ENM 531: Data-driven Modeling and Probabilistic Scientific Computing

Lecture #22: Gaussian process regression

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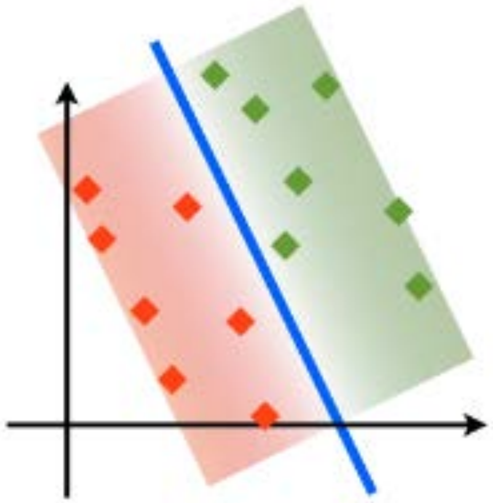
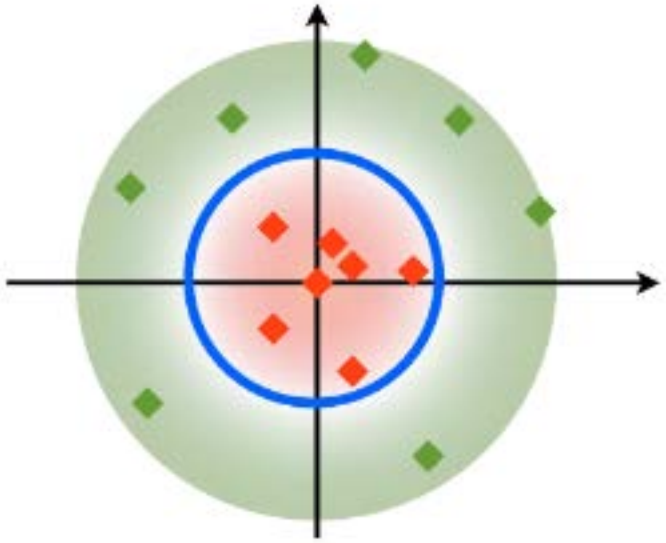
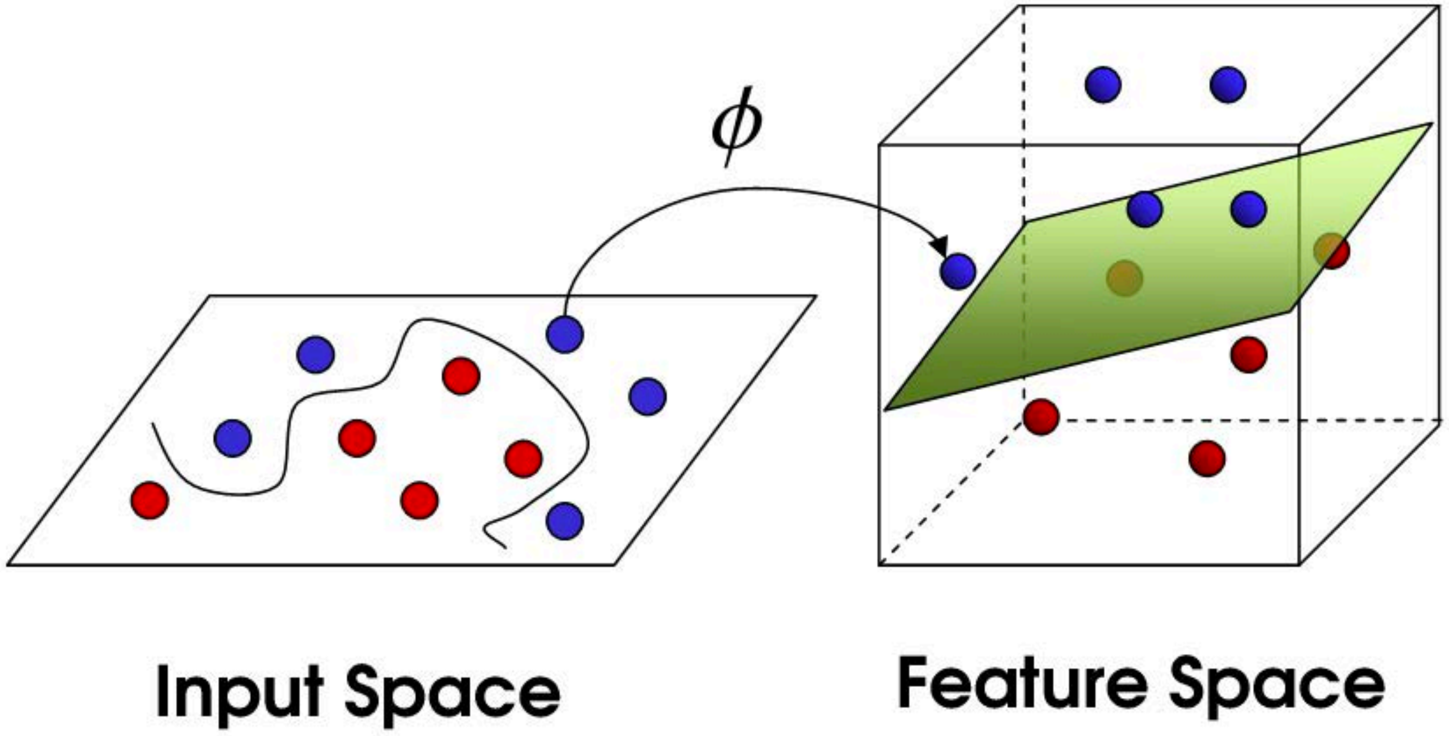
“Linearization” by embedding to higher dimensions

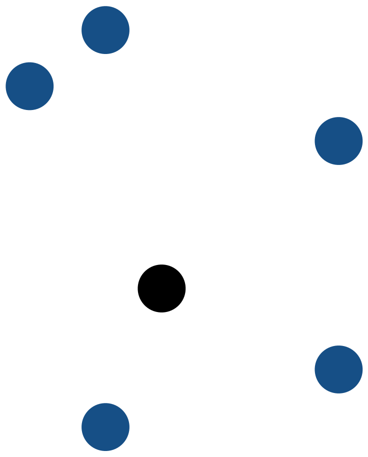
$$f(\boldsymbol{x}) = \langle \theta, \phi(\boldsymbol{x}) \rangle_{\mathcal{H}}, \quad \phi : \mathbb{R}^d \to \mathbb{R}^m$$







Kernel methods



$$\begin{tikzcd}
f(\boldsymbol{x}) = \langle \theta, \phi(\boldsymbol{x}) \rangle_{\mathcal{H}}, \quad \phi : \mathbb{R}^d \to \mathbb{R}^m \arrow[d, "m \to \infty"', "k(\boldsymbol{x}, \boldsymbol{x}') = \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{x}') \rangle_{\mathcal{H}}"] \\
f(\boldsymbol{x}) = \sum_{i=1}^{n} (\boldsymbol{K}^{-1} \boldsymbol{y})_i k(\boldsymbol{x}_i, \boldsymbol{x}), \quad \boldsymbol{K}_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)
\end{tikzcd}$$

$$\begin{tikzcd}
p(\theta|\mathcal{D}) = \dfrac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})} \arrow[d] \\
p(f|\mathcal{D}) = \dfrac{p(\mathcal{D}|f)p(f)}{p(\mathcal{D})}
\end{tikzcd}$$

$$f(\boldsymbol{x}) \sim \mathcal{GP}(0, k(\boldsymbol{x}, \boldsymbol{x}'))$$

Key take-away points:

-Kernels and representer theorems: learning with infinite-dimensional linear models can be done in time that depend on the number of observations by using a kernel function.

-Kernels on $\mathbb{R}^d$: such models include polynomials and classical Sobolev spaces (functions with square-integrable partial derivatives).

