ENM 531: Data-driven Modeling and Probabilistic Scientific Computing

Lecture #21: Kernel methods

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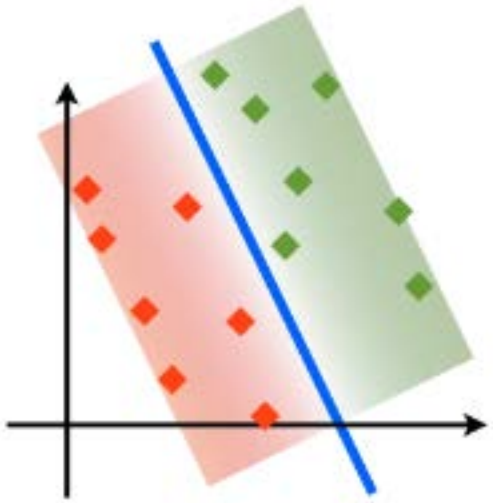
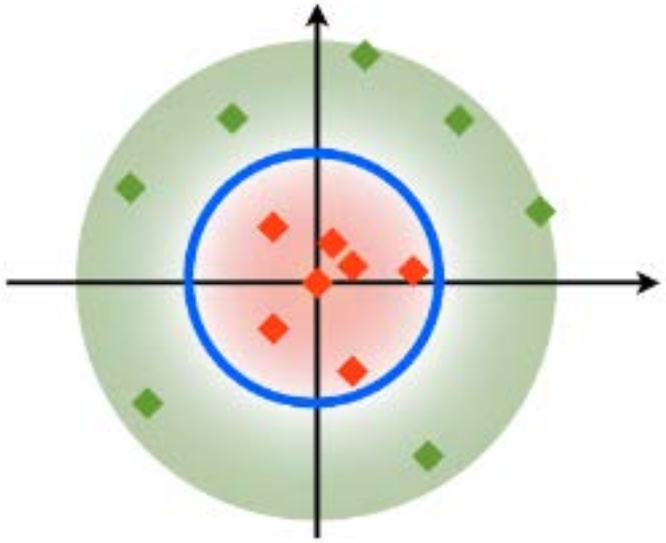
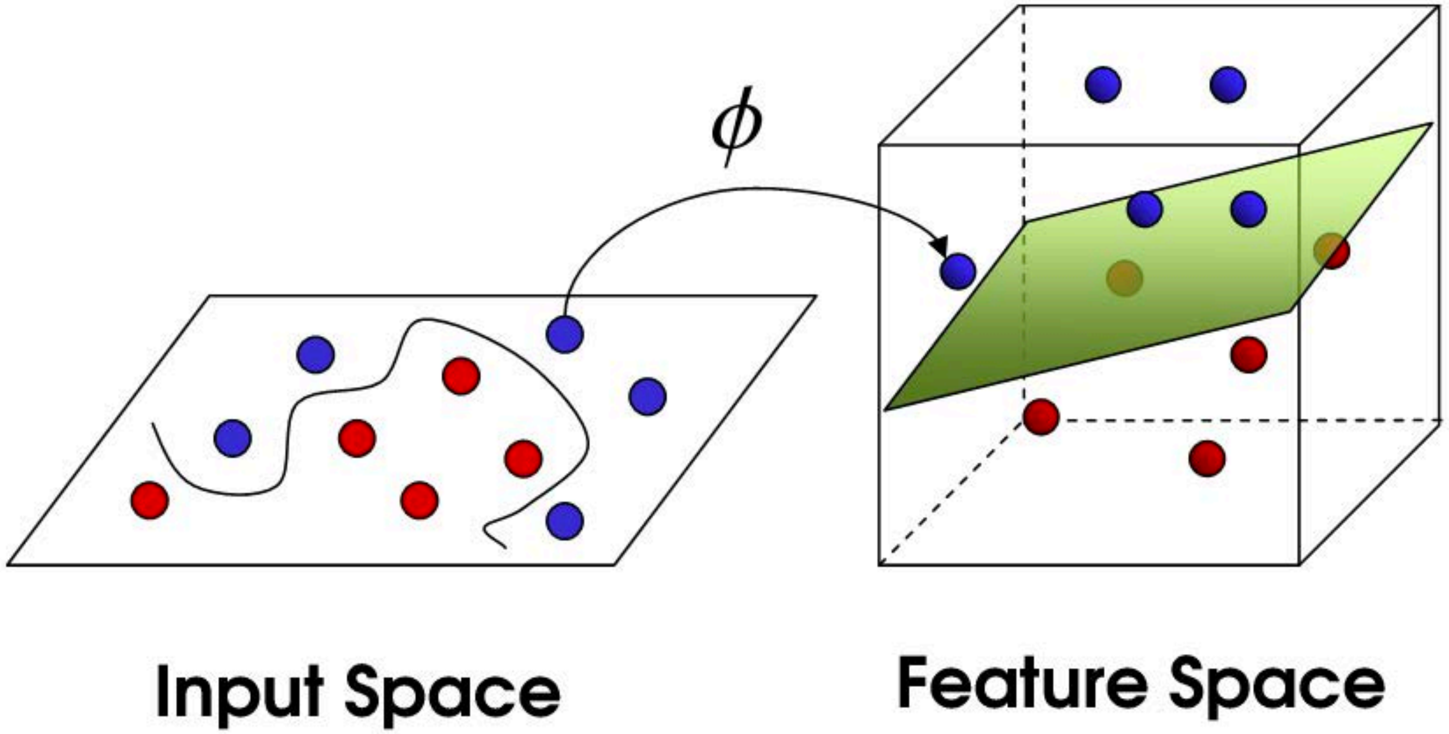
“Linearization” by embedding to higher dimensions

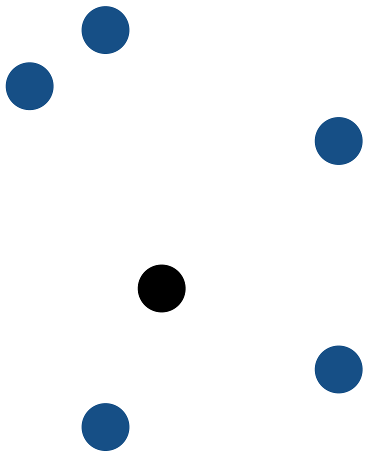
$$f(\boldsymbol{x}) = \langle \theta, \phi(\boldsymbol{x}) \rangle_{\mathcal{H}}, \quad \phi : \mathbb{R}^d \to \mathbb{R}^m$$







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.

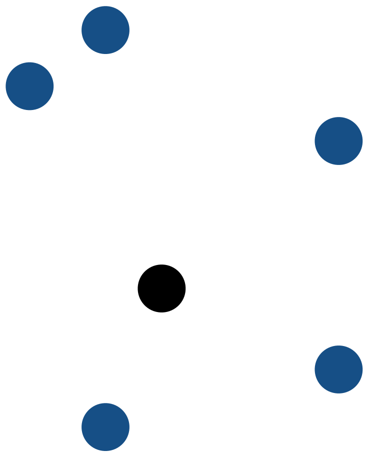
-Analysis of well-specified models: When the target function is in the associated function space, learning can be done with rates that are independent of dimension.

-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

Kernel methods



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

Why is this relevant? The study of infinite-dimensional linear methods is important for several reasons:

