An introduction to Gaussian processes

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Why Gaussian processes?

- So far: linear models with a finite number of basis functions, e.g. $\boldsymbol{\phi}(x) = (1, x, x^2, \ldots, x^K)$
- Open questions:
  - How to design a suitable basis?
  - How many basis functions to pick?
- Gaussian processes: accurate and flexible regression method yielding predictions alongside with error bars.

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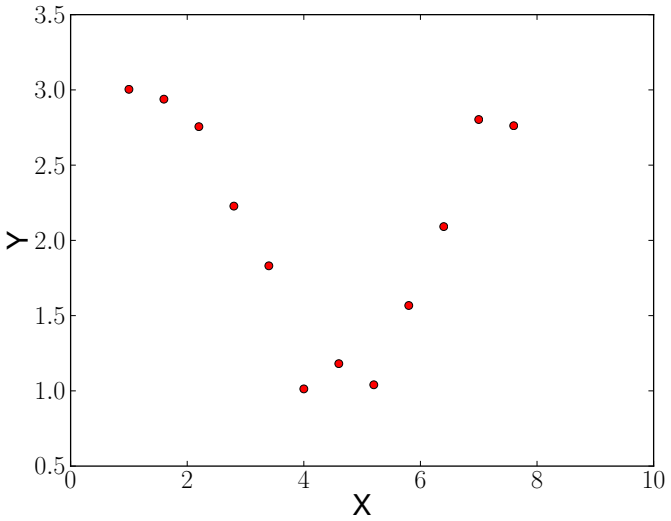

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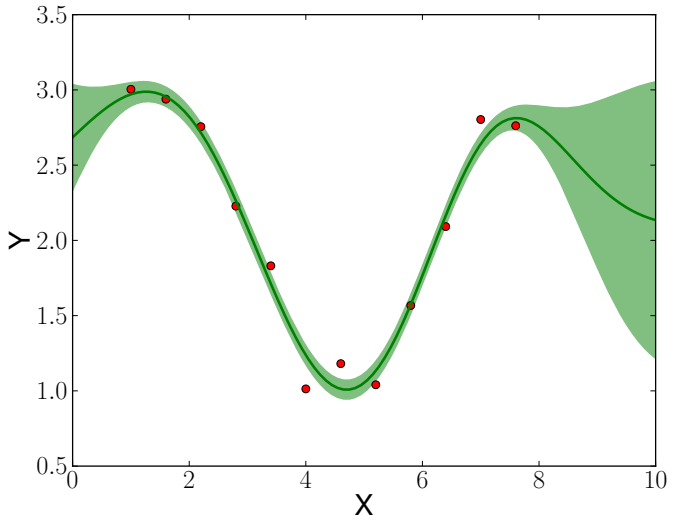


Further reading

- A comprehensive and very good introduction to Gaussian processes
  C. E. Rasmussen, C. K. Williams
  Gaussian proceesses for machine learning
  - Free download: `http://www.gaussianprocess.org/gpml/`
- A really good introductory movie to watch
  `http://videolectures.net/gpip06_mackay_gpb/`
  - Many ideas used in this course are borrowed from this lecture.

Outline

Outline

The Gaussian distribution

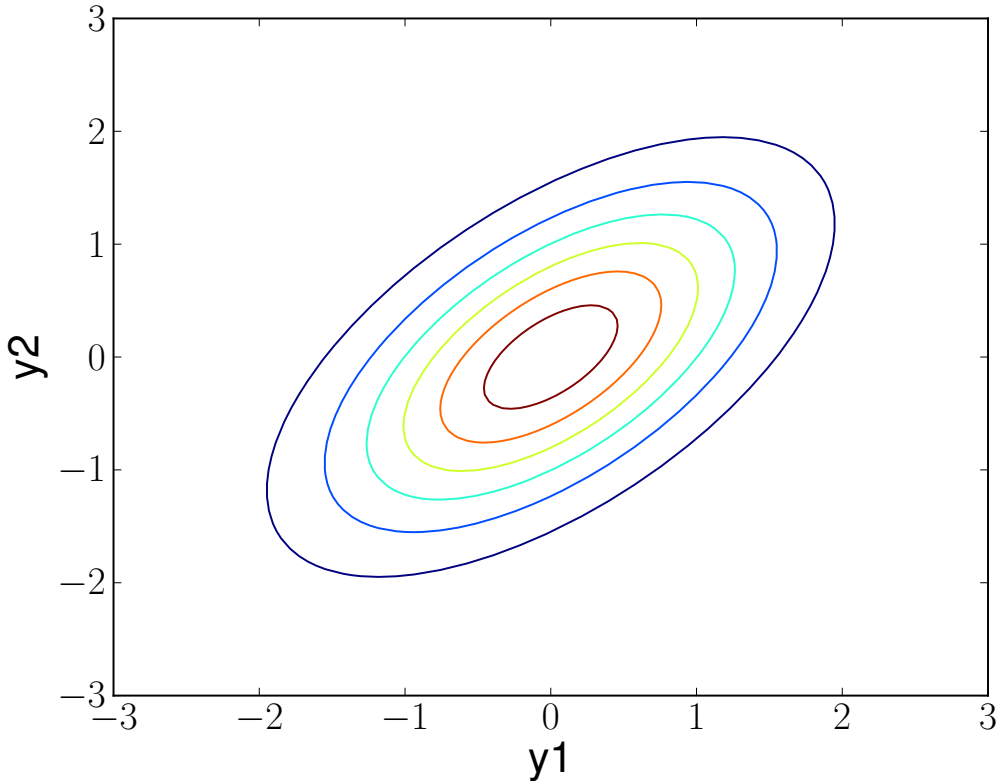
- Gaussian processes are merely based on the good old Gaussian

$$\mathcal{N}\left(\mathbf{x}\,\middle|\,\boldsymbol{\mu}, \mathbf{K}\right) = \frac{1}{\sqrt{|2\pi\,\mathbf{K}|}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\,\mathbf{K}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

- Covariance matrix or kernel matrix

A 2D Gaussian

- Probability contour
- Samples



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A 2D Gaussian

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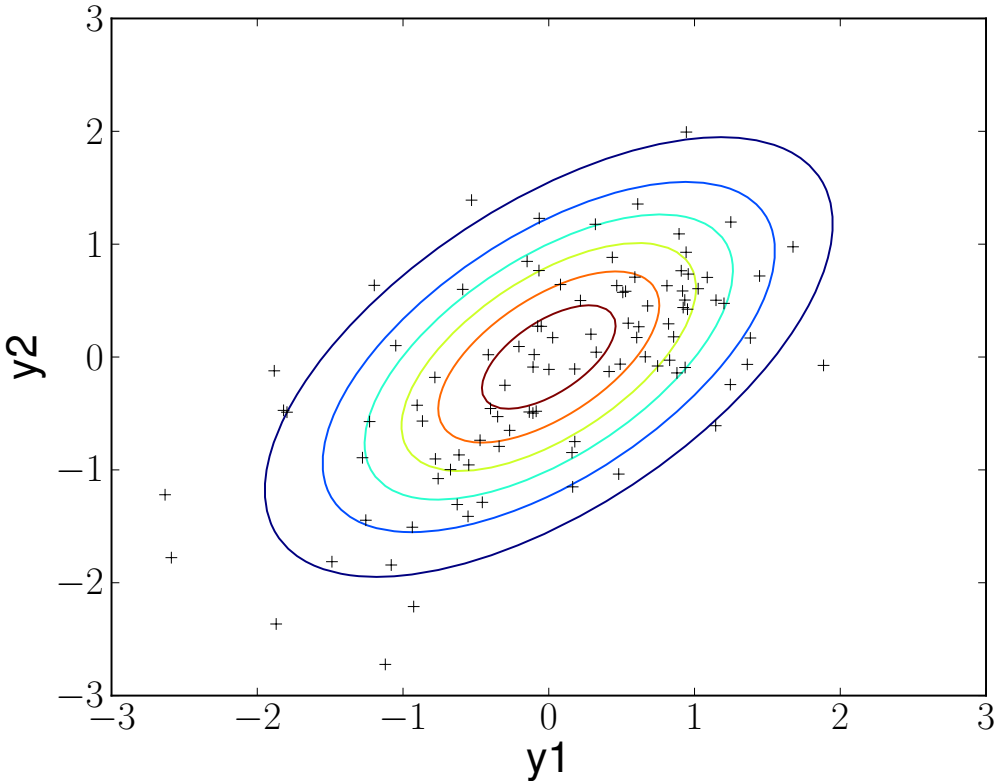

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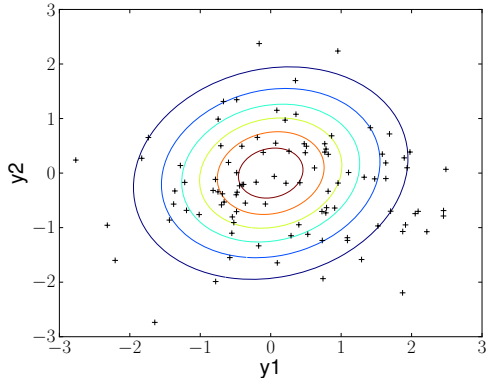
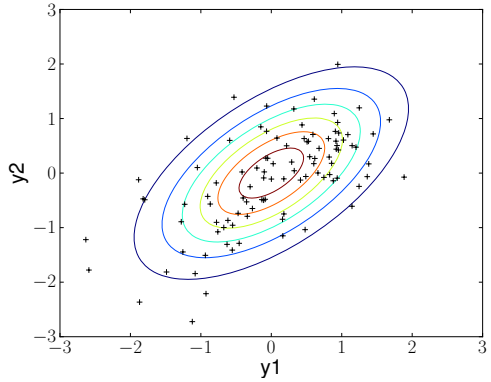
A 2D Gaussian

