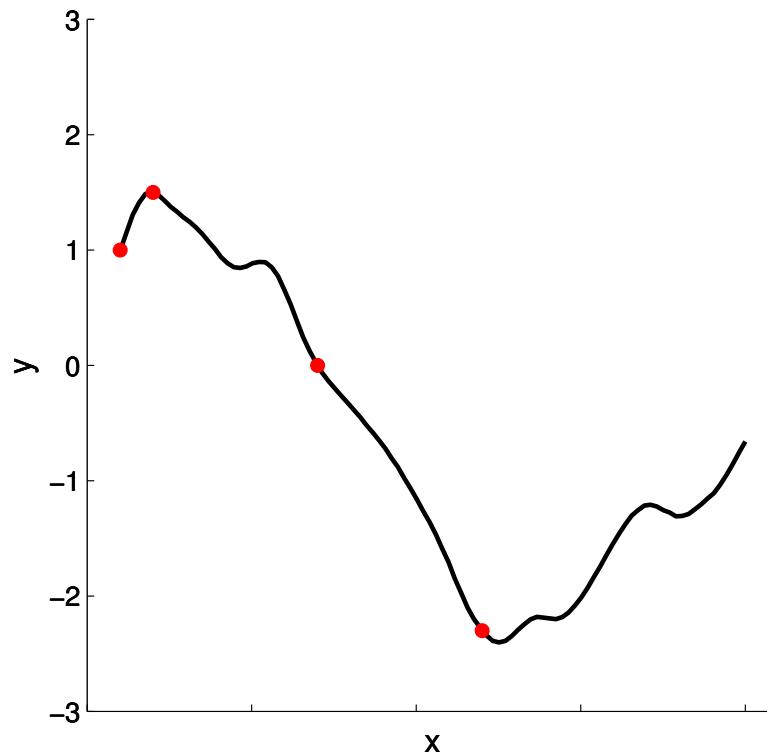
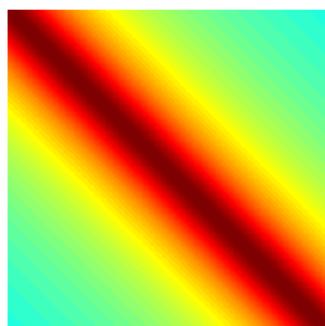


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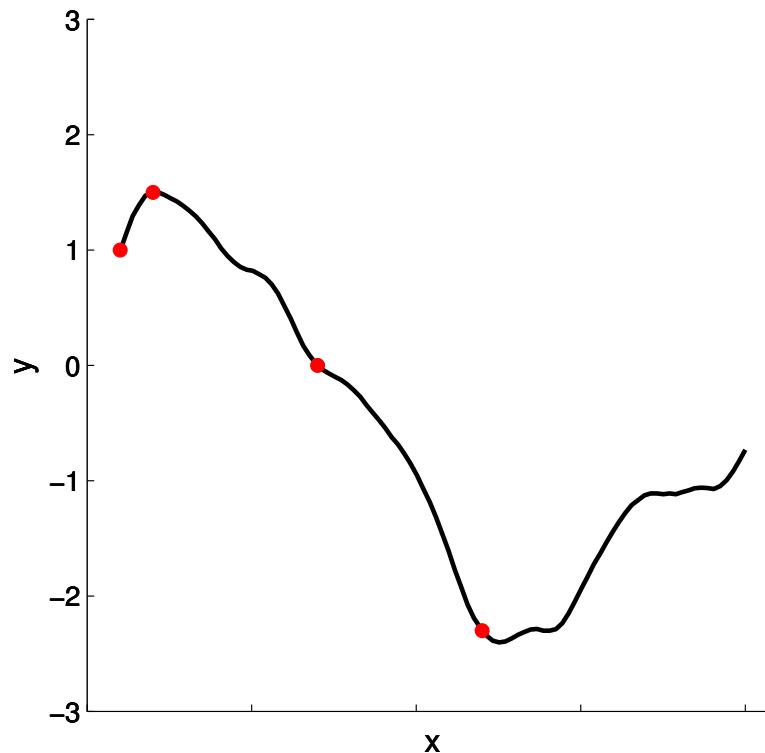
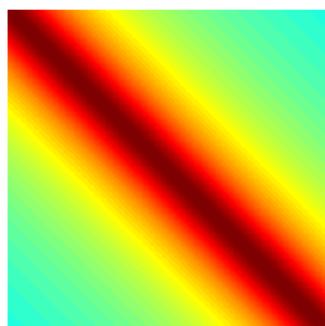


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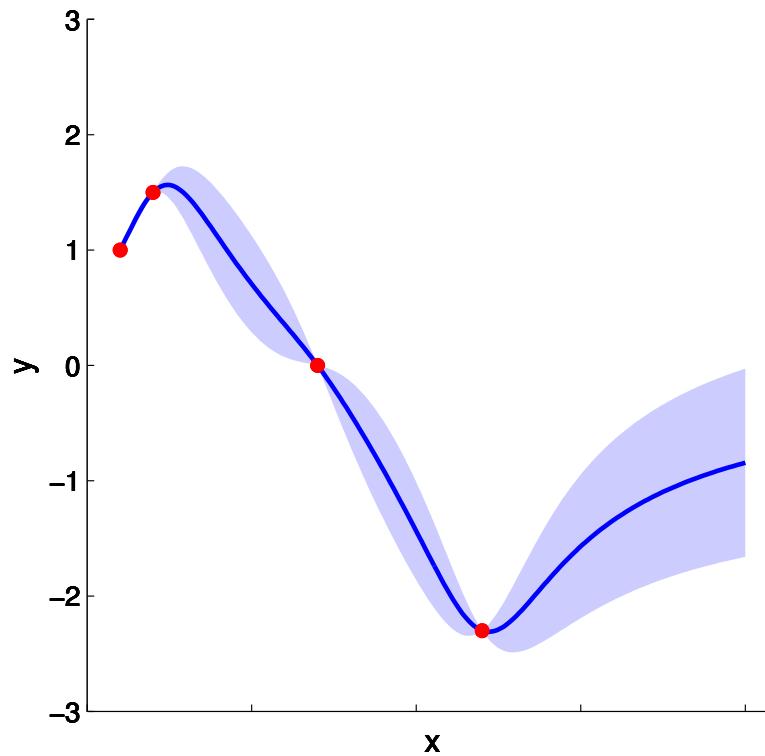
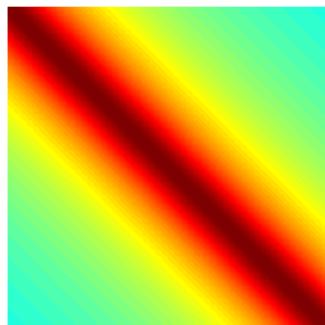


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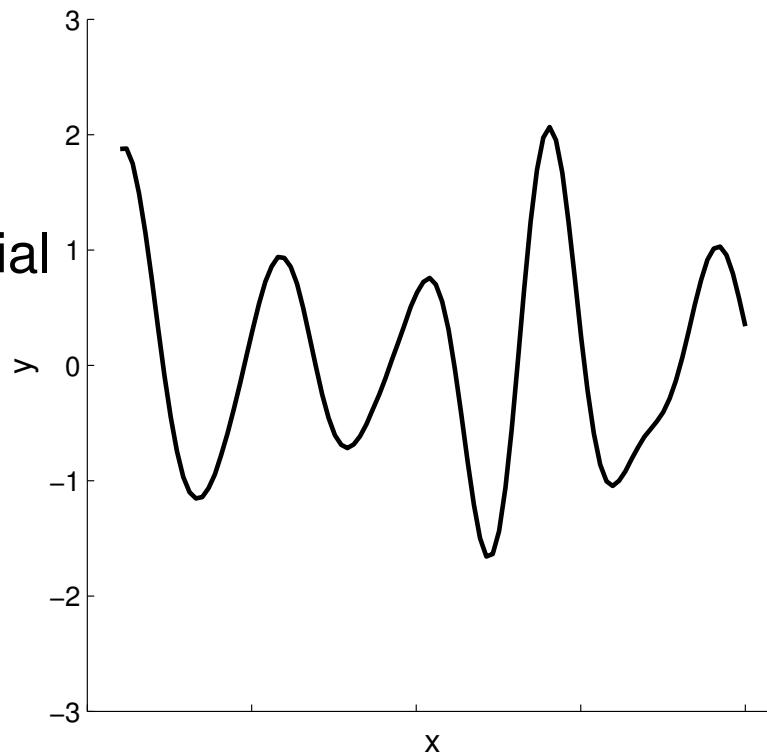
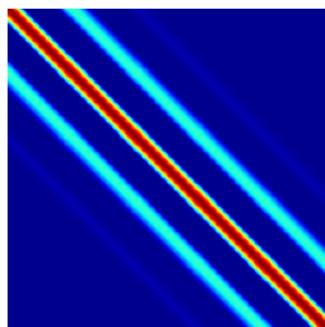
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Periodic

sinusoid \times squared exponential

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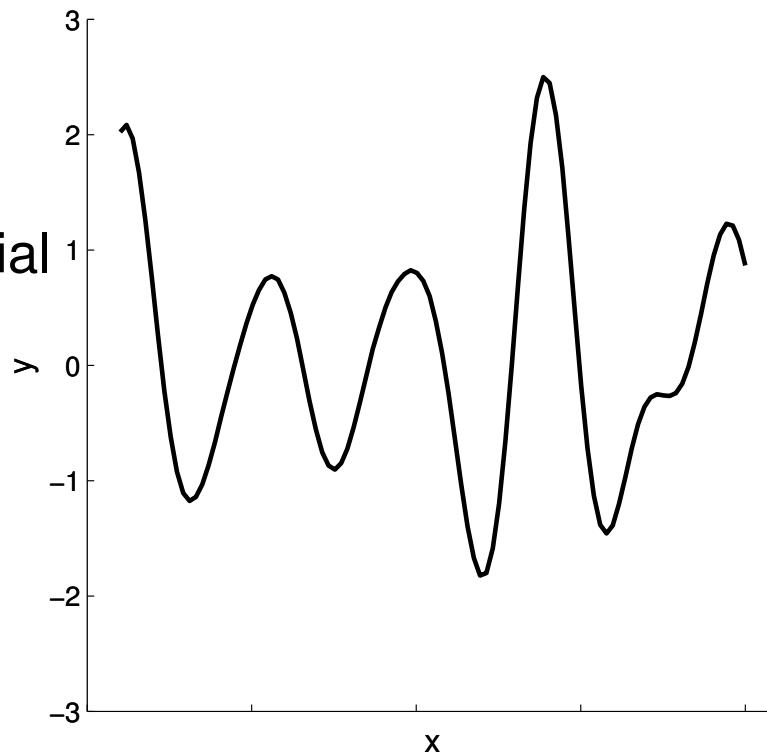
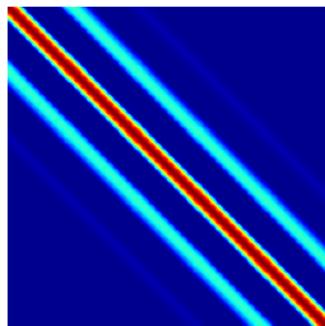
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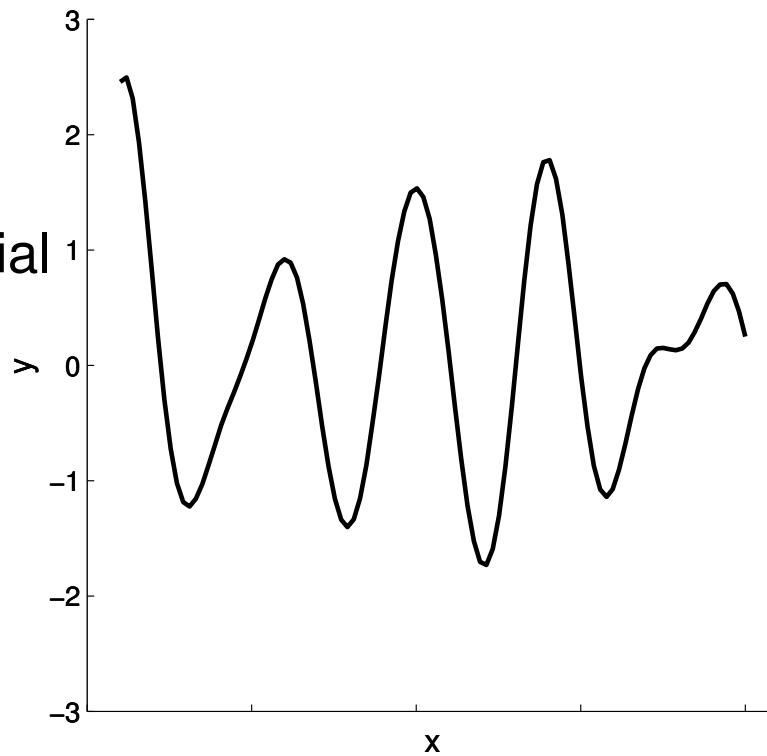
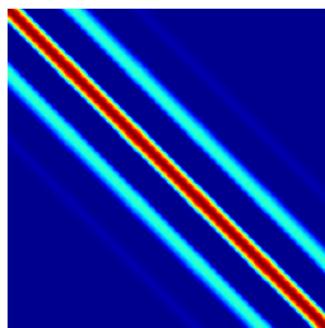
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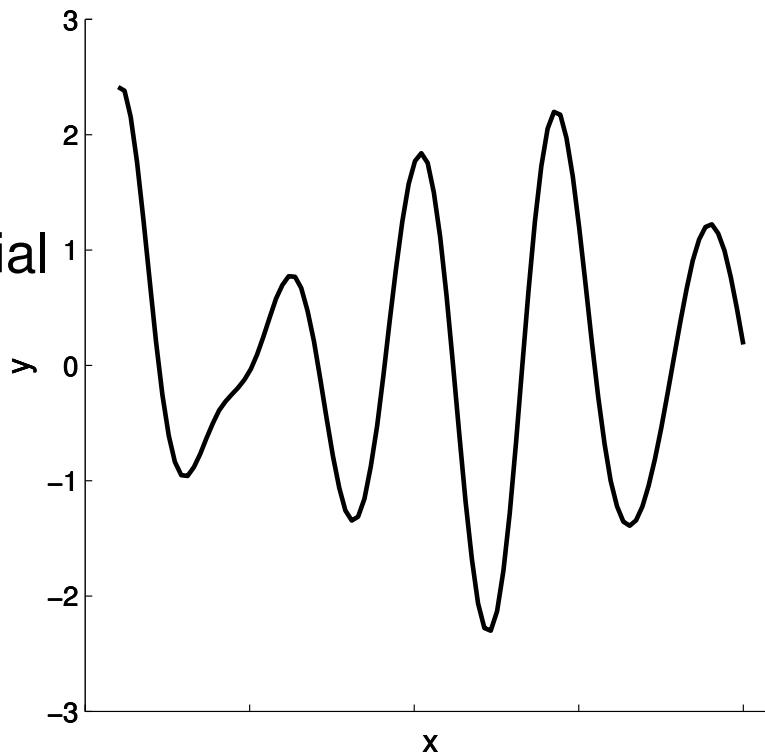
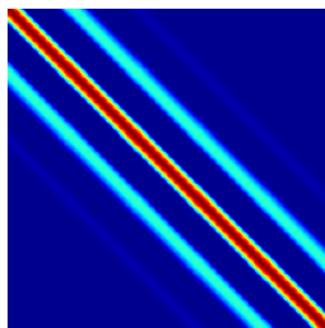
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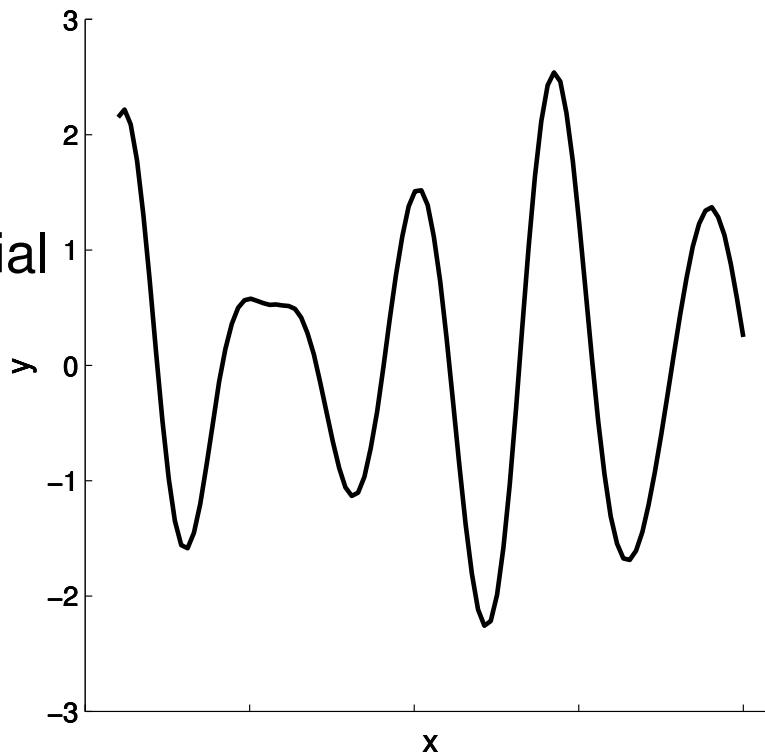
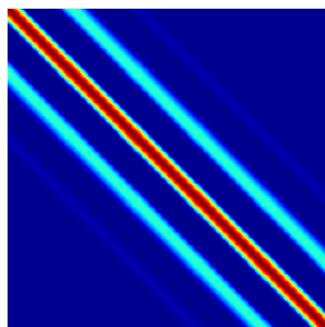
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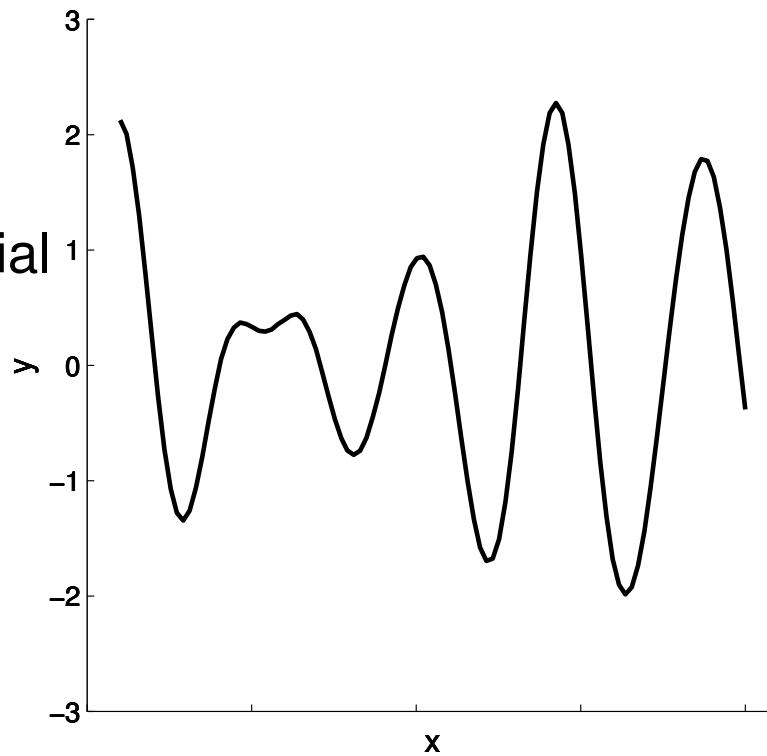
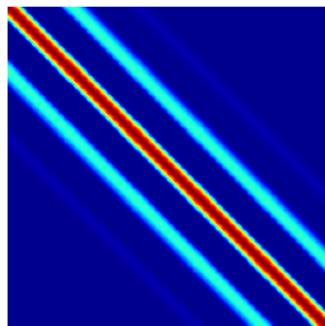
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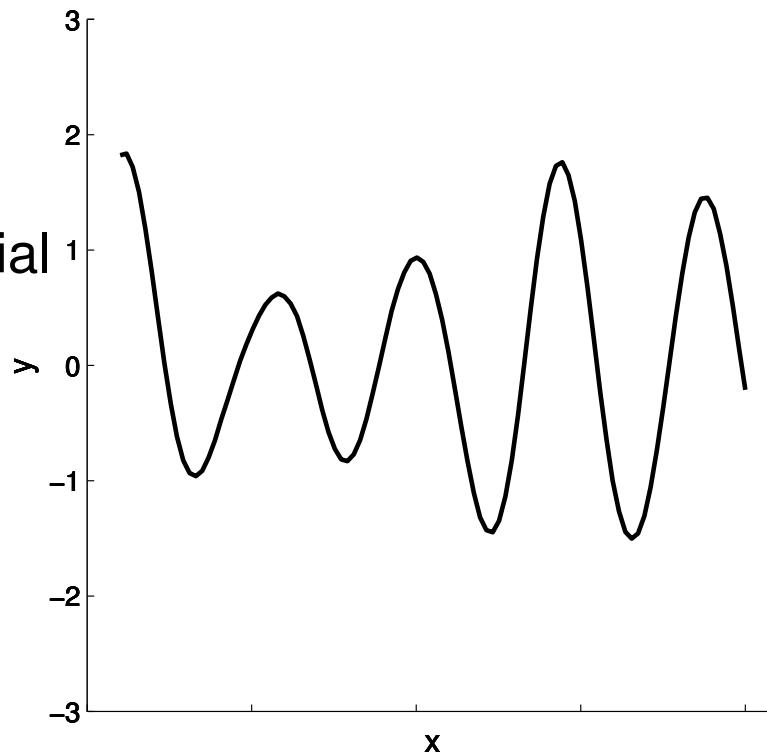
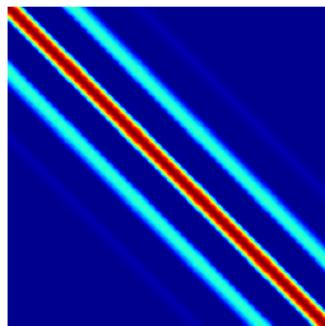
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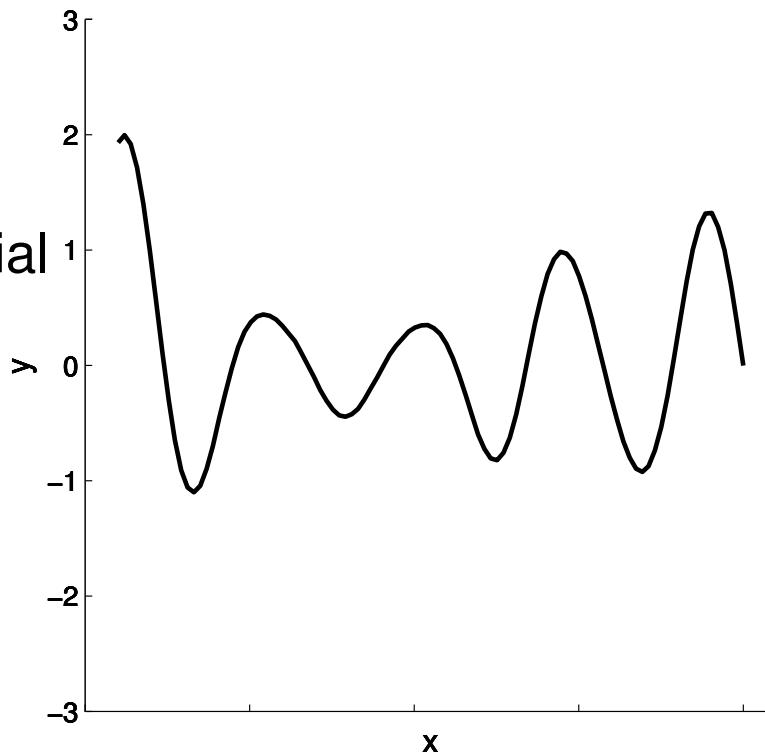
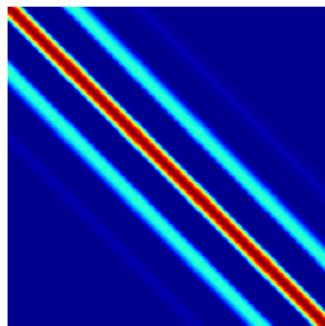
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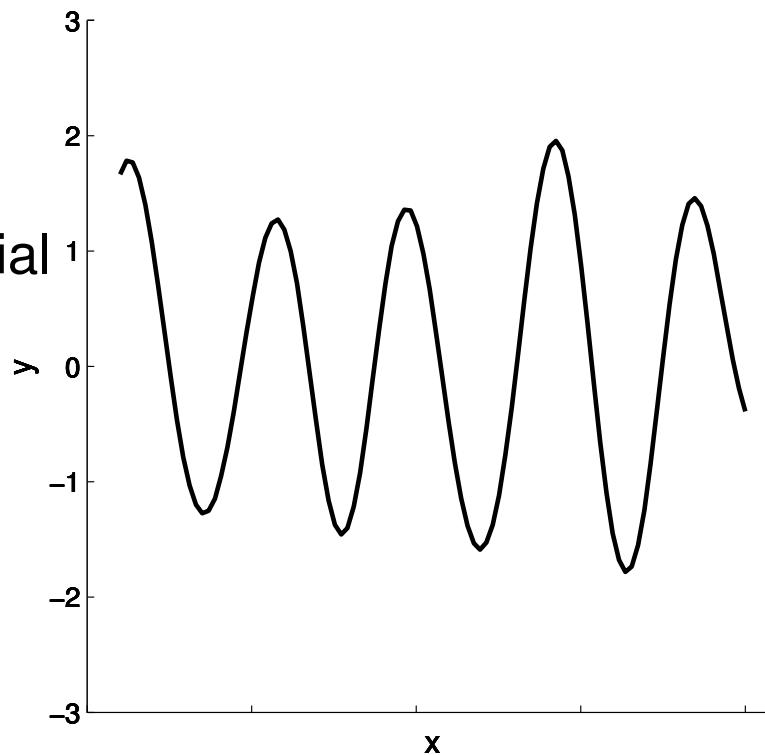
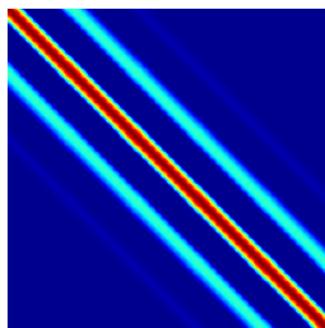
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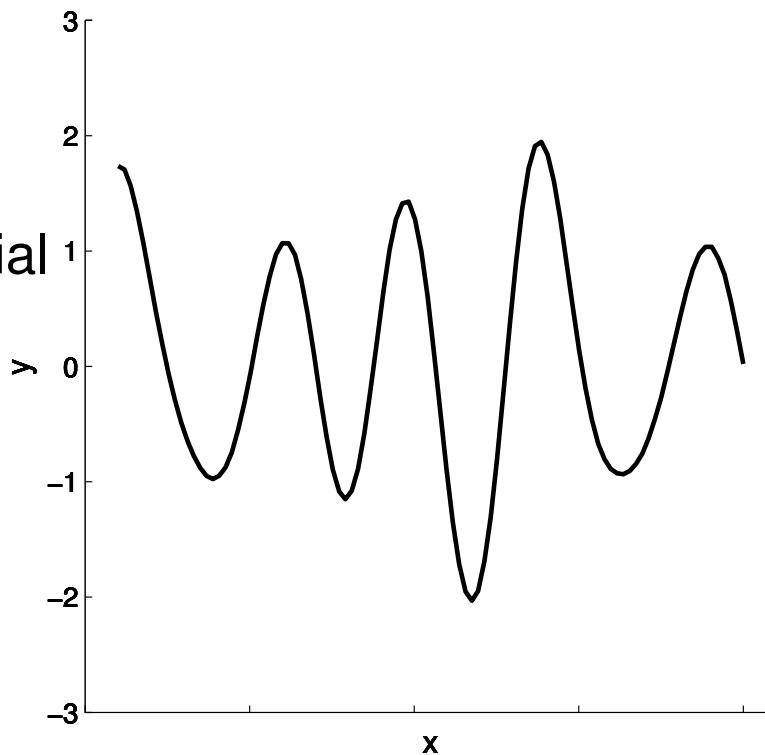
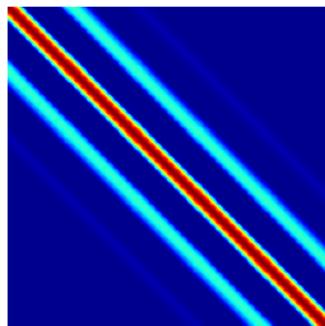
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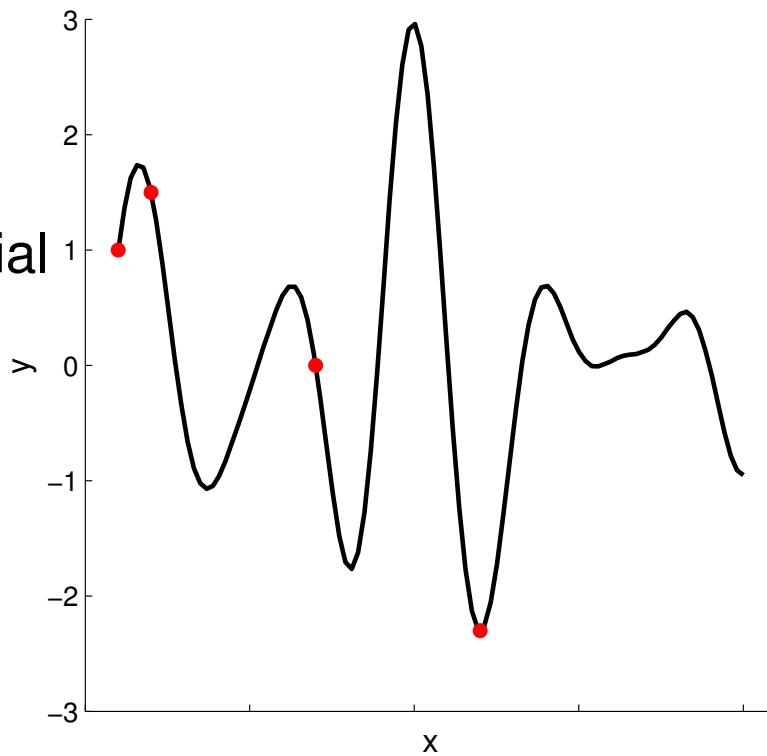
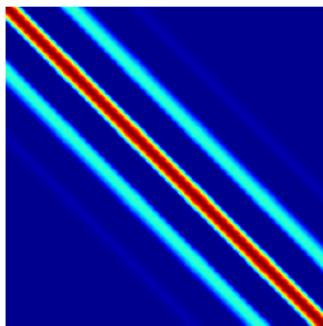