-Algorithms: convex optimization algorithms can be applied with theoretical guarantees and many dedicated developments to avoid the quadratic complexity of computing the kernel matrix.

-Analysis of well-specified models: When the target function is in the associated function space, learning can be done with rates that are independent of dimension.

-Analysis of mis-specified models: if the target is not in the the RKHS, the curse of dimensionality cannot be avoided in the worst case situations of few existing derivatives of the target function, but the methods are adaptive to any amount of intermediate smoothness.

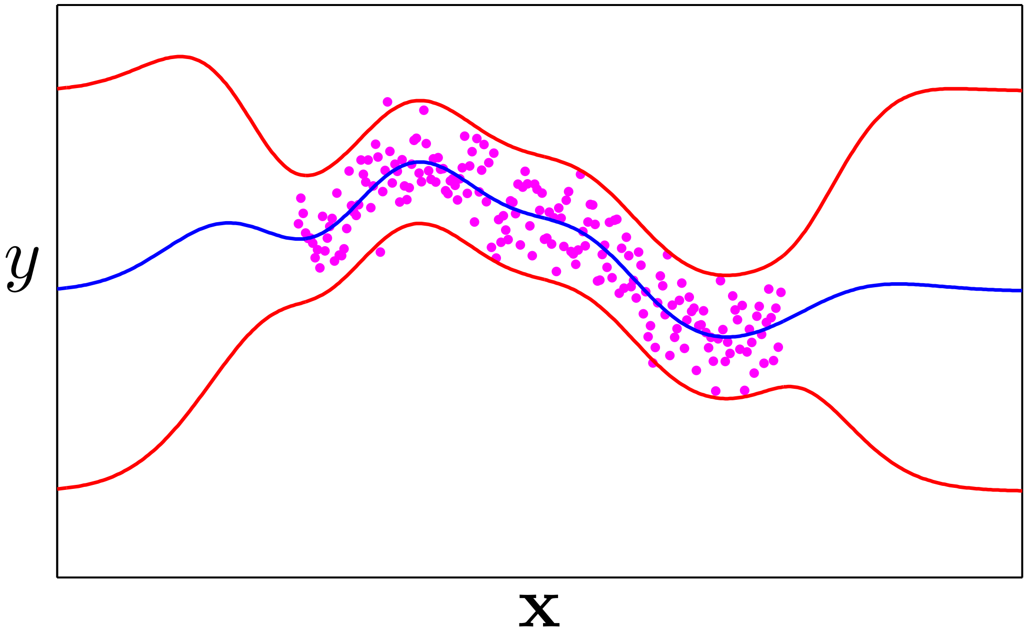
-Sharp analysis of ridge regression: for the square loss, a more involded analysis leads to optimal rates in a variety of situations in $\mathbb{R}^d$.

https://www.di.ens.fr/~fbach/ltfp_book.pdf

Nonlinear regression

Consider the problem of nonlinear regression:

You want to learn a function f with error bars from data $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$



A Gaussian process defines a distribution over functions $p(f)$ which can be used for Bayesian regression:

$$p(f|\mathcal{D}) = \frac{p(f)p(\mathcal{D}|f)}{p(\mathcal{D})}$$

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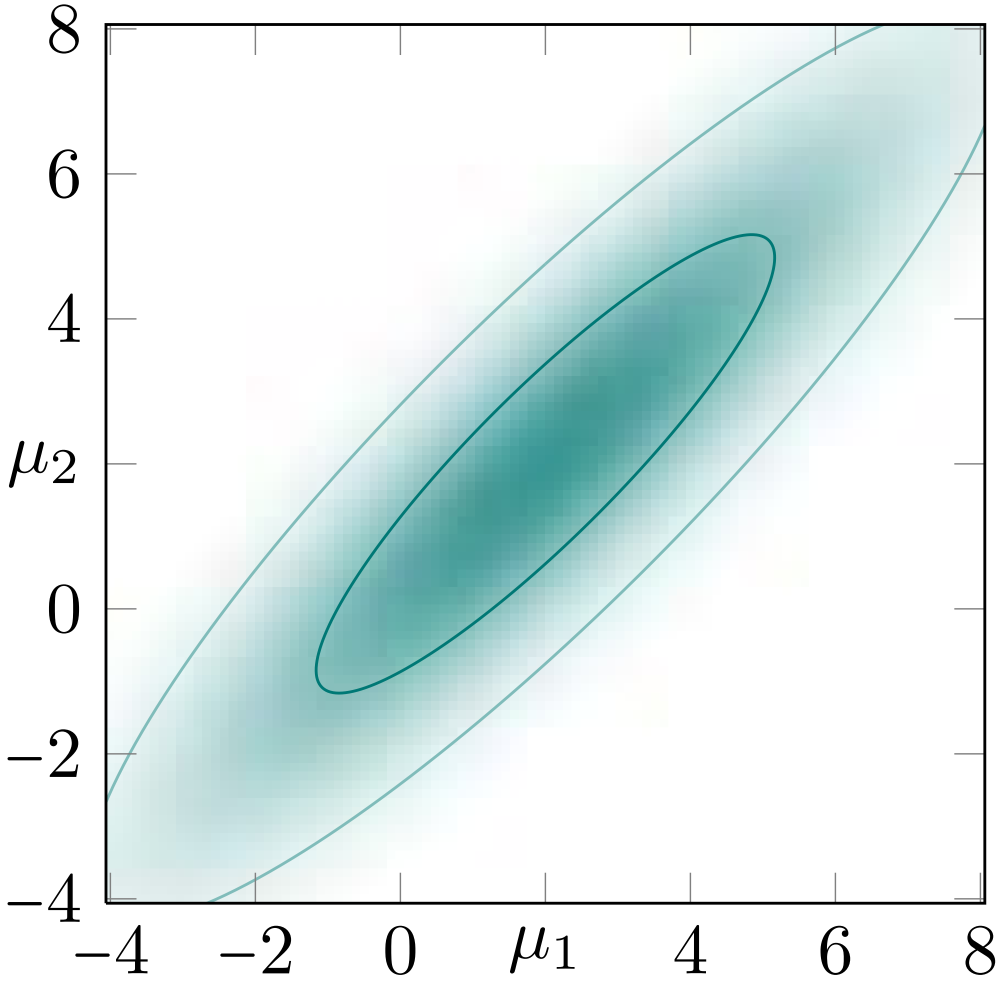
The Gaussian distribution