Varying the covariance matrix



$$\mathbf{K} = \begin{bmatrix} 1 & 0.14 \\ 0.14 & 1 \end{bmatrix}$$



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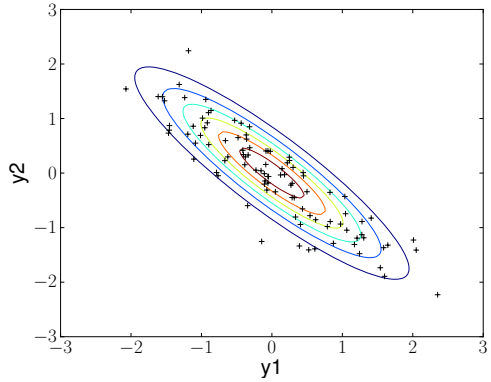
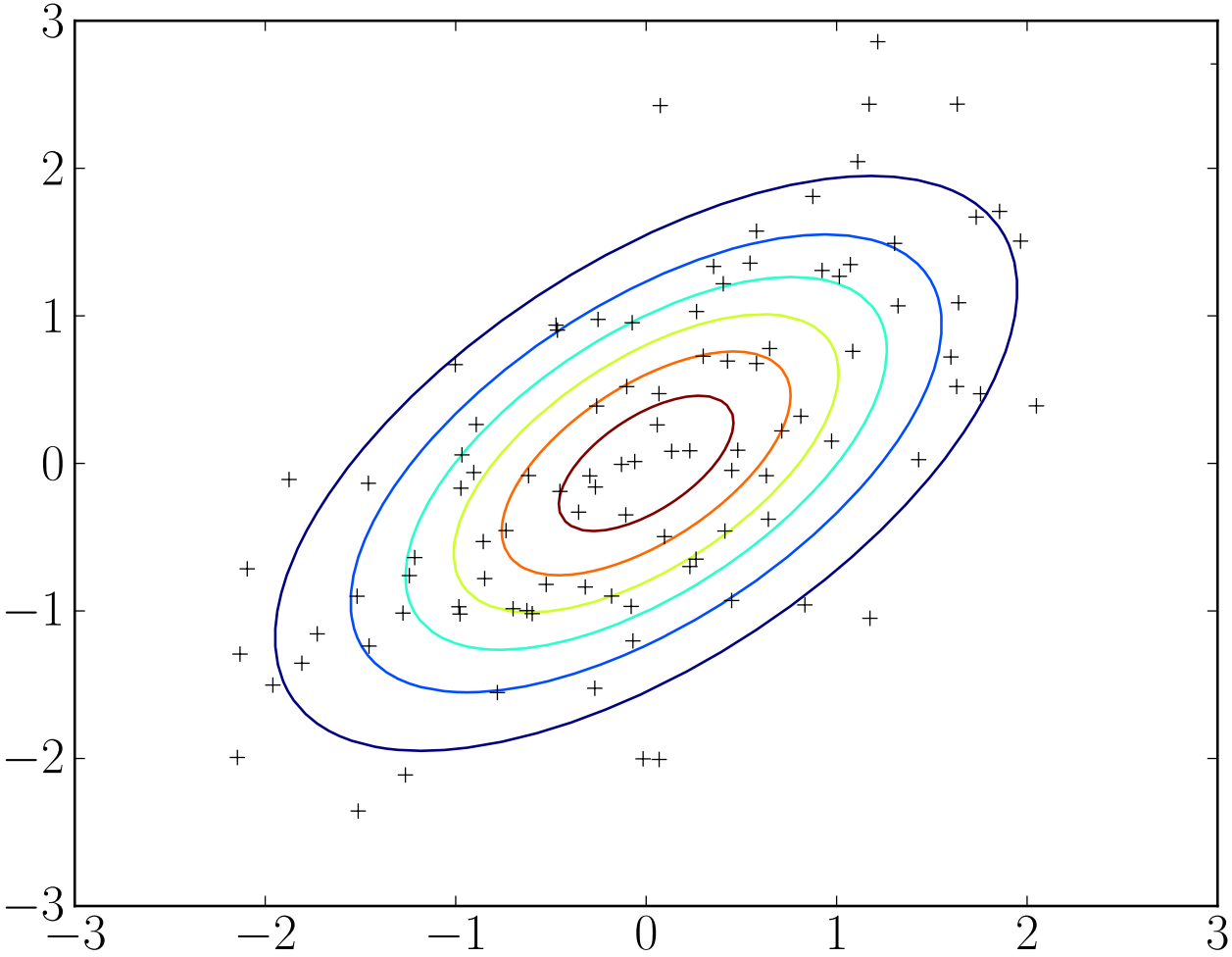


$$\mathbf{K} = \begin{bmatrix} 1 & -0.9 \\ -0.9 & 1 \end{bmatrix}$$

A 2D Gaussian

Inference



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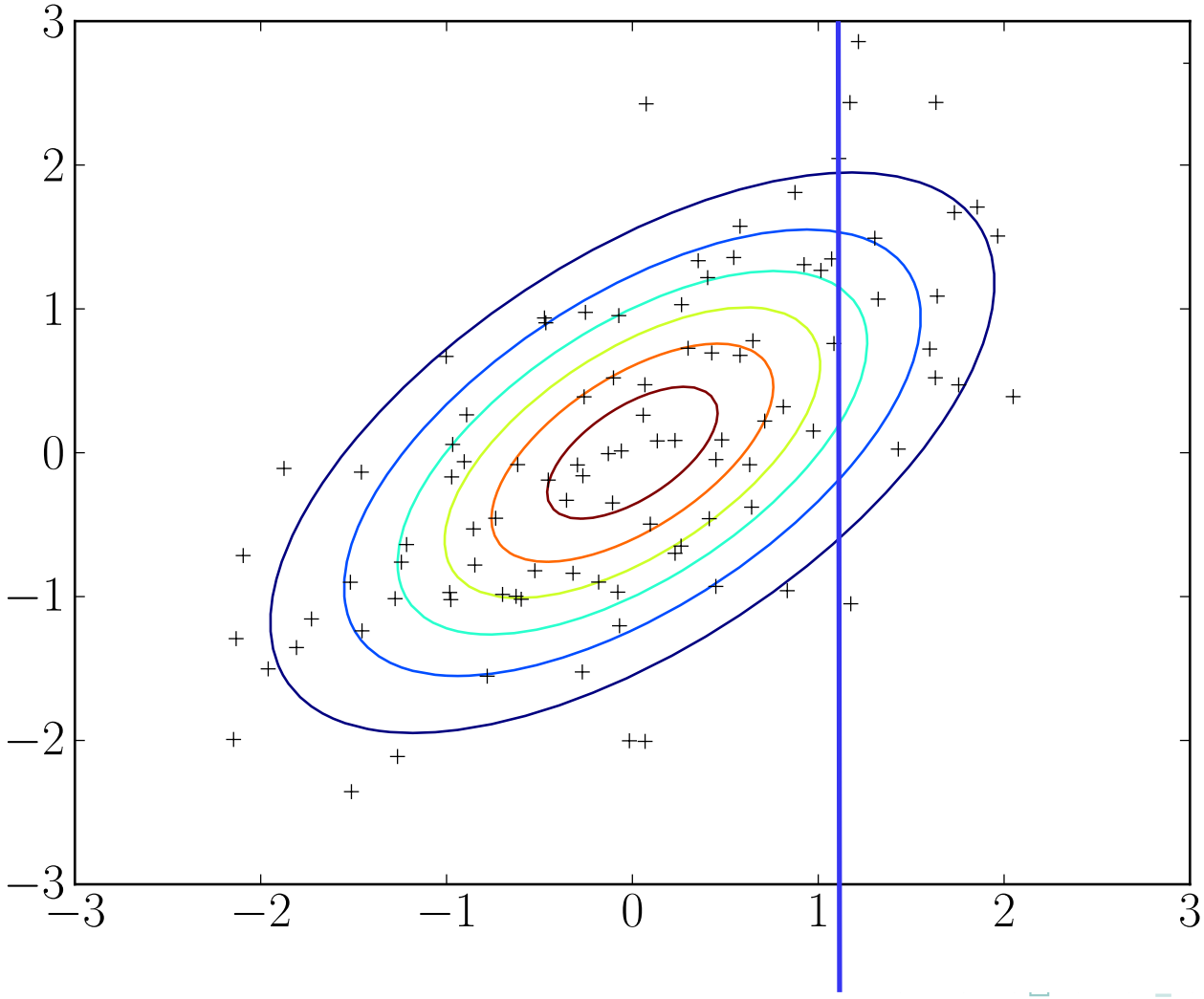

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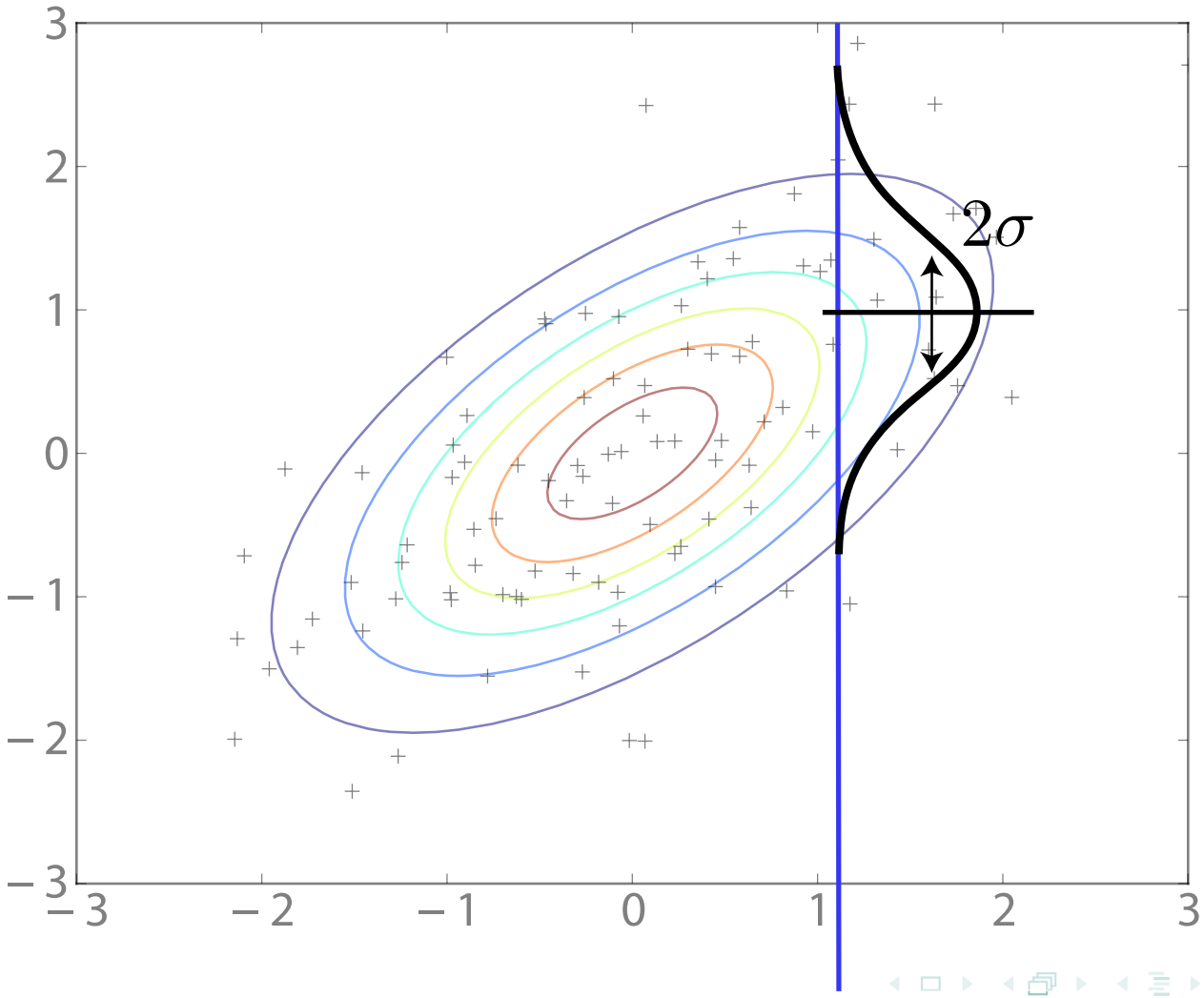