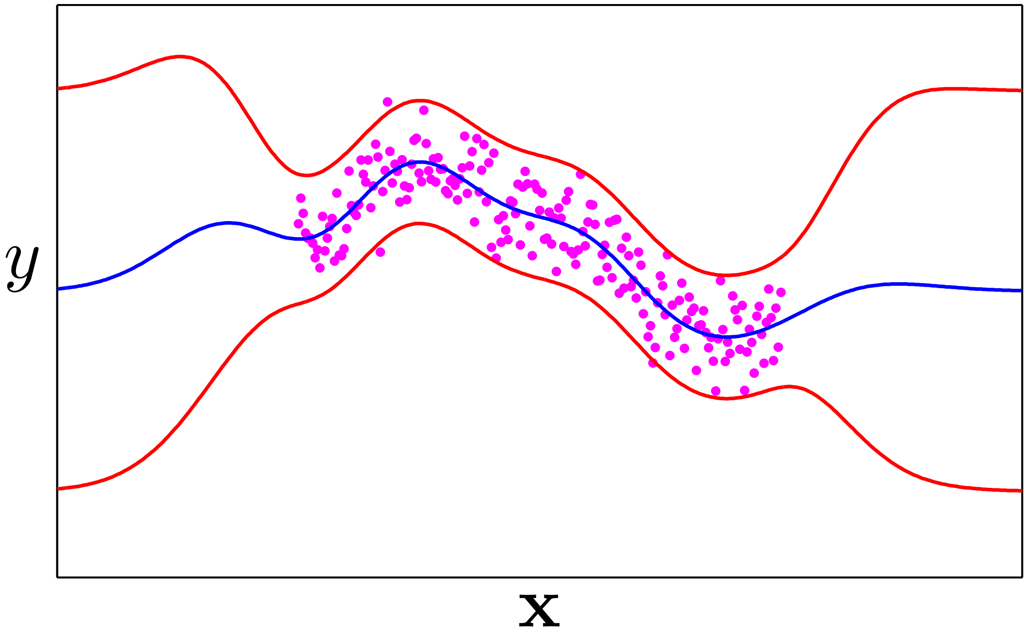
- Understanding linear models in finite but very large input dimensions requires tools from infinite-dimensional analysis.
- Kernel methods lead to simple and stable algorithms, with theoretical guarantees, and adaptivity to smoothness of the target functon (as opposed to local averaging techniques). They can be applied in high dimensions, with good practical performance (note that for supervised learning problems with many observations in domains such as computer vision and natural language processing, they do not achieve the state of the art anymore, which is achieved by neural networks presented in Chapter 9).
- They can be easily applied when input observations are not vectors.
- They are useful to understand other models such as neural networks (see Chapter 9).

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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Carl Friedrich Gauss (1777–1855)

Paying Tolls with A Bell

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

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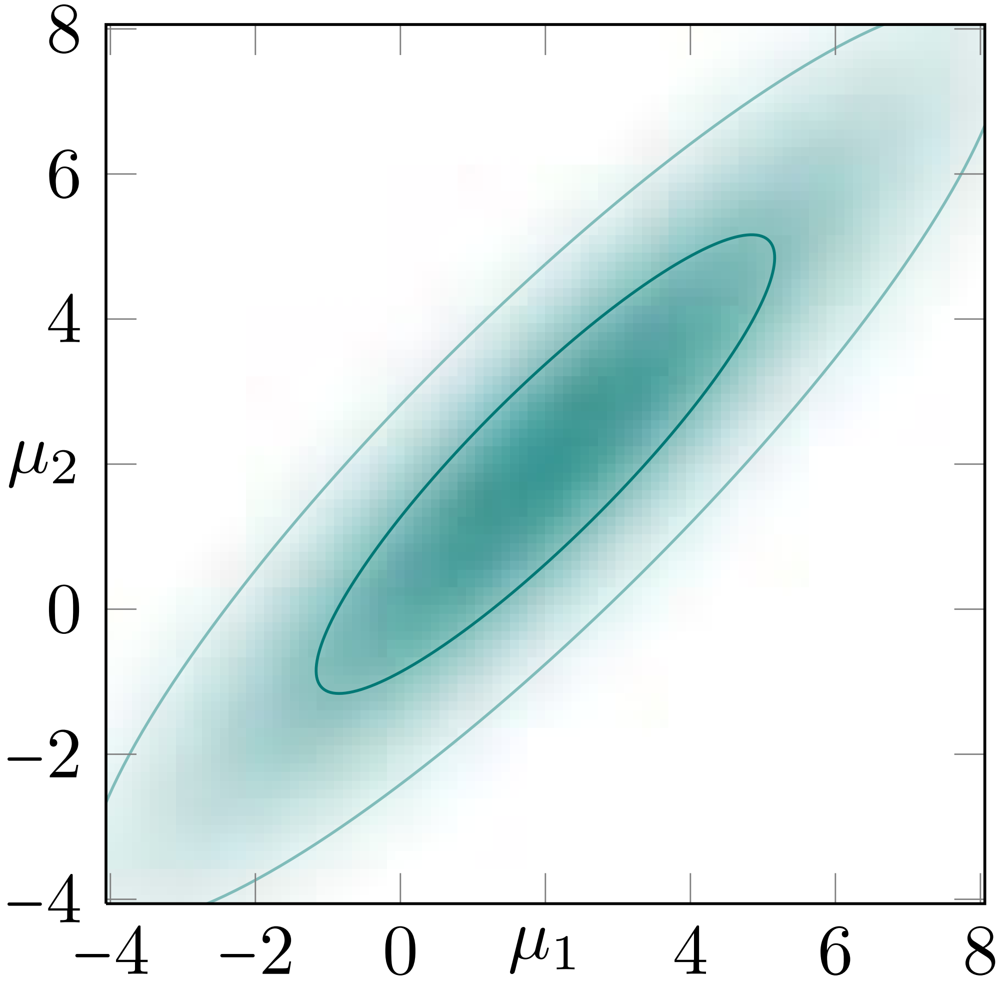
The Gaussian distribution