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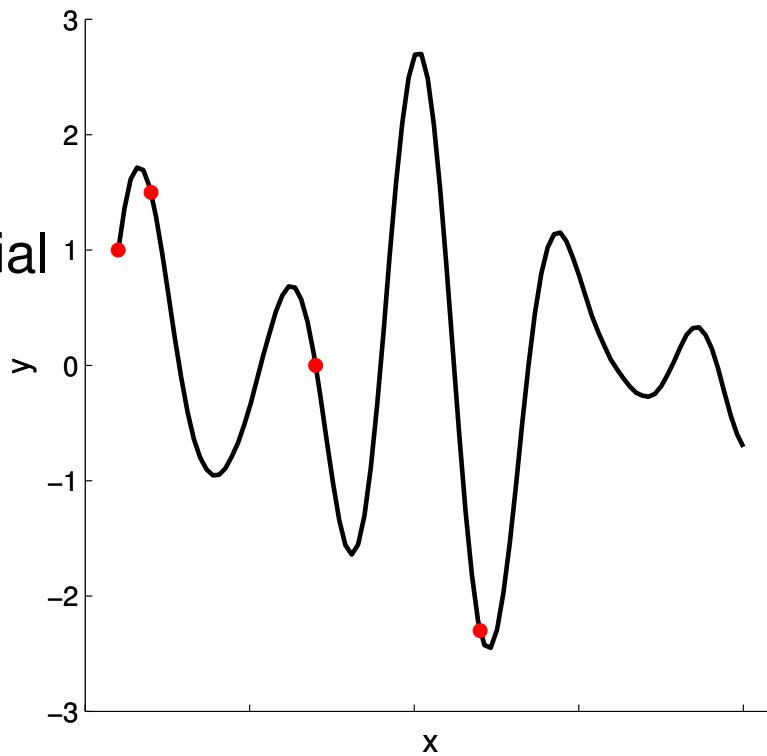
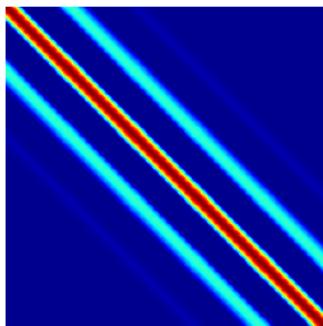
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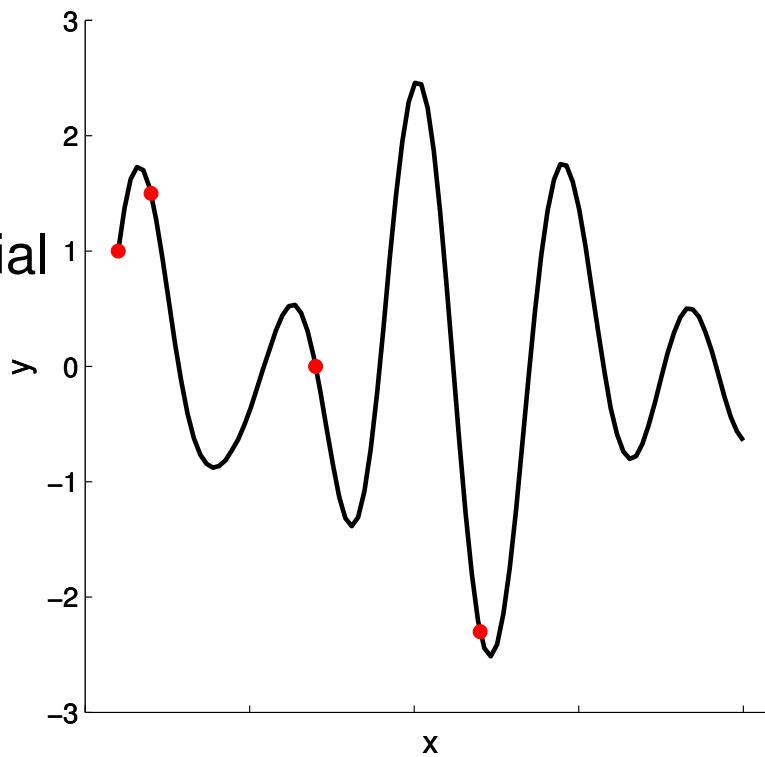
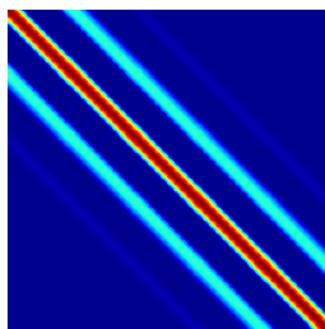
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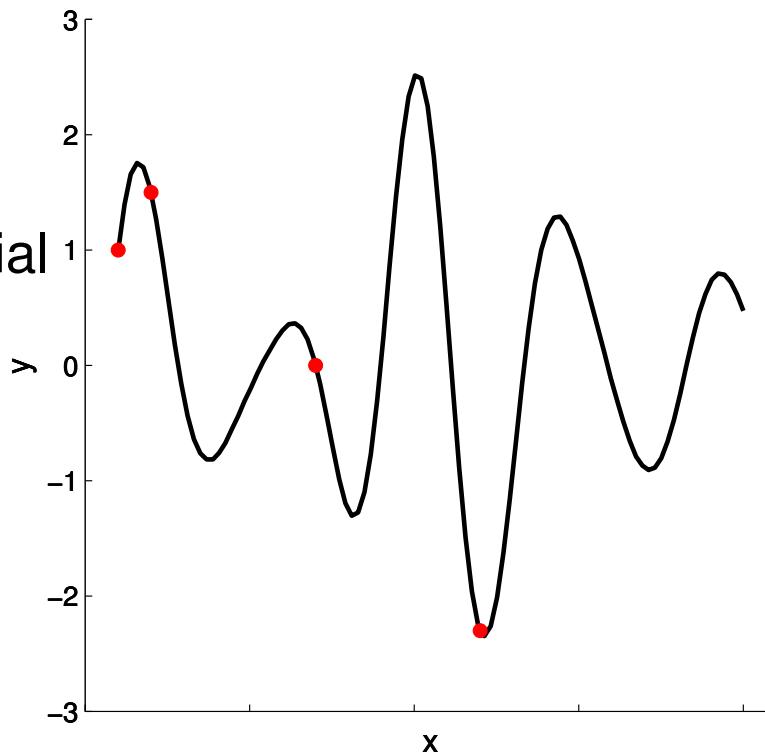
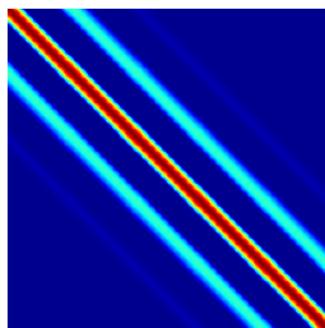
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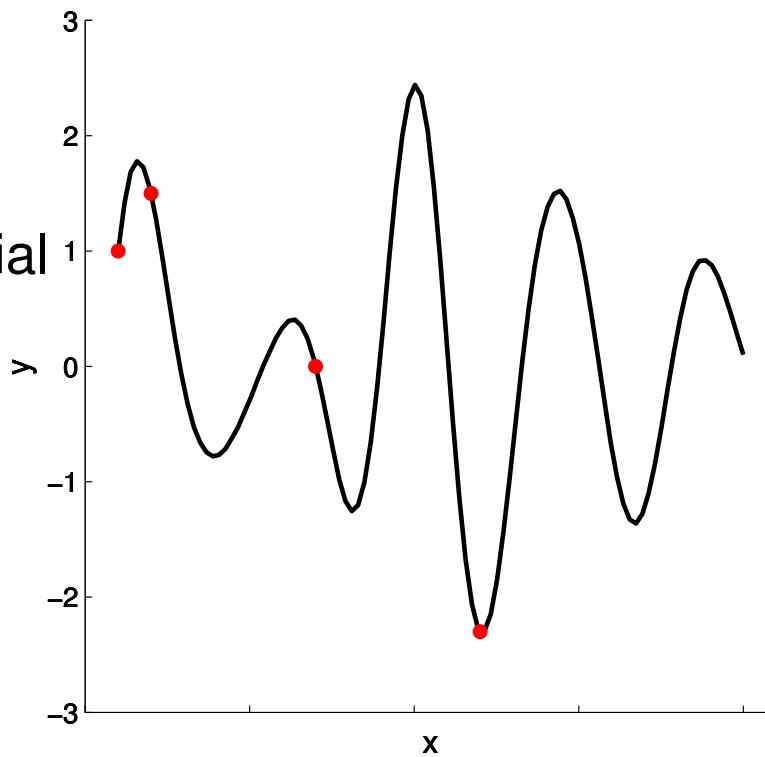
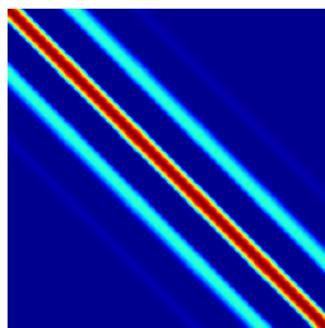
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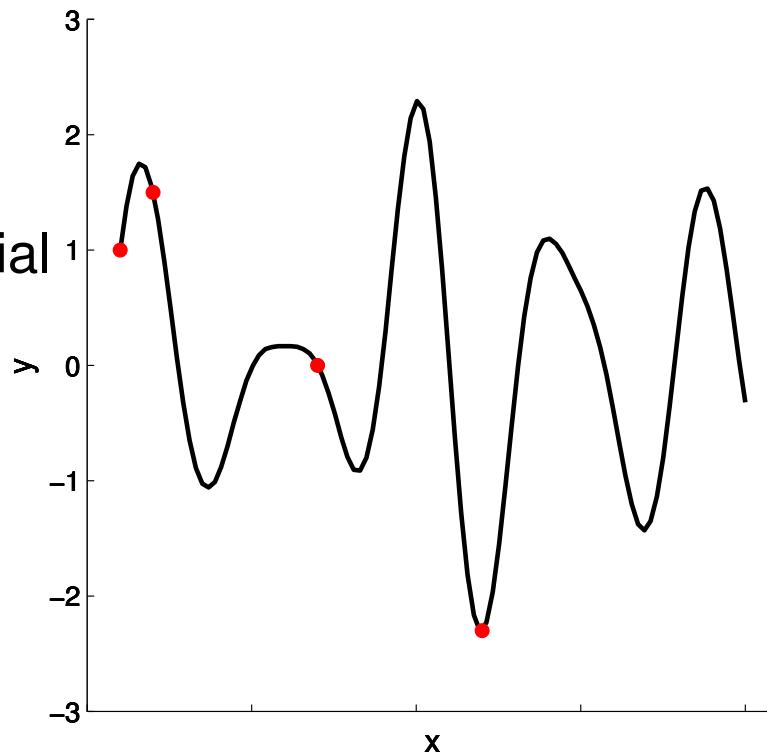
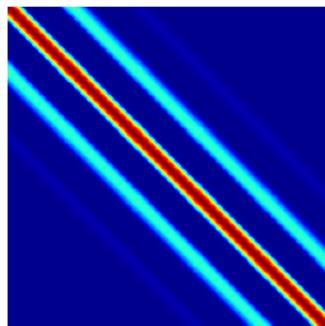
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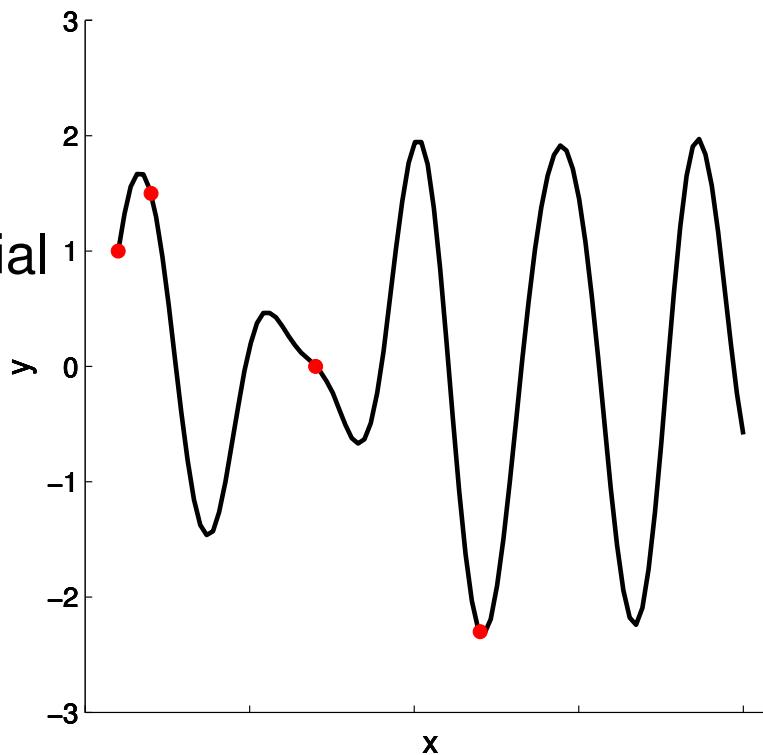
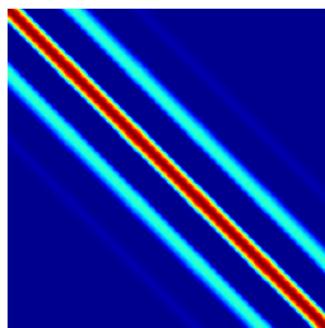
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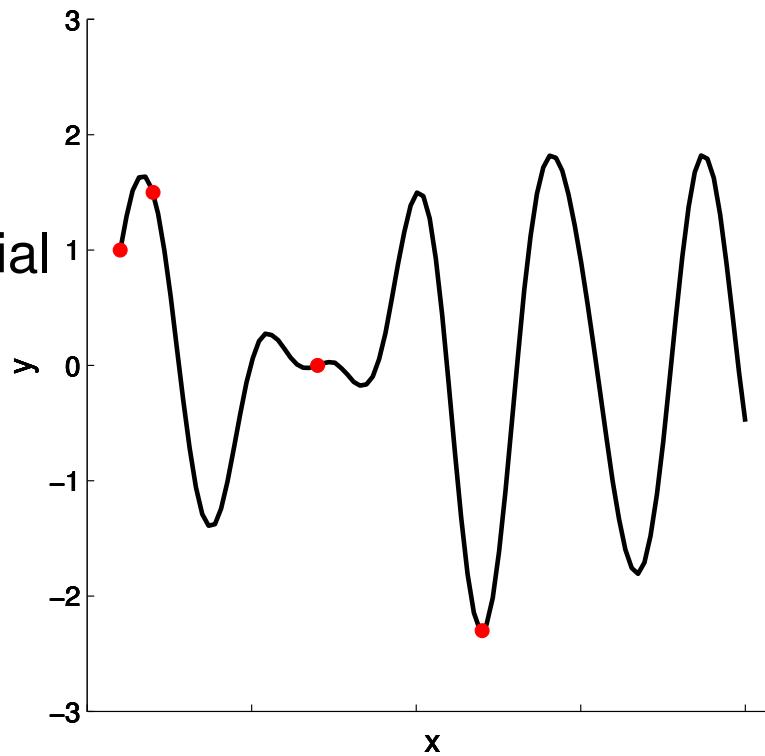
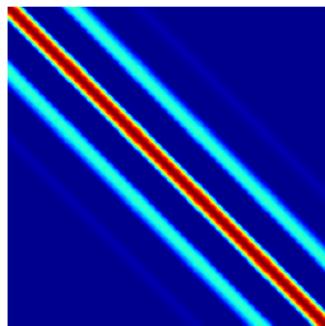
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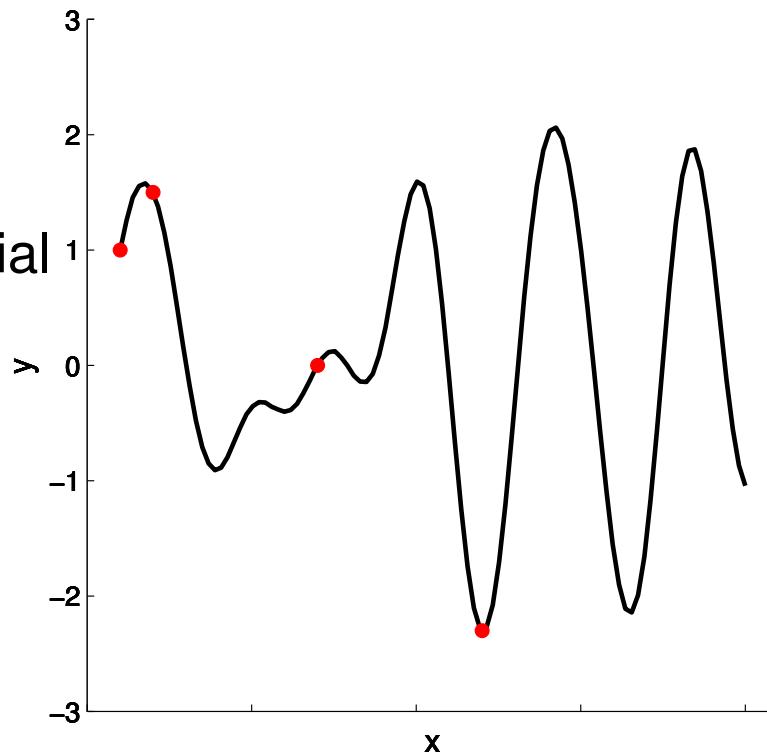
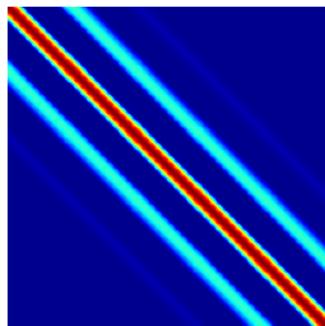
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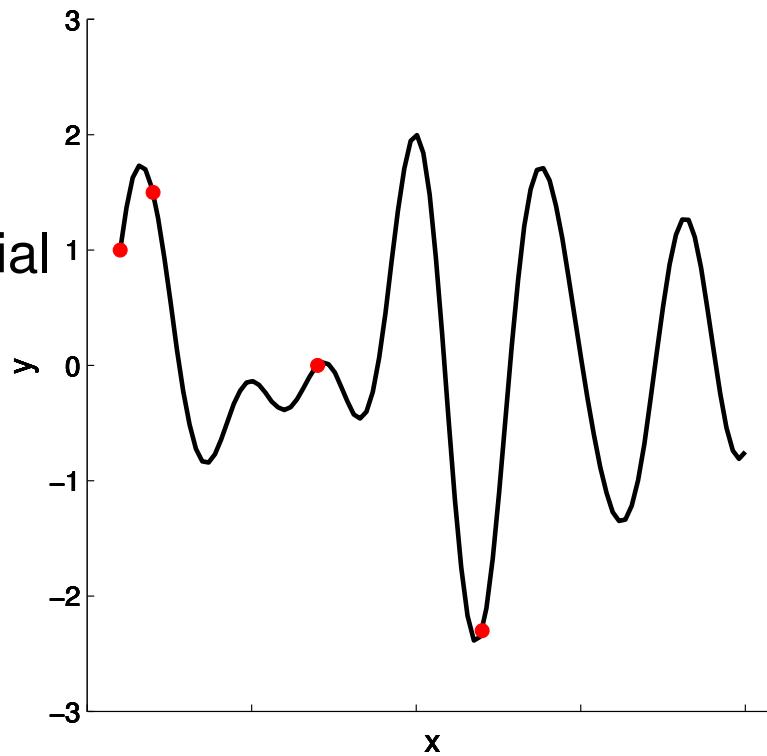
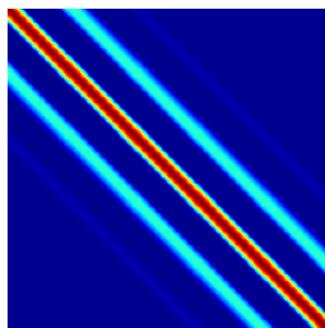
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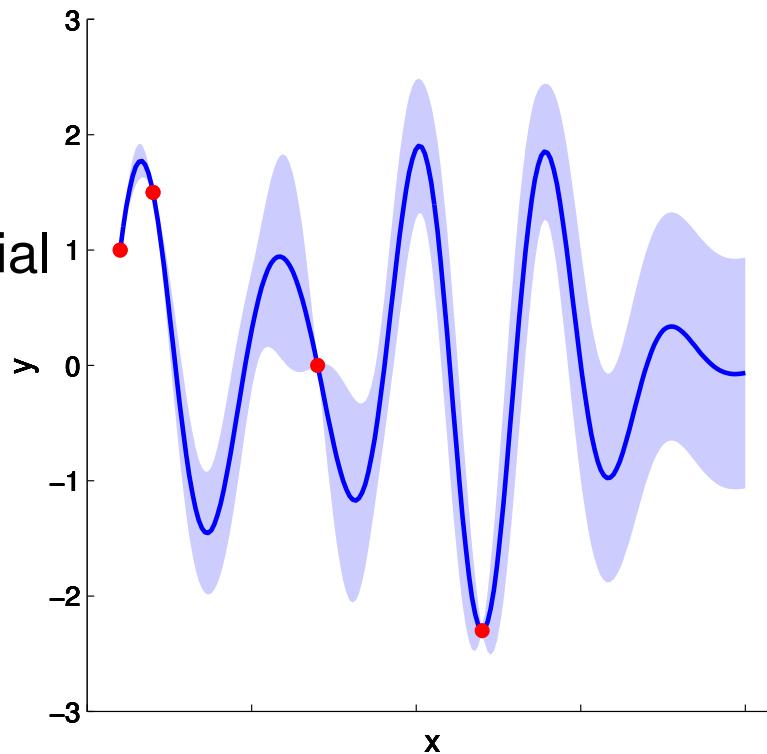
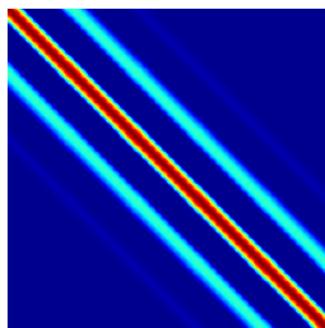
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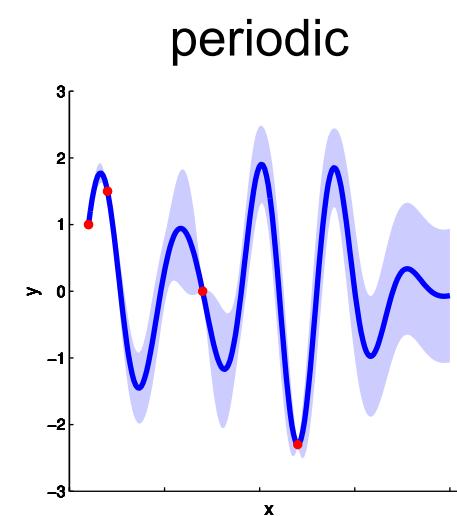
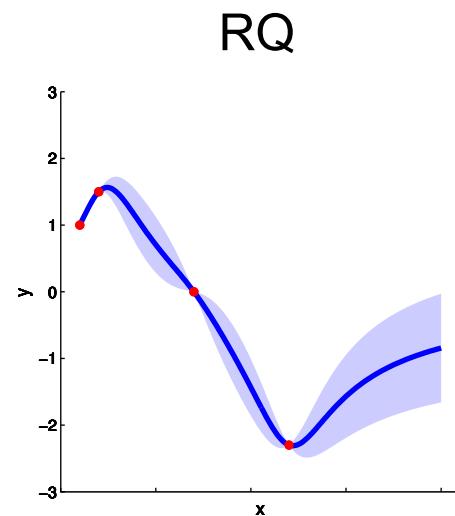
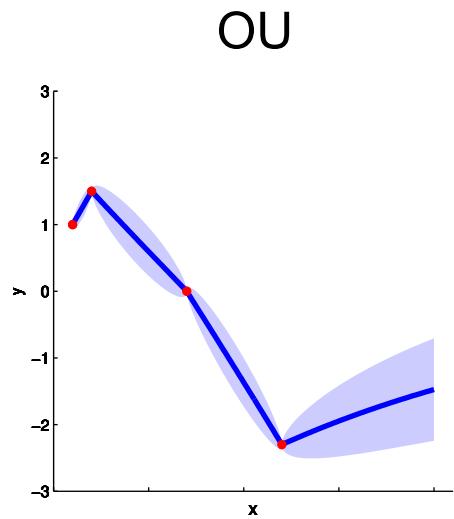
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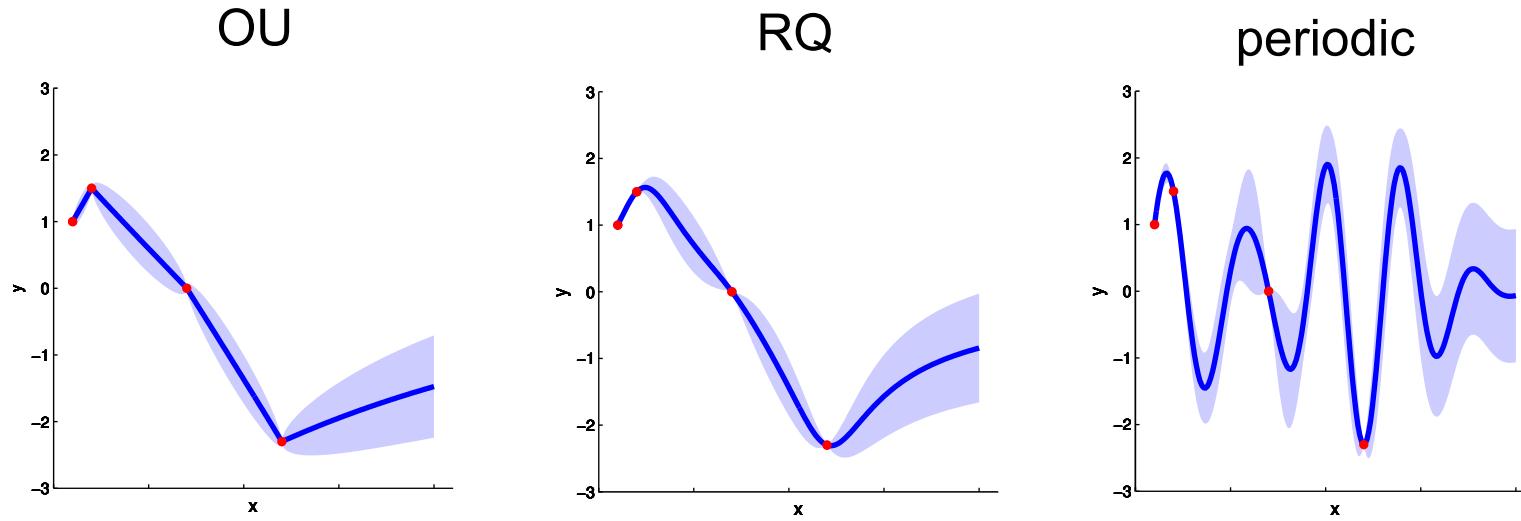
$\Sigma =$