Inference

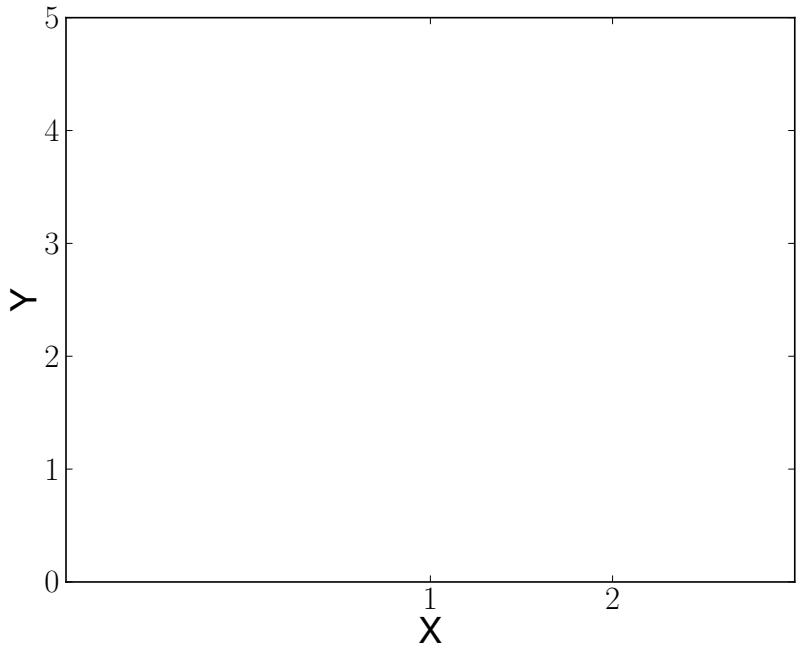
- Joint probability $p(y_1, y_2 \,|\, \mathbf{K}) = \mathcal{N}\left([y_1, y_2] \,|\, \mathbf{0}, \mathbf{K}\right)$
- Conditional probability

$$p(y_2 \,|\, y_1, \mathbf{K}) = \frac{p(y_1, y_2 \,|\, \mathbf{K})}{p(y_1 \,|\, \mathbf{K})}$$
$$\propto \exp\left\{-\frac{1}{2}[y_1, y_2]\,\mathbf{K}^{-1}\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}\right\}$$

- Completing the square yields a Gaussian with non-zero as posterior for y_2.

Extending the idea to higher dimensions

- Let us interpret y_1 and y_2 as outputs in a regression setting.
- We can introduce an additional 3rd point.



- Now $P([y_1, y_2, y_3] \,|\, \mathbf{K}_3) = \mathcal{N}([y_1, y_2, y_3] \,|\, \mathbf{0}, \mathbf{K}_3)$, where $\mathbf{K}_3$ is now a 3 x 3 covariance matrix!

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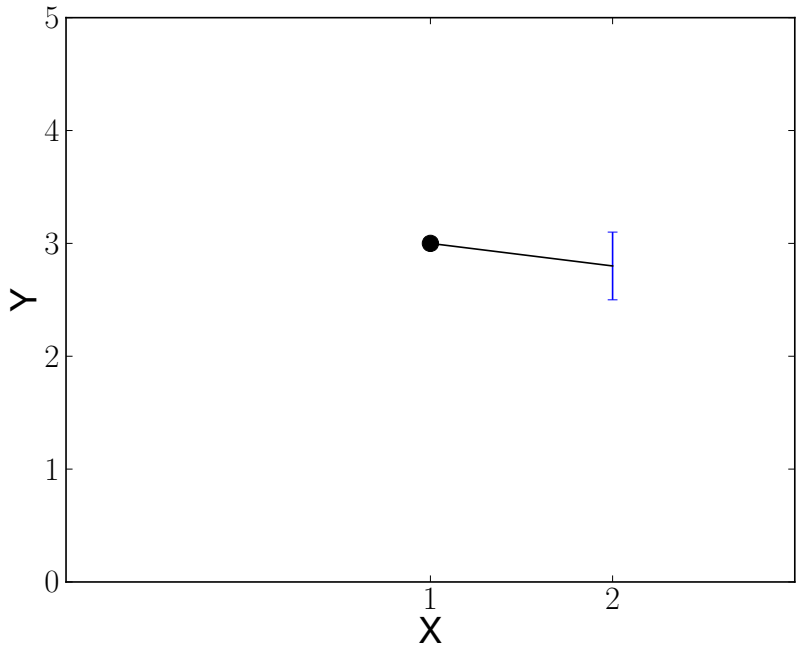

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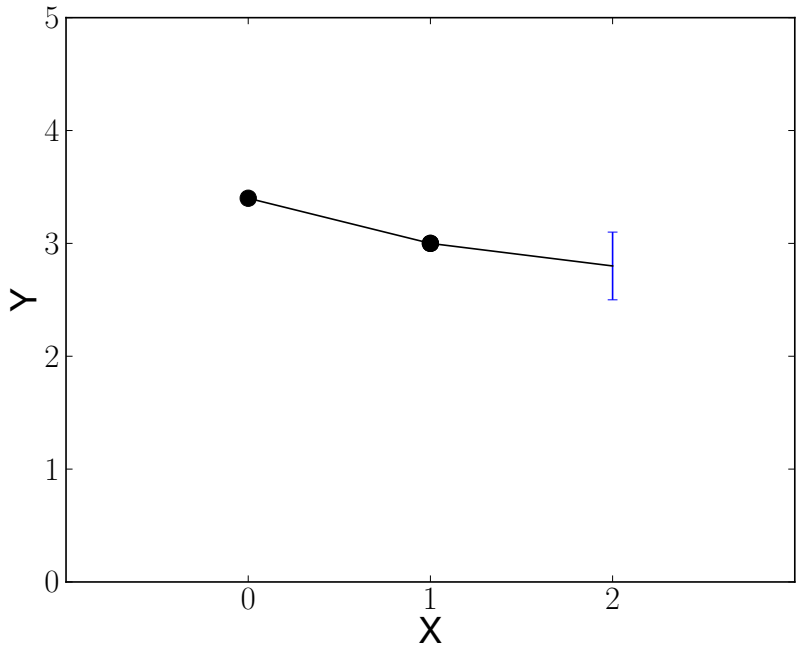

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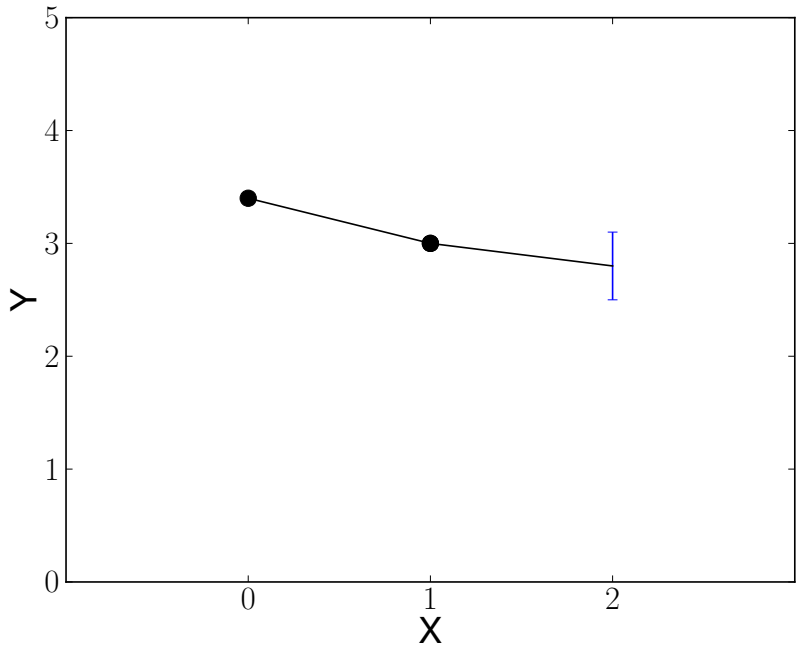

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Constructing Covariance Matrices

- Analogously we can look at the joint probability for arbitrary many points and obtain predictions.
- Issue: how to construct a good covariance matrix?
- A simple heuristics

$$\mathbf{K}_2 = \begin{bmatrix} 1 & 0.6 \\ 0.6 & 1 \end{bmatrix}$$

$$\mathbf{K}_3 = \begin{bmatrix} 1 & 0.6 & 0 \\ 0.6 & 1 & 0.6 \\ 0 & 0.6 & 1 \end{bmatrix}$$

- Note:
  - The ordering of the points y_1, y_2, y_3 matters.
  - Important to ensure that covariance matrices remain positive definite (matrix inversion).

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Constructing Covariance Matrices

A general recipe

- Use a covariance function (kernel function) to construct $\mathbf{K}$:

$$\mathbf{K}_{i,j} = k(x_i, x_j; \boldsymbol{\theta}_\mathsf{K})$$

- For example: The squared exponential covariance function embodies the belief that points further apart are less correlated:

$$k_{\mathsf{SE}}(x_i, x_j, ; A, L) = A^2 \exp\left\{-0.5 \cdot \frac{(x_i - x_j)^2}{L^2}\right\}$$

  - Overall correlation, amplitude
  - Scaling parameter, smoothness

- $\theta_\mathsf{K} = \{A, L\}$ are called hyperparameters.
- We denote the covariance matrix for a set of inputs $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ as: $\mathbf{K}_{\mathbf{X},\mathbf{X}}(\theta_\mathsf{K})$

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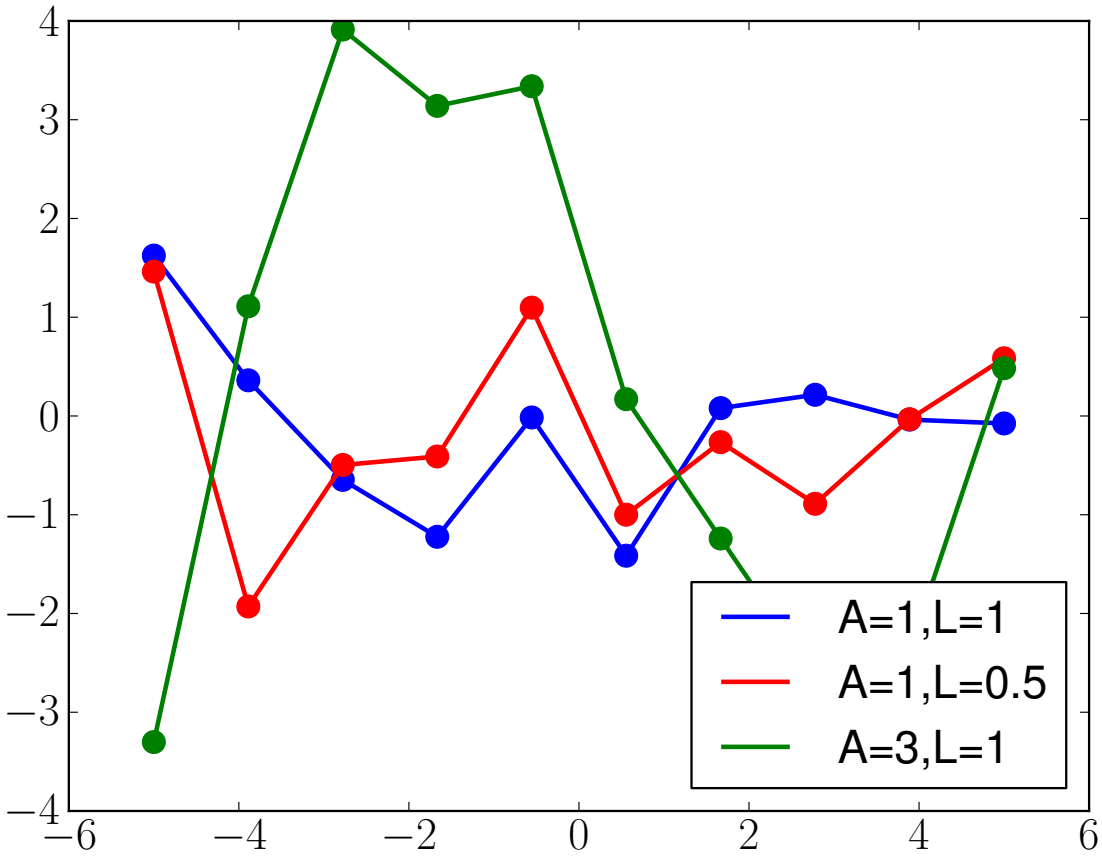
Constructing Covariance Matrices