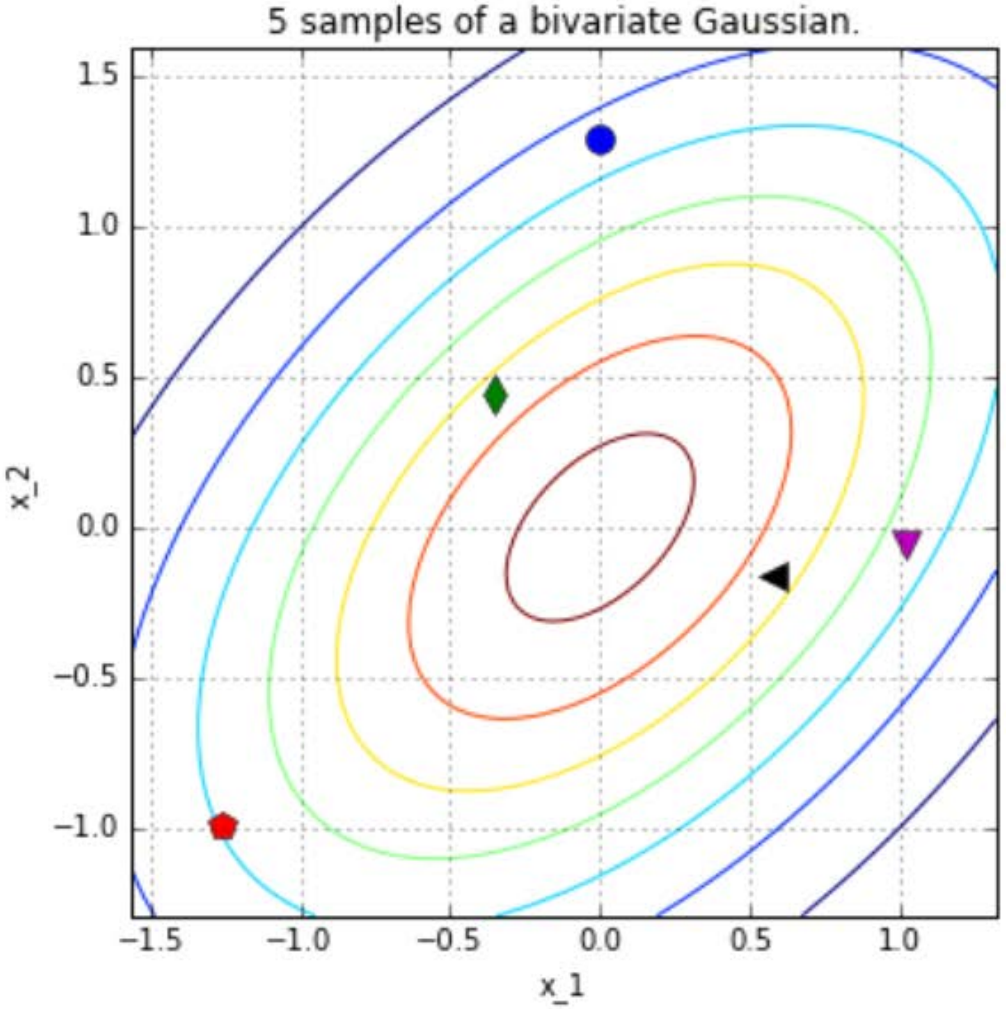
Multivariate Form

$$\mathcal{N}(x;\mu,\Sigma) = \frac{1}{(2\pi)^{N/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right]$$

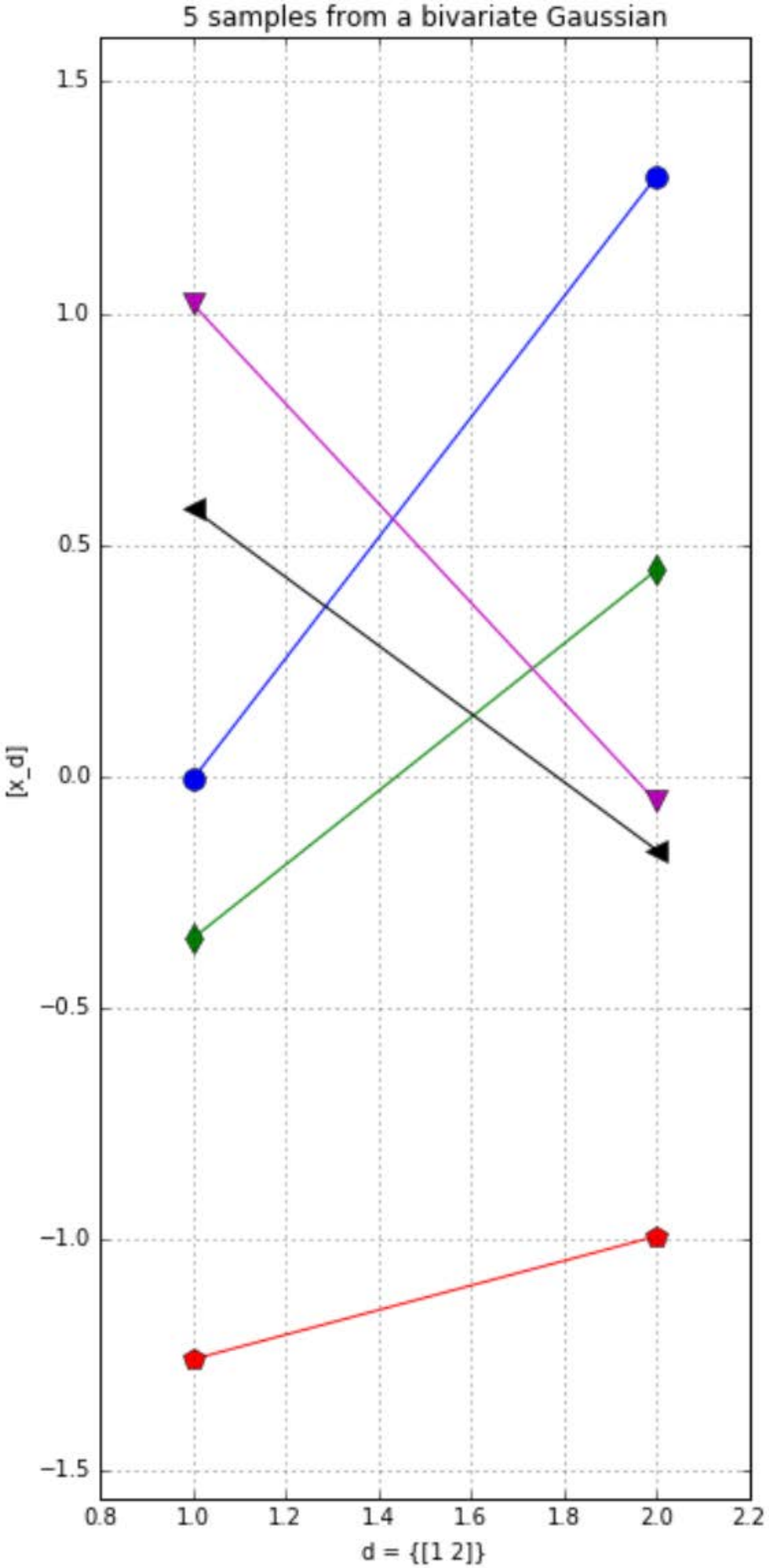


- $x, \mu \in \mathbb{R}^N$, $\Sigma \in \mathbb{R}^{N\times N}$
- Σ is positive semidefinite, i.e.
  - $v^\top \Sigma v \geq 0$ for all $v \in \mathbb{R}^N$
  - Hermitian, all eigenvalues ≥ 0