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

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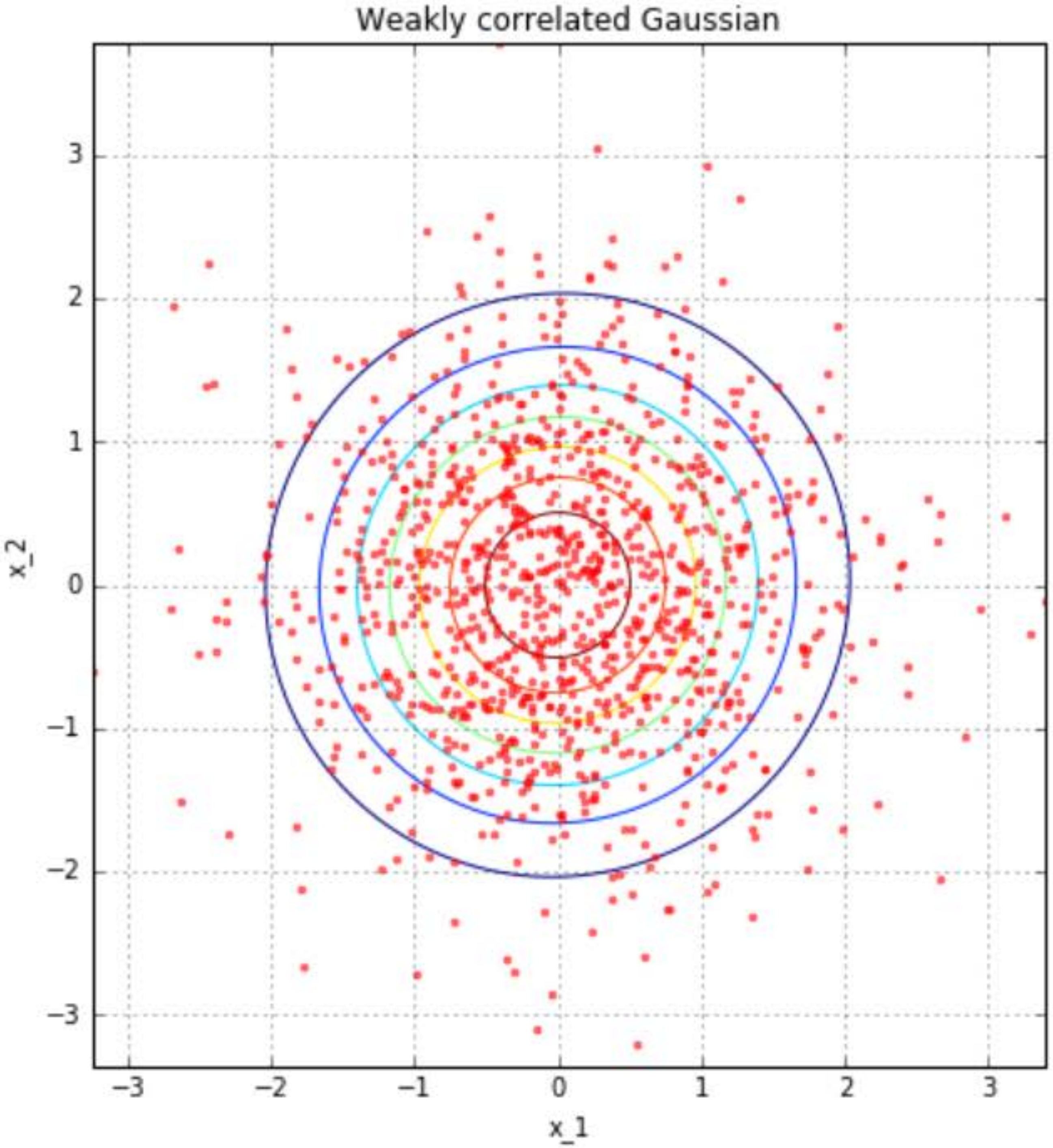