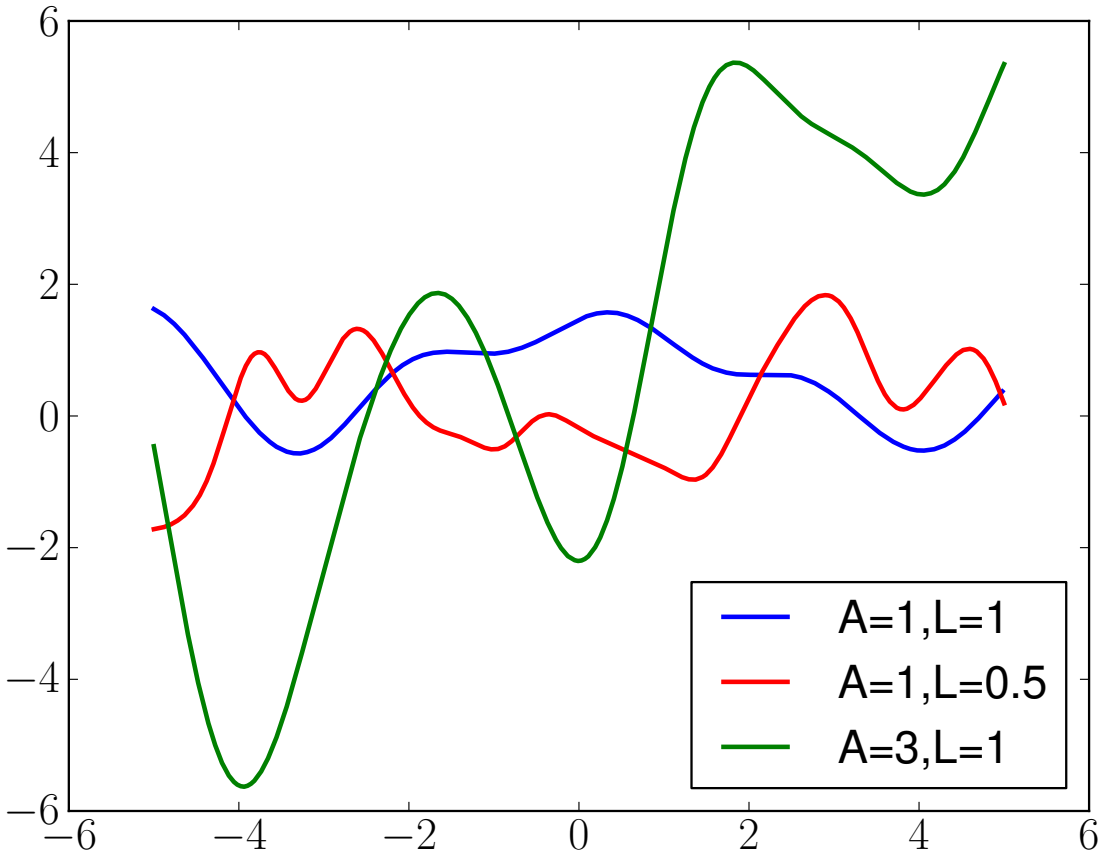
GP samples using the squared exponential covariance function



10D Gaussian

Constructing Covariance Matrices

GP samples using the squared exponential covariance function



500D Gaussian

Constructing Covariance Matrices

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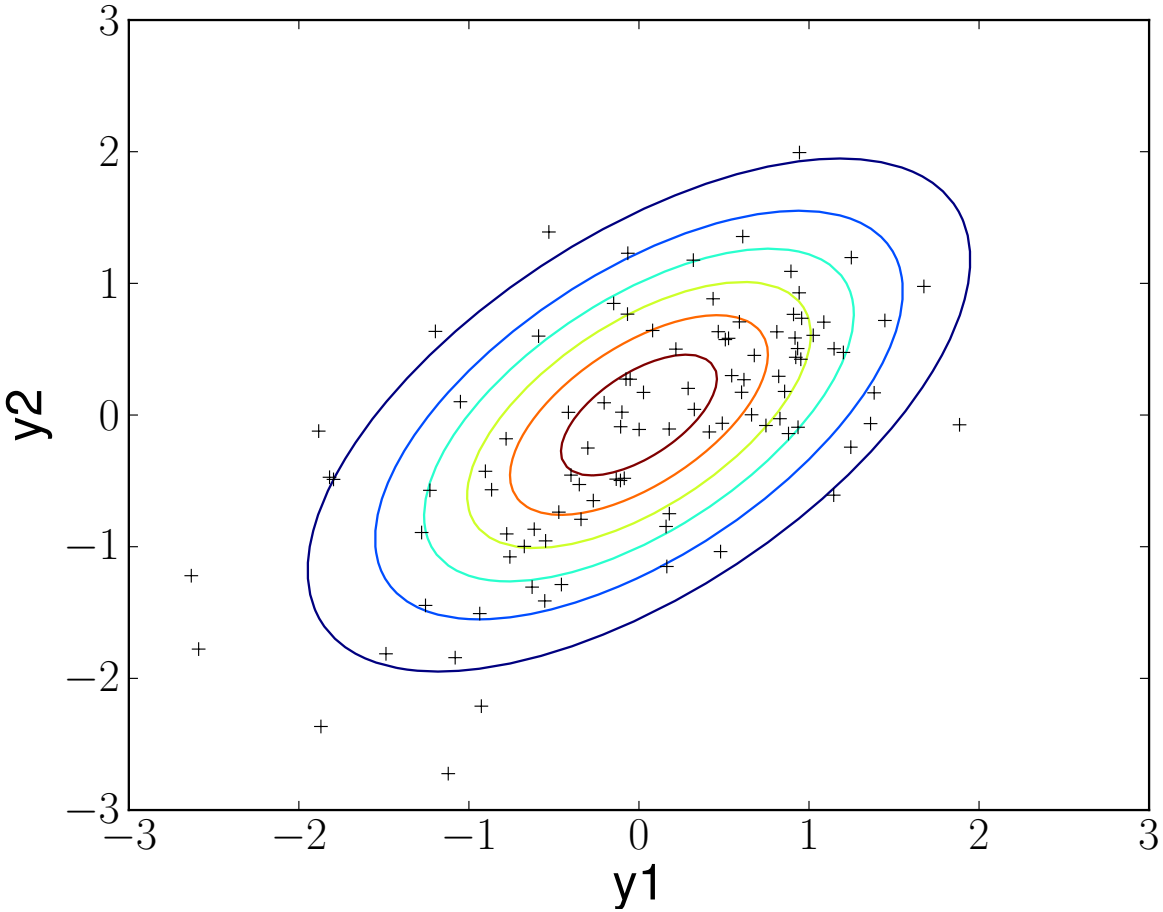

Reminder: Every function line corresponds to a sample drawn from this 2D Gaussian!

Why this all works

- Consistency of the 10D and 500D Gaussian.
- A small quizz:
  - Let y_1, y_2, y_3 have covariance matrix

$$\mathbf{K}_3 = \begin{bmatrix} 1 & 5 & 0 \\ 5 & 1 & 5 \\ 0 & 5 & 1 \end{bmatrix} \text{ and inverse } \mathbf{K}_3^{-1} = \begin{bmatrix} 1.5 & -1 & 5 \\ -1 & 2 & -1 \\ 5 & -1 & 1.5 \end{bmatrix}$$

  - Now focus on the variables y_1, y_2, integrating out y_3. Which of the following statements is true

$$\text{a) } \mathbf{K}_2 = \begin{bmatrix} 1 & 5 \\ 5 & 1 \end{bmatrix} \qquad \text{b) } \mathbf{K}_2^{-1} = \begin{bmatrix} 1.5 & -1 \\ -1 & 2 \end{bmatrix}$$

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Function space view

So far

1. Joint Gaussian distribution over the set of all outputs $\mathbf{y}$.
2. Covariance function as a recipe to construct a suitable covariance matrices from the corresponding inputs $\mathbf{X}$.

Function space view

The Gaussian process as a prior on functions

- Covariance function and hyperparameters reflect the prior belief on function smoothness, lengthscales etc.
- The general recipe allows a joint Gaussian to be constructed for an arbitrary selection of input locations $\mathbf{X}$.

Prior on infinite function $f(x)$

$$p(f(x)) = \mathsf{GP}(f(x) \,|\, k)$$

Prior on function values $\mathbf{f} = (f_1, \ldots, f_N)$

$$p(\mathbf{f} \,|\, \mathbf{X}, \boldsymbol{\theta}_\mathsf{K}) = \mathcal{N}\left(\mathbf{f} \,|\, \mathbf{0}, \mathbf{K}_{\mathbf{X},\mathbf{X}}(\boldsymbol{\theta}_\mathsf{K})\right)$$

Noise-free observations

- Given noise-free training data $\mathcal{D} = \{\mathbf{x}_n, f_n\}_{n=1}^N$
- Want to make predictions $\mathbf{f}^\star$ at test points $\mathbf{X}^\star$
- Joint distribution of $\mathbf{f}$ and $\mathbf{f}^\star$ is

$$p([\mathbf{f}, \mathbf{f}^\star] \,|\, \mathbf{X}, \mathbf{X}^\star, \boldsymbol{\theta}_\mathsf{K}) = \mathcal{N}\left([\mathbf{f}, \mathbf{f}^\star] \,\middle|\, \mathbf{0}, \begin{bmatrix} \mathbf{K}_{\mathbf{X},\mathbf{X}} & \mathbf{K}_{\mathbf{X},\mathbf{X}^\star} \\ \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}} & \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}^\star} \end{bmatrix}\right)$$

(All kernel matrices $\mathbf{K}$ depend on hyperparameters $\boldsymbol{\theta}_\mathsf{K}$ which are dropped for brevity.)