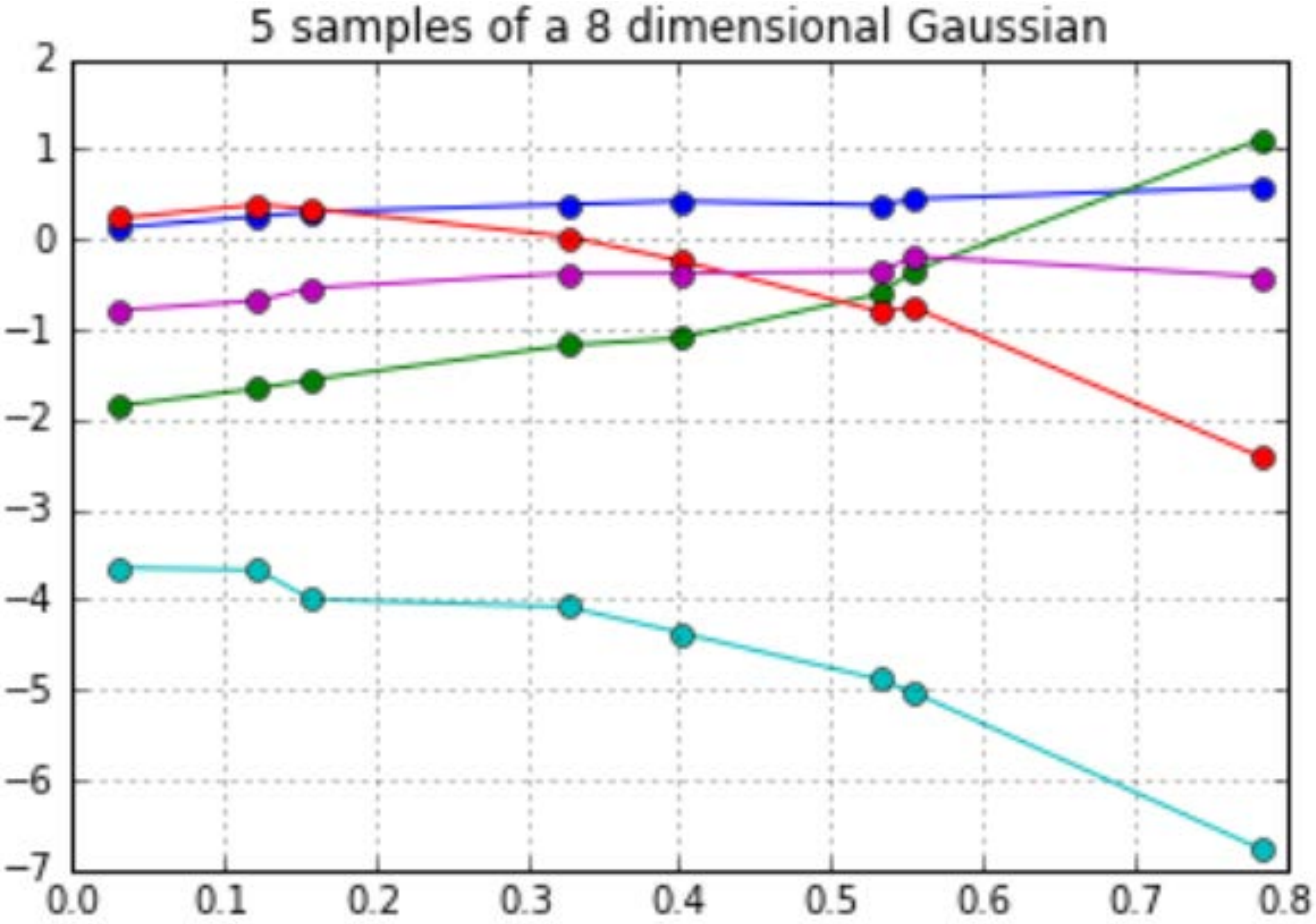
http://mlss.tuebingen.mpg.de/2013/2013/hennig_slides1.pdf