The covariance function has a large effect



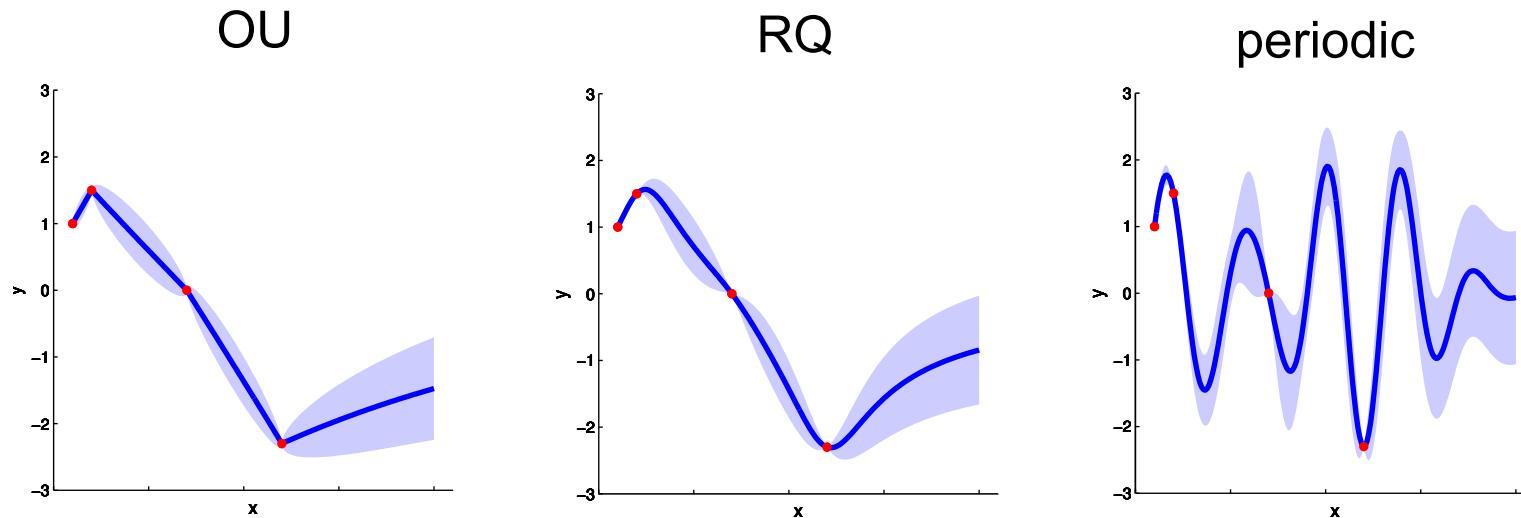
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Bayesian model comparison:

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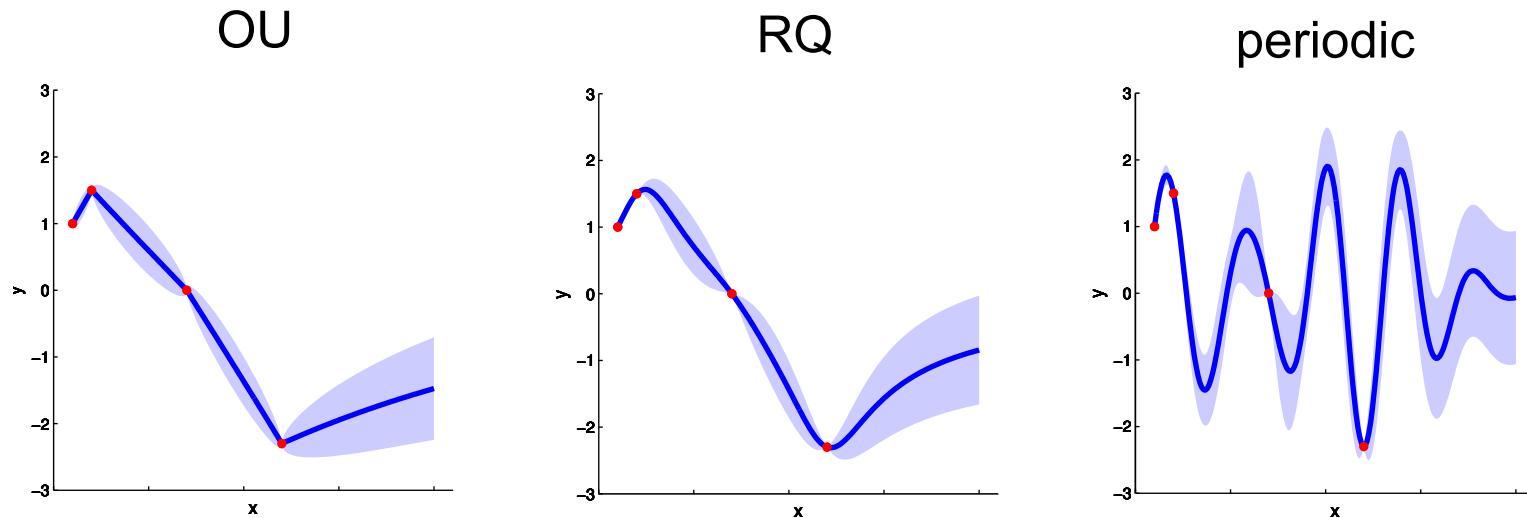


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prior over models

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

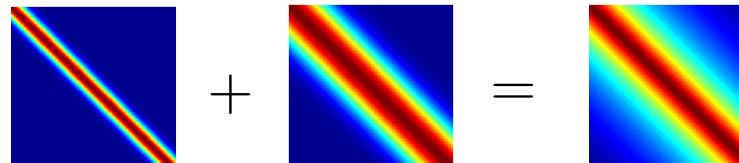
prior over models

Making new covariance functions from old

(positive) linear combinations
of covariance functions

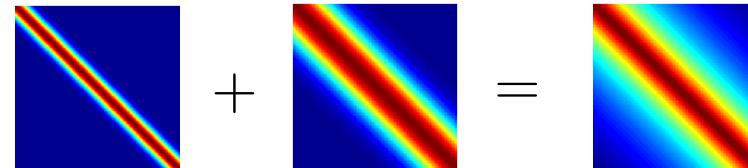
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$$\begin{array}{ccc} \text{e.g.} & \begin{array}{c} \text{scale mixture of SE} \\ + \end{array} & = \end{array} \quad \begin{array}{c} \text{rational} \\ \text{quadratic} \end{array}$$


Making new covariance functions from old

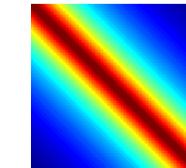
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e.g.

scale mixture of SE

=

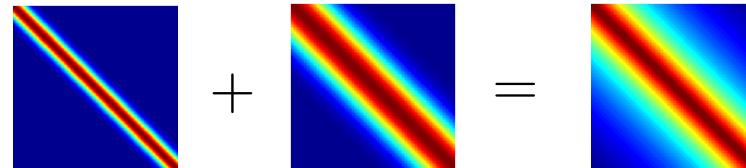


rational
quadratic

multiplication of covariance
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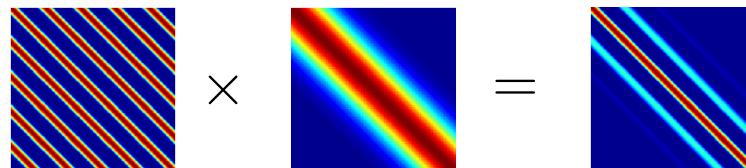
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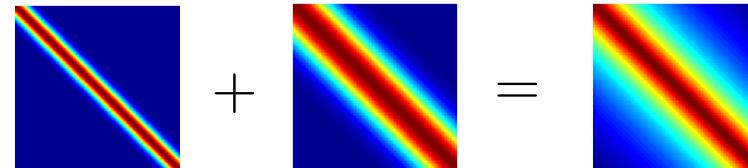
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e.g. periodic SE $\cos(\omega \Delta x) \exp(-\frac{1}{2l^2} \Delta x^2)$

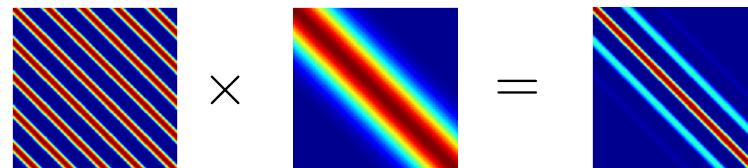
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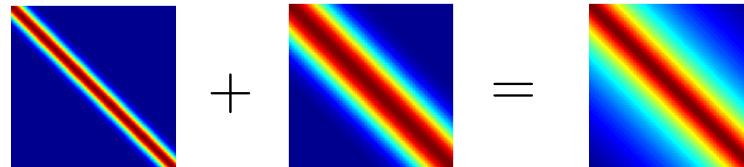
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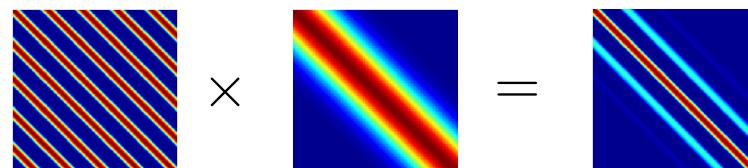
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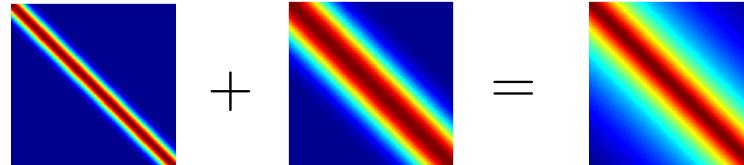
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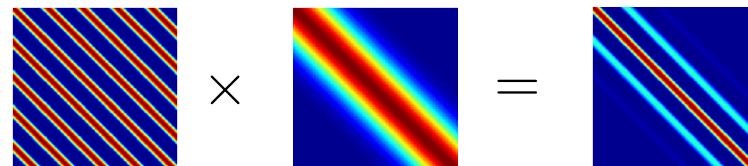
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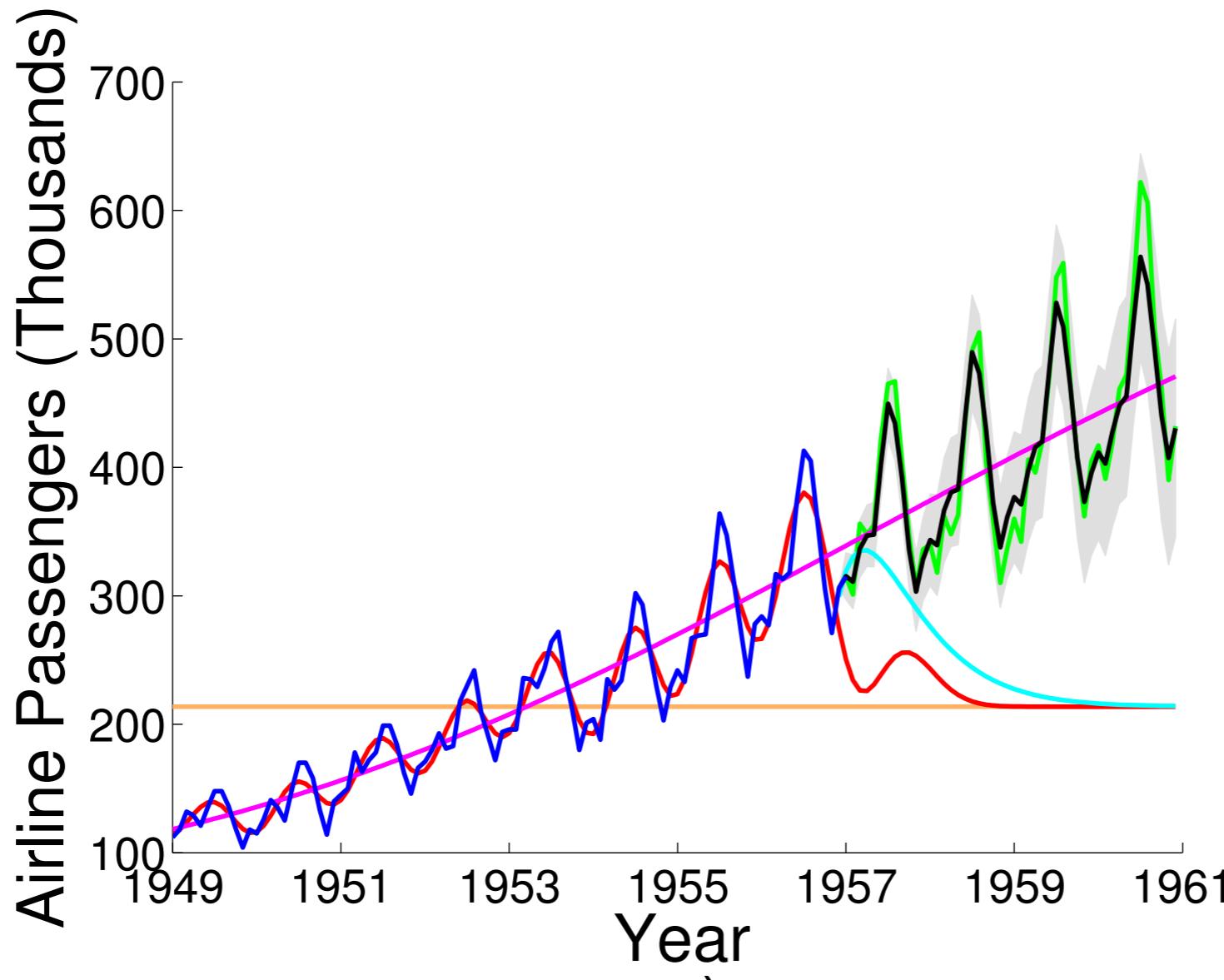
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Meta-kernel, learn which is right directly

$$k(\tau) = \sum_{q=1}^Q w_q \prod_{p=1}^P \exp\{-2\pi^2 \tau_p^2 v_q^{(p)}\} \cos(2\pi \tau_p \mu_q^{(p)}).$$

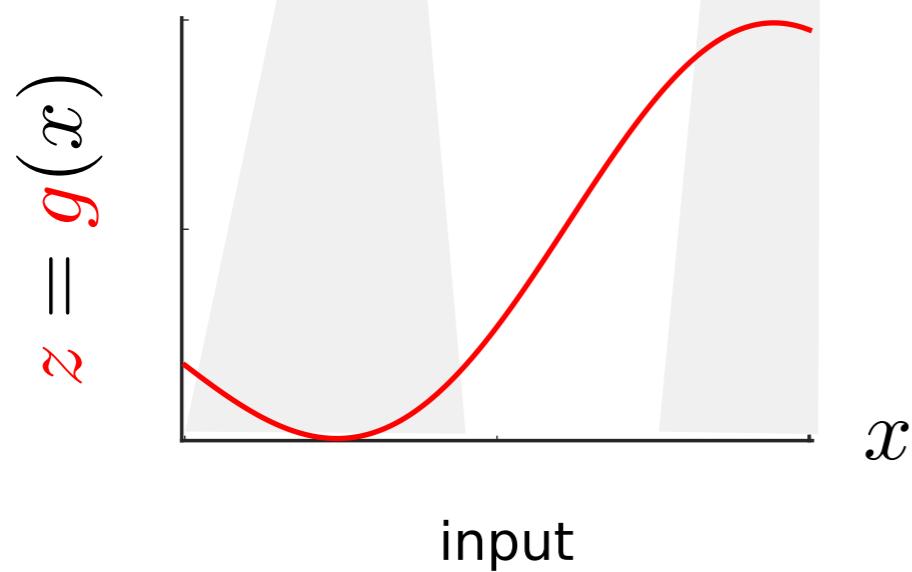
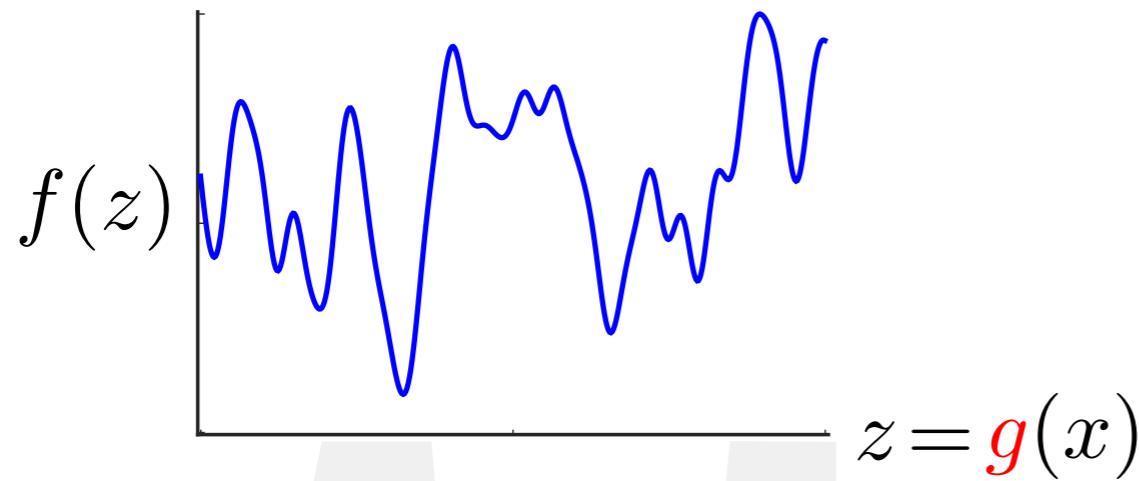