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Inference

- Given observed noisy data $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$, the joint probability over latent function values $\mathbf{f}$ and $\mathbf{f}^\star$ given $\mathbf{y}$ is

$$p([\mathbf{f}, \mathbf{f}^\star] \,|\, \mathbf{X}, \mathbf{X}^\star, \mathbf{y}, \boldsymbol{\theta}_\mathrm{K}, \sigma^2) \propto \overbrace{\mathcal{N}\left([\mathbf{f}, \mathbf{f}^\star] \,|\, \mathbf{0}, \mathbf{K}\right)}^{\text{Prior}} \times \underbrace{\prod_{n=1}^{N} \mathcal{N}\left(y_n \,|\, f_n, \sigma^2\right)}_{\text{Likelihood}},$$

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- Applying "Gaussian calculus", integrating out $\mathbf{f}$ yields

$$p([\mathbf{y}, \mathbf{f}^\star] \,|\, \mathbf{X}, \mathbf{X}^\star, \mathbf{y}, \boldsymbol{\theta}_\mathsf{K}, \sigma^2) \propto \mathcal{N}\left([\mathbf{y}, \mathbf{f}^\star] \,\middle|\, \mathbf{0}, \begin{bmatrix} \mathbf{K}_{\mathbf{X},\mathbf{X}} + \sigma^2 \mathbf{I} & \mathbf{K}_{\mathbf{X},\mathbf{X}^\star} \\ \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}} & \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}^\star} \end{bmatrix}\right)$$

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Making predictions

- The predictive distribution follows from the joint distribution by completing the square (conditioning)

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- Gaussian predictive distribution for $\mathbf{f}^\star$

$$p(\mathbf{f}^\star \,|\, \mathbf{X}, \mathbf{y}, \mathbf{X}^\star, \boldsymbol{\theta}_\mathsf{K}, \sigma^2) = \mathcal{N}(\mathbf{f}^\star \,|\, \boldsymbol{\mu}^\star, \boldsymbol{\Sigma}^\star) \text{ with}$$

$$\boldsymbol{\mu}^\star = \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}} \left[\mathbf{K}_{\mathbf{X},\mathbf{X}} + \sigma^2\mathbf{I}\right]^{-1} \mathbf{y}$$

$$\boldsymbol{\Sigma}^\star = \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}^\star} - \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}} \left[\mathbf{K}_{\mathbf{X},\mathbf{X}} + \sigma^2\mathbf{I}\right]^{-1} \mathbf{K}_{\mathbf{X},\mathbf{X}^\star}$$

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$$p([\mathbf{y}, \mathbf{f}^\star] \,|\, \mathbf{X}, \mathbf{X}^\star, \mathbf{y}, \boldsymbol{\theta}_\mathsf{K}, \sigma^2) \propto \mathcal{N}\left([\mathbf{y}, \mathbf{f}^\star] \middle| \mathbf{0}, \begin{bmatrix} \mathbf{K}_{\mathbf{X},\mathbf{X}} + \sigma^2\mathbf{I} & \mathbf{K}_{\mathbf{X},\mathbf{X}^\star} \\ \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}} & \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}^\star} \end{bmatrix}\right)$$

- Gaussian predictive distribution for $\mathbf{f}^\star$

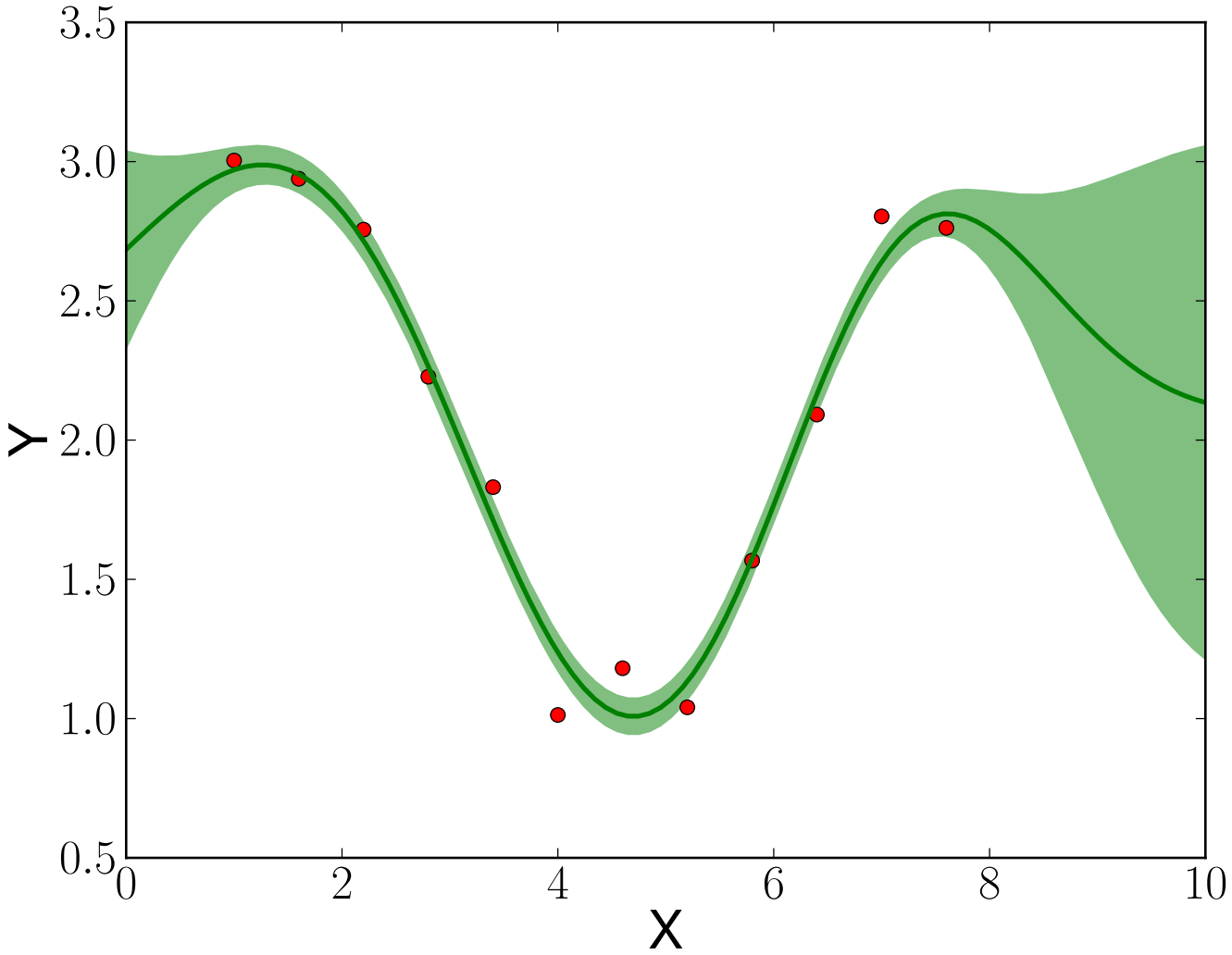
$$p(\mathbf{f}^\star \,|\, \mathbf{X}, \mathbf{y}, \mathbf{X}^\star, \boldsymbol{\theta}_\mathsf{K}, \sigma^2) = \mathcal{N}(\mathbf{f}^\star \,|\, \boldsymbol{\mu}^\star, \boldsymbol{\Sigma}^\star) \text{ with}$$

$$\boldsymbol{\mu}^\star = \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}} \left[\mathbf{K}_{\mathbf{X},\mathbf{X}} + \sigma^2\mathbf{I}\right]^{-1} \mathbf{y}$$

$$\boldsymbol{\Sigma}^\star = \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}^\star} - \mathbf{K}_{\mathbf{X}^\star,\mathbf{X}} \left[\mathbf{K}_{\mathbf{X},\mathbf{X}} + \sigma^2\mathbf{I}\right]^{-1} \mathbf{K}_{\mathbf{X},\mathbf{X}^\star}$$

Making predictions

Example



Making predictions

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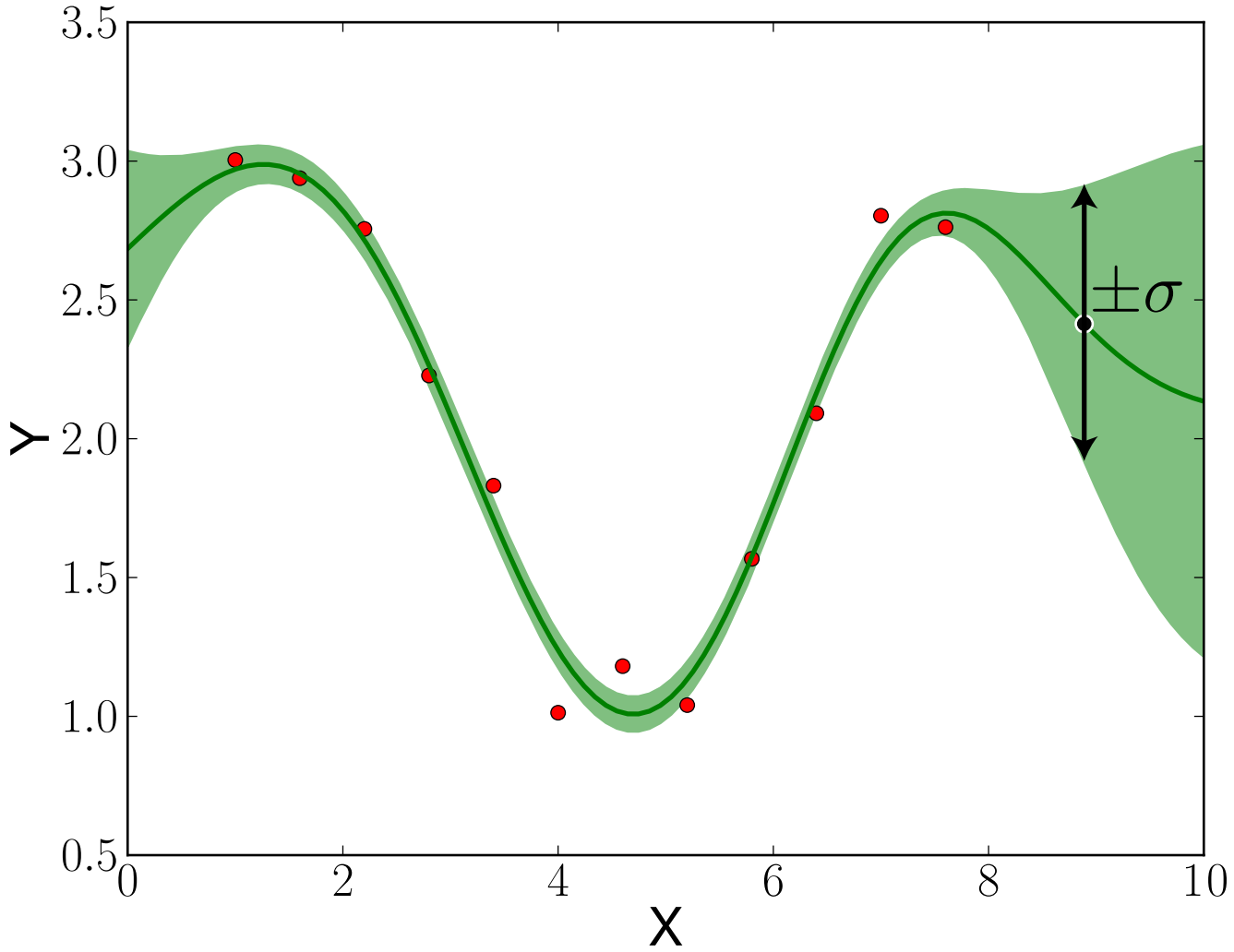

Learning hyperparameters

1. Fixed covariance matrix: $p(\mathbf{y} \mid \mathbf{K})$
2. Constructed covariance matrix: $\{\mathbf{K}\}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j; \boldsymbol{\theta}_\mathsf{K})$
3. Can we learn the hyperparameters $\boldsymbol{\theta}_\mathsf{K}$?