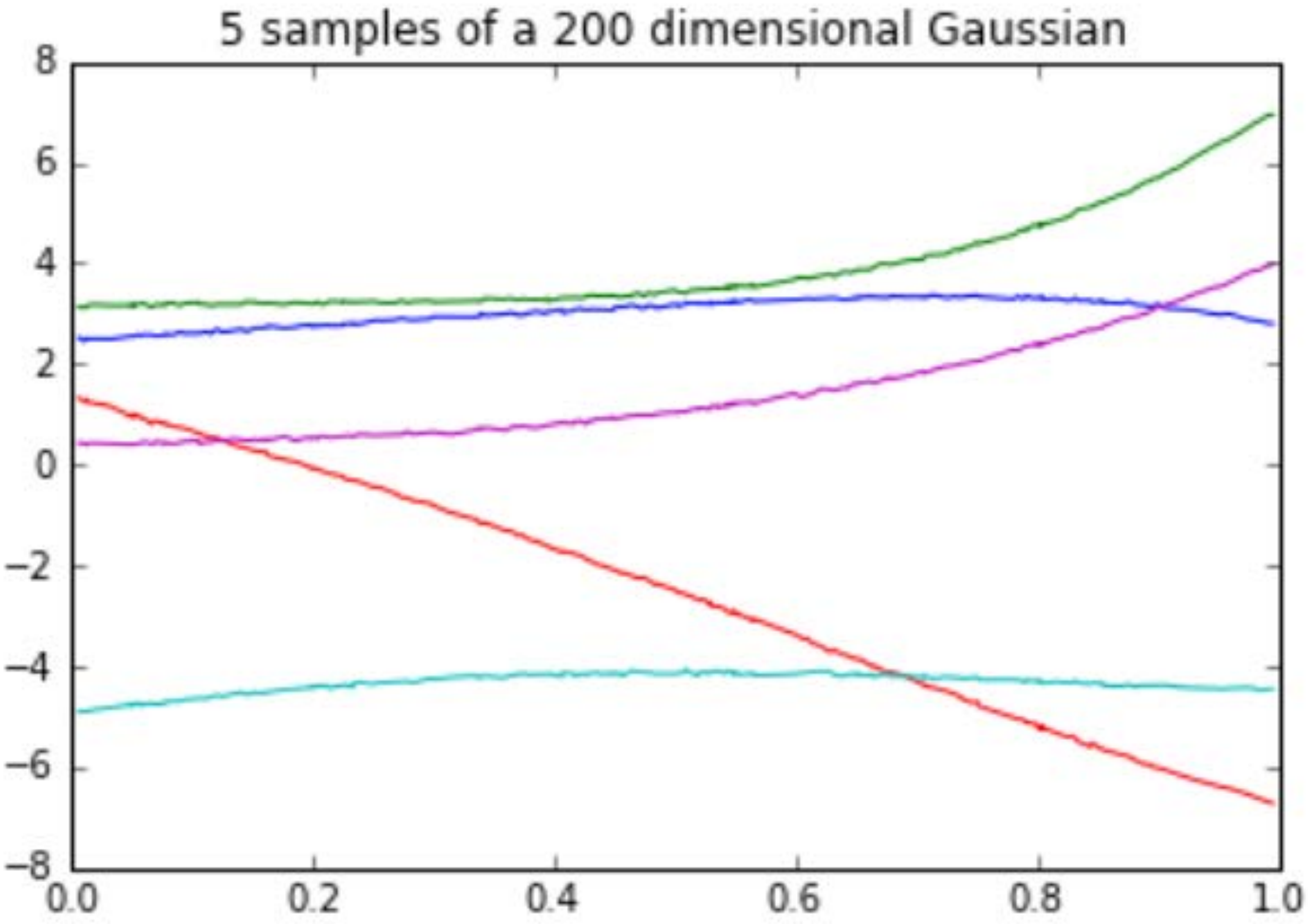


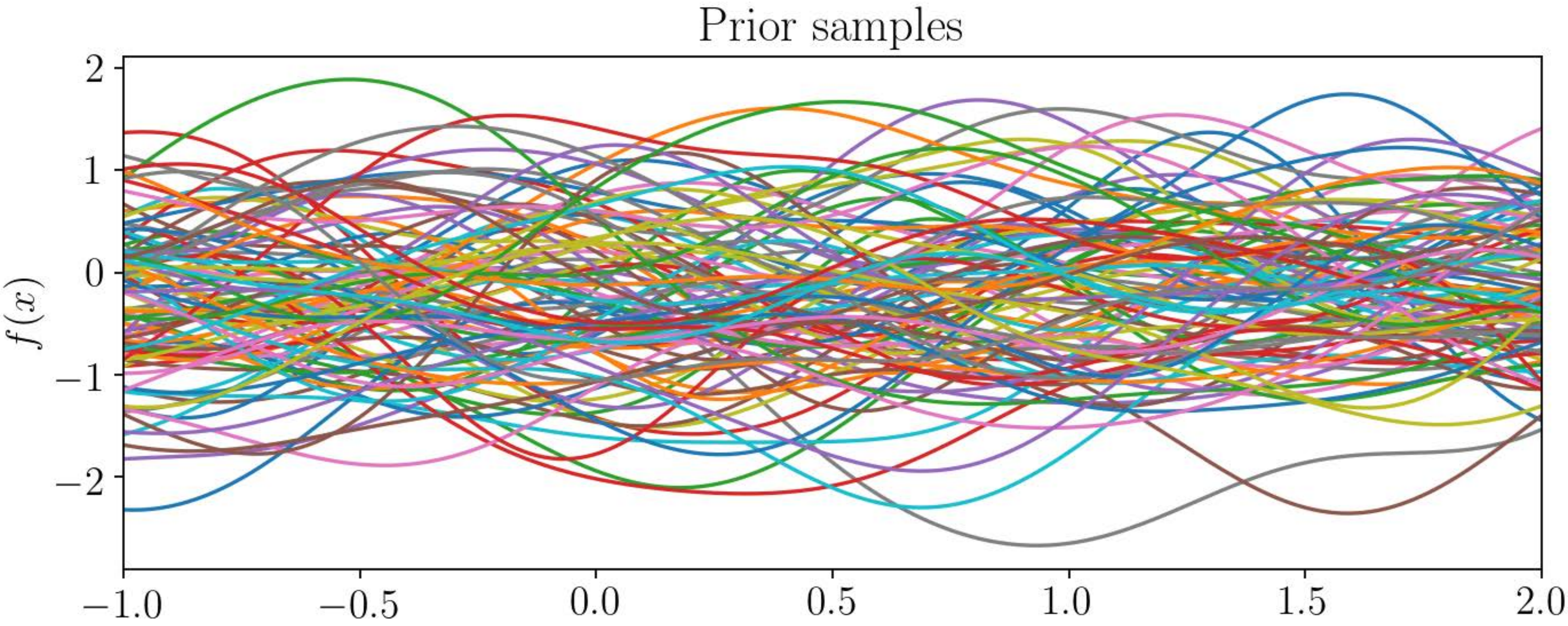
5 samples of a bivariate Gaussian.



5 samples from a bivariate Gaussian


5 samples of a 8 dimensional Gaussian
2
1
0
−1
−2
−3
−4
−5
−6
−7
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8


5 samples of a 200 dimensional Gaussian
8
6
4
2
0
−2
−4
−6
−8
0.0
0.2
0.4
0.6
0.8
1.0


Prior samples
f(x)
2
1
0
−1
−2
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

From linear regression to GPs:

- Linear regression with inputs x_i and outputs y_i: $$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$
- Linear regression with M basis functions: $$y_i = \sum_{m=1}^{M} \beta_m \, \phi_m(x_i) + \epsilon_i$$
- Bayesian linear regression with basis functions:

$$\beta_m \sim \mathrm{N}(\cdot|0, \lambda_m) \quad \text{(independent of } \beta_\ell,\ \forall \ell \neq m\text{)}, \qquad \epsilon_i \sim \mathrm{N}(\cdot|0, \sigma^2)$$

- Integrating out the coefficients, β_j, we find:

$$E[y_i] = 0, \qquad Cov(y_i, y_j) = K_{ij} \overset{\text{def}}{=} \sum_{m=1}^{M} \lambda_m \, \phi_m(x_i) \, \phi_m(x_j) + \delta_{ij}\sigma^2$$

This is a Gaussian process with covariance function $K(x_i, x_j) = K_{ij}$.

This GP has a finite number (M) of basis functions. Many useful GP kernels correspond to infinitely many basis functions (i.e. infinite-dim feature spaces).

A multilayer perceptron (neural network) with infinitely many hidden units and Gaussian priors on the weights → a GP (Neal, 1996)

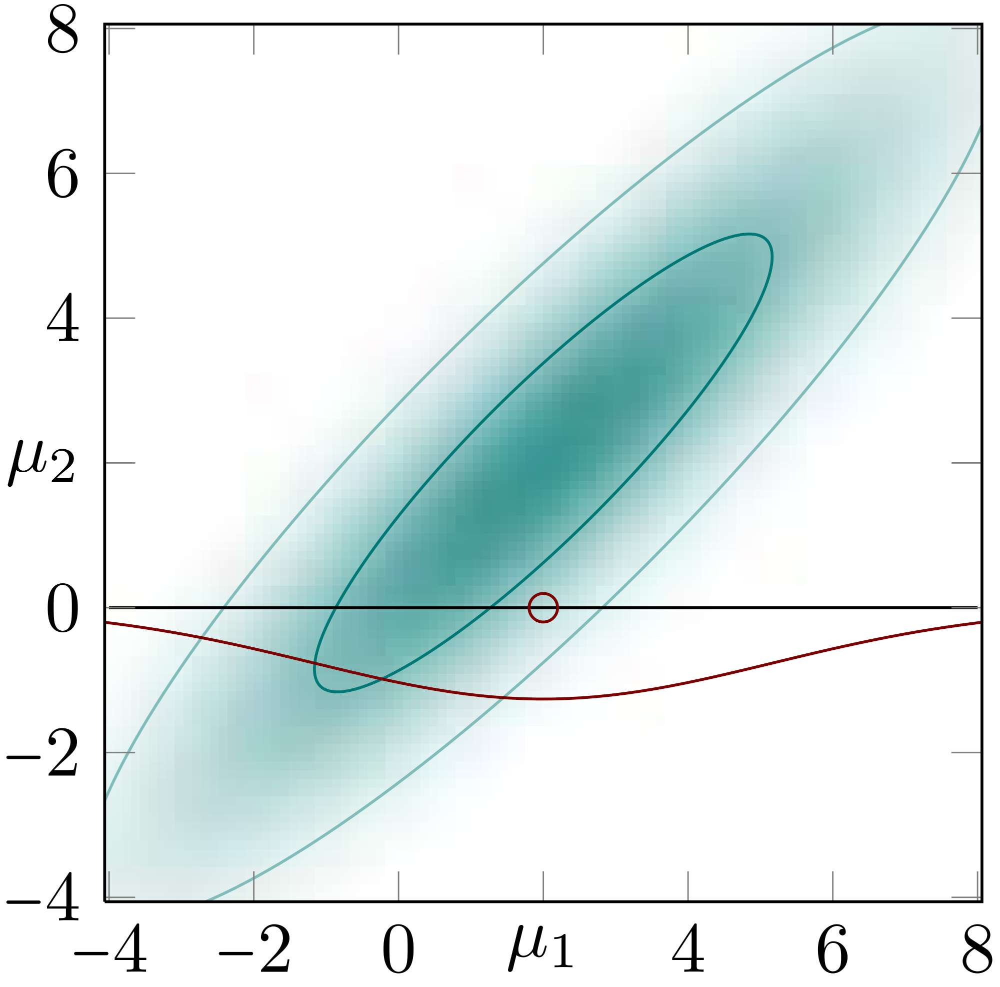
http://mlss2011.comp.nus.edu.sg/uploads/Site/lect1gp.pdf

Closure under Marginalization

projections of Gaussians are Gaussian

- projection with $A = \begin{pmatrix} 1 & 0 \end{pmatrix}$

$$\int \mathcal{N}\left[\begin{pmatrix} x \\ y \end{pmatrix}; \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix}\right] \mathrm{d}y = \mathcal{N}(x; \mu_x, \Sigma_{xx})$$