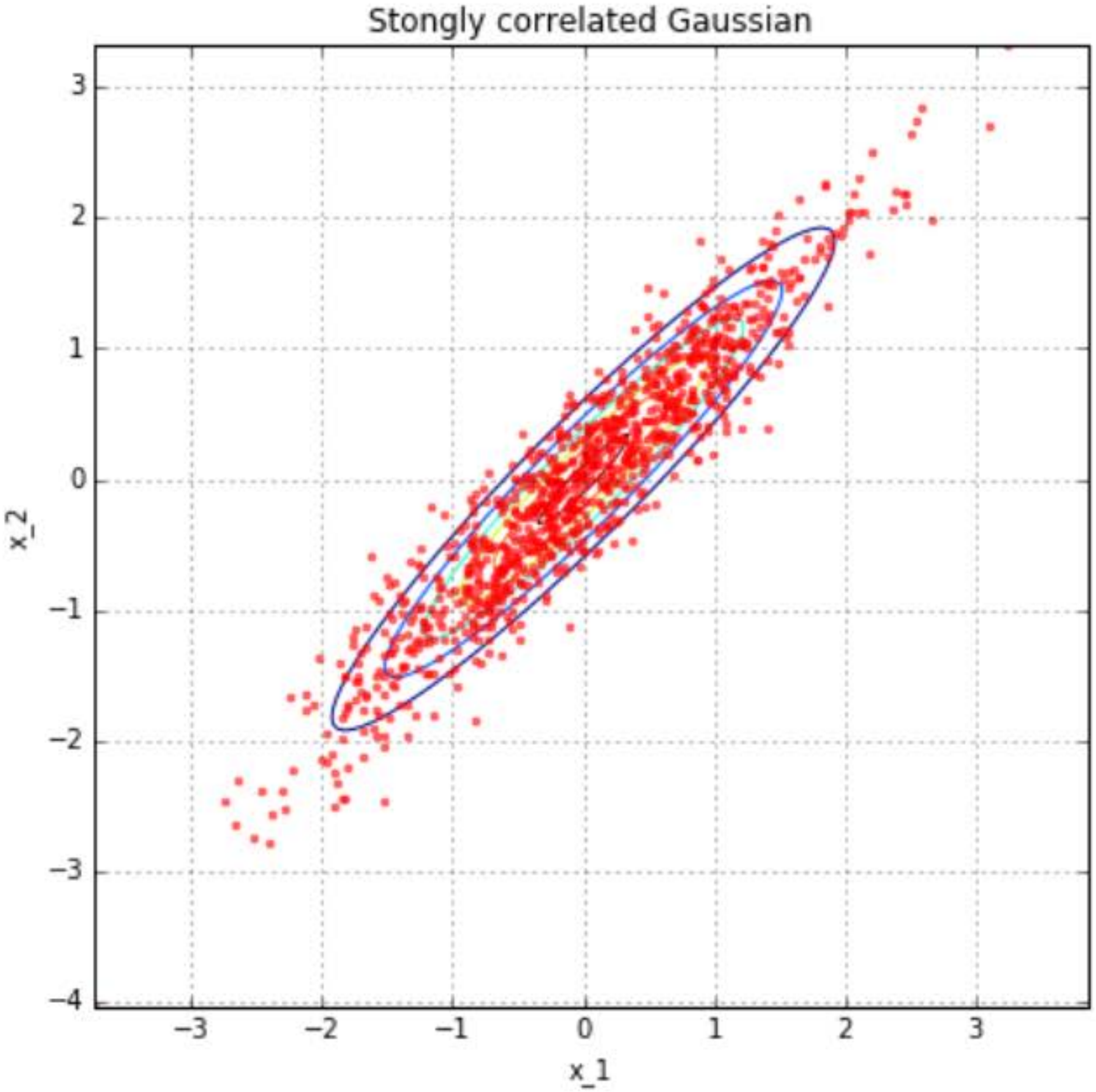
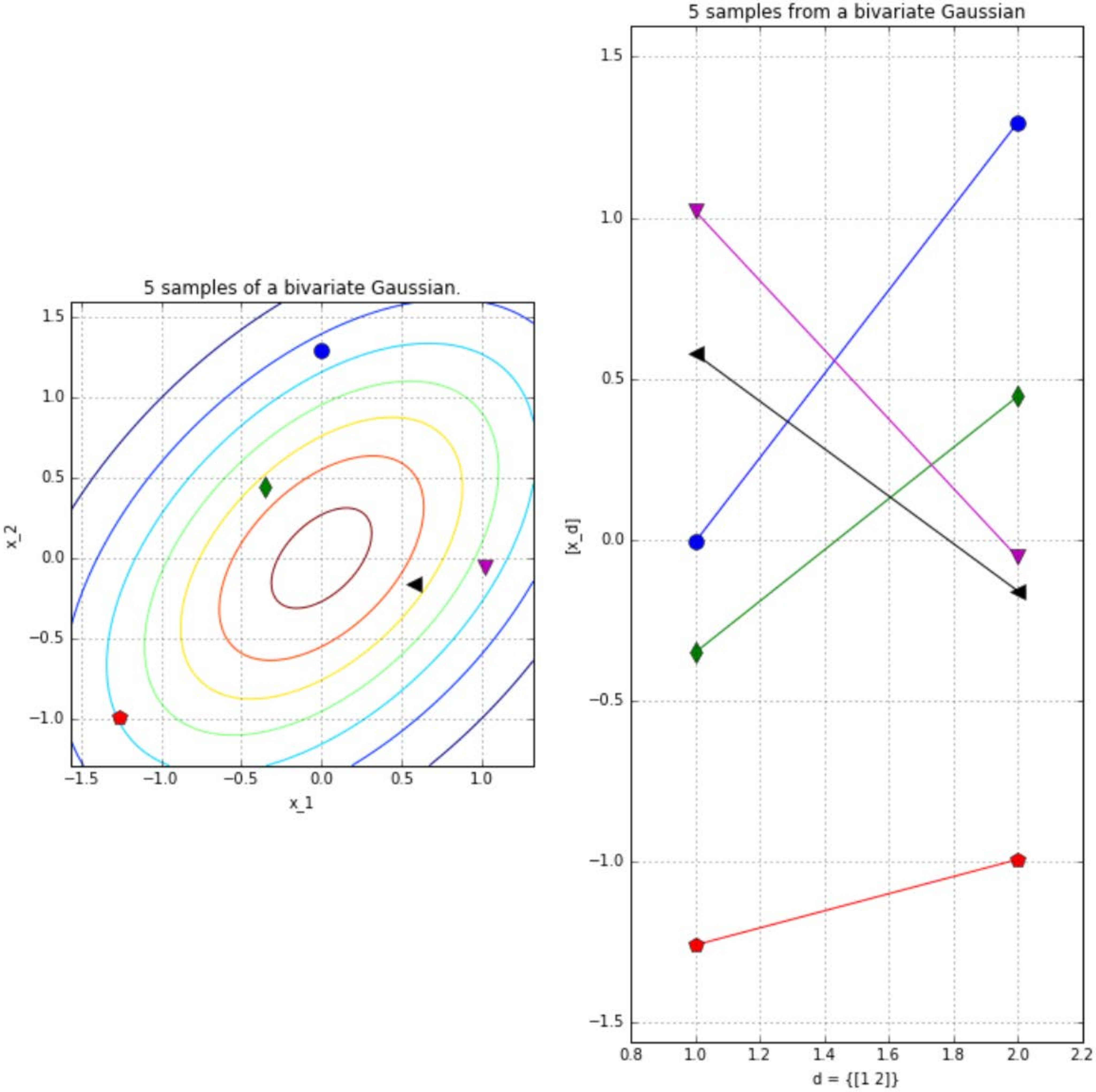
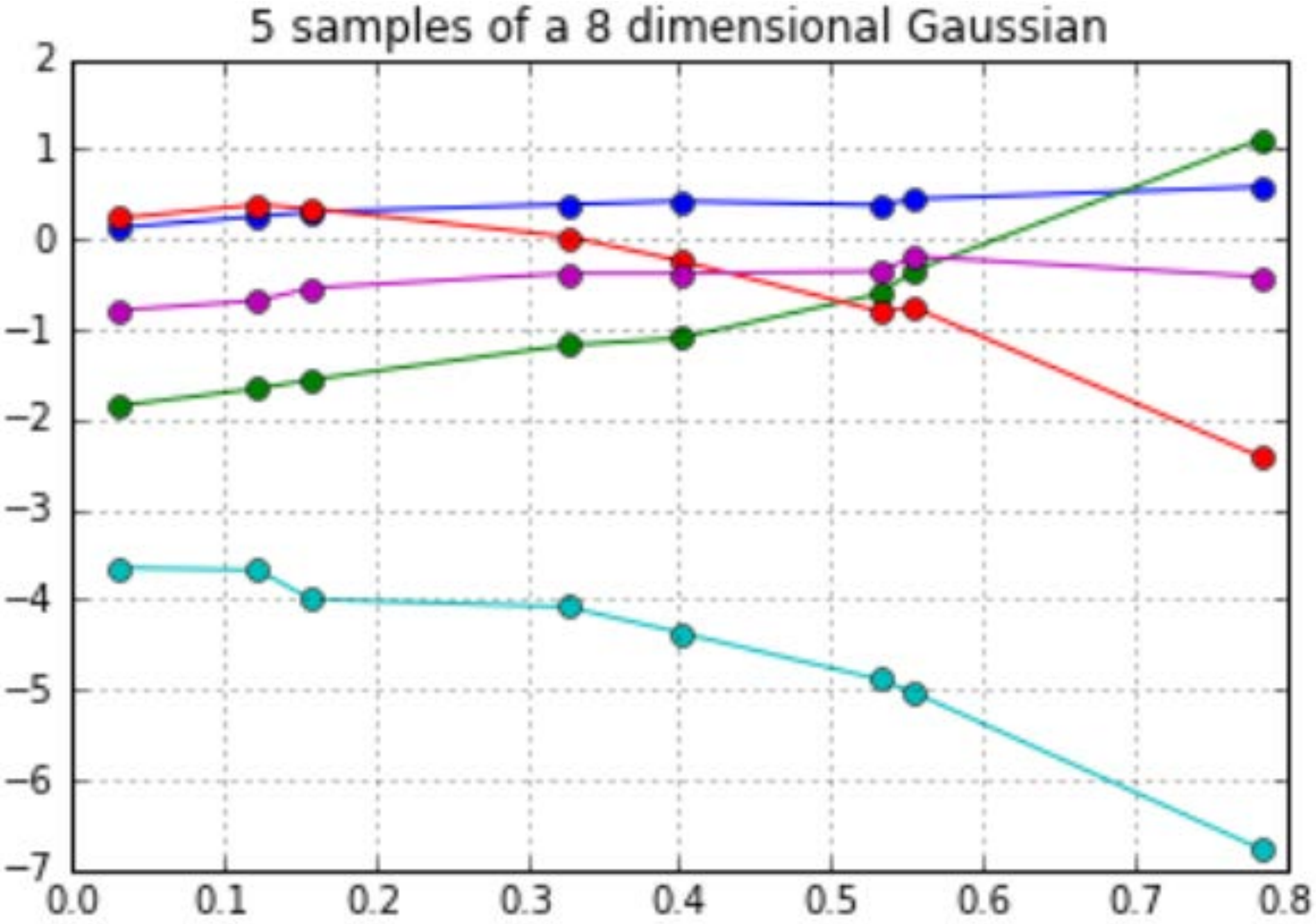