Learning hyperparameters

- Formally we are interested in the posterior

$$p(\boldsymbol{\theta}_K \mid \mathcal{D}) \propto p\left(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\theta}_K\right) p(\boldsymbol{\theta}_K)$$

- Inference is analytically intractable!
- MAP estimate instead of a full posterior. Set θ_K to the most probable hyperparameter settings:

$$\begin{aligned}
\hat{\boldsymbol{\theta}_K} &= \operatorname*{argmax}_{\boldsymbol{\theta}_K} \ln \left[p\left(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\theta}_K\right) p(\boldsymbol{\theta}_K)\right] \\
&= \operatorname*{argmax}_{\boldsymbol{\theta}_K} \ln \mathcal{N}\left(\mathbf{y} \mid \mathbf{0}, \mathbf{K}_{\mathbf{X},\mathbf{X}}(\boldsymbol{\theta}_K) + \sigma^2 \mathbf{I}\right) + \ln p(\boldsymbol{\theta}_K) \\
&= \operatorname*{argmax}_{\boldsymbol{\theta}_K} \Bigg[-\frac{1}{2} \log \det[\mathbf{K}_{\mathbf{X},\mathbf{X}}(\boldsymbol{\theta}_K) + \sigma^2 \mathbf{I}] \\
&\quad - \frac{1}{2} \mathbf{y}^{\mathrm{T}} [\mathbf{K}_{\mathbf{X},\mathbf{X}}(\boldsymbol{\theta}_K) + \sigma^2 \mathbf{I}]^{-1} \mathbf{y} - \frac{N}{2} \log 2\pi + \ln p(\boldsymbol{\theta}_K) \Bigg]
\end{aligned}$$

- Optimization can be carried out using standard optimization techniques.

Learning hyperparameters

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- Optimization can be carried out using standard optimization techniques.

Choosing covariance functions

- The covariance function embodies the prior belief about functions.
- Example: linear regression

$$y_n = wx_n + c + \psi_n$$

- Covariance function denote covariation

$$\begin{aligned} k(x_n, x'_n) &= \langle y_n y'_n \rangle \\ &= \langle (wx_n + c + \psi_n)(wx'_n + c + \psi'_n) \rangle \\ &= \underbrace{w^2 \cdot x_n x'_n + c^2}_{\text{kernel: } k(x_n, x'_n)} + \delta_{n,n'} \psi_n^2 \end{aligned}$$

Choosing covariance functions

Multidimensional input space

- Generalise squared exponential covariance function to multiple dimensions
  - 1 Dimension $k_{\mathsf{SE}}(x_i, x_j, ; A, L) = A^2 \exp\left\{-0.5 \cdot \frac{(x_i - x_j)^2}{L^2}\right\}$
  - D Dimensions dD

$$k_{\mathsf{SE}}(\mathbf{x}_i, \mathbf{x}_j, ; A, \mathbf{L}) = A^2 \exp\left\{-0.5 \sum_{d=1}^{D} \frac{(x_i^d - x_j^d)^2}{L_d^2}\right\}$$

- Lengthscale parameters L_d denote "relevance" of a particular data dimension.
  - Large L_d correspond to irrelevant dimensions.

Choosing covariance functions

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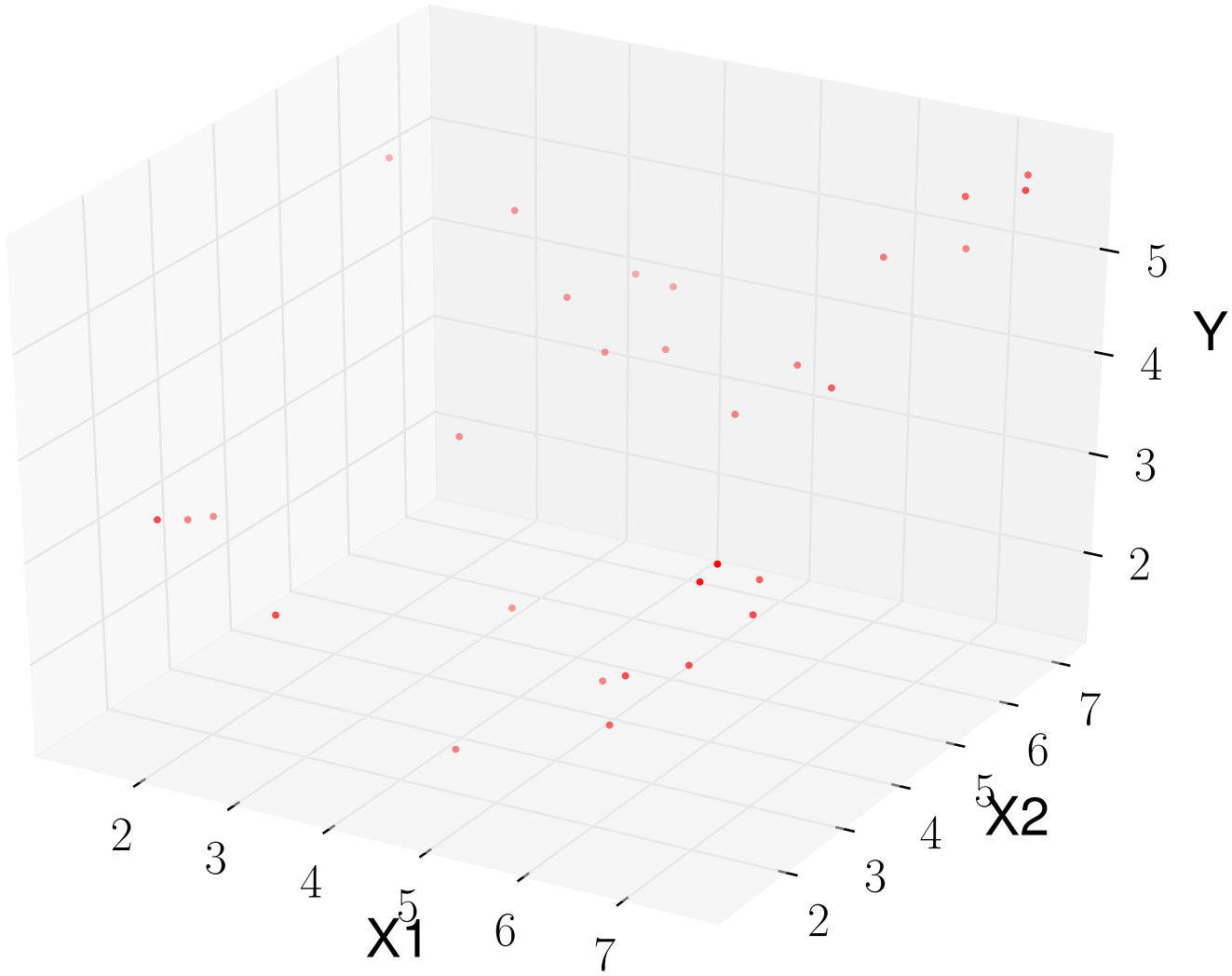
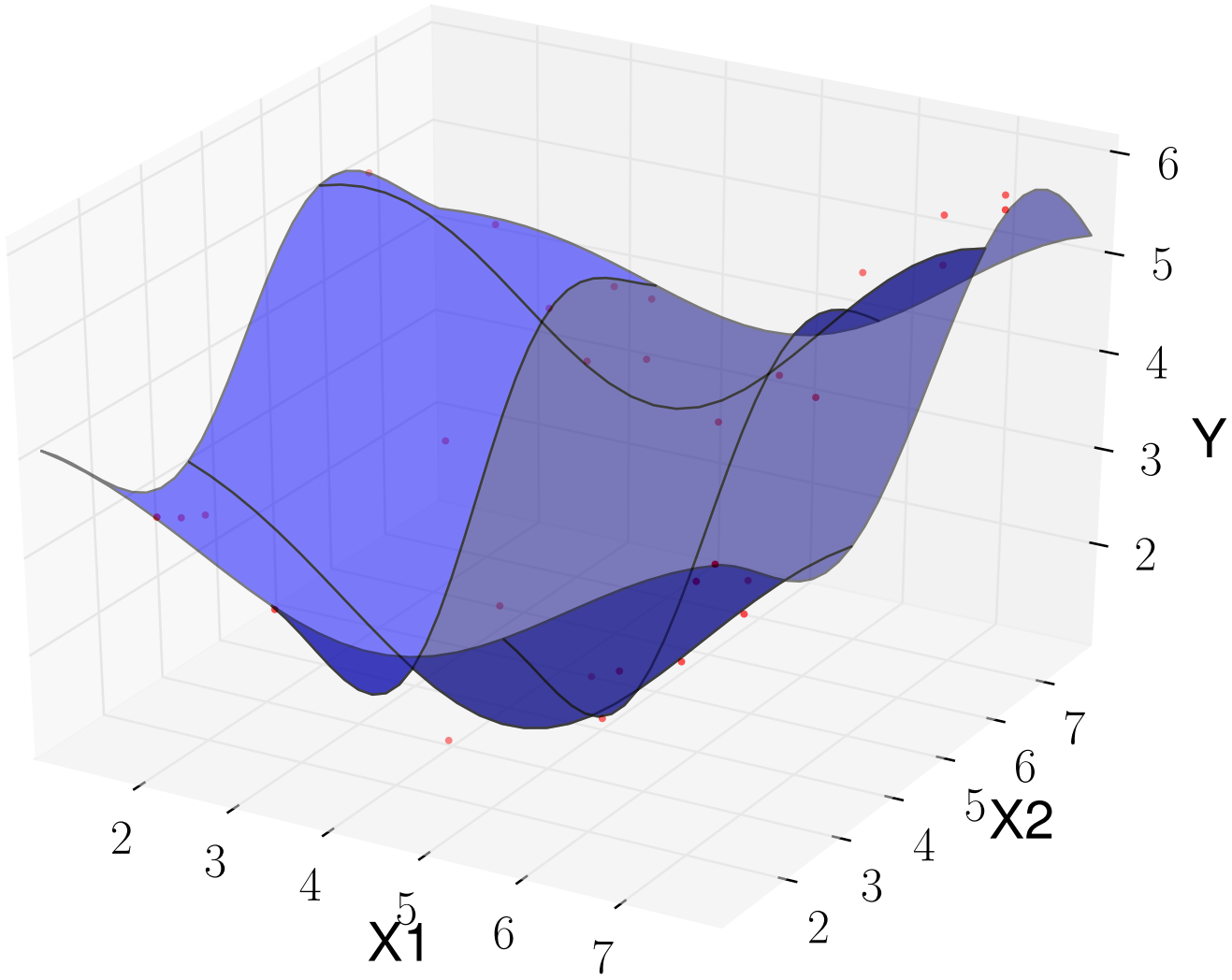
Choosing covariance functions