Deep GPs

$$y(x) = \textcolor{blue}{f}(\textcolor{red}{g}(x)) + \sigma_y \epsilon$$

$$f(x) = \mathcal{GP}(0, K_f(x, x'))$$

$$g(x) = \mathcal{GP}(0, K_g(x, x'))$$

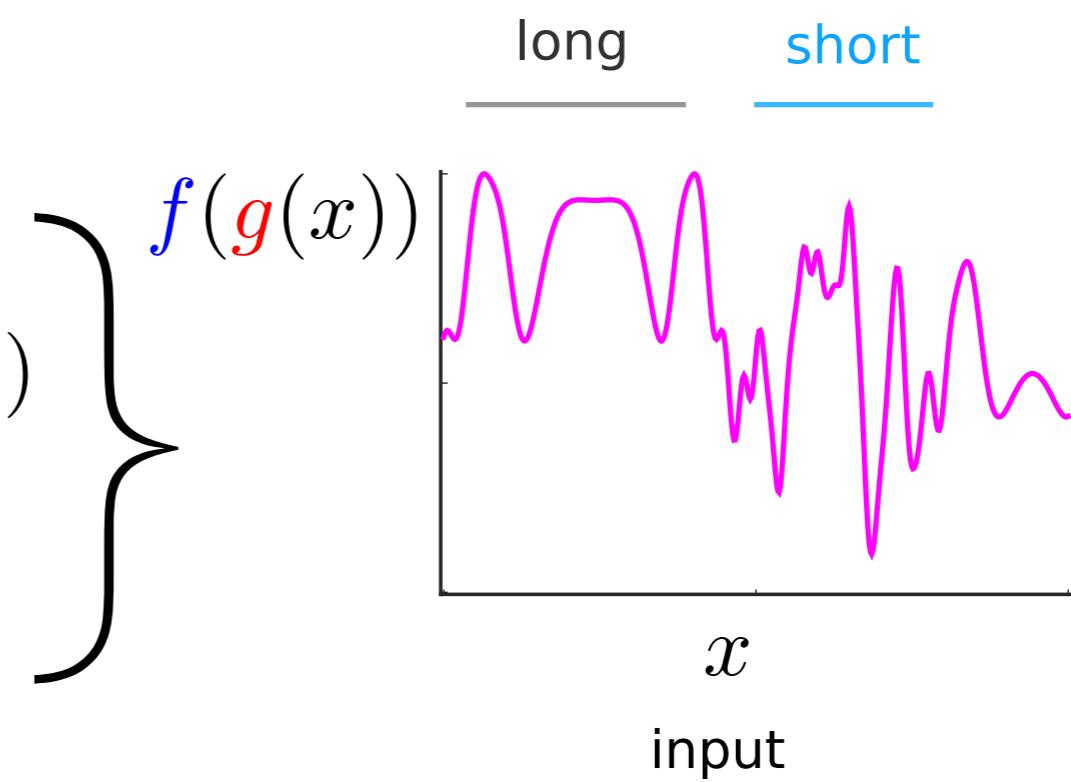
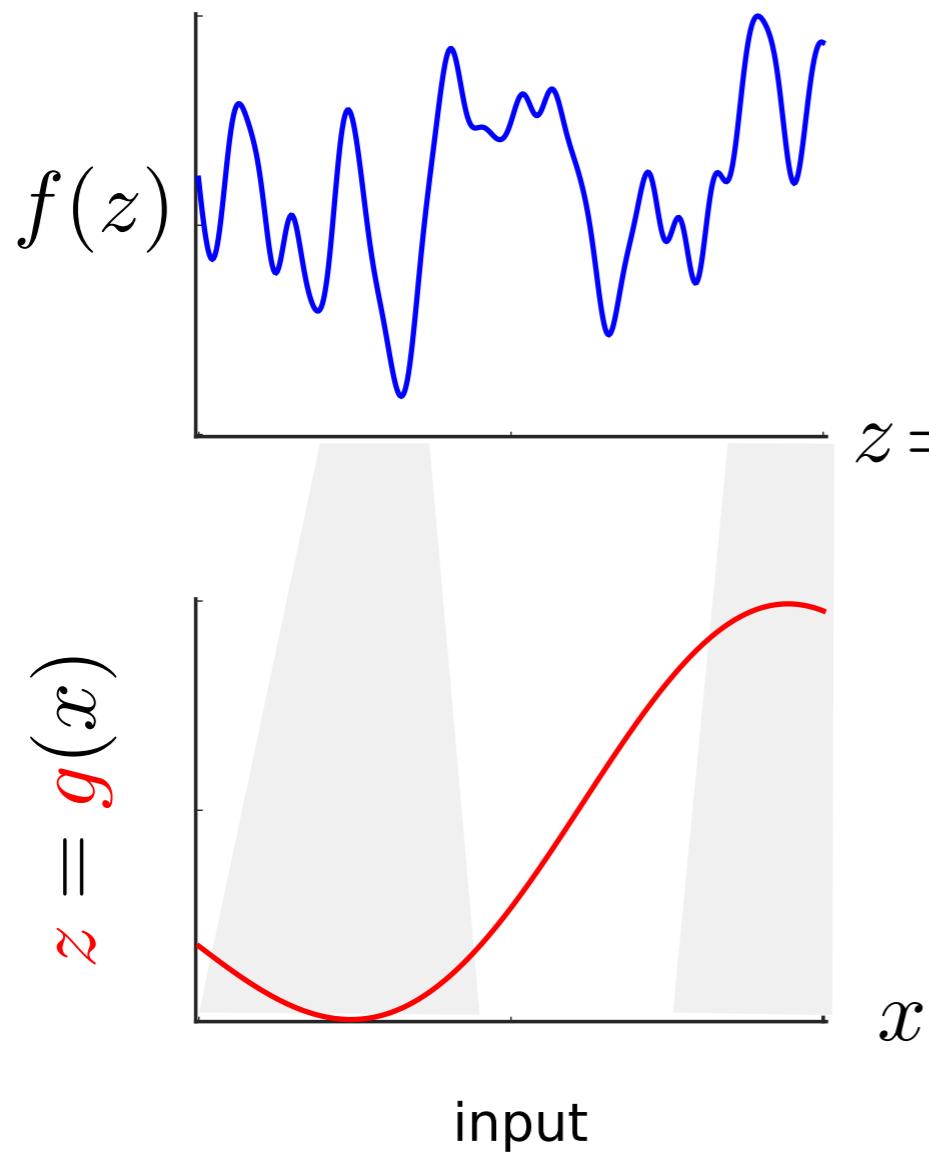


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DGP = multi-layer neural network,
infinitely wide hidden layer

How do we choose the hyper-parameters?

idea: use probability distributions to represent plausibility
of hyper-parameters (uncertainty) given the data

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$$\text{what we know after seeing the data} \propto \text{what the data tell us} \times \text{what we knew before seeing the data}$$

(likelihood) (prior)

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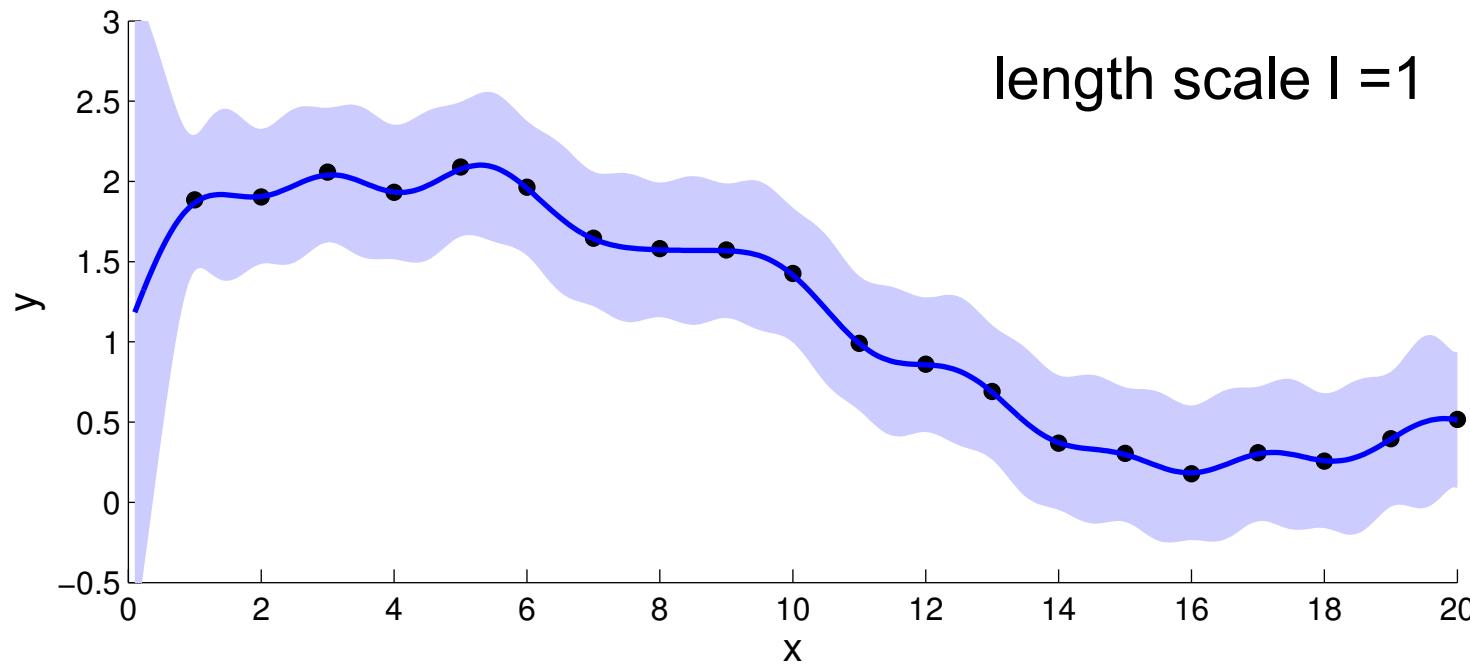
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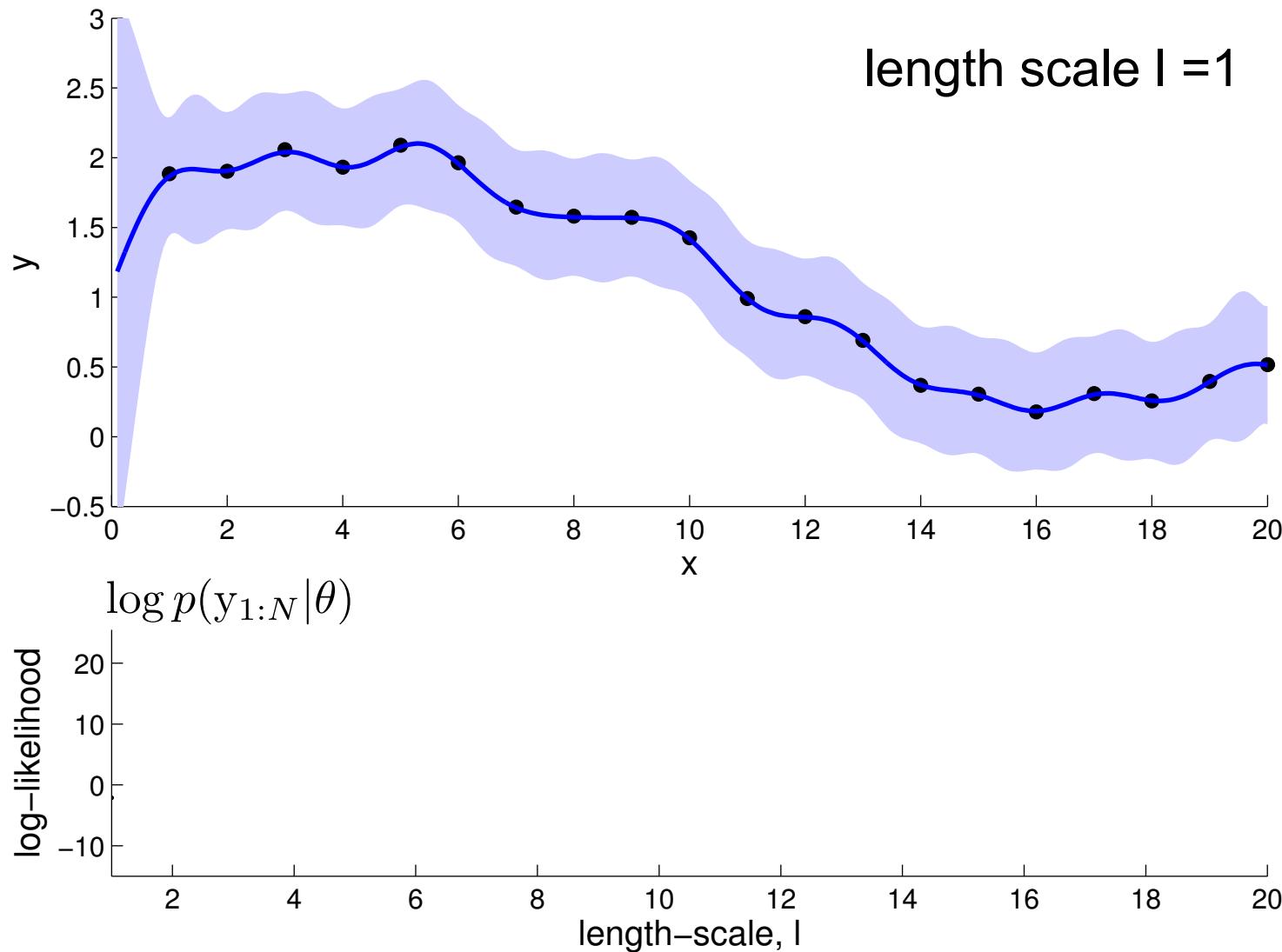
$p(\mathbf{y}_{1:N} | \theta)$ = likelihood of the parameters
= how well did θ predict the data we observed