- this is the sum rule

$$\int p(x,y)\,\mathrm{d}y = \int p(y \mid x)p(x)\,\mathrm{d}y = p(x)$$

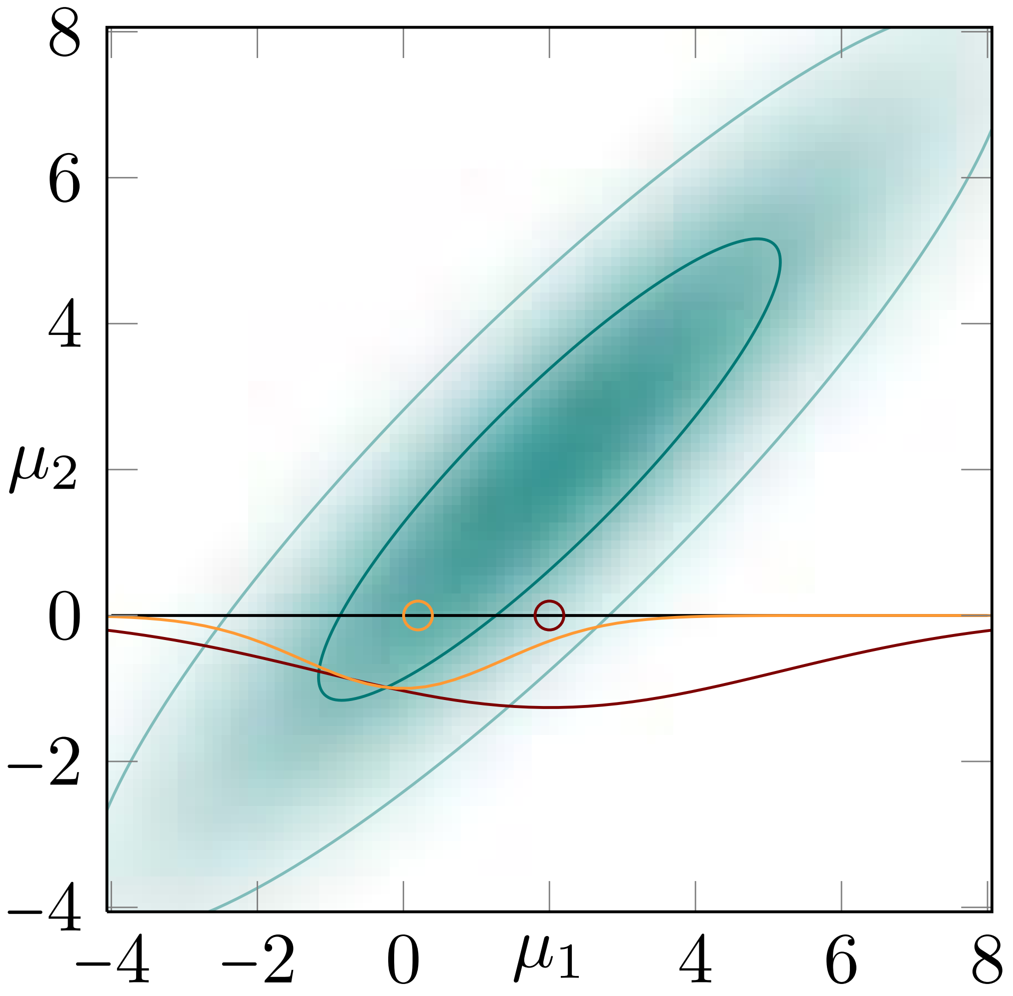
- so every finite-dim Gaussian is a marginal of infinitely many more

http://mlss.tuebingen.mpg.de/2013/2013/hennig_slides1.pdf

Closure under Conditioning

cuts through Gaussians are Gaussians

$$p(x \mid y) = \frac{p(x,y)}{p(y)} = \mathcal{N}\left(x; \mu_x + \Sigma_{xy}\Sigma_{yy}^{-1}(y - \mu_y), \Sigma_{xx} - \Sigma_{xy}\Sigma_{yy}^{-1}\Sigma_{yx}\right)$$



- this is the product rule
- so Gaussians are closed under the rules of probability

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Using Gaussian processes for nonlinear regression

Imagine observing a data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)_{i=1}^n\} = (\mathbf{X}, \mathbf{y})$.

Model:

$$\begin{aligned} y_i &= f(\mathbf{x}_i) + \epsilon_i \\ f &\sim \mathsf{GP}(\cdot|0, K) \\ \epsilon_i &\sim \mathsf{N}(\cdot|0, \sigma^2) \end{aligned}$$

Prior on f is a GP, likelihood is Gaussian, therefore posterior on f is also a GP.

We can use this to make predictions

$$p(y_*|\mathbf{x}_*, \mathcal{D}) = \int p(y_*|\mathbf{x}_*, f, \mathcal{D})\, p(f|\mathcal{D})\, df$$

We can also compute the marginal likelihood (evidence) and use this to compare or tune covariance functions

$$p(\mathbf{y}|\mathbf{X}) = \int p(\mathbf{y}|f, \mathbf{X})\, p(f)\, df$$

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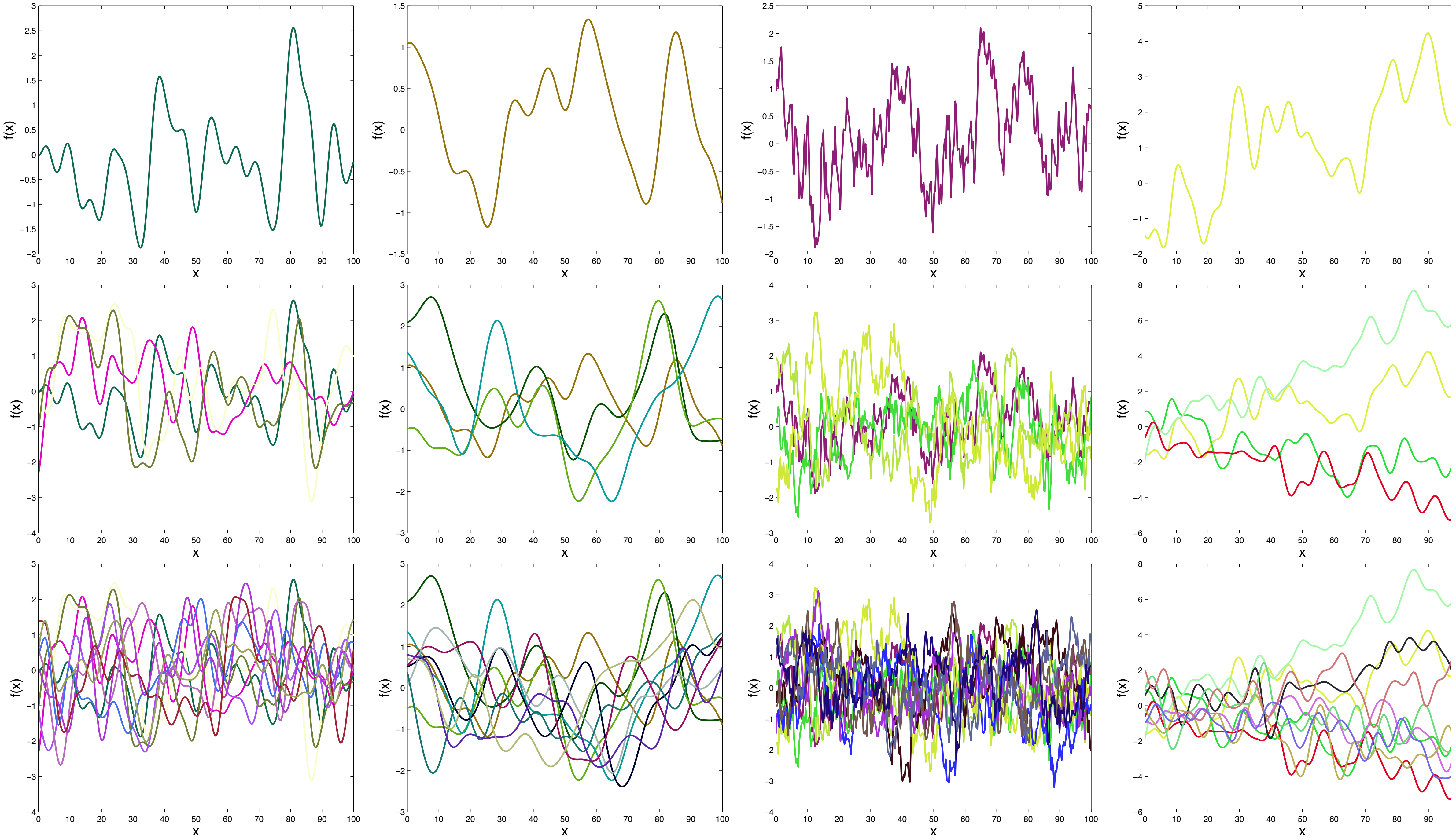
Samples from GPs with different $K(x, x')$