2D regression



Choosing covariance functions

2D regression



Choosing covariance functions

Any kernel will do

- Established kernels are all valid covariance functions, allowing for a wide range of possible input domains $\mathbf{X}$:
  - Graph kernels (molecules)
  - Kernels defined on strings (DNA sequences)

Choosing covariance functions

Combining existing covariance functions

- The sum of two covariances functions is itself a valid covariance function

$$k_S(x, x') = k_1(x, x') + k_2(x, x')$$

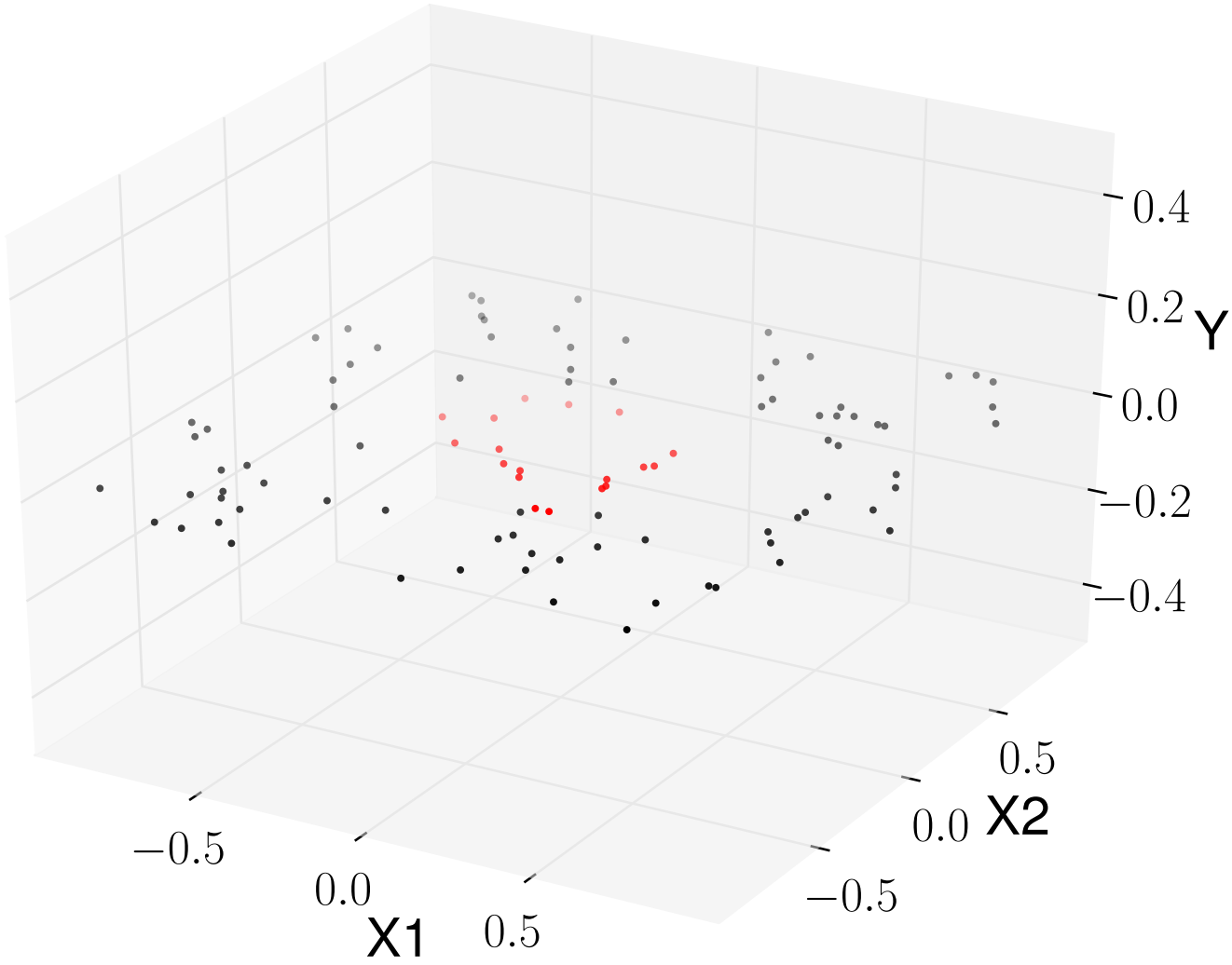
- The product of two covariance functions is itself a valid covariance function

$$k_P(x, x') = k_1(x, x') \cdot k_2(x, x')$$

Outline

GPs for classification

- How to deal with binary observations?



GPs for classification

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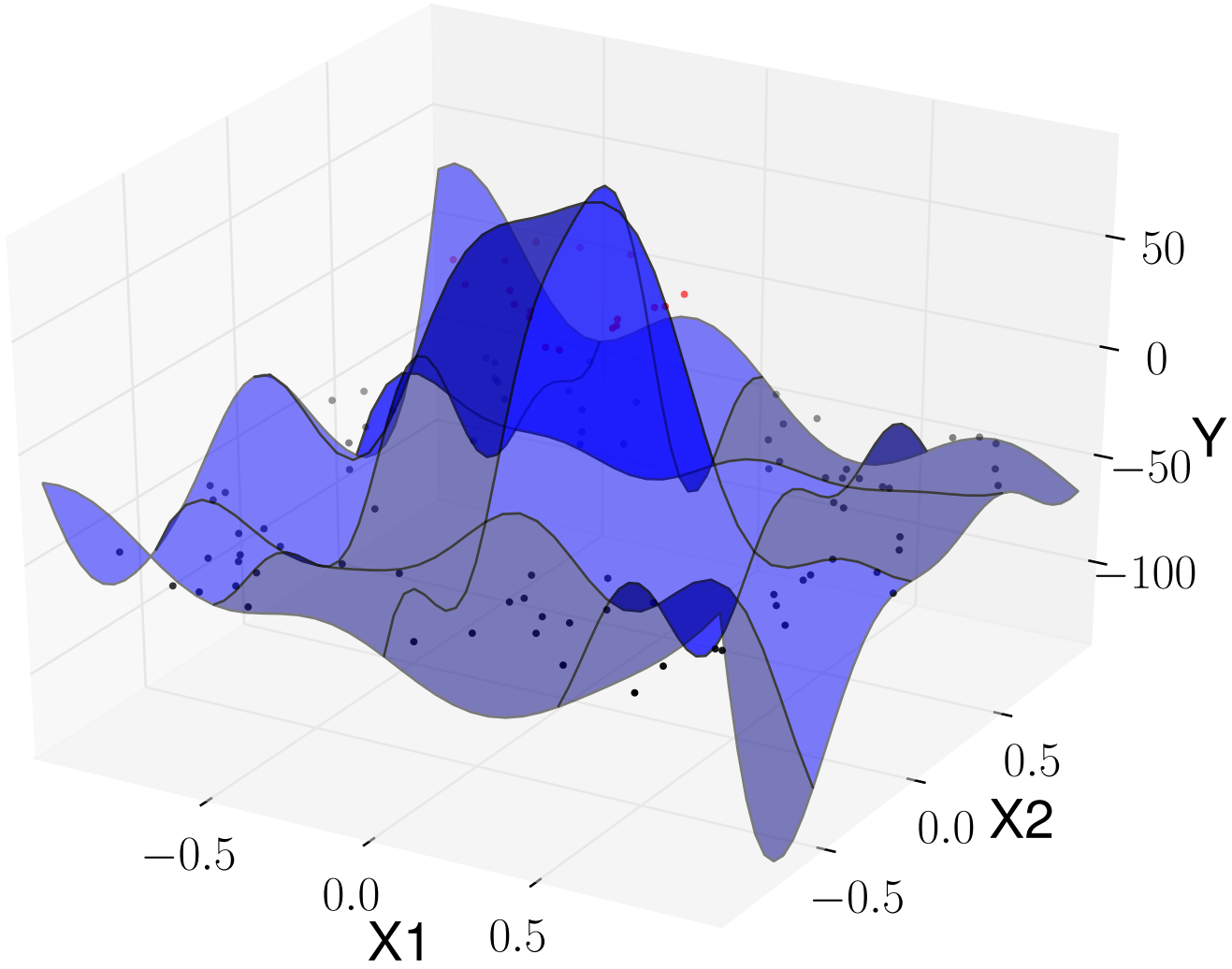

GPs for classification

Probit likelihood model

- Posterior with a general likelihood model

$$p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}, \boldsymbol{\theta}_{\mathsf{K}}, \sigma^2) \propto \overbrace{\mathcal{N}\left(\mathbf{f} \mid \mathbf{0}, \mathbf{K}_{\mathbf{X},\mathbf{X}}(\boldsymbol{\theta}_{\mathsf{K}})\right)}^{\text{Prior}} \times \overbrace{\prod_{n=1}^{N} p(y_n \mid f_n)}^{\text{Likelihood}}$$

- Classification: probit link model

$$p(y_n = 1 \mid f_n) = \frac{1}{1 + exp(-f_n)}$$

GPs for classification

Inference

- Inference with non-Gaussian likelihood is analytically intractable.
- Idea: approximate the true likelihood terms each with a Gaussian

$$KL\Bigg[\overbrace{\mathcal{N}\left(\mathbf{f} \,|\, \mathbf{0}, \mathbf{K}_{\mathbf{X},\mathbf{K}}(\boldsymbol{\theta}_\mathsf{K})\right)}^{\text{Prior}} \times \overbrace{\prod_{n=1}^{N} p(y_n \,|\, f_n)}^{\text{exact likelihood}} \,\Big|\Big|$$

$$\underbrace{\mathcal{N}\left(\mathbf{f} \,|\, \mathbf{0}, \mathbf{K}_{\mathbf{X},\mathbf{X}}(\boldsymbol{\theta}_\mathsf{K})\right)}_{\text{Prior}} \times \underbrace{\prod_{n=1}^{N} \mathcal{N}\left(f_n \,|\, \tilde{\mu}_n, \tilde{\sigma}_n\right)}_{\text{approximation}} \Bigg]$$

- The KL divergence is a common measure of approximation accuracy

$$KL[P||Q] = \int_{\boldsymbol{\theta}} P(\boldsymbol{\theta}) \frac{P(\boldsymbol{\theta} \,|\, \mathcal{D})}{Q(\boldsymbol{\theta})}$$