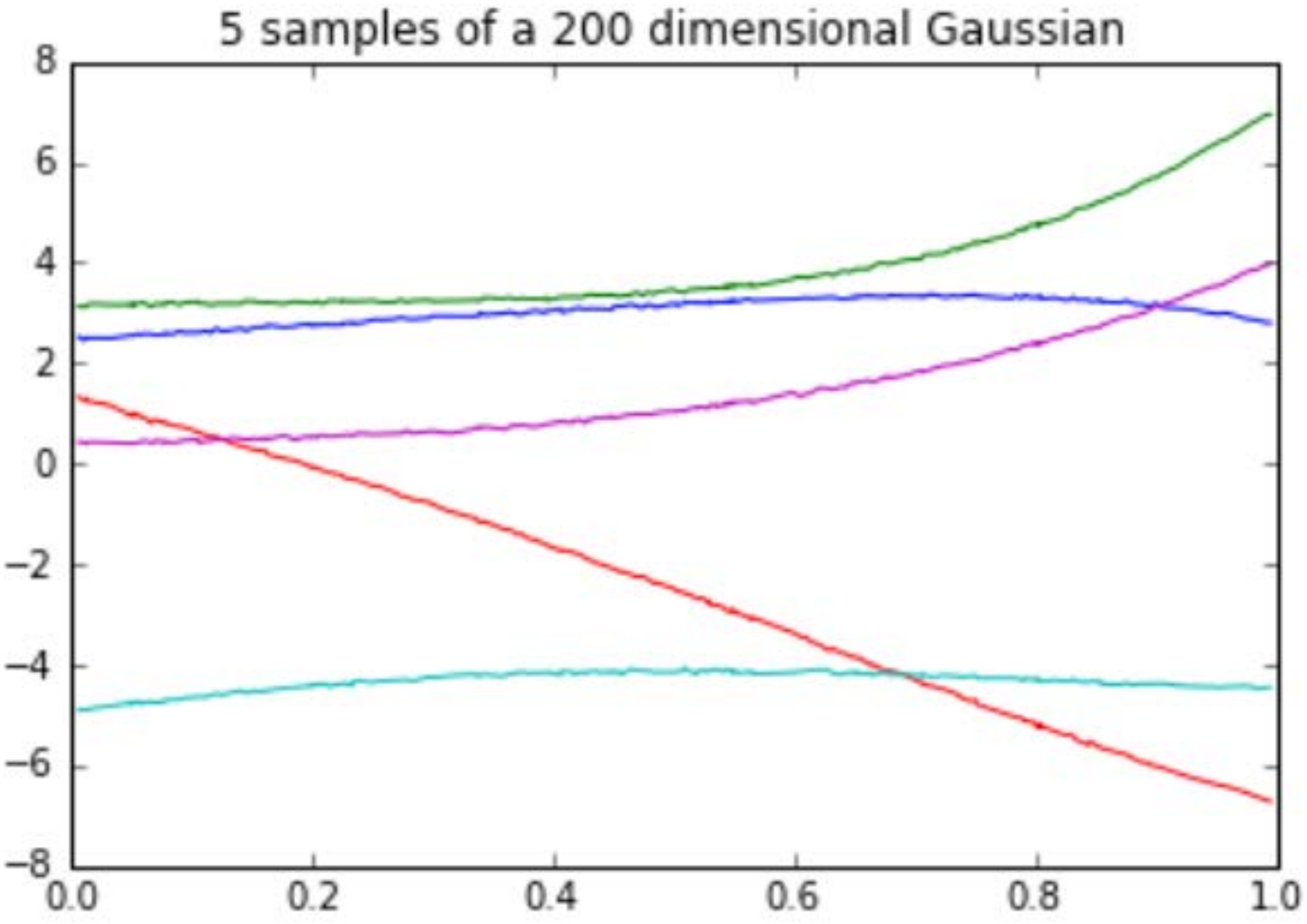
Weakly correlated Gaussian

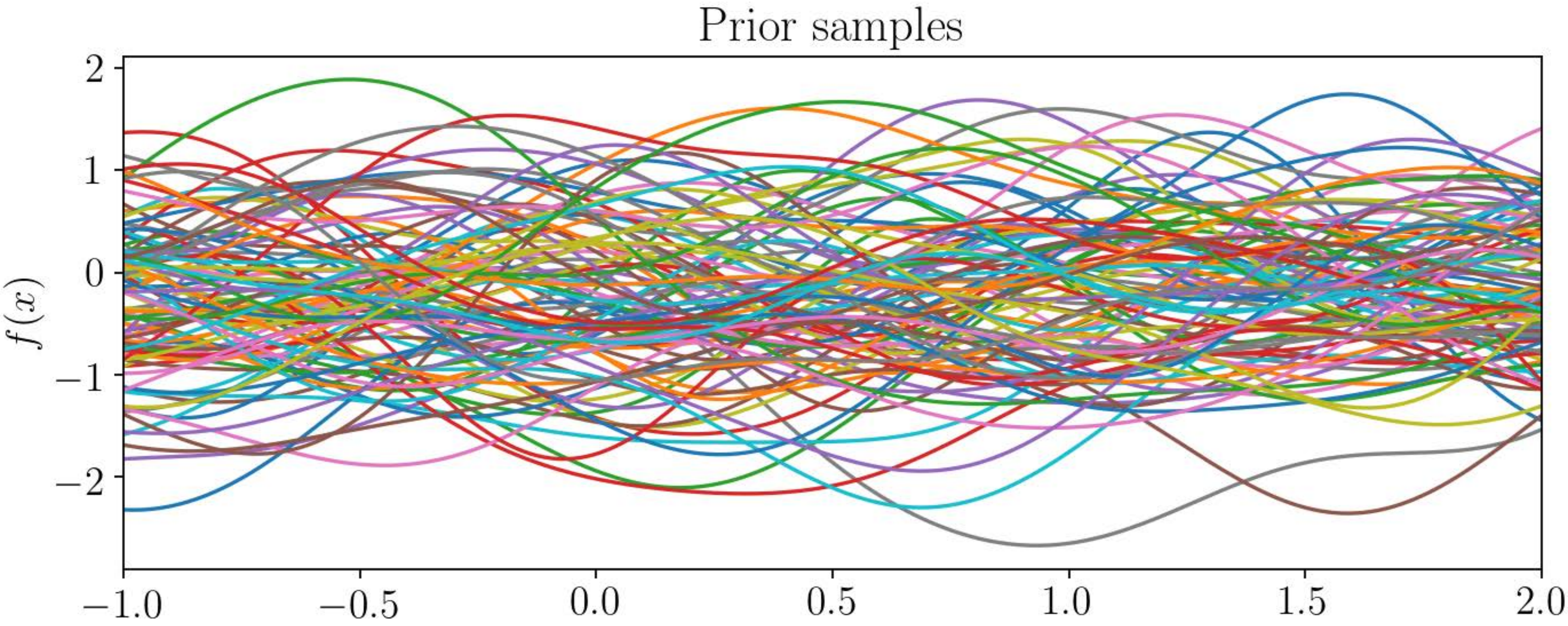


Stongly correlated Gaussian


5 samples of a bivariate Gaussian.
x_2
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
x_1
5 samples from a bivariate Gaussian
[x_d]
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
d = {[1 2]}


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:

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

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)

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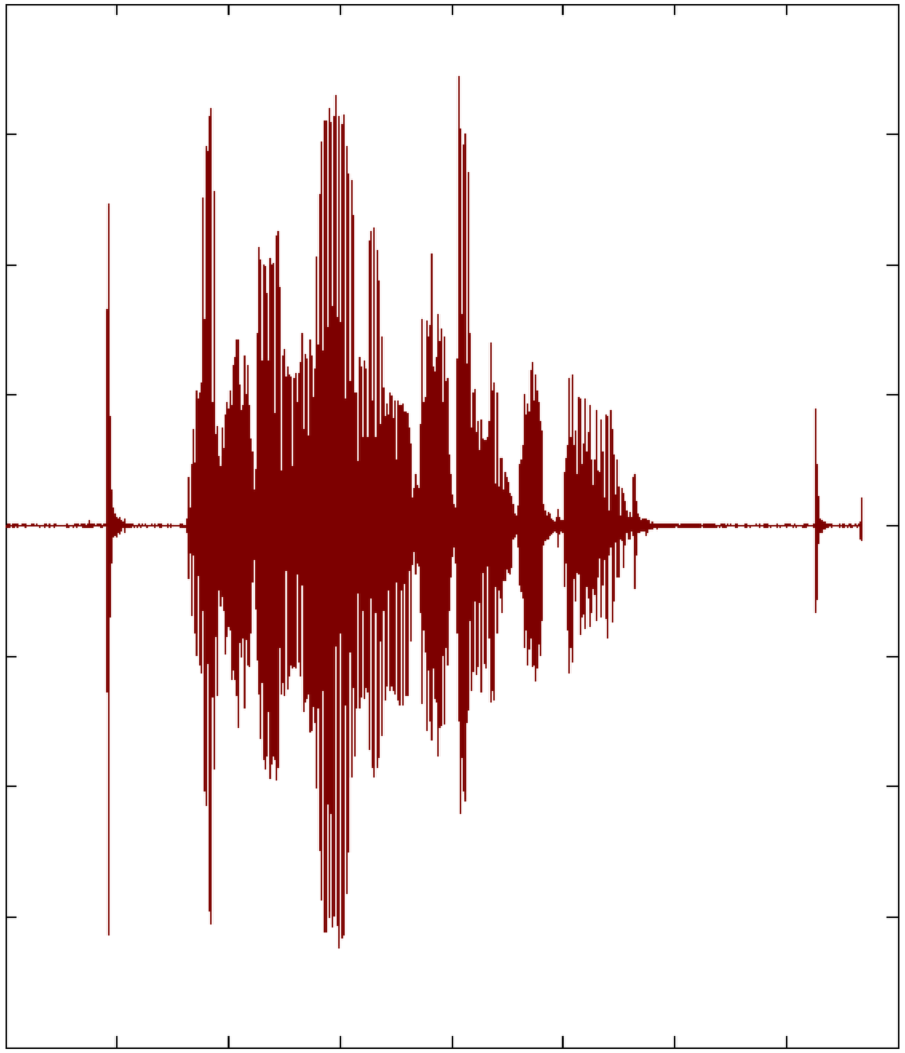
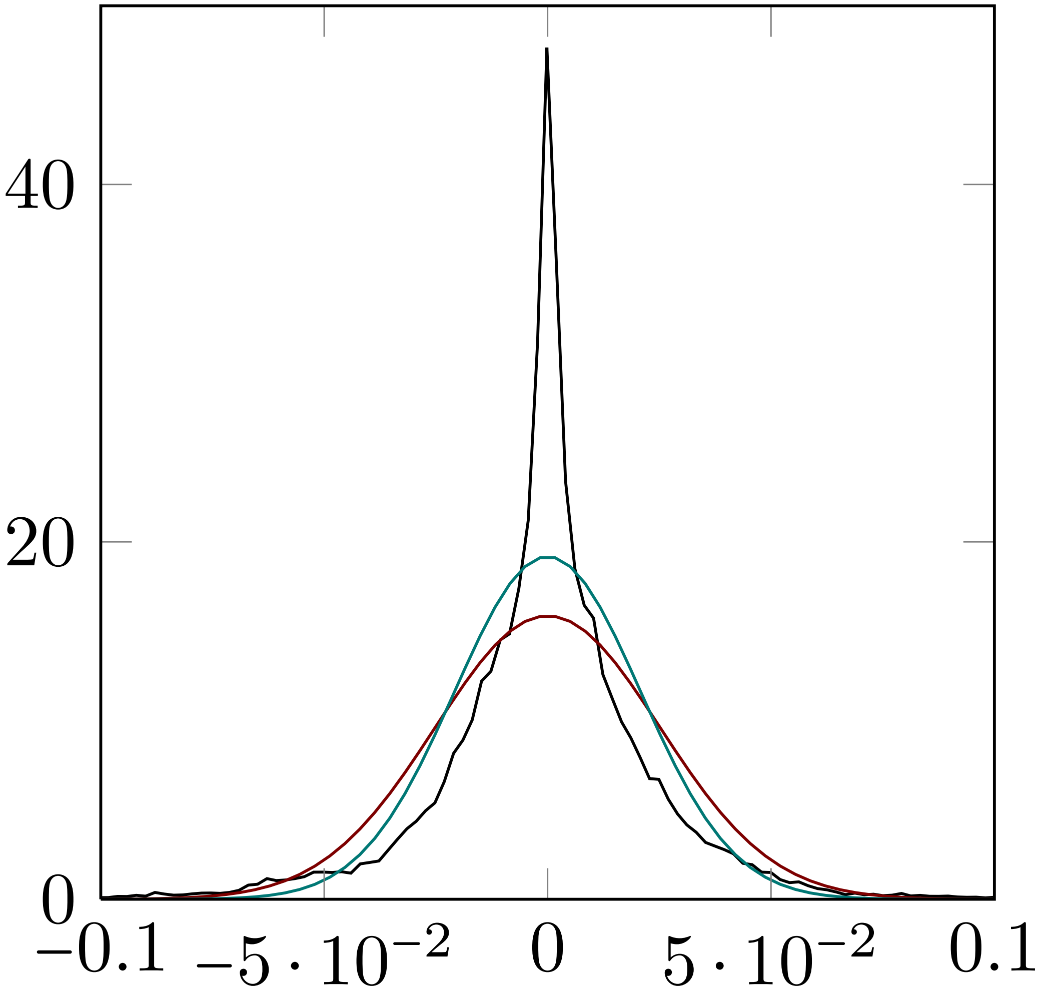
Why Gaussian?

an experiment





- nothing in the real world is Gaussian (except sums of i.i.d. variables)
- But nothing in the real world is linear either!

Gaussians are for inference what linear maps are for algebra.

