ENM 531: Data-driven modeling and probabilistic scientific computing

Lecture #5: Bayesian linear regression

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$$f : \mathcal{X} \to \mathcal{Y}$$

Example #1: Atmospheric science

	δ_K			
Latitude	$K = 0.67$	$K = 1.5$	$K = 2.0$	$K = 3.0$
65	-3.1	3.52	6.05	9.3
55	-3.22	3.62	6.02	9.3
45	-3.3	3.65	5.92	9.17
35	-3.32	3.52	5.7	8.82
25	-3.17	3.47	5.3	8.1
15	-3.07	3.25	5.02	7.52
5	-3.02	3.15	4.95	7.3
-5	-3.02	3.15	4.97	7.35
-15	-3.12	3.2	5.07	7.62
-25	-3.2	3.27	5.35	8.22
-35	-3.35	3.52	5.62	8.8
-45	-3.37	3.7	5.95	9.25
-55	-3.25	3.7	6.1	9.5

Table 3.1. Variation of the average yearly temperature on the Earth for four different values of the concentration K of carbon acid at different latitudes

Example #2: Finance