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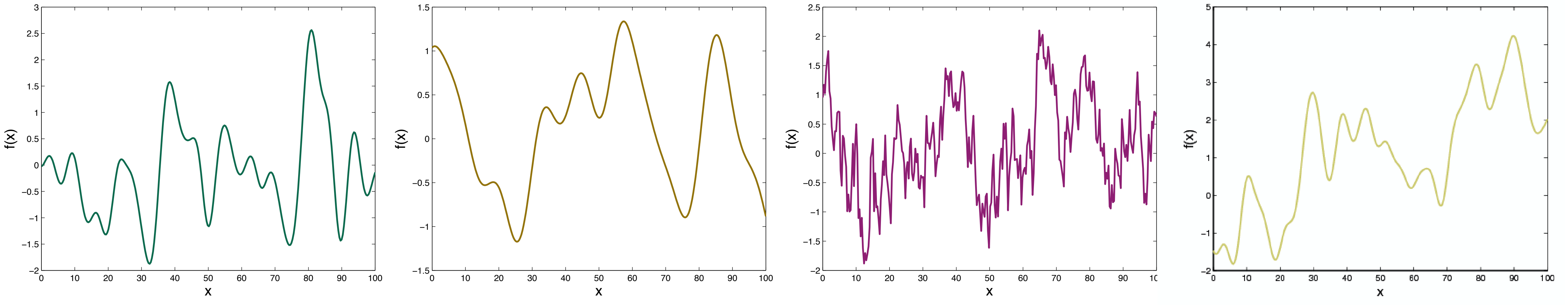
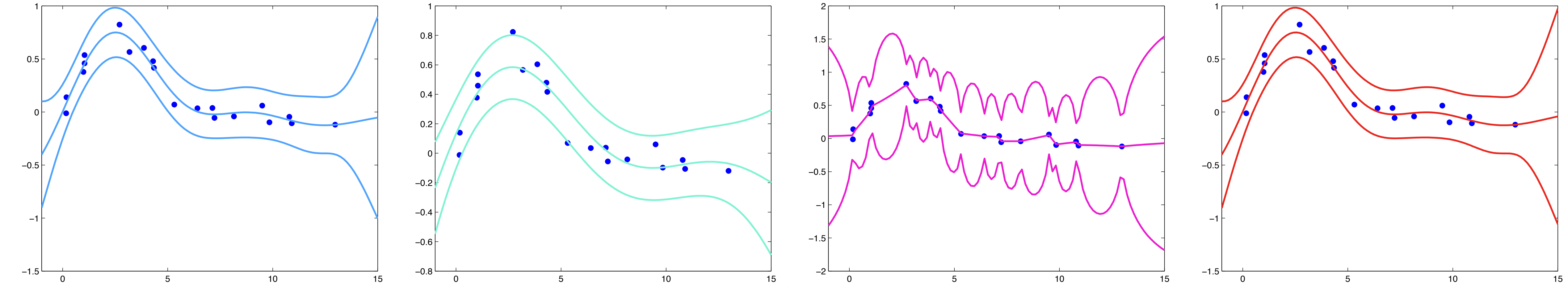
Prediction using GPs with different $K(x, x')$

A sample from the prior for each covariance function:



Corresponding predictions, mean with two standard deviations:



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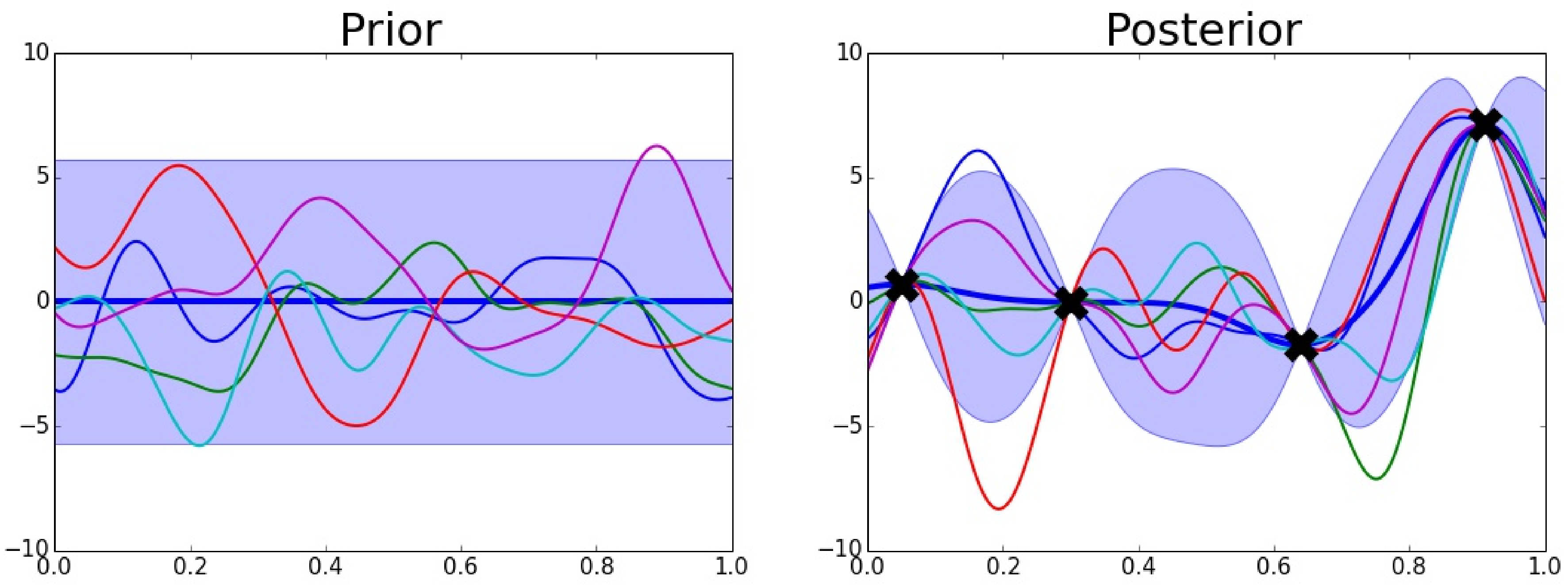
Data-driven modeling with Gaussian processes

$$y = f(\boldsymbol{x}) + \epsilon \qquad f \sim \mathcal{GP}(0, k(\boldsymbol{x}, \boldsymbol{x}'; \boldsymbol{\theta}))$$



<u>Training via maximizing the marginal likelihood</u>

$$\log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) = -\frac{1}{2}\log|\boldsymbol{K} + \sigma_\epsilon^2 \boldsymbol{I}| - \frac{1}{2}\boldsymbol{y}^T(\boldsymbol{K} + \sigma_\epsilon^2 \boldsymbol{I})^{-1}\boldsymbol{y} - \frac{N}{2}\log 2\pi$$