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

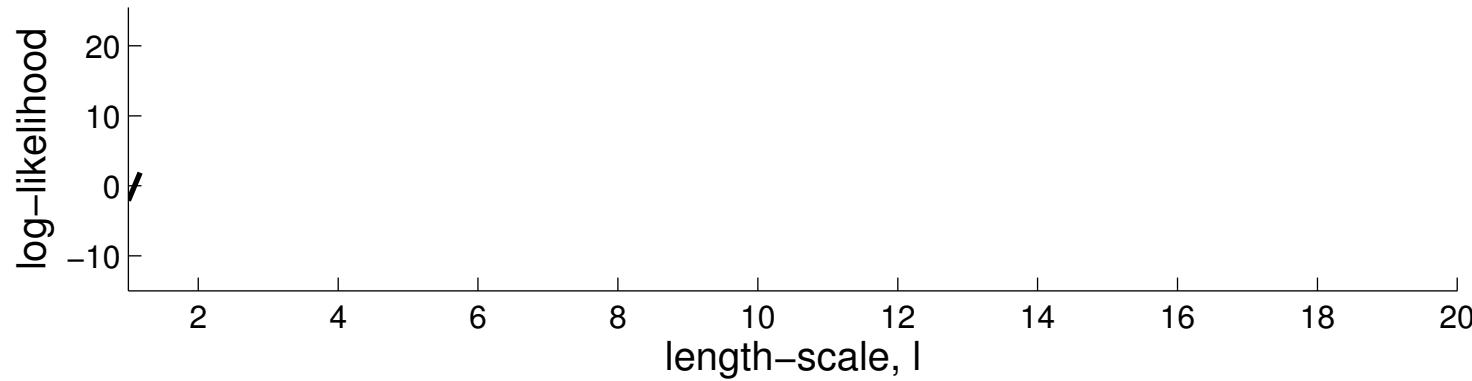
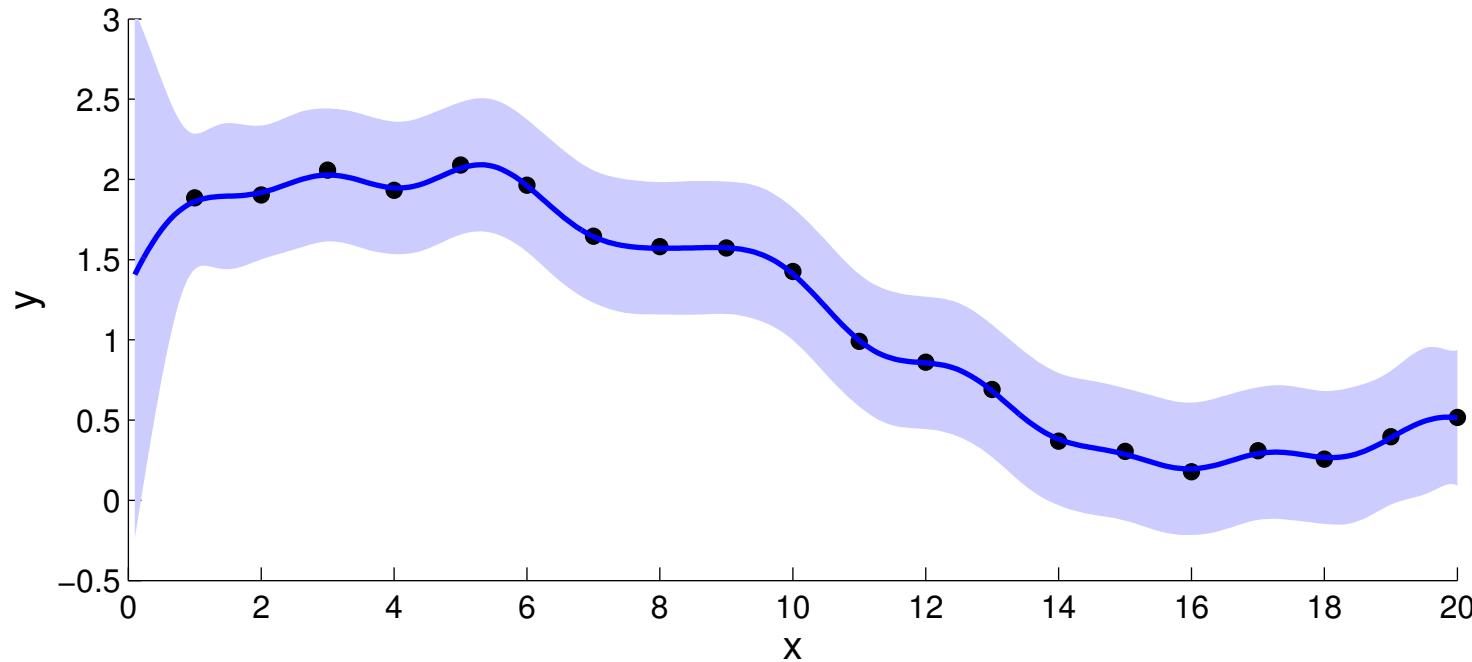
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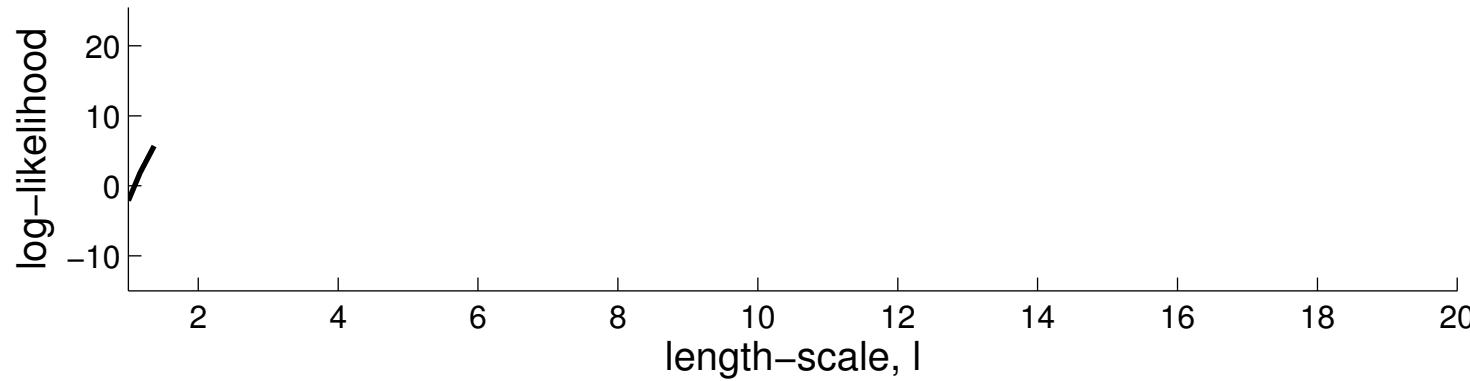
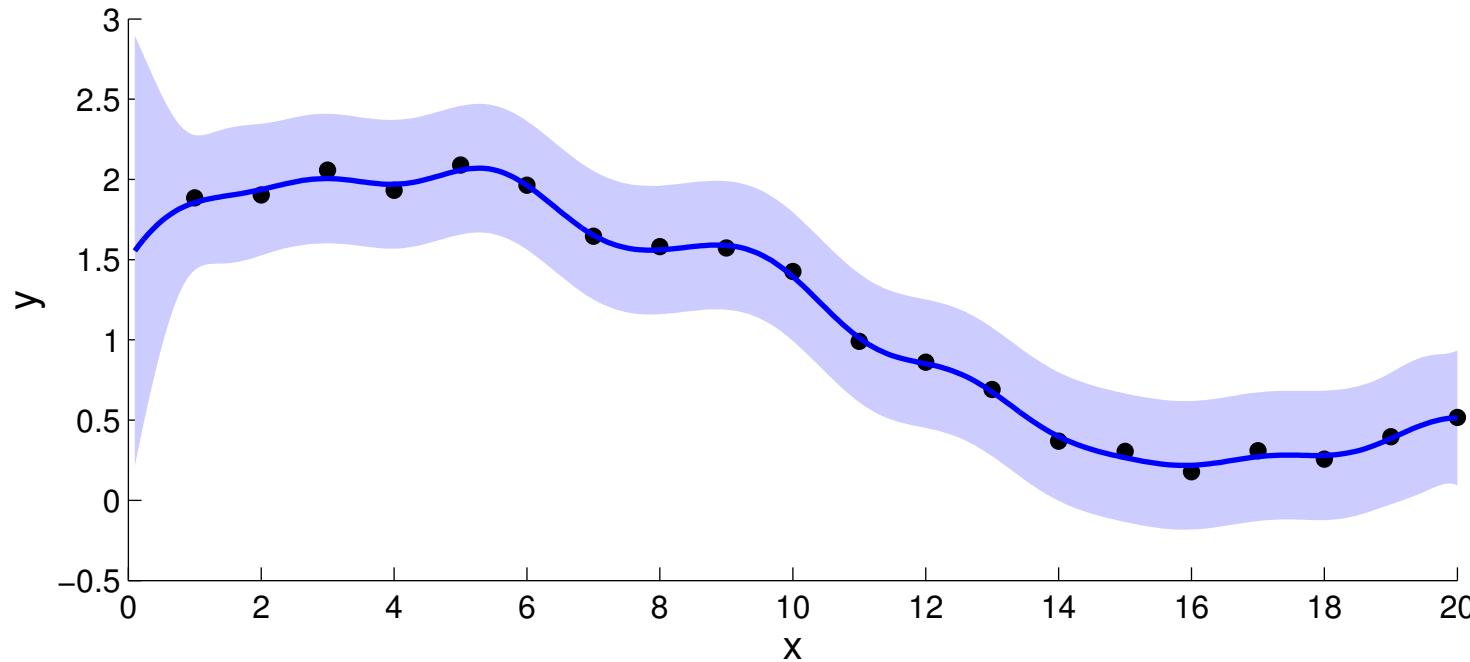
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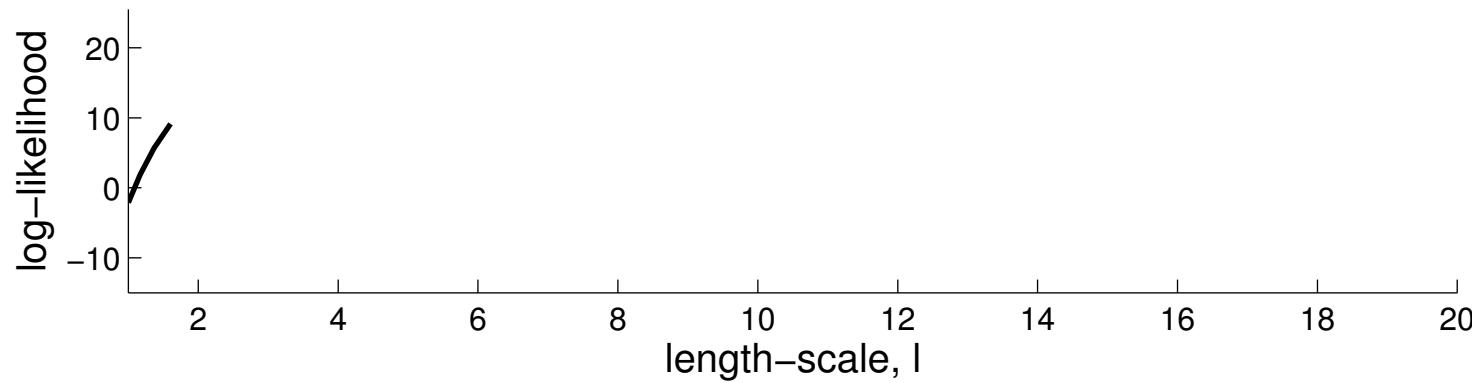
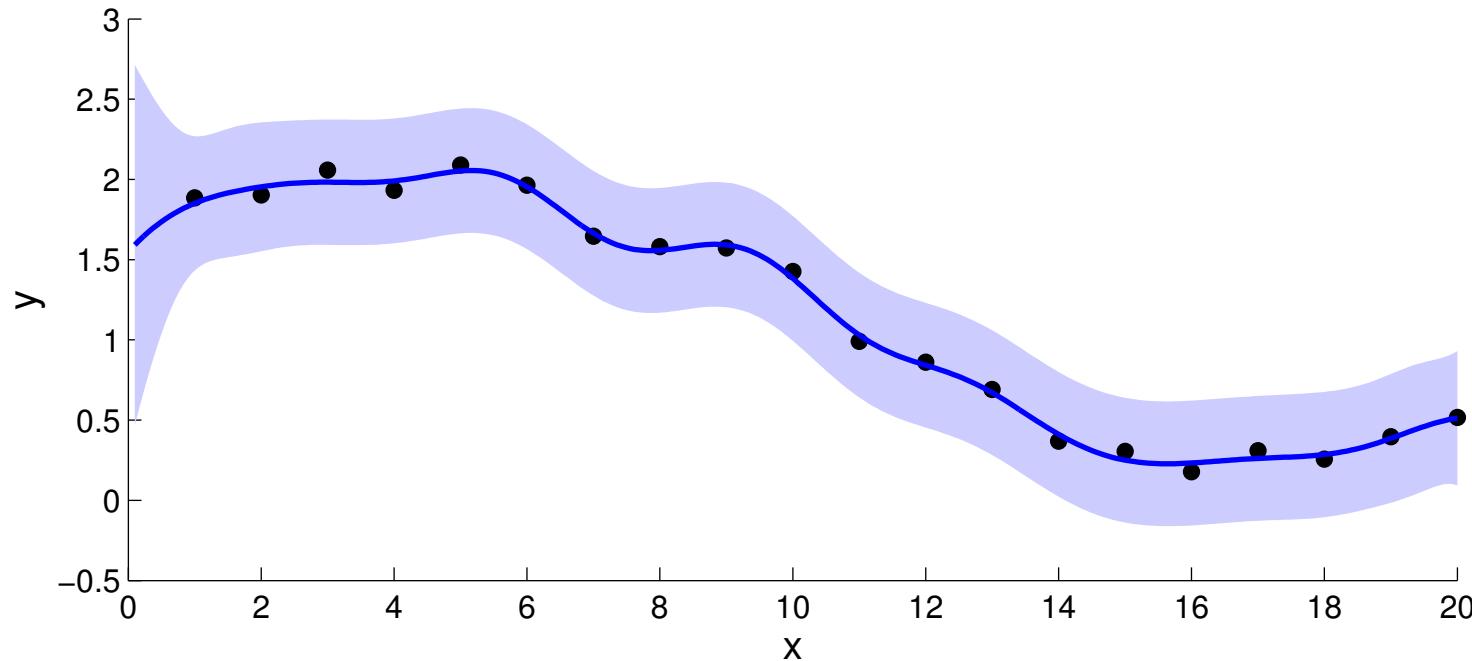
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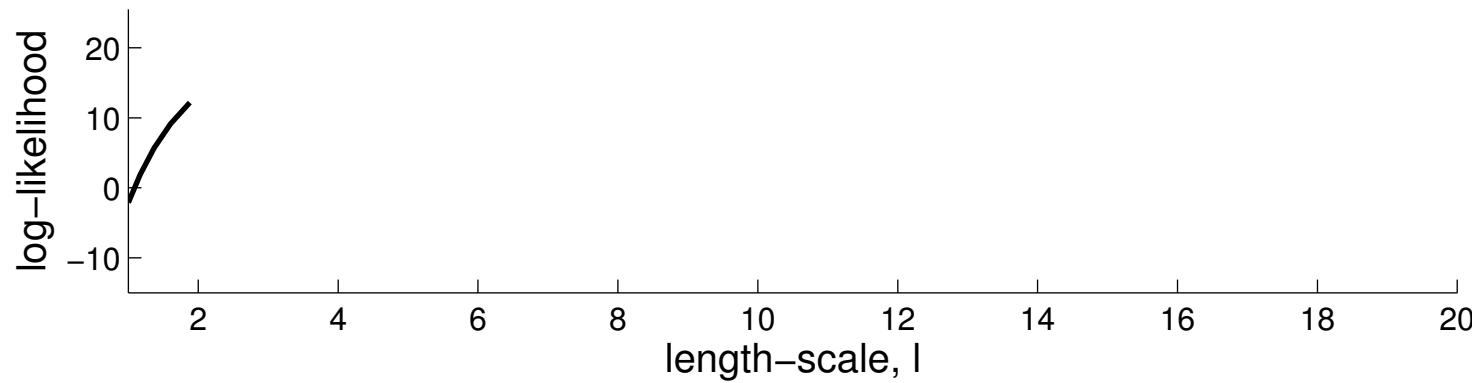
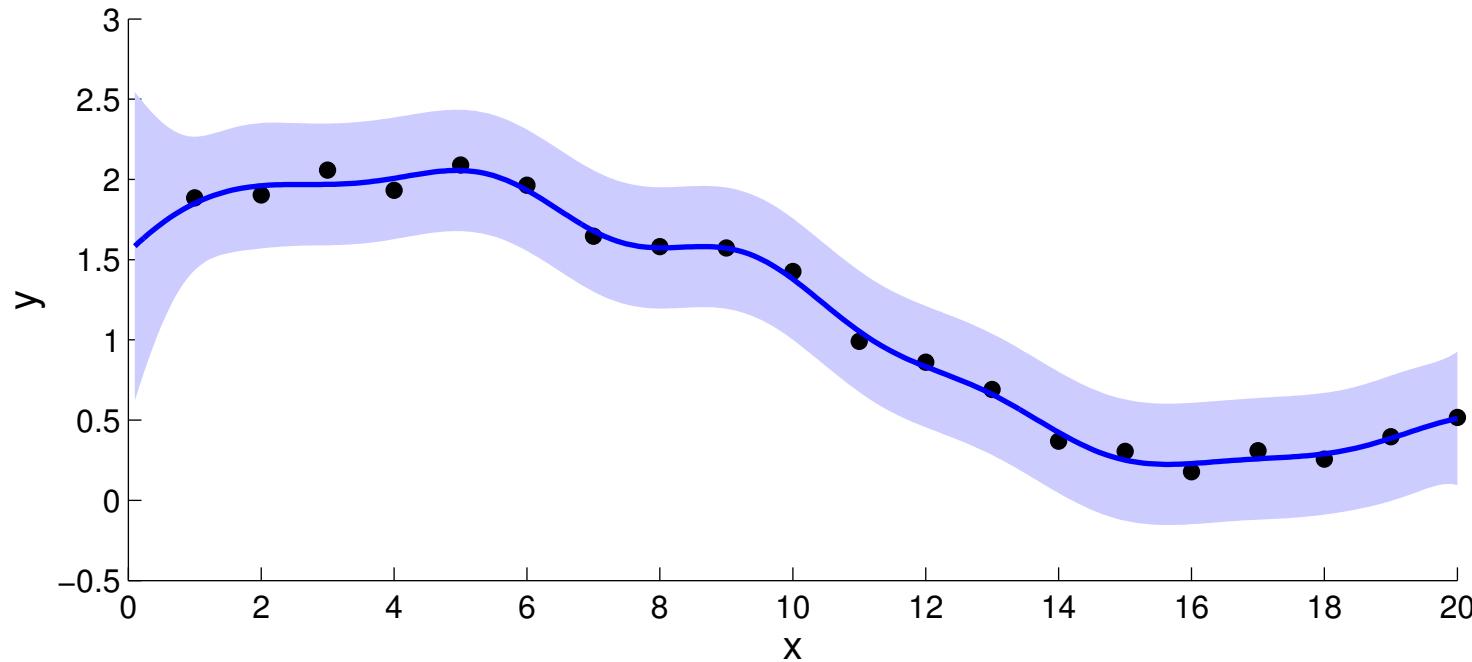
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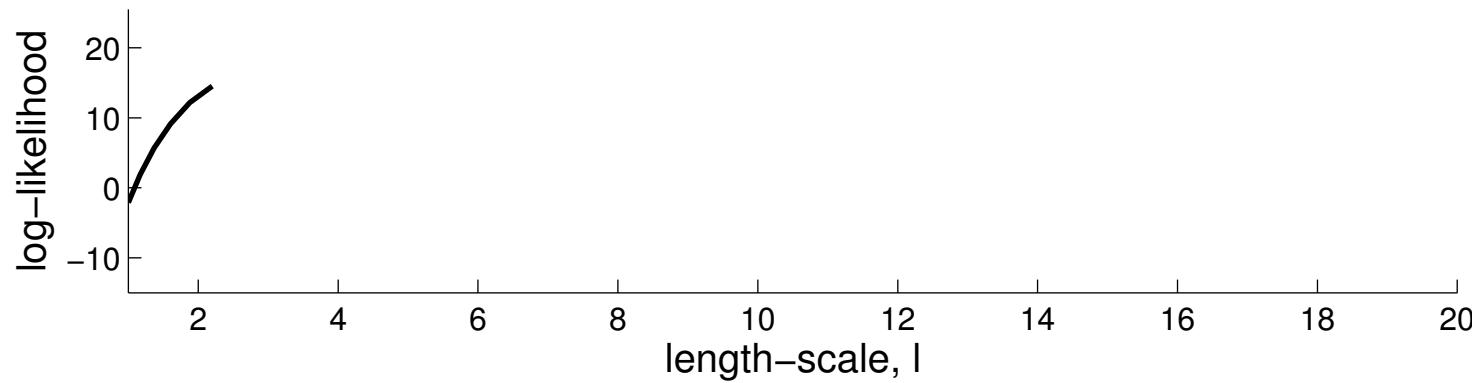
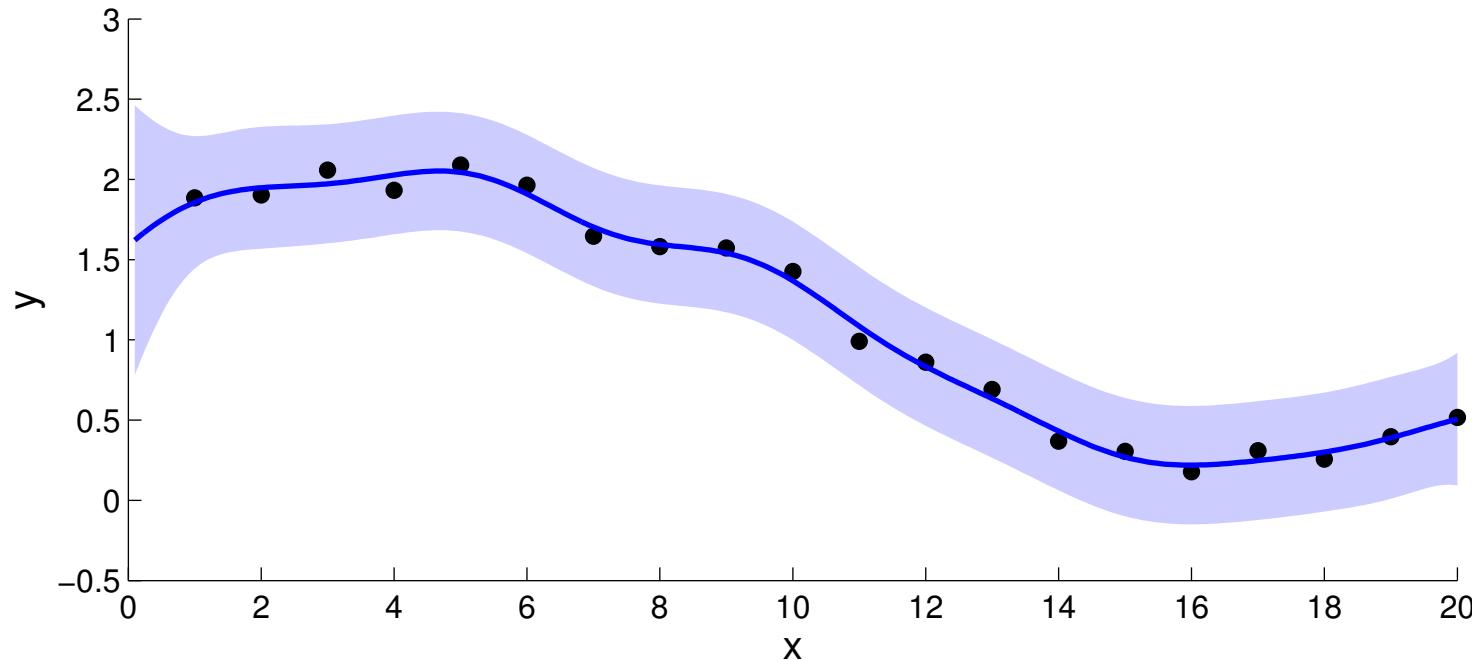
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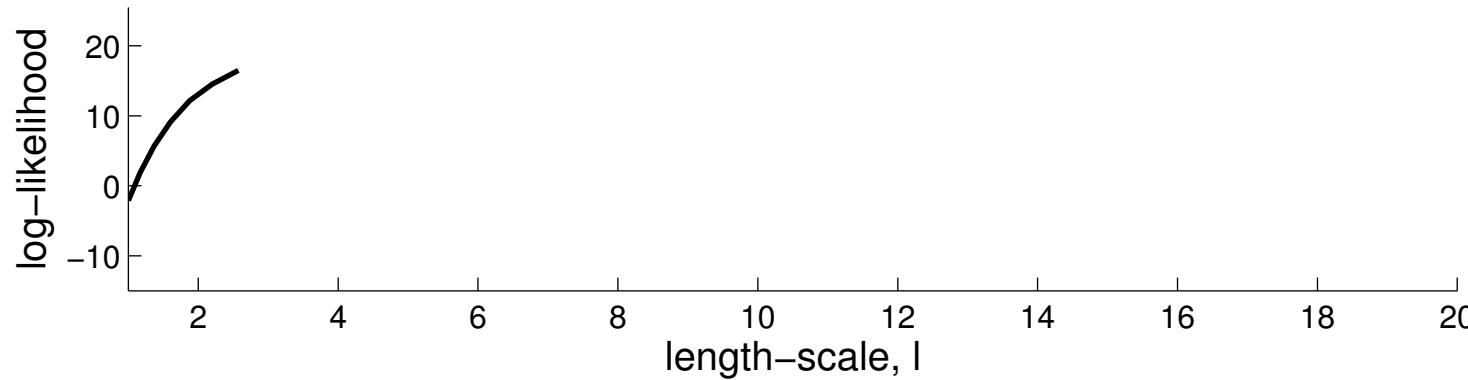
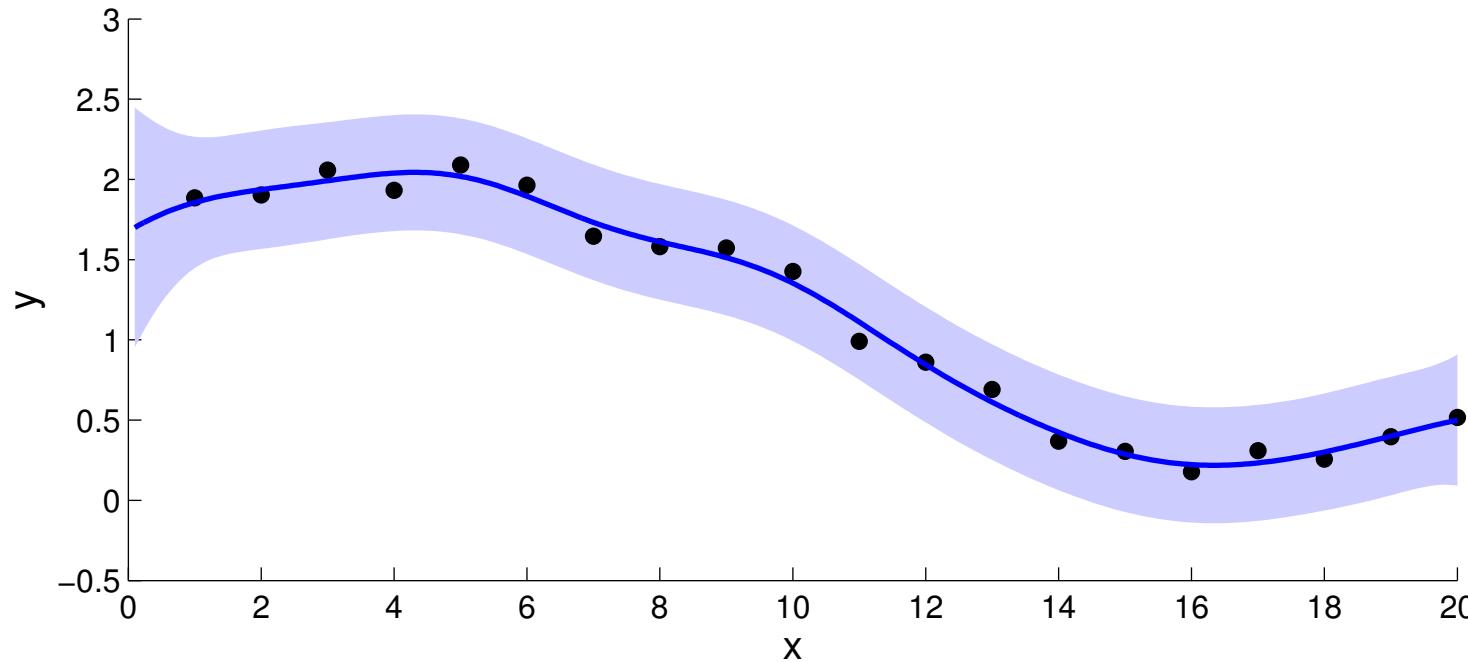
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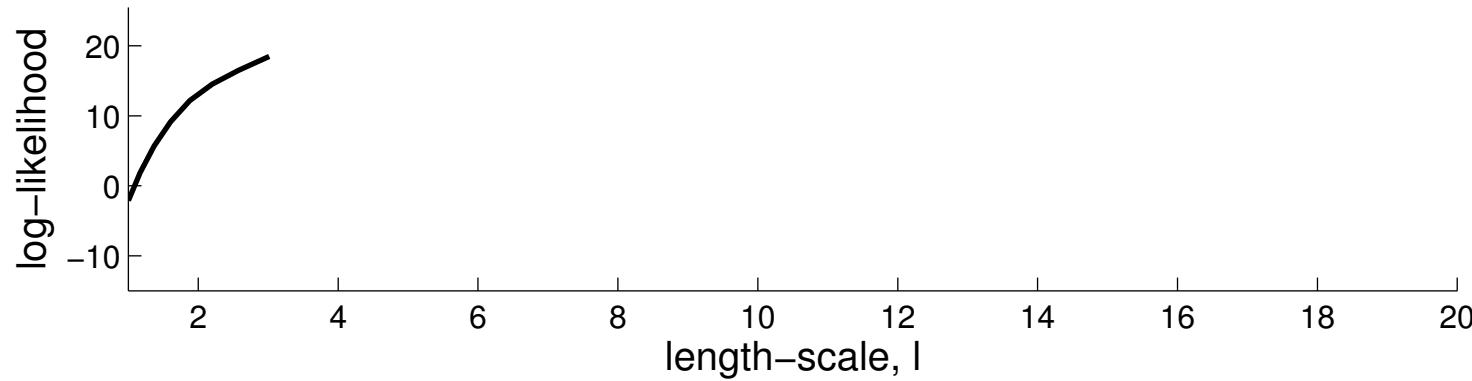
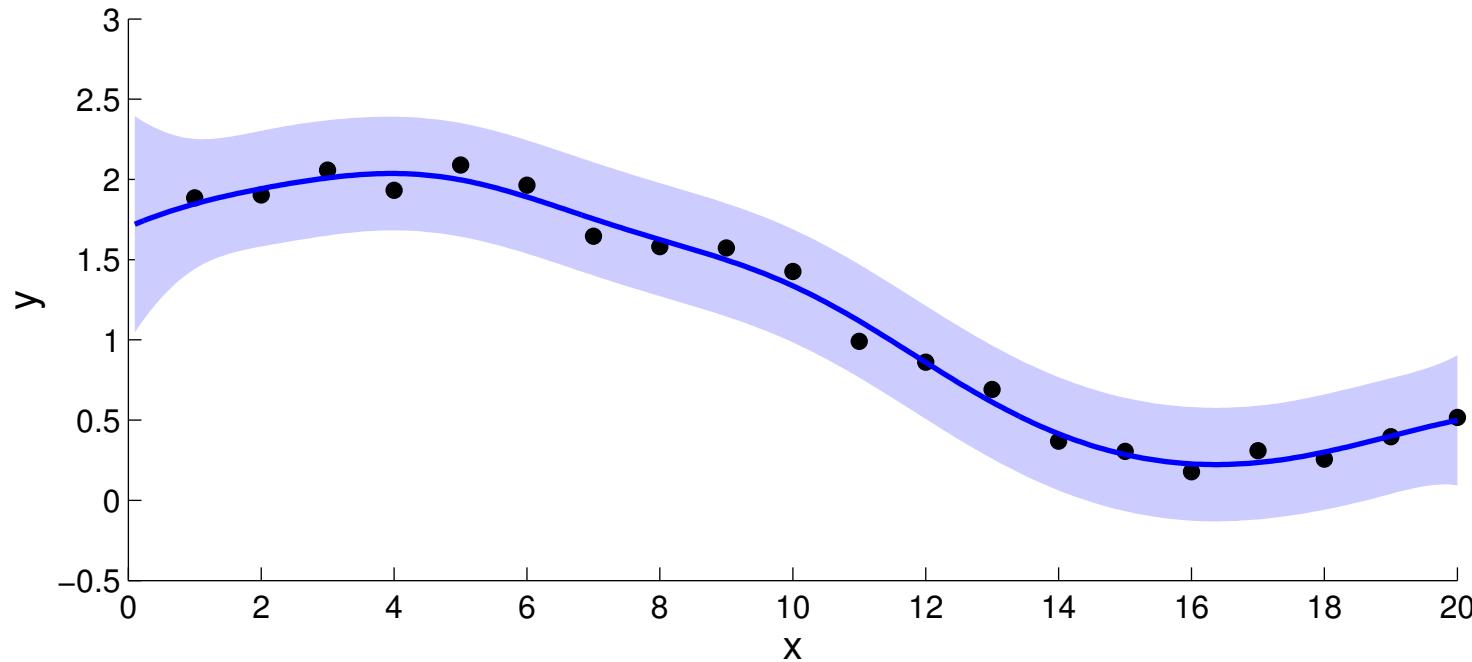