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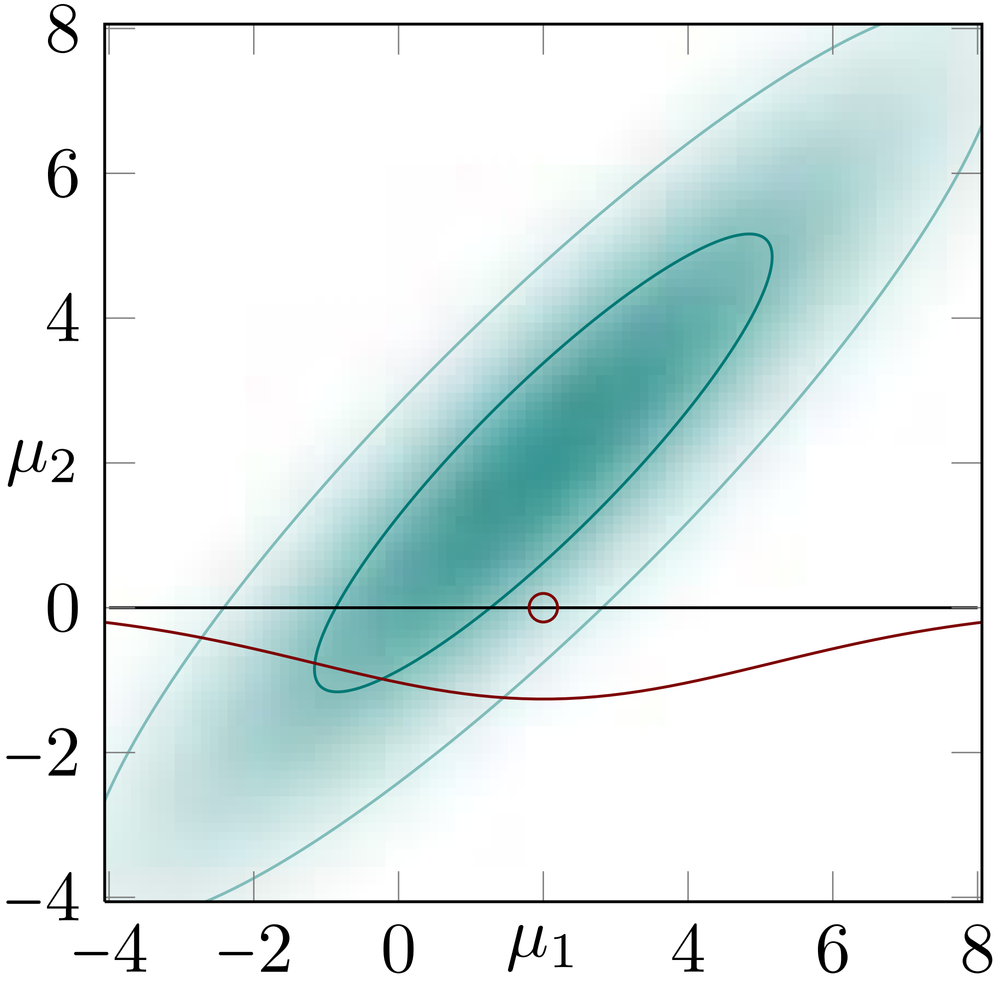
Closure under Marginalization

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

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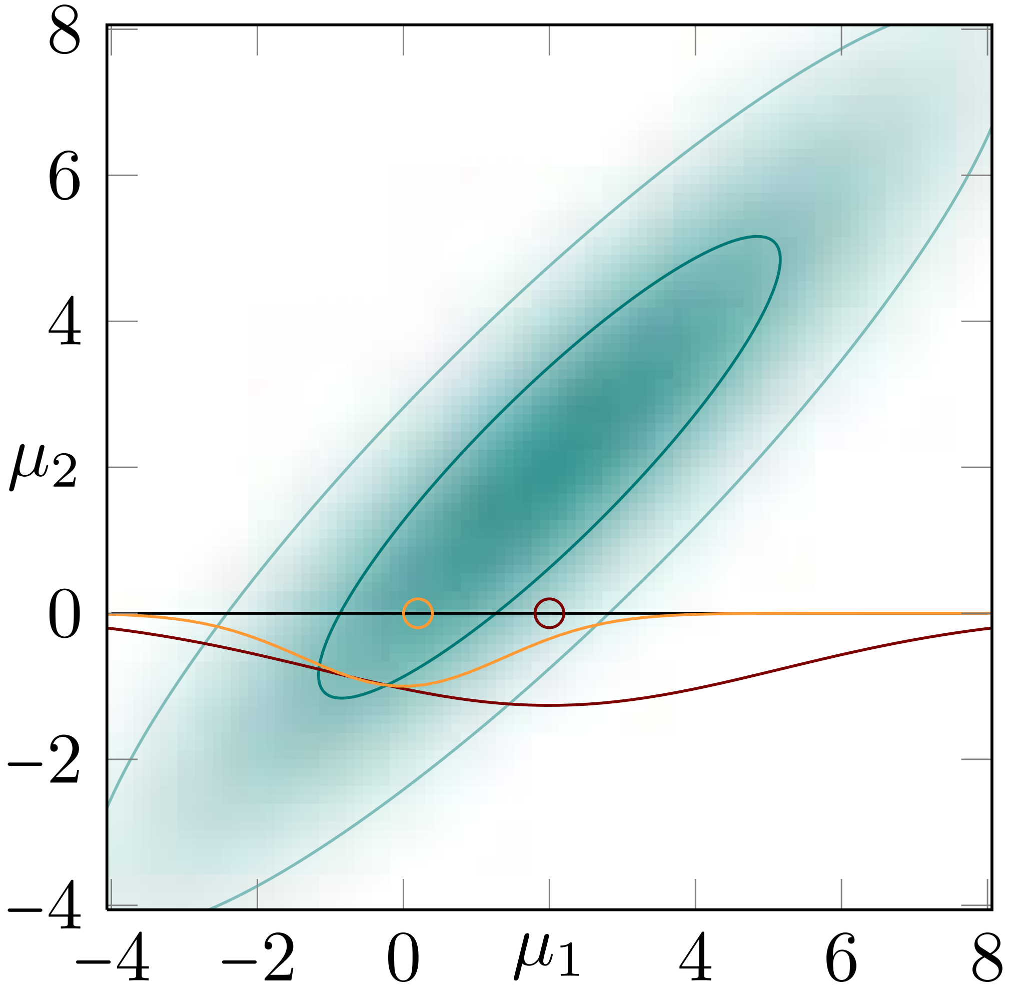
Closure under Conditioning

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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Gaussian process covariance functions (kernels)

$p(f)$ is a Gaussian process if for *any* finite subset $\{x_1, \ldots, x_n\} \subset \mathcal{X}$, the marginal distribution over that finite subset $p(\mathbf{f})$ has a multivariate Gaussian distribution.

Gaussian processes (GPs) are parameterized by a mean function, $\mu(x)$, and a covariance function, or kernel, $K(x, x')$.

$$p(f(x), f(x')) = \mathsf{N}(\mu, \Sigma)$$

where

$$\mu = \begin{bmatrix} \mu(x) \\ \mu(x') \end{bmatrix} \quad \Sigma = \begin{bmatrix} K(x, x) & K(x, x') \\ K(x', x) & K(x', x') \end{bmatrix}$$

and similarly for $p(f(x_1), \ldots, f(x_n))$ where now μ is an $n \times 1$ vector and Σ is an $n \times n$ matrix.

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Gaussian process covariance functions

Gaussian processes (GPs) are parameterized by a mean function, $\mu(x)$, and a covariance function, $K(x, x')$.

An example covariance function:

$$K(x_i, x_j) = v_0 \exp\left\{ - \left(\frac{|x_i - x_j|}{r} \right)^{\alpha} \right\} + v_1 + v_2\, \delta_{ij}$$

with parameters $(v_0, v_1, v_2, r, \alpha)$

These kernel parameters are interpretable and can be learned from data:

v_0	signal variance
v_1	variance of bias
v_2	noise variance
r	lengthscale
α	roughness

Once the mean and covariance functions are defined, everything else about GPs follows from the basic rules of probability applied to mutivariate Gaussians.