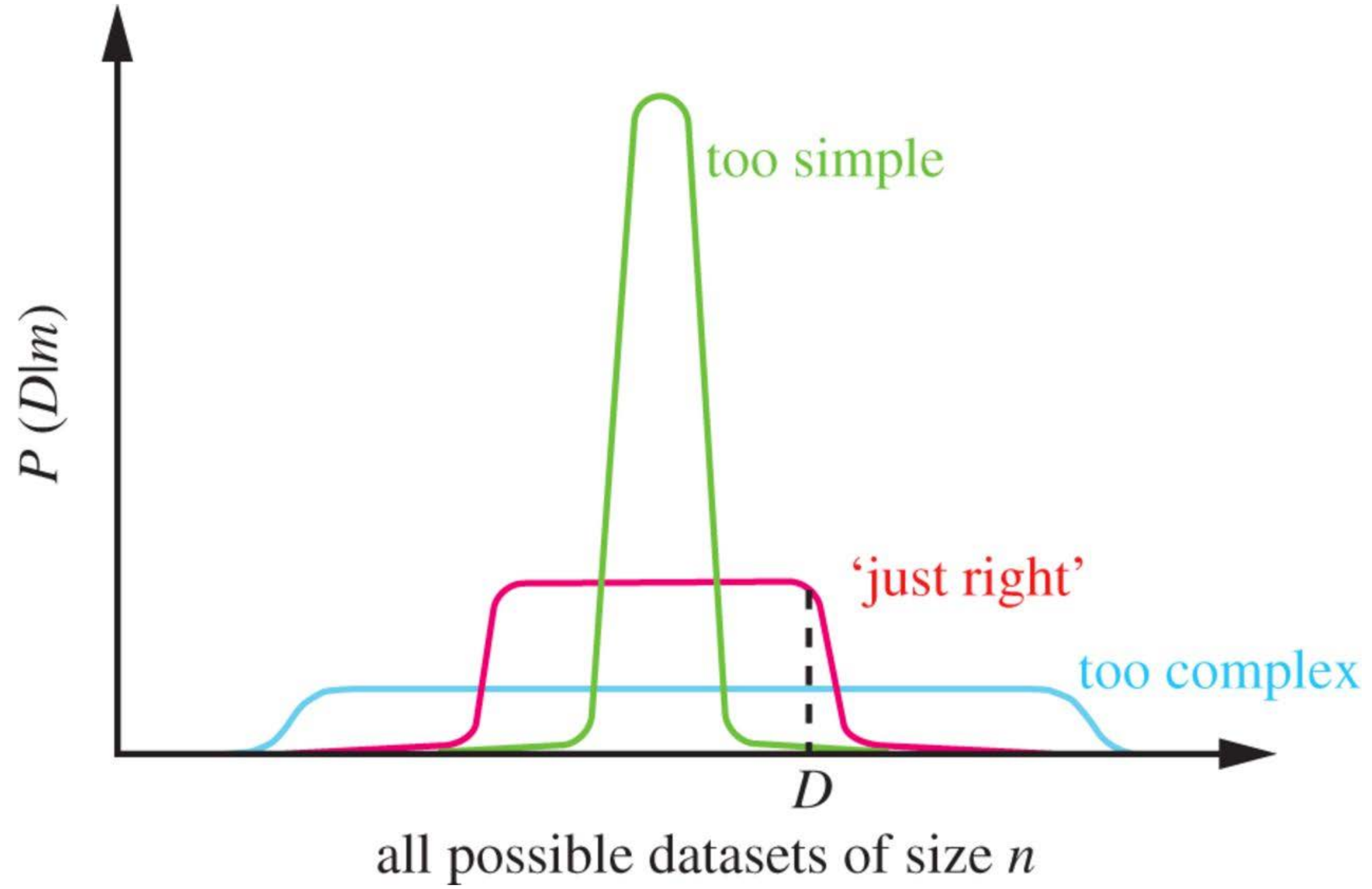
<u>Prediction via conditioning on available data</u>

$$\begin{aligned} p(f_*|\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{x}_*) &= \mathcal{N}(f_*|\mu_*, \sigma_*^2), \\ \mu_*(\boldsymbol{x}_*) &= \boldsymbol{k}_{*N}(\boldsymbol{K} + \sigma_\epsilon^2 \boldsymbol{I})^{-1}\boldsymbol{y}, \\ \sigma_*^2(\boldsymbol{x}_*) &= \boldsymbol{k}_{**} - \boldsymbol{k}_{*N}(\boldsymbol{K} + \sigma_\epsilon^2 \boldsymbol{I})^{-1}\boldsymbol{k}_{N*}, \end{aligned}$$

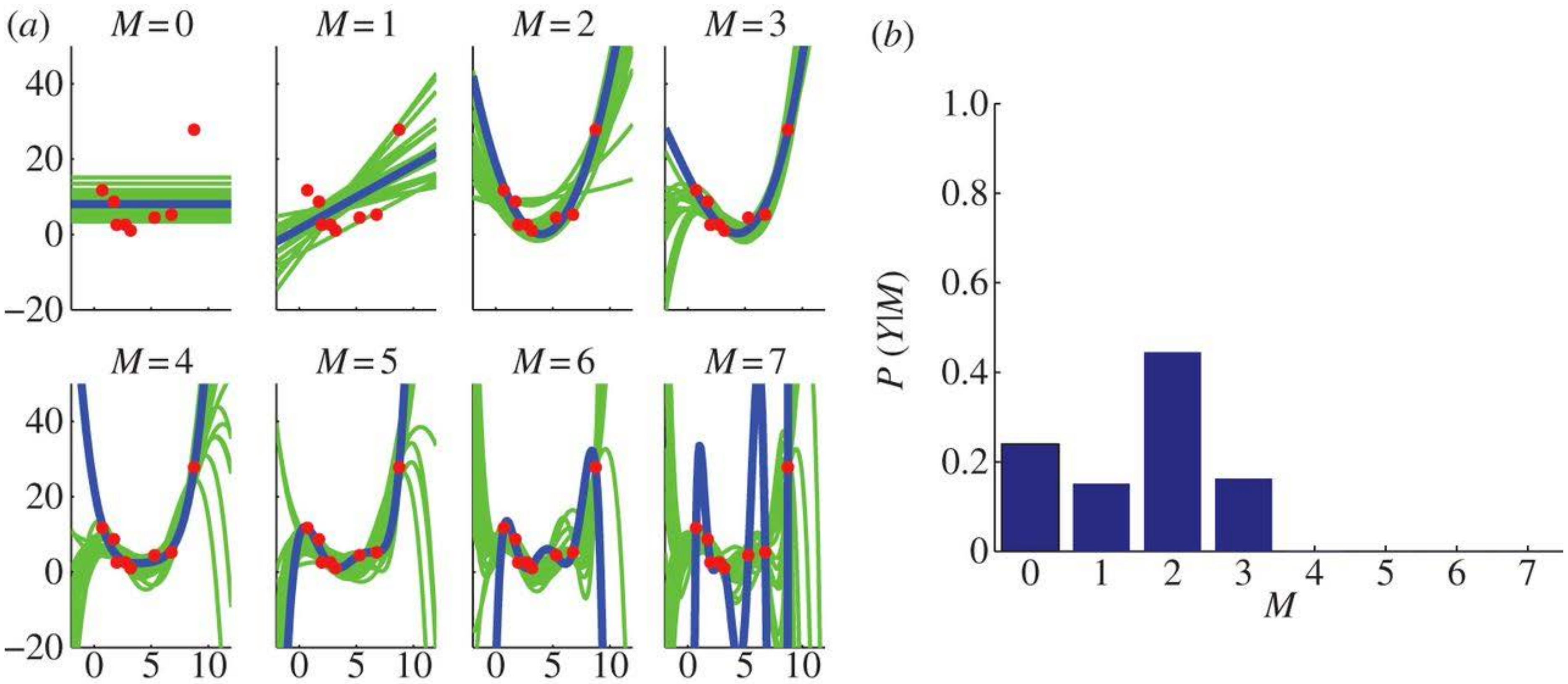
Demo code: https://github.com/PredictiveIntelligenceLab/GPTutorial

Occam's razor

William of Ockham (~1285-1347 A.D)



"plurality should not be posited without necessity."



Ghahramani, Z. (2013). Bayesian non-parametrics and the probabilistic approach to modelling. Phil. Trans. R. Soc. A, 371(1984), 20110553.