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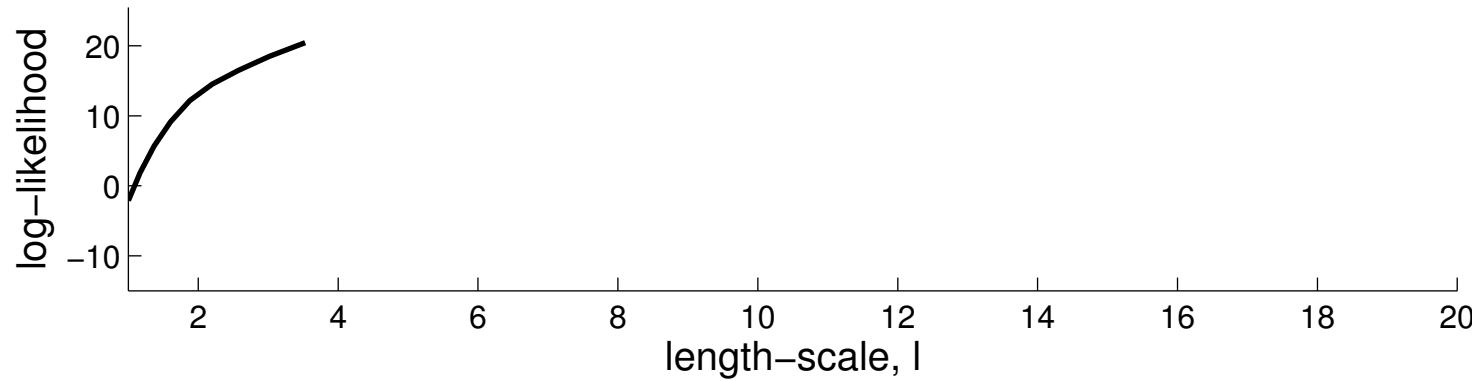
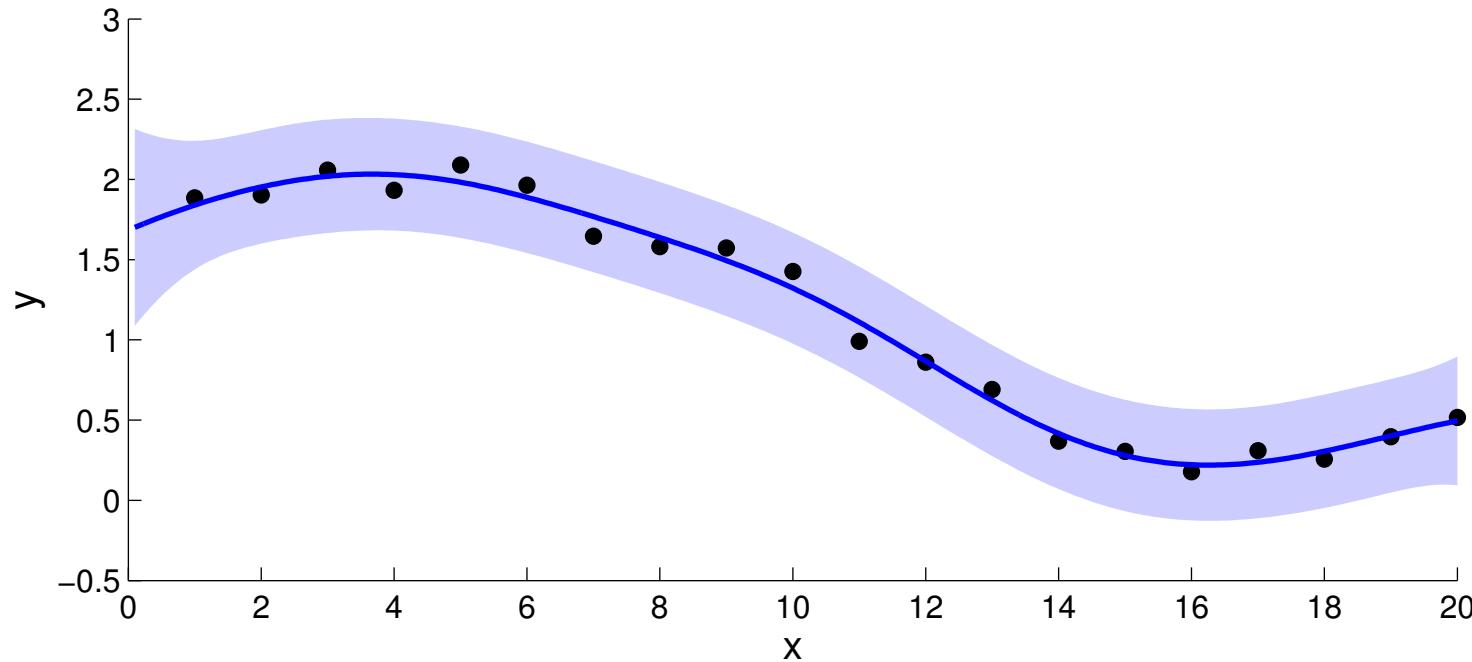
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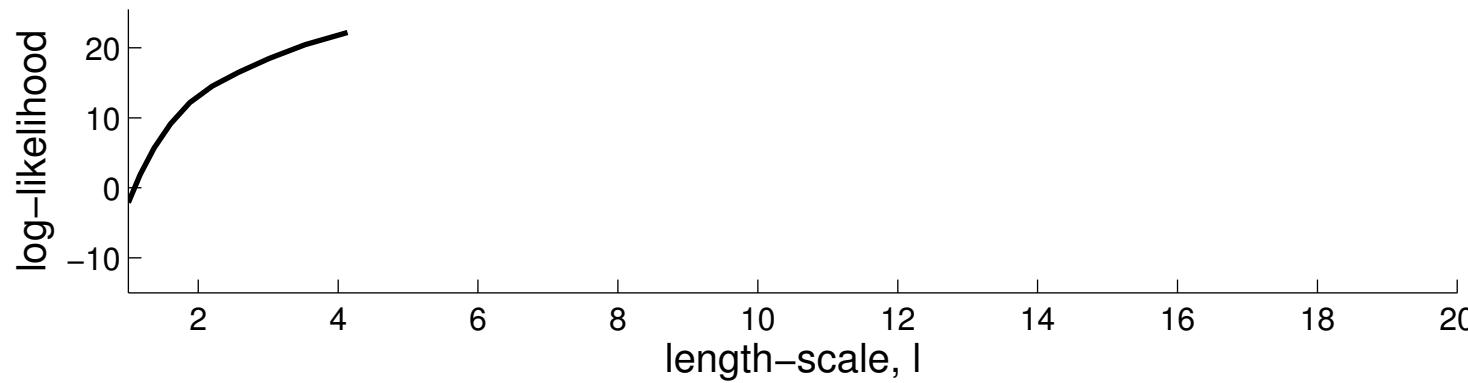
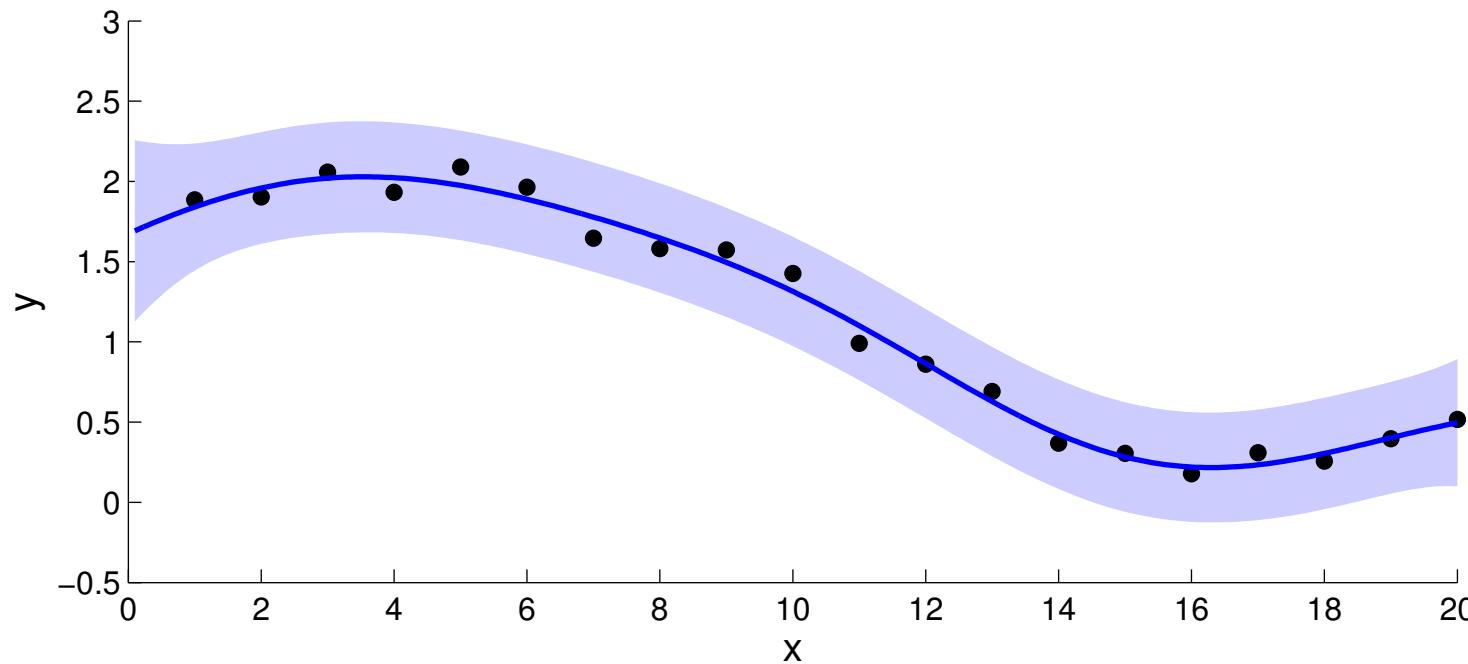
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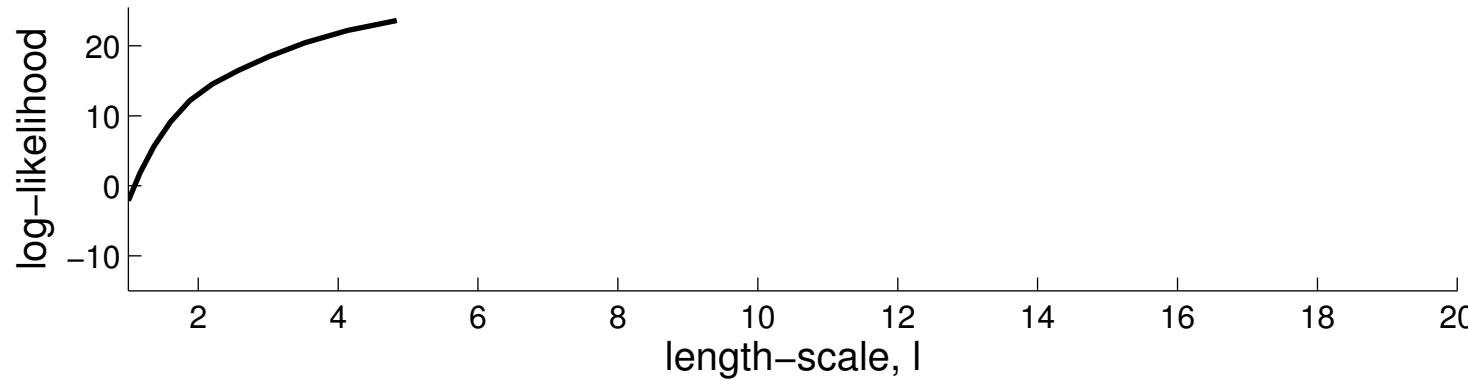
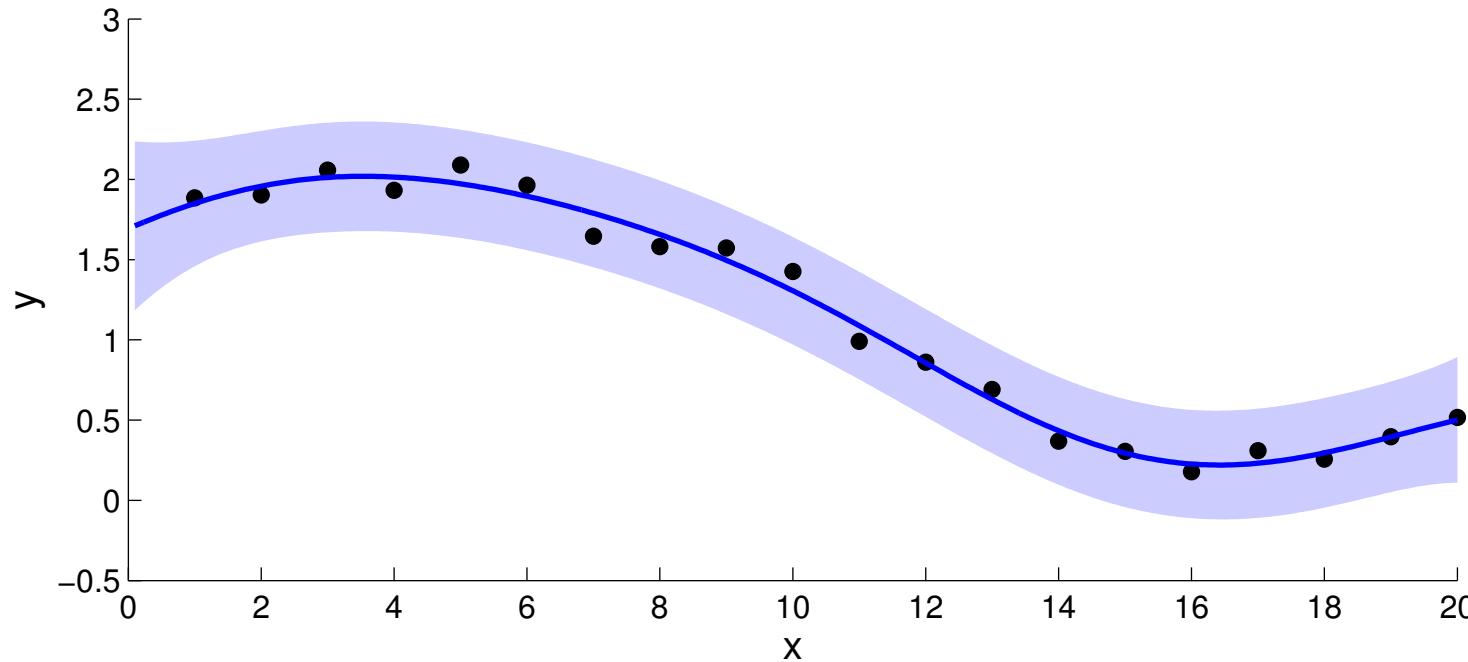
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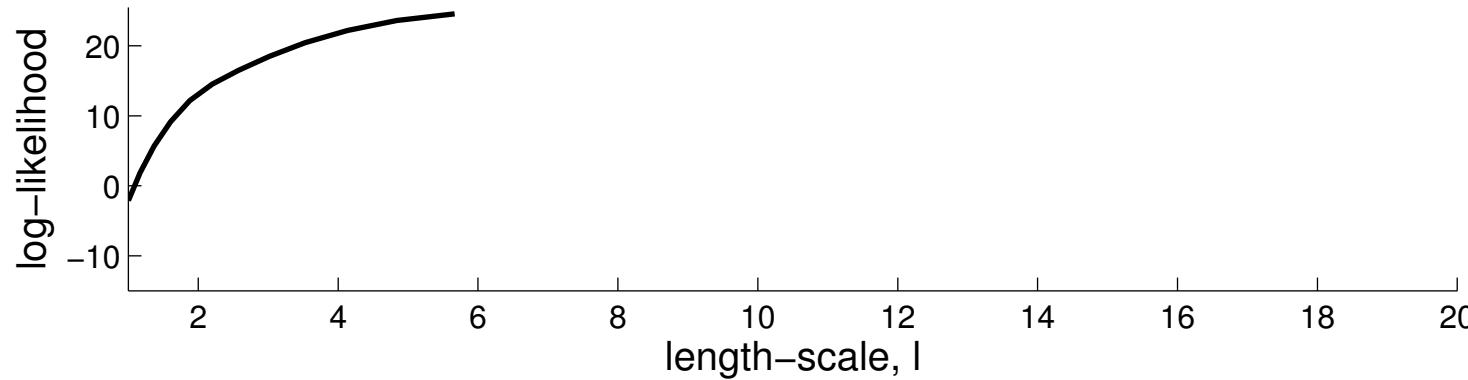
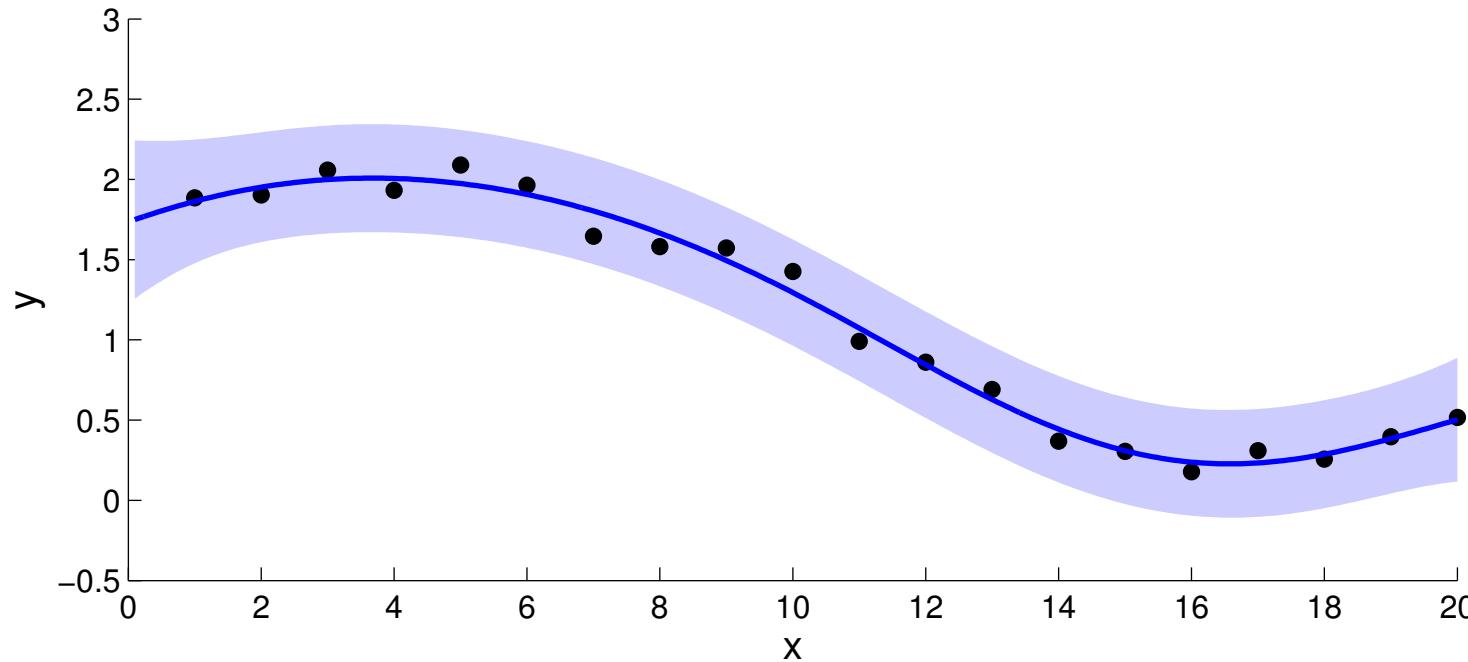
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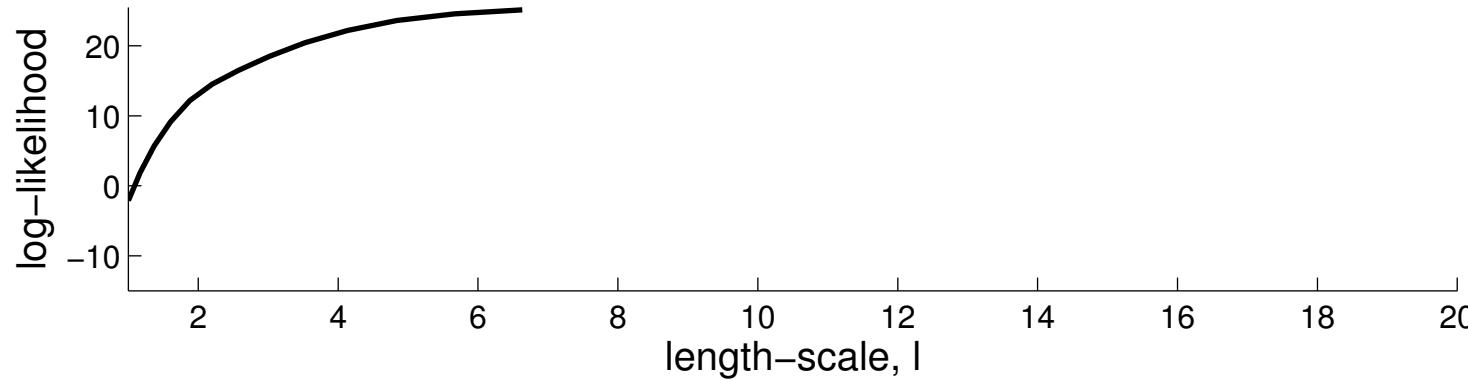
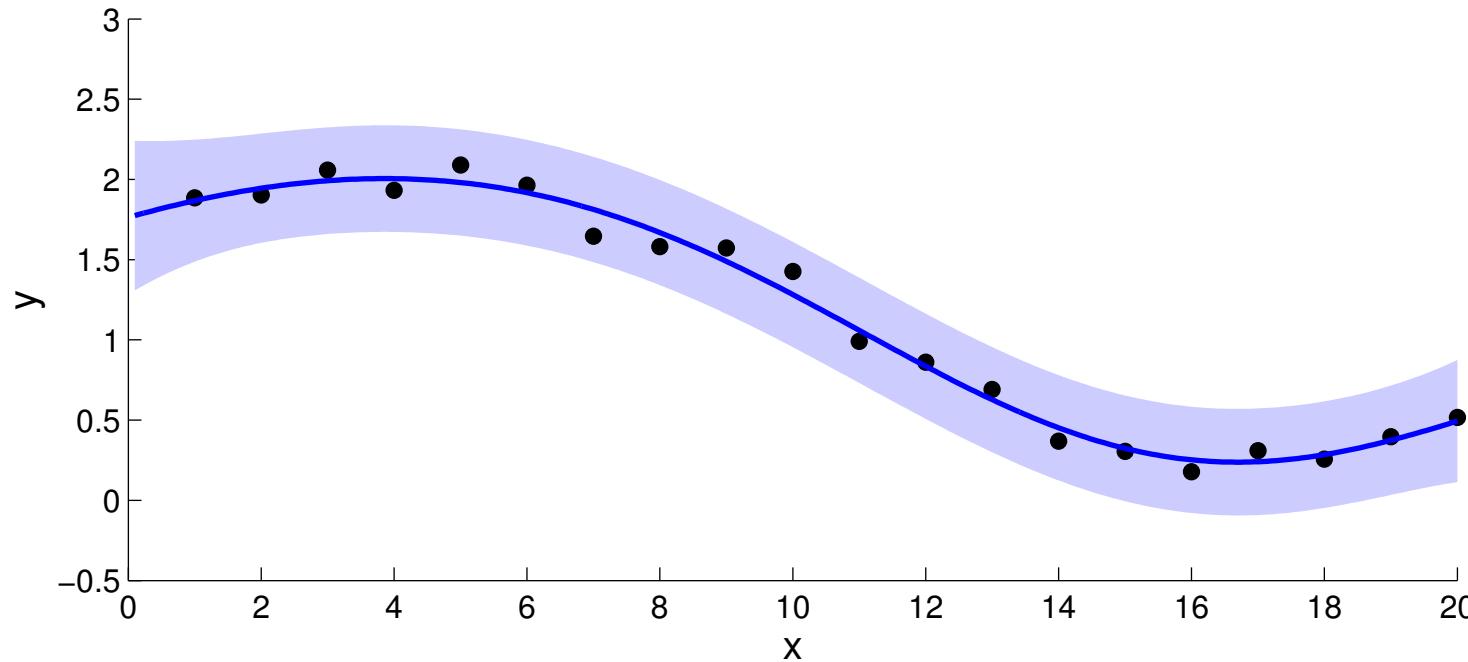
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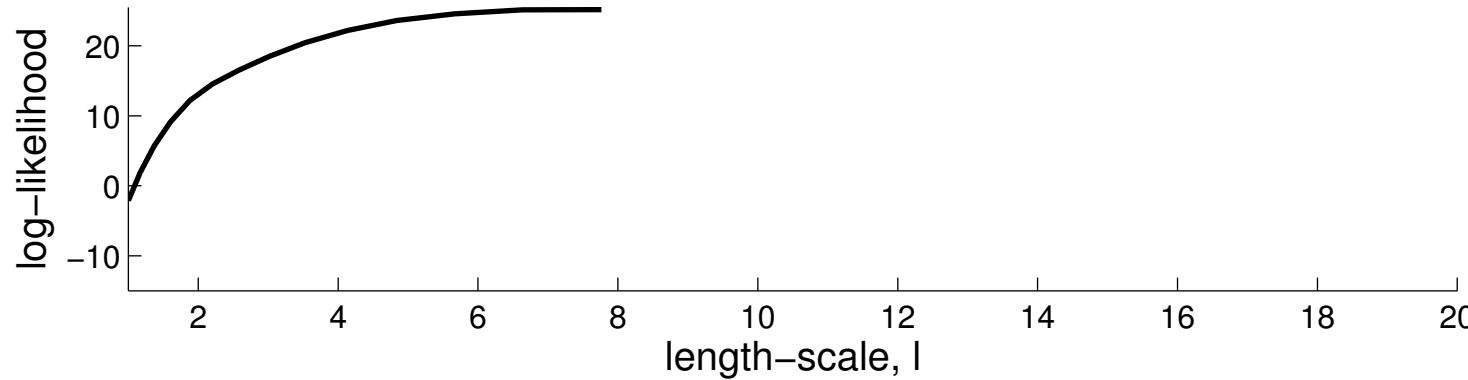
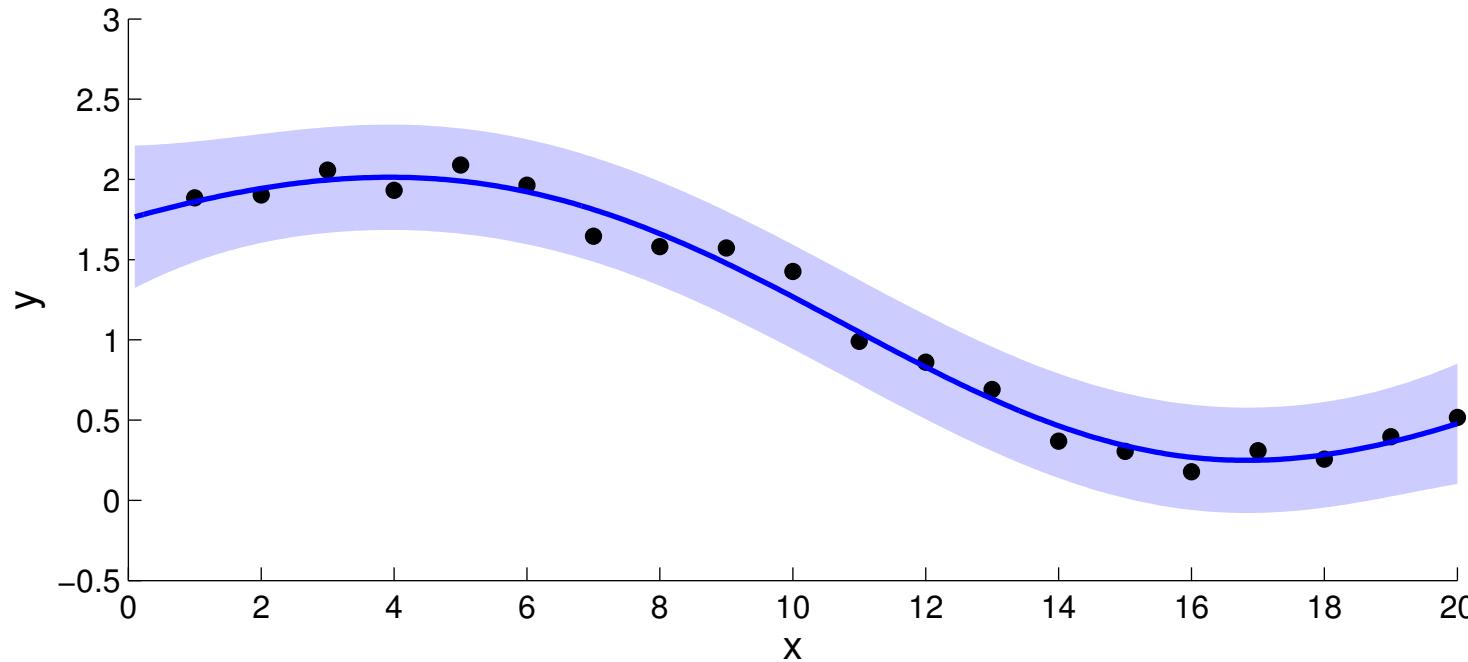
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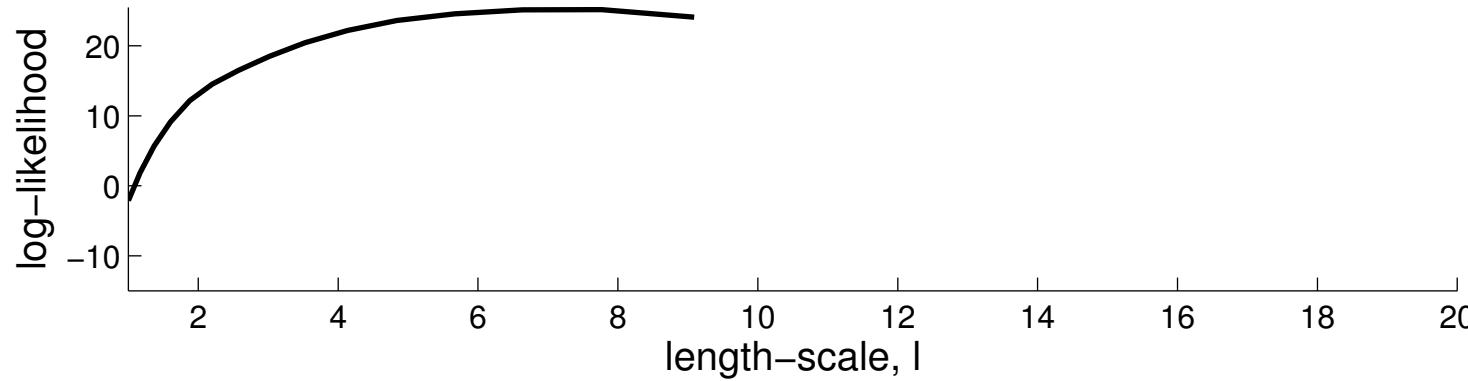
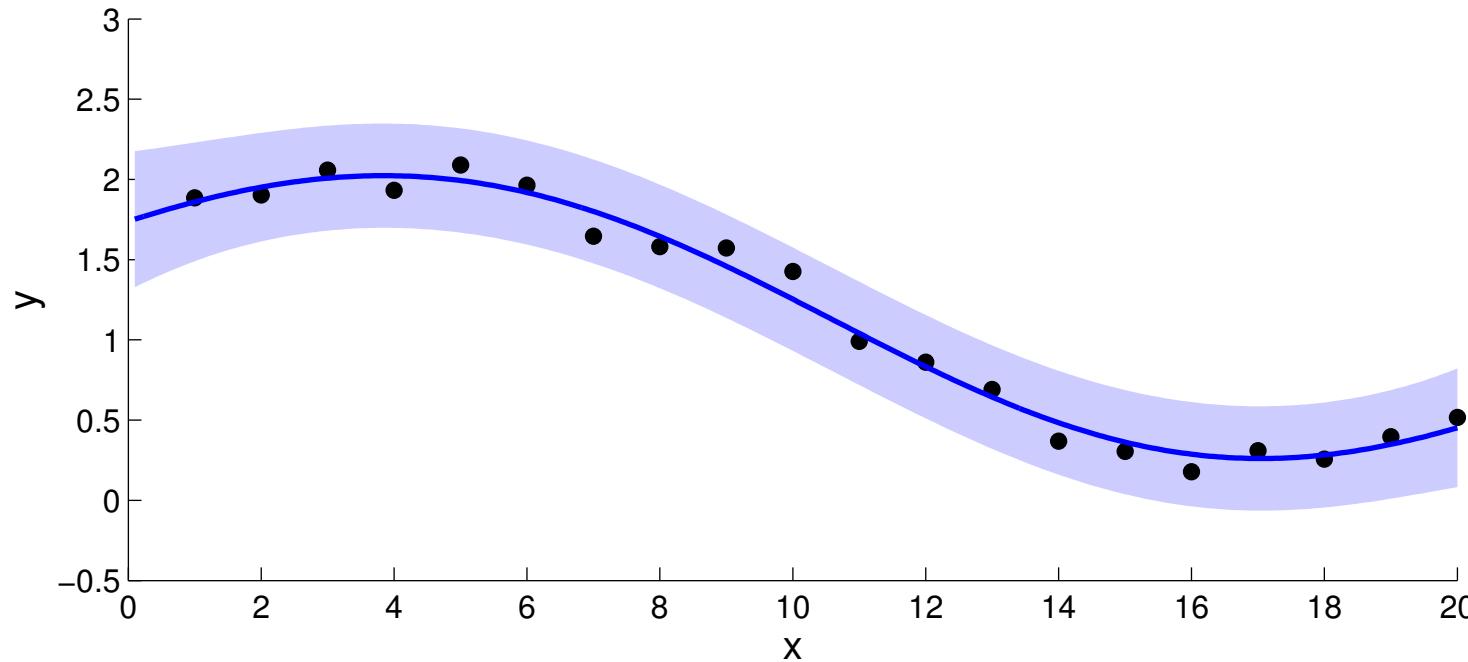