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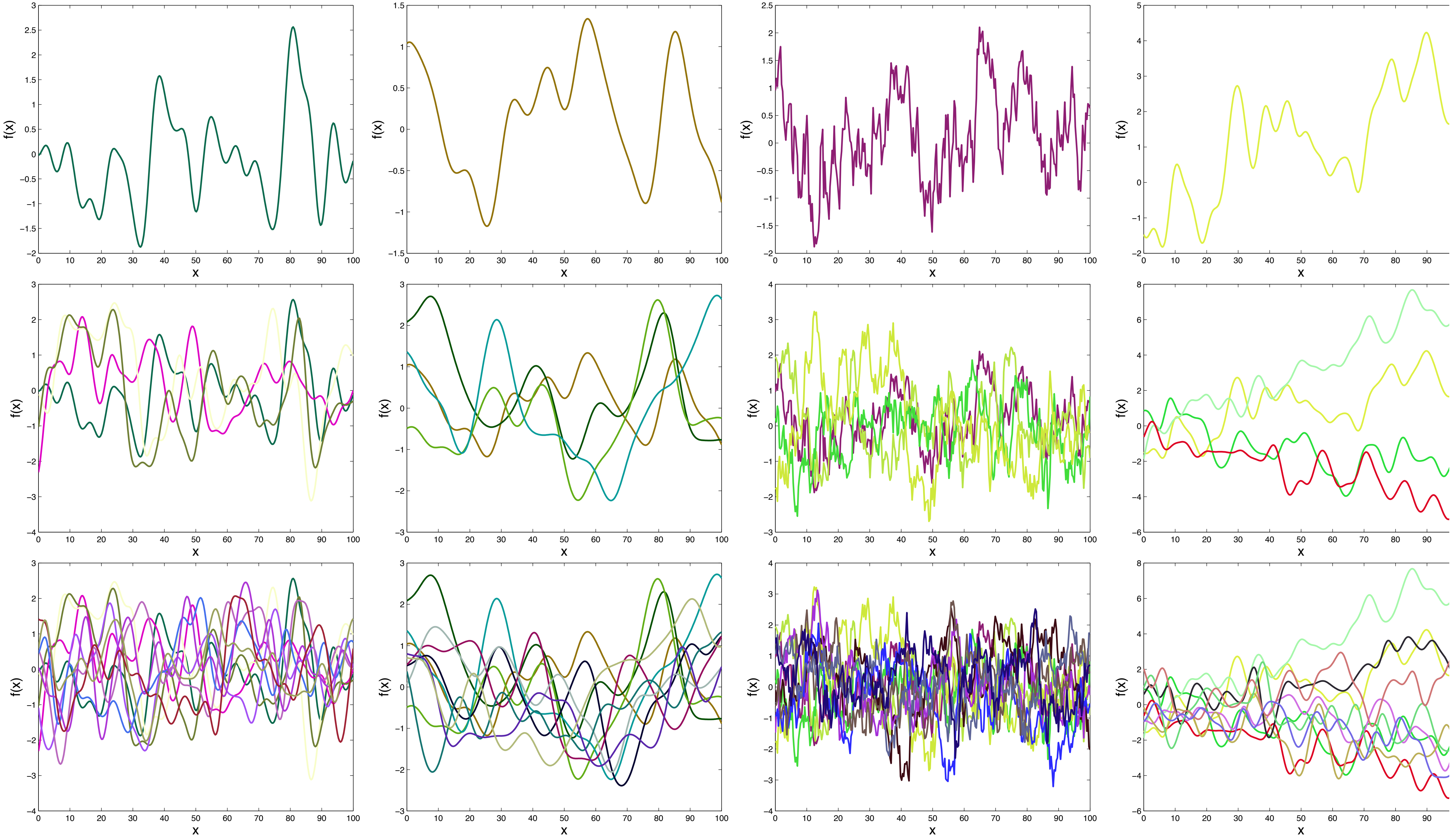
Samples from GPs with different $K(x, x')$



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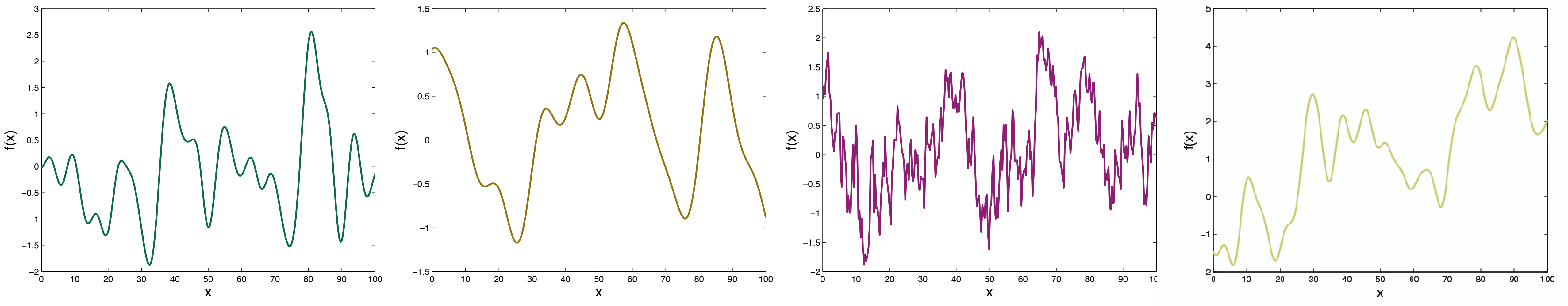
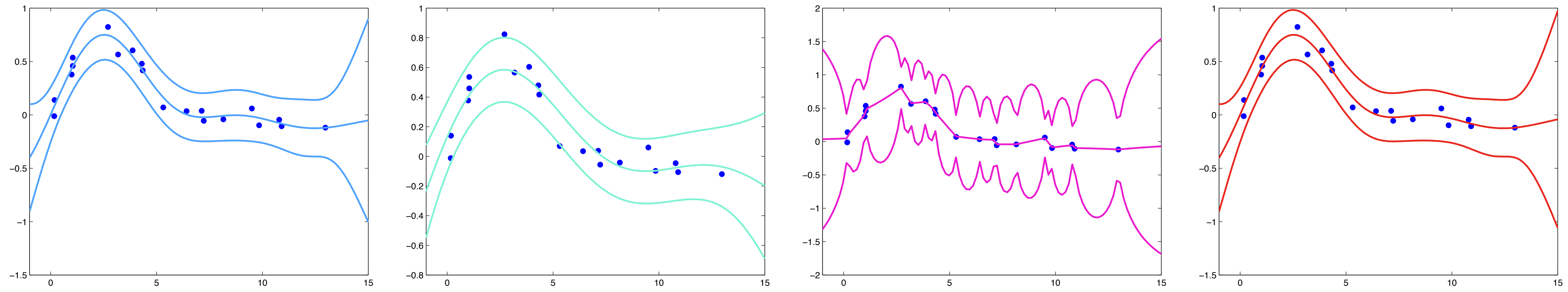
Prediction using GPs with different $K(x, x')$

A sample from the prior for each covariance function:



Corresponding predictions, mean with two standard deviations:



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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:

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

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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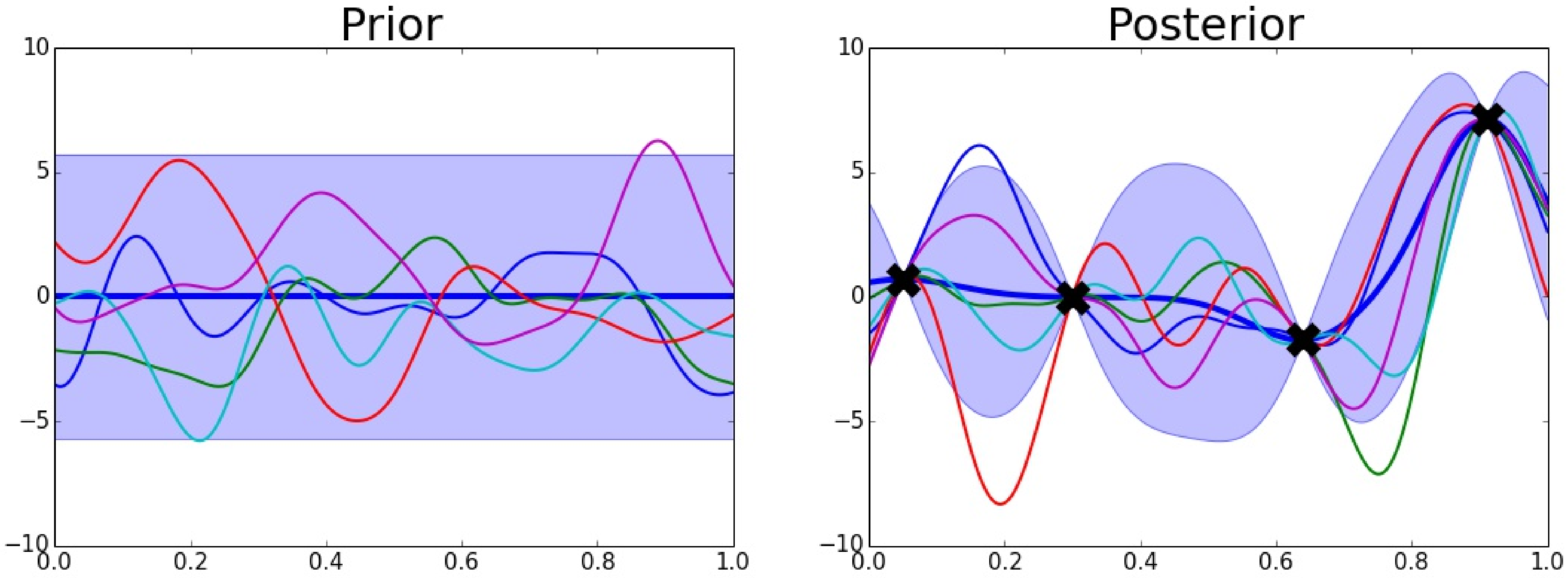
Data-driven modeling with Gaussian processes