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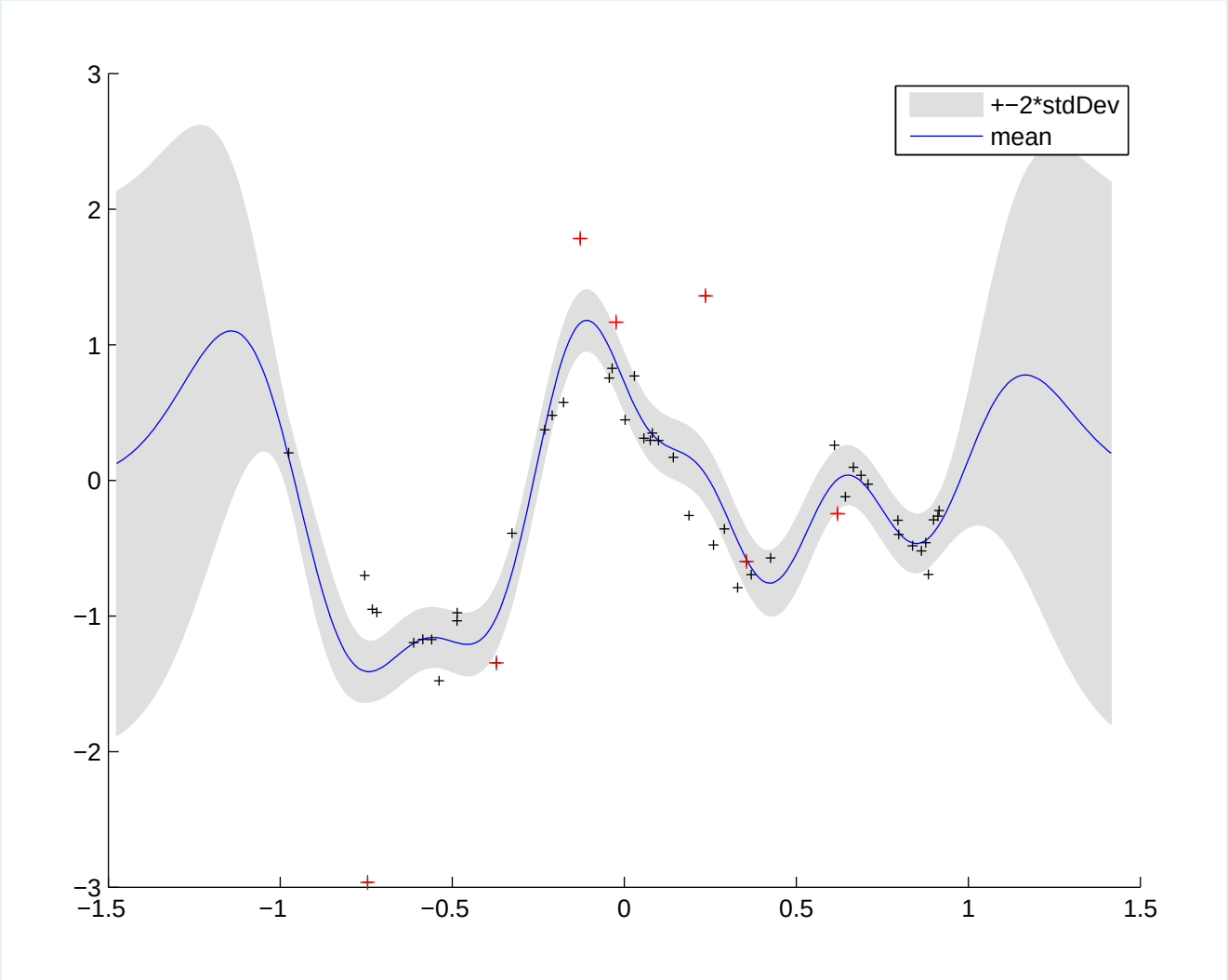
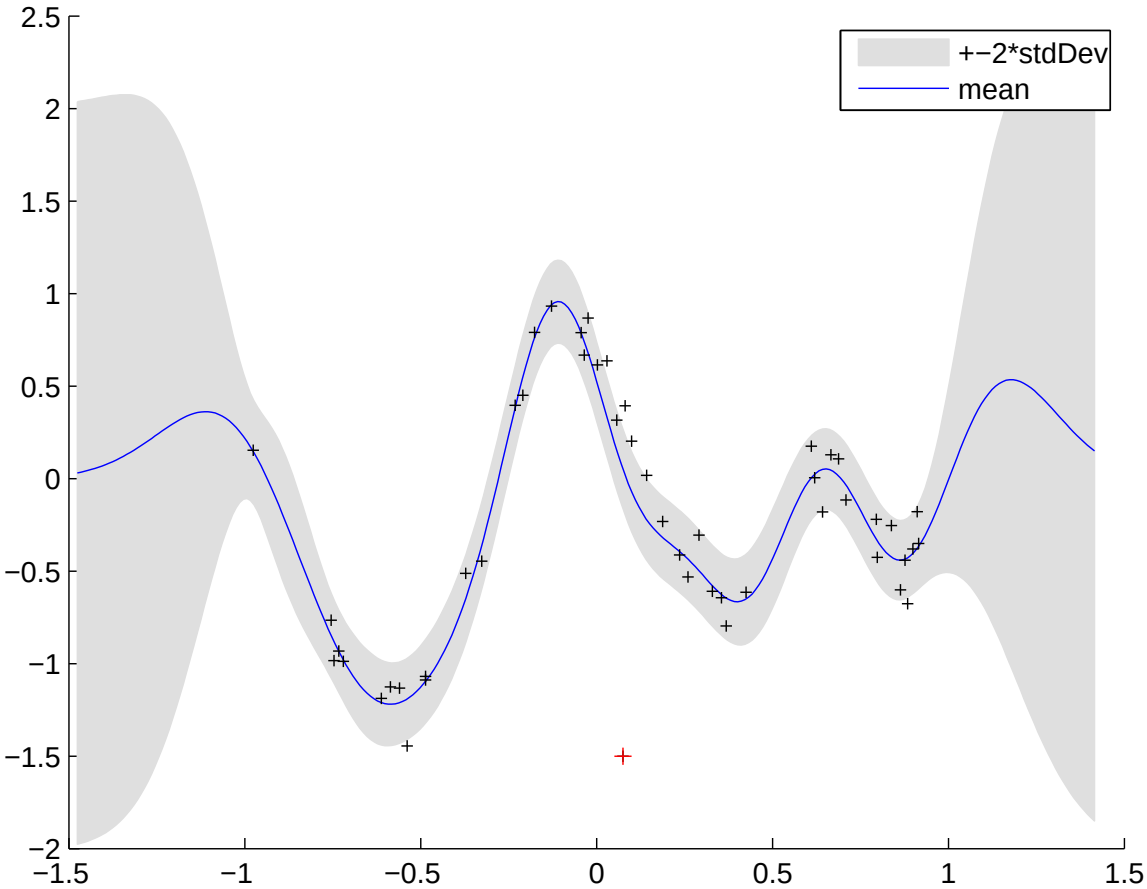
Robust regression

Regression with 15% outliers



Robust regression

Regression with 1% outliers



Robust regression

Mixture likelihood model

- Naive: filtering.
- We rather would like the likelihood model to empobdy the belief that a fraction of datapoints is "useless".

$$p(y_n \mid f_n) = \pi_{ok} \mathcal{N}\left(y_n \mid f_n, \sigma^2\right) + (1 - \pi_{ok}) \mathcal{N}\left(y_n \mid f_n, \sigma^2_\infty\right)$$

Robust regression

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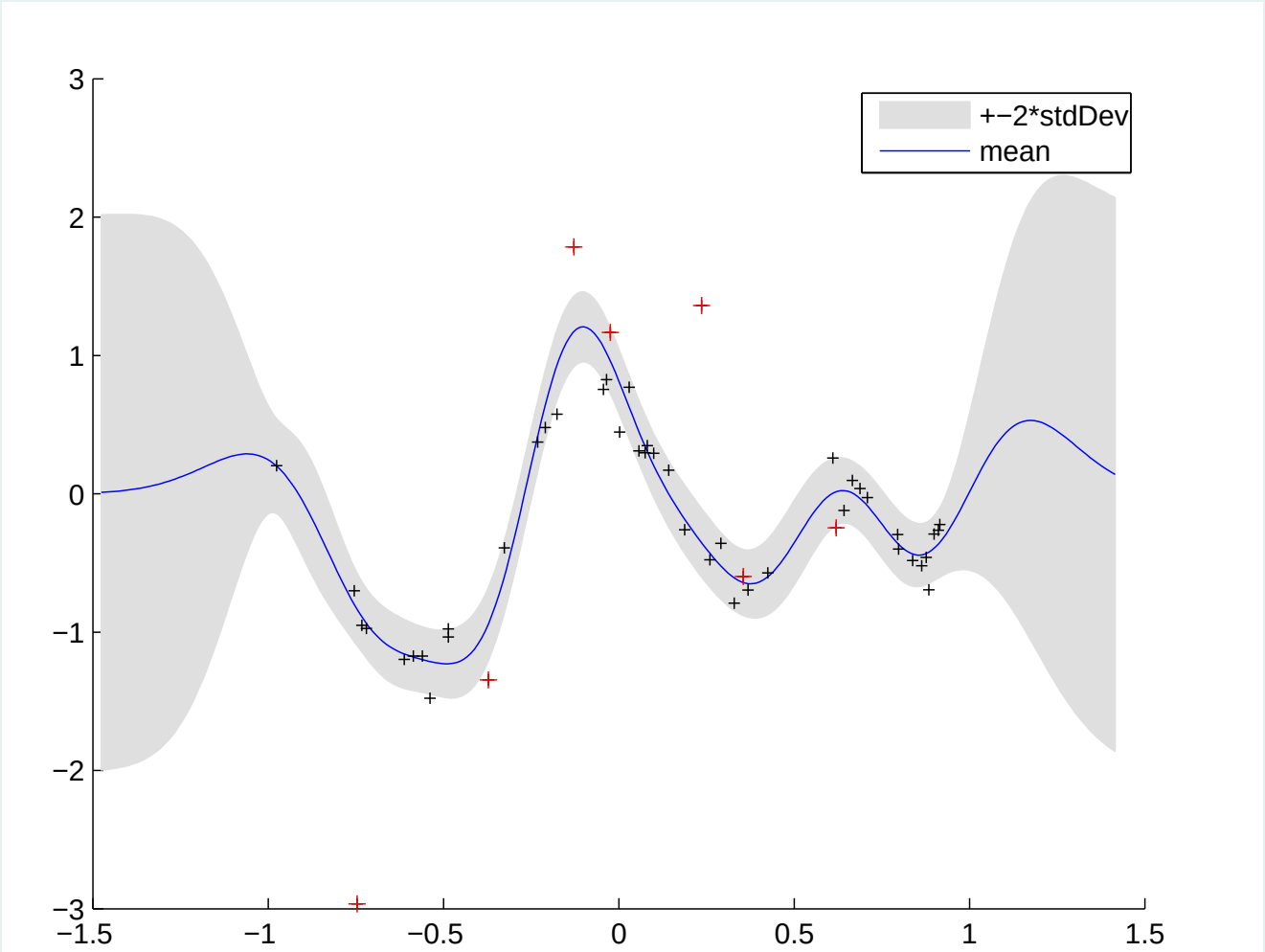
Robust regression

Mixture likelihood in action

Robust noise model



Why Gaussian processes and not something else?

- Tractable probabilistic model; uncertainty estimates
- Equal or better performance than other methods.
- Many other approaches as special case
  - Linear regression
  - Splines
  - Neural networks
- Kernel method; flexible choice of covariance functions.

- Major limitation: inversion of $N \times N$ matrix; scaling $\mathrm{O}(N^3)$.

Outline

Summary

- The key ingredient of a Gaussian processes is the covariance function; a recipe to construct covariance matrices.
- GP predictions boil down to conditioning joint Gaussian distributions.
- Most probable covariance function hyperparameters can be derived from the marginal likelihood.
- Non-Gaussian likelihood models allow for classification and robust regression, however require approximate inference techniques.