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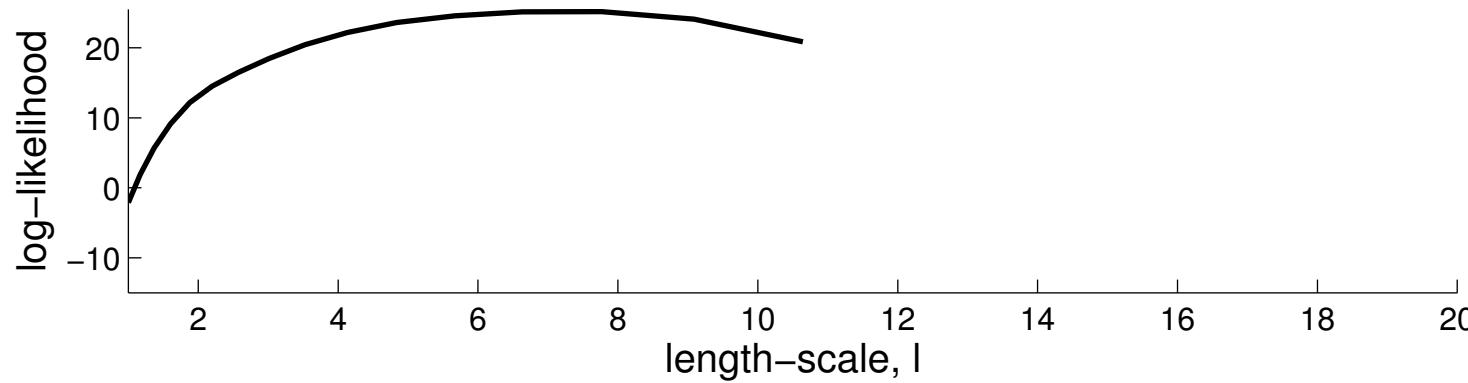
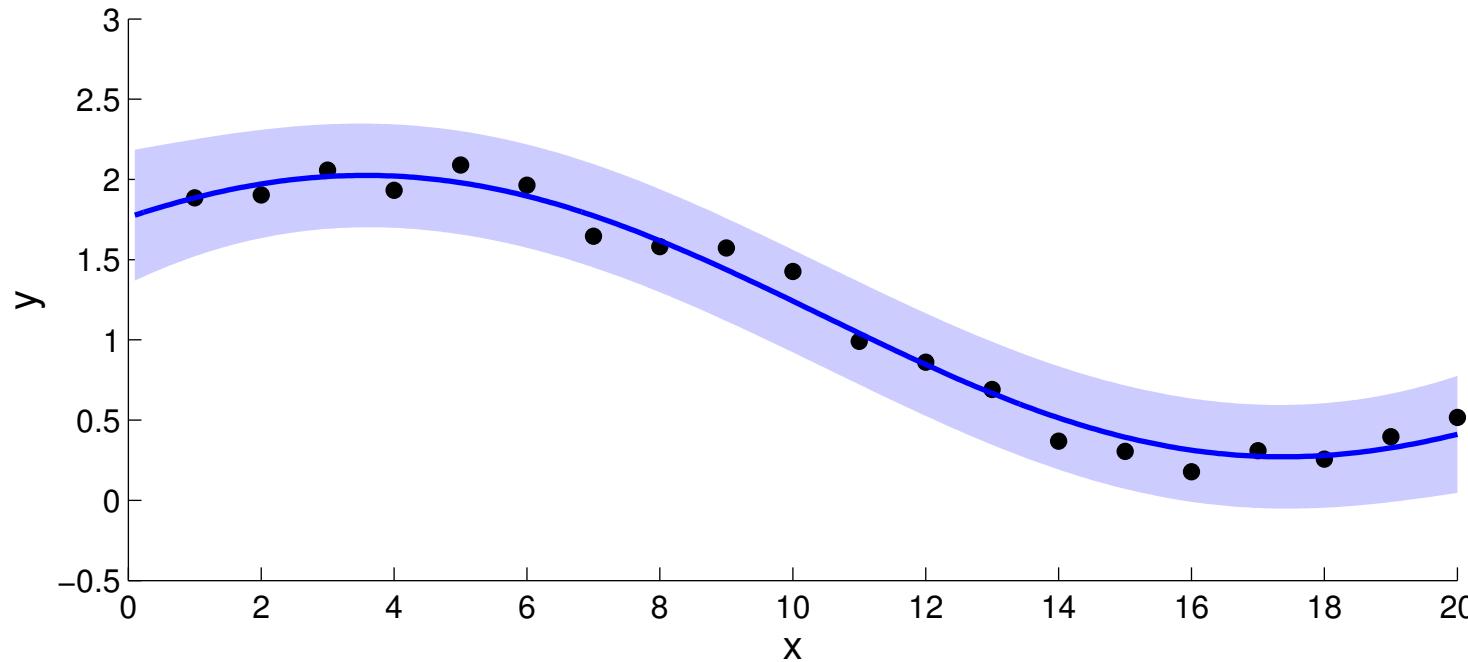
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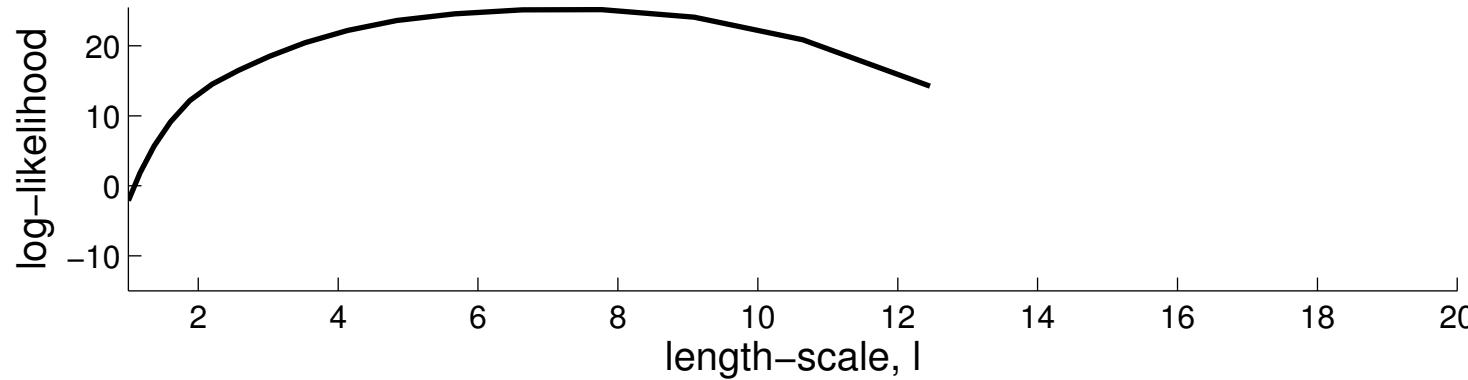
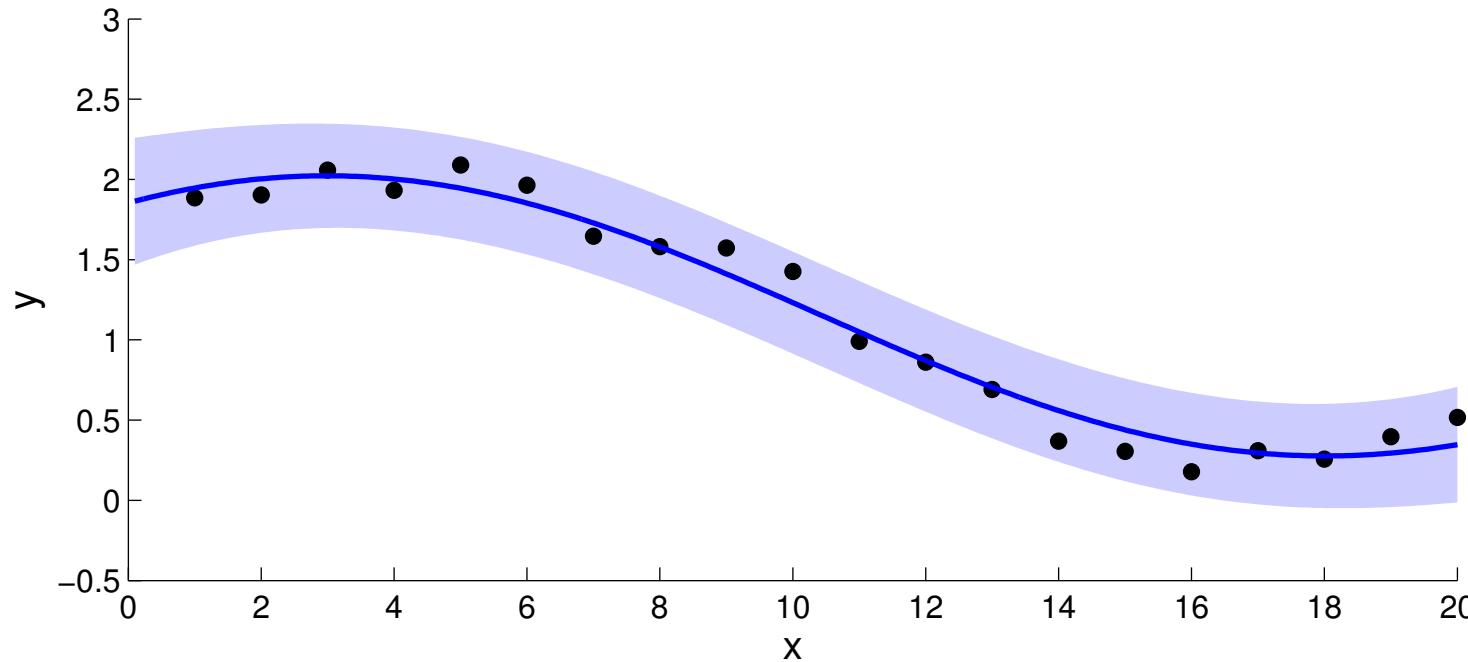
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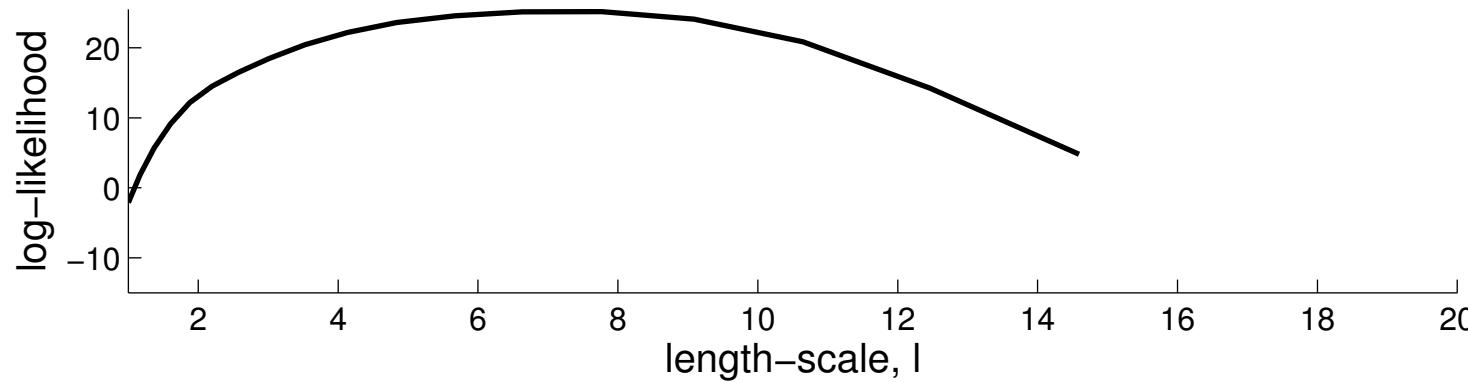
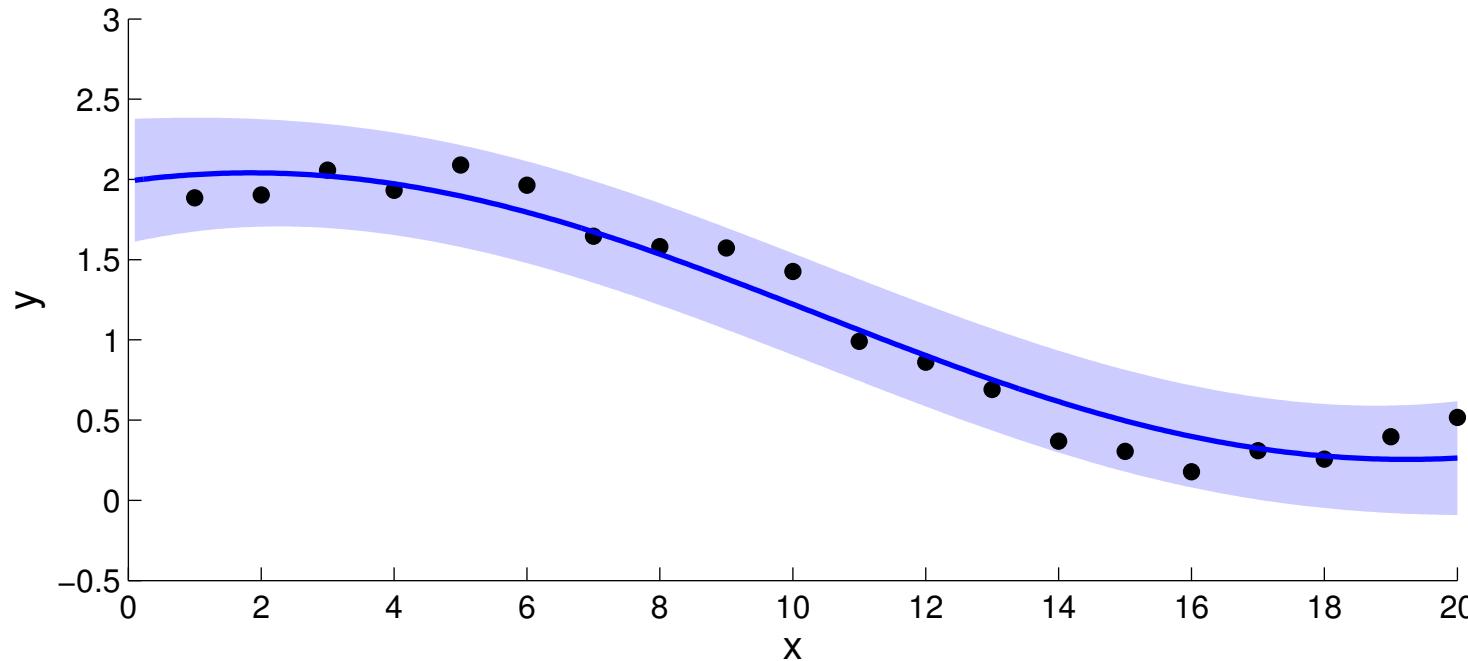
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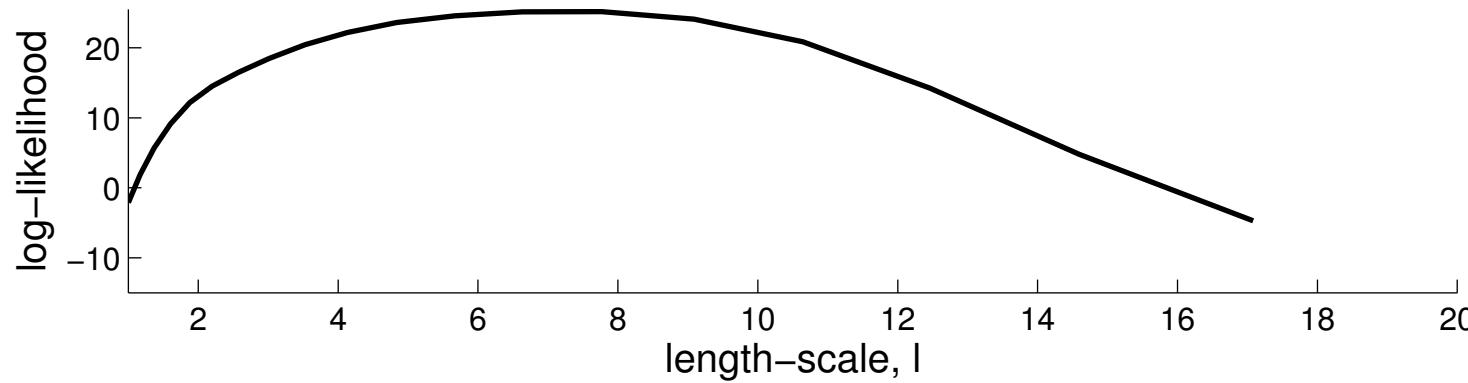
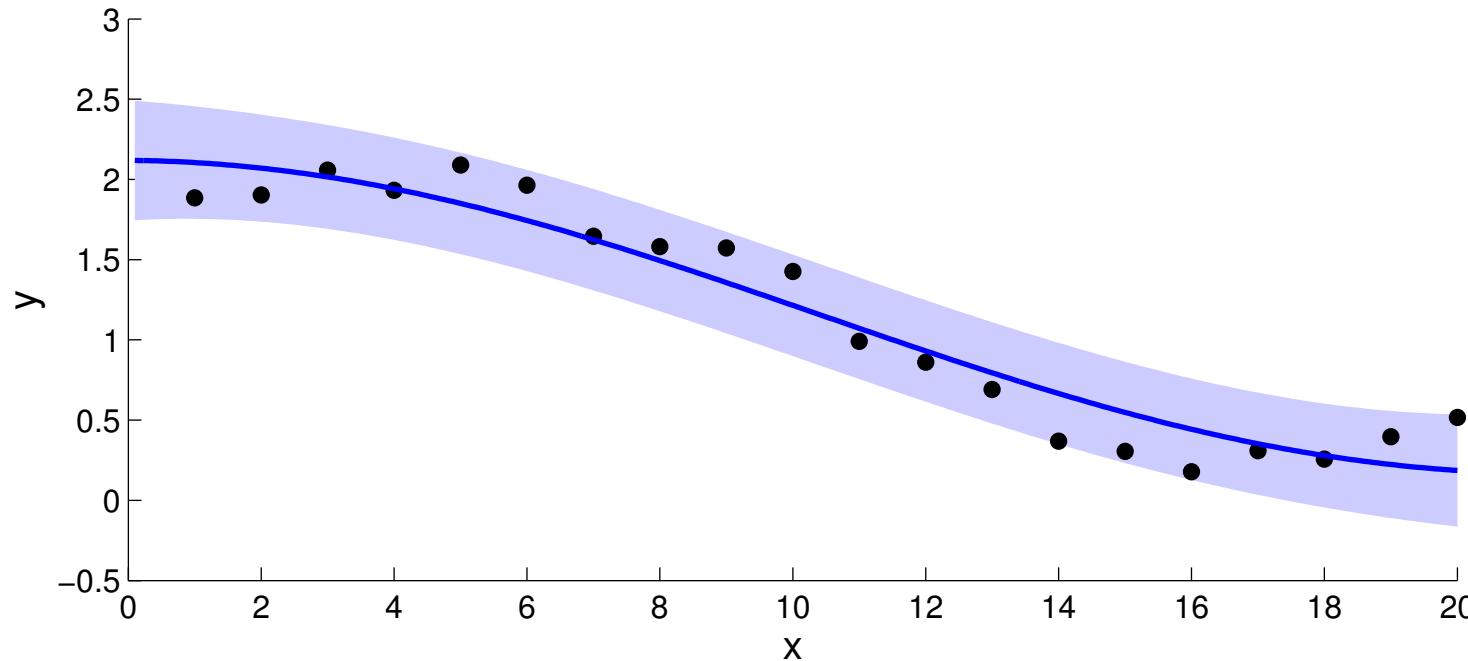
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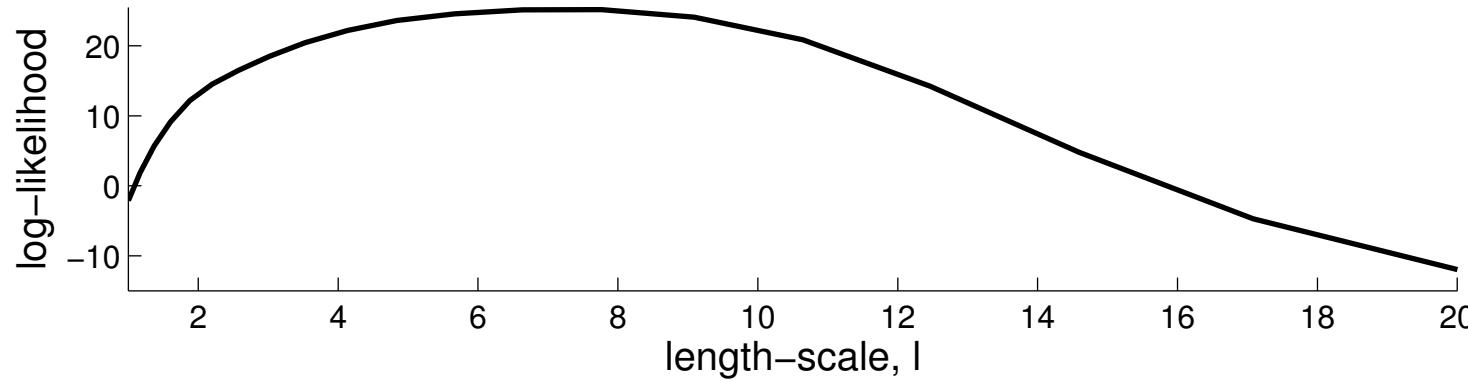
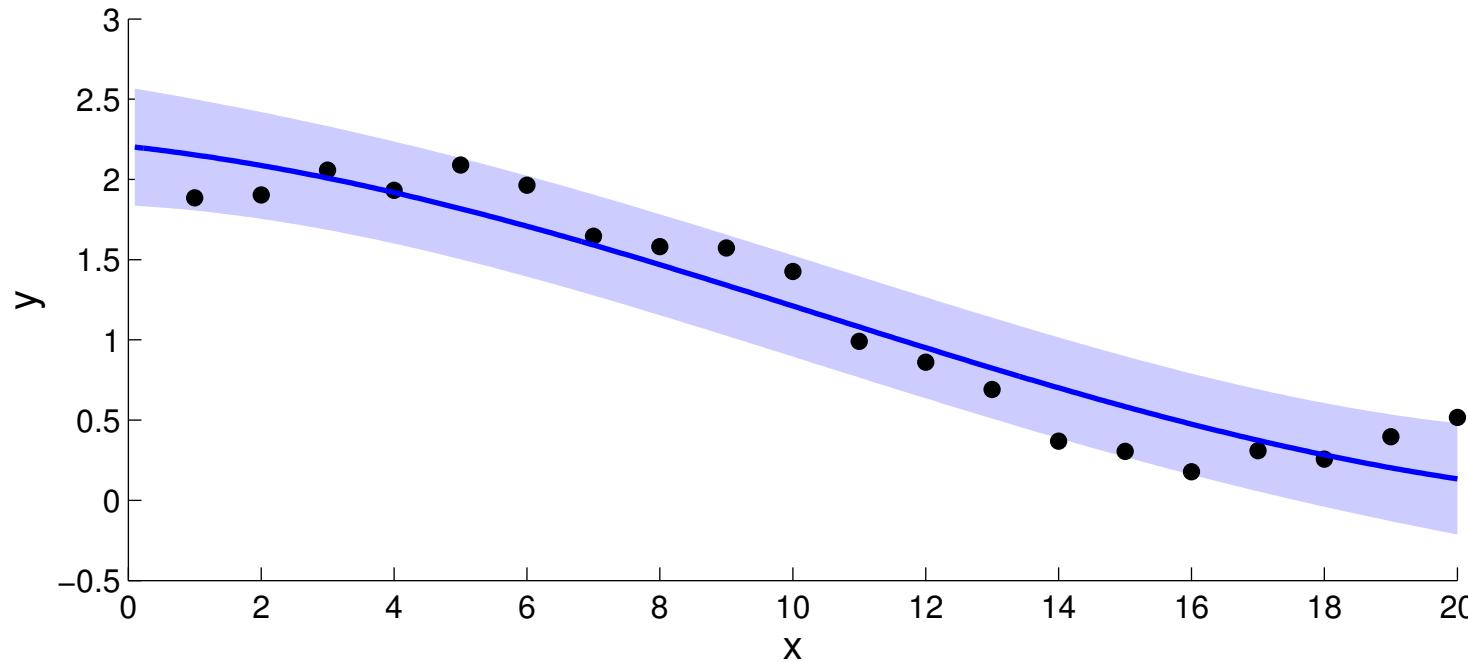
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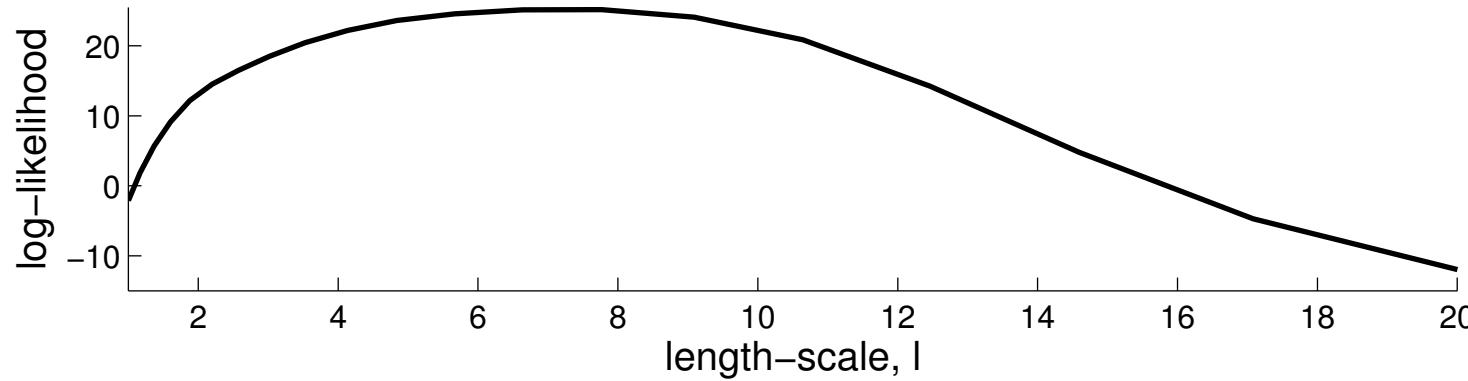
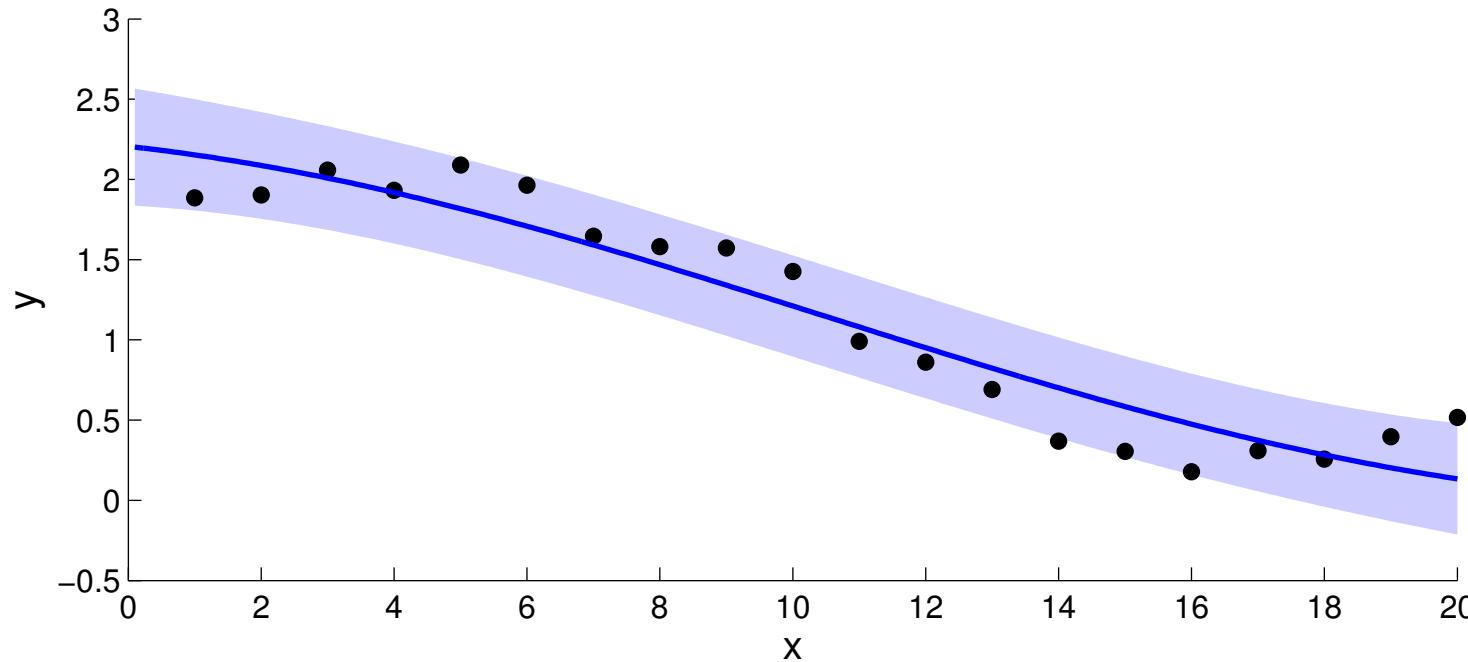
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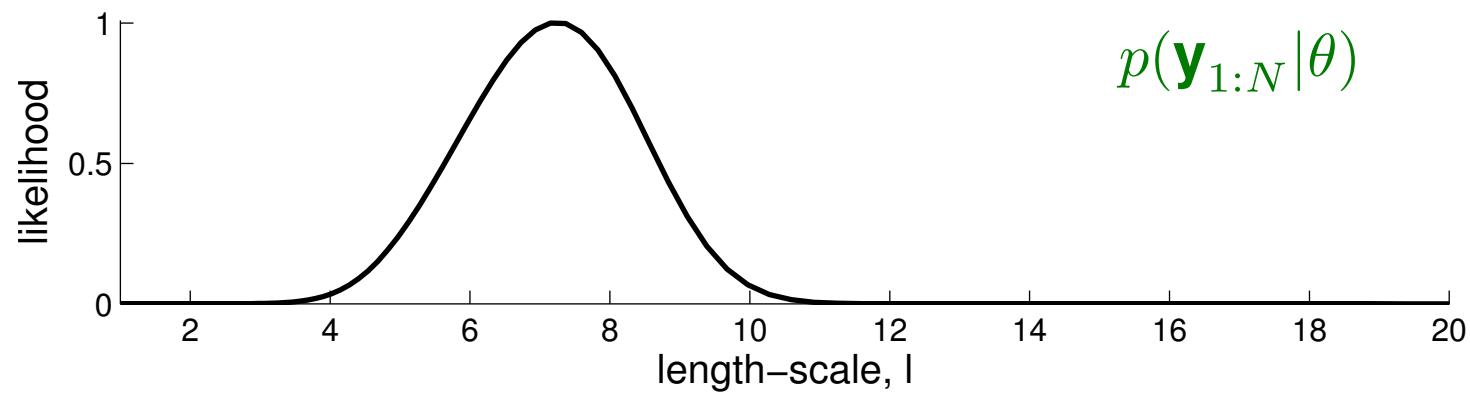
How do we choose the hyper-parameters?