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



Training via maximizing the marginal likelihood

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

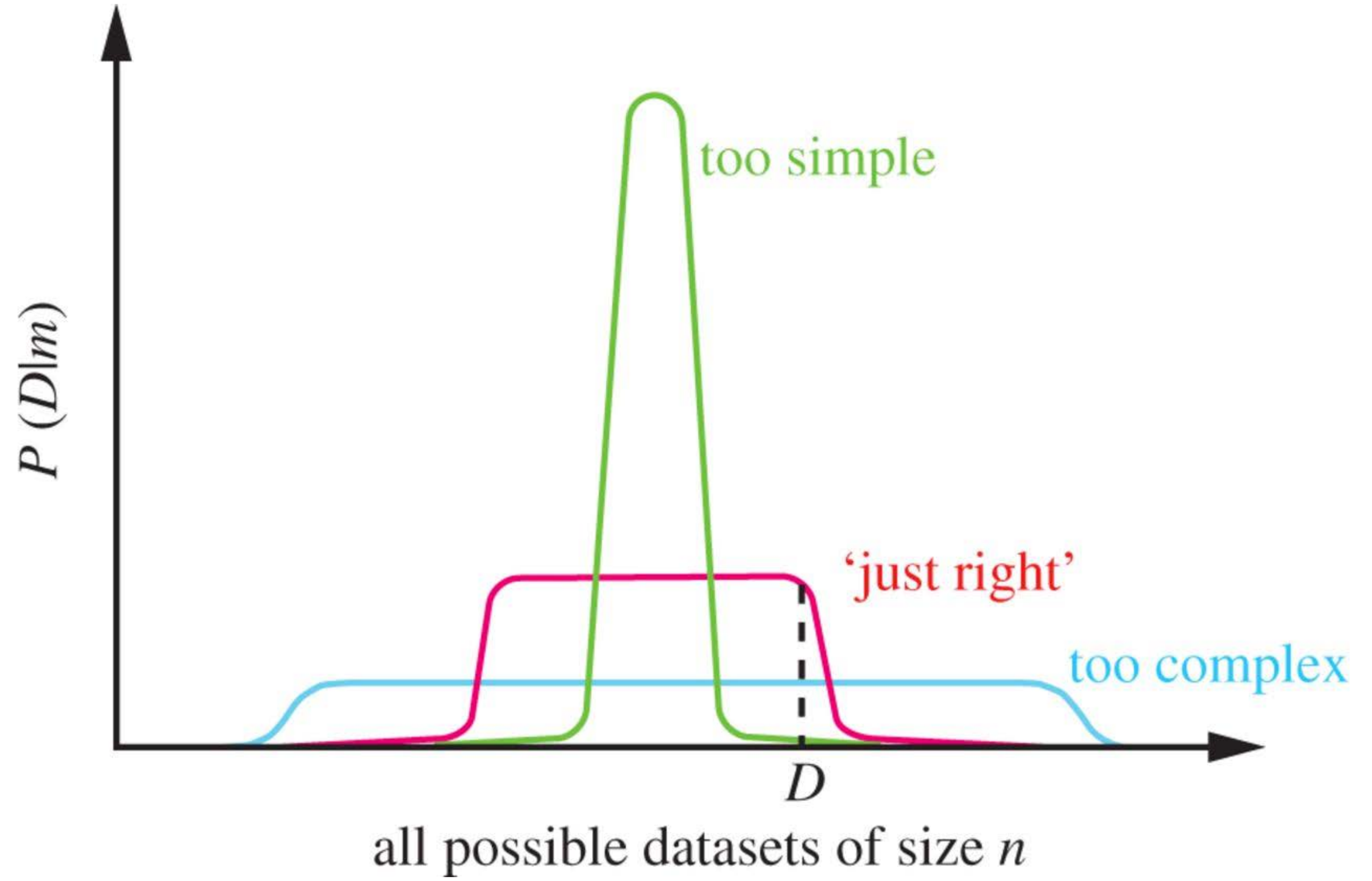
Prediction via conditioning on available data

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

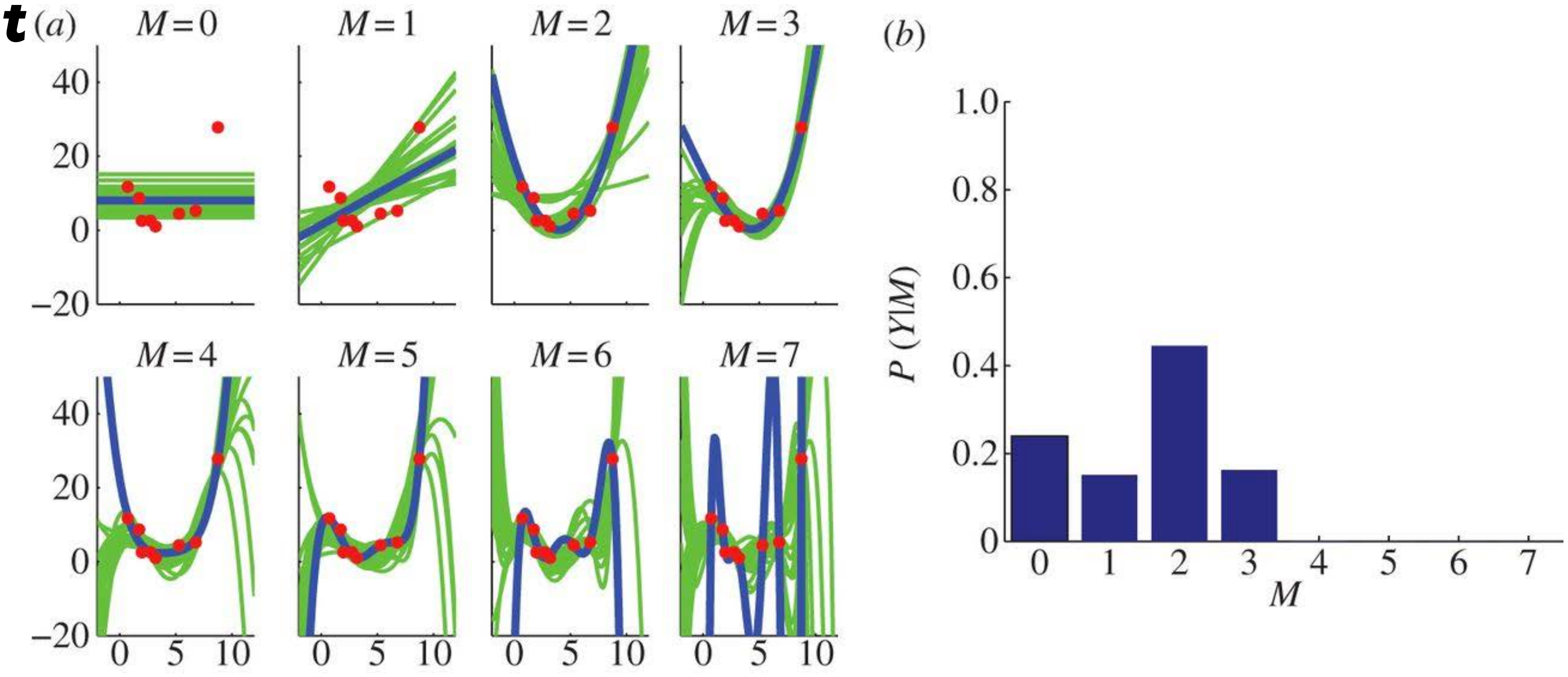
Demo code: https://github.com/PredictiveIntelligenceLab/GPTutorial

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.