How do we choose the hyper-parameters?

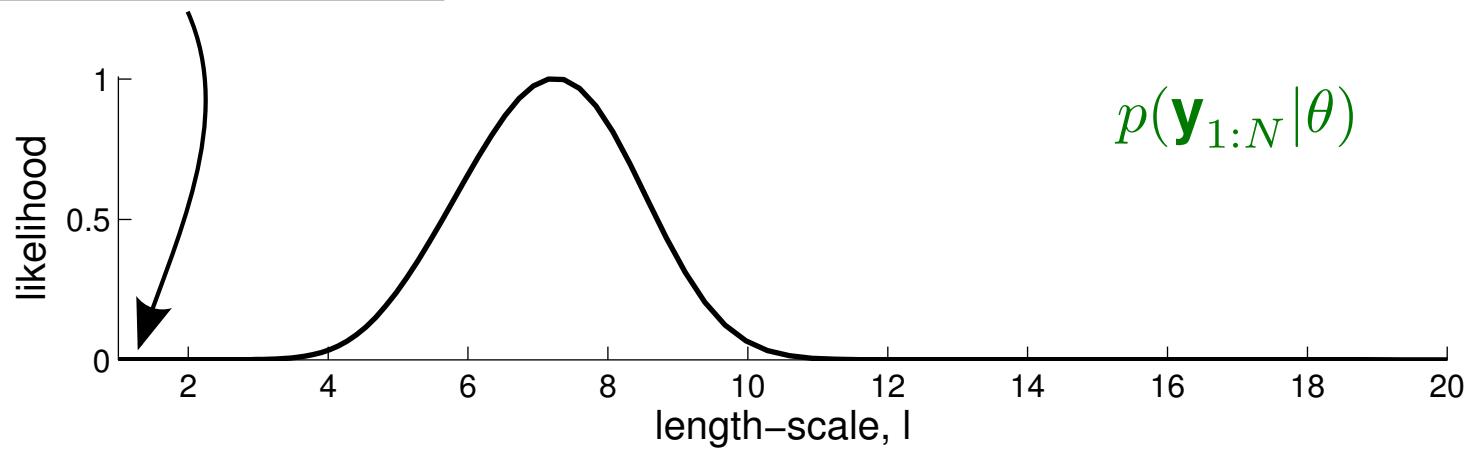
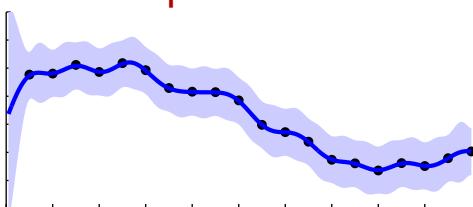


How do we choose the hyper-parameters?



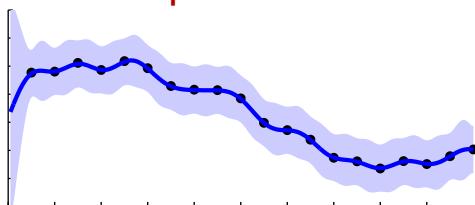
Why does Bayesian inference work?

fits every training point
"complex" model

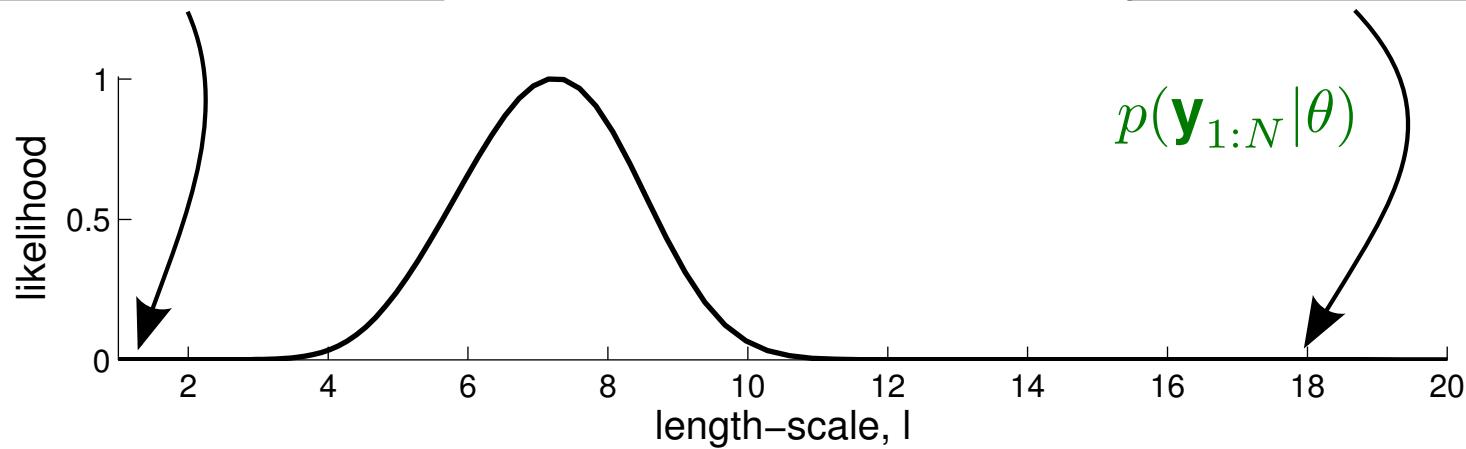
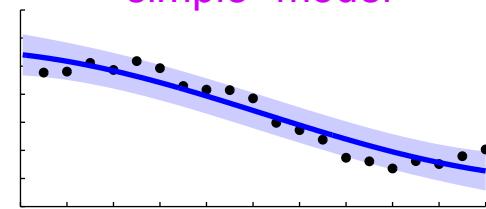


Why does Bayesian inference work?

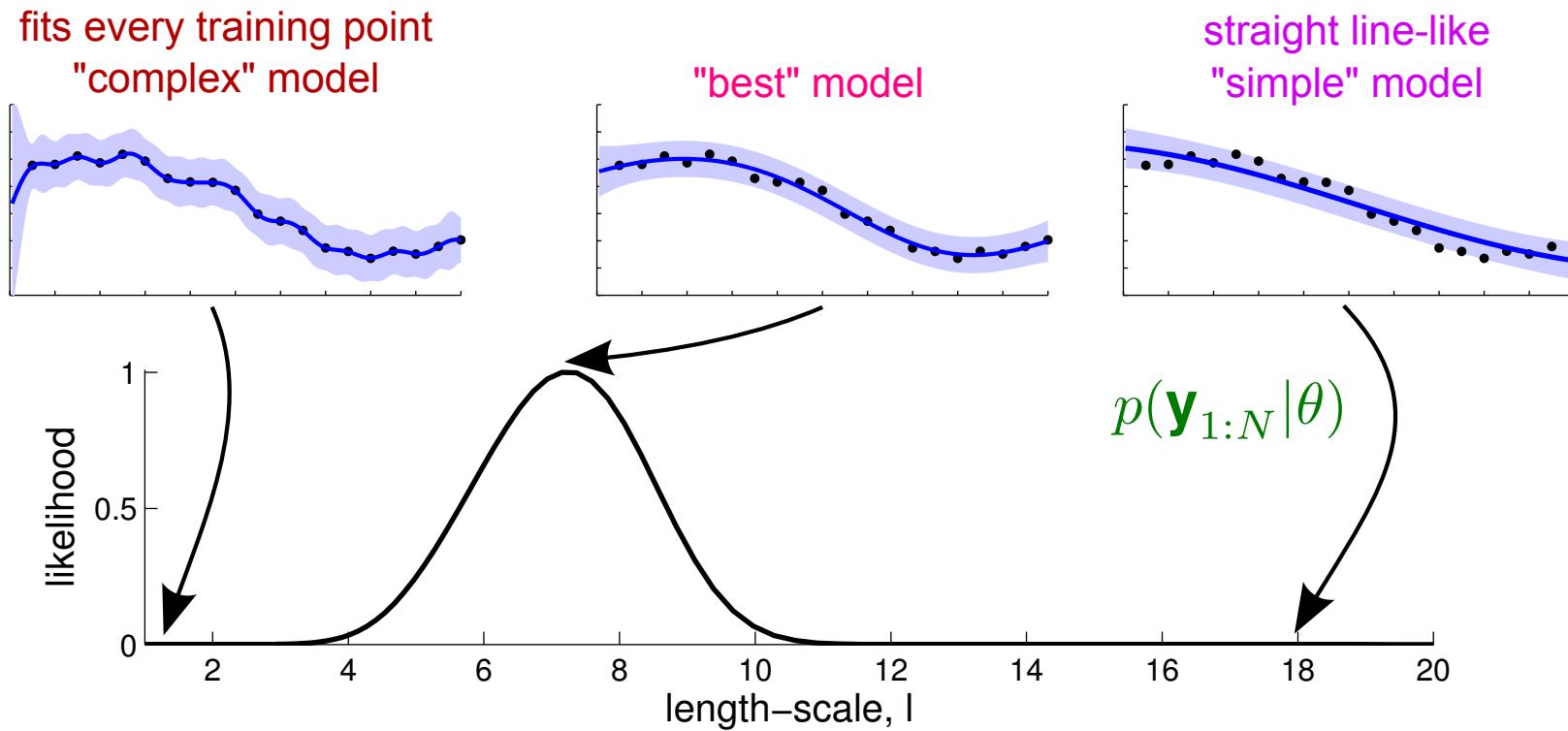
fits every training point
"complex" model



straight line-like
"simple" model



Why does Bayesian inference work?



Why does Bayesian inference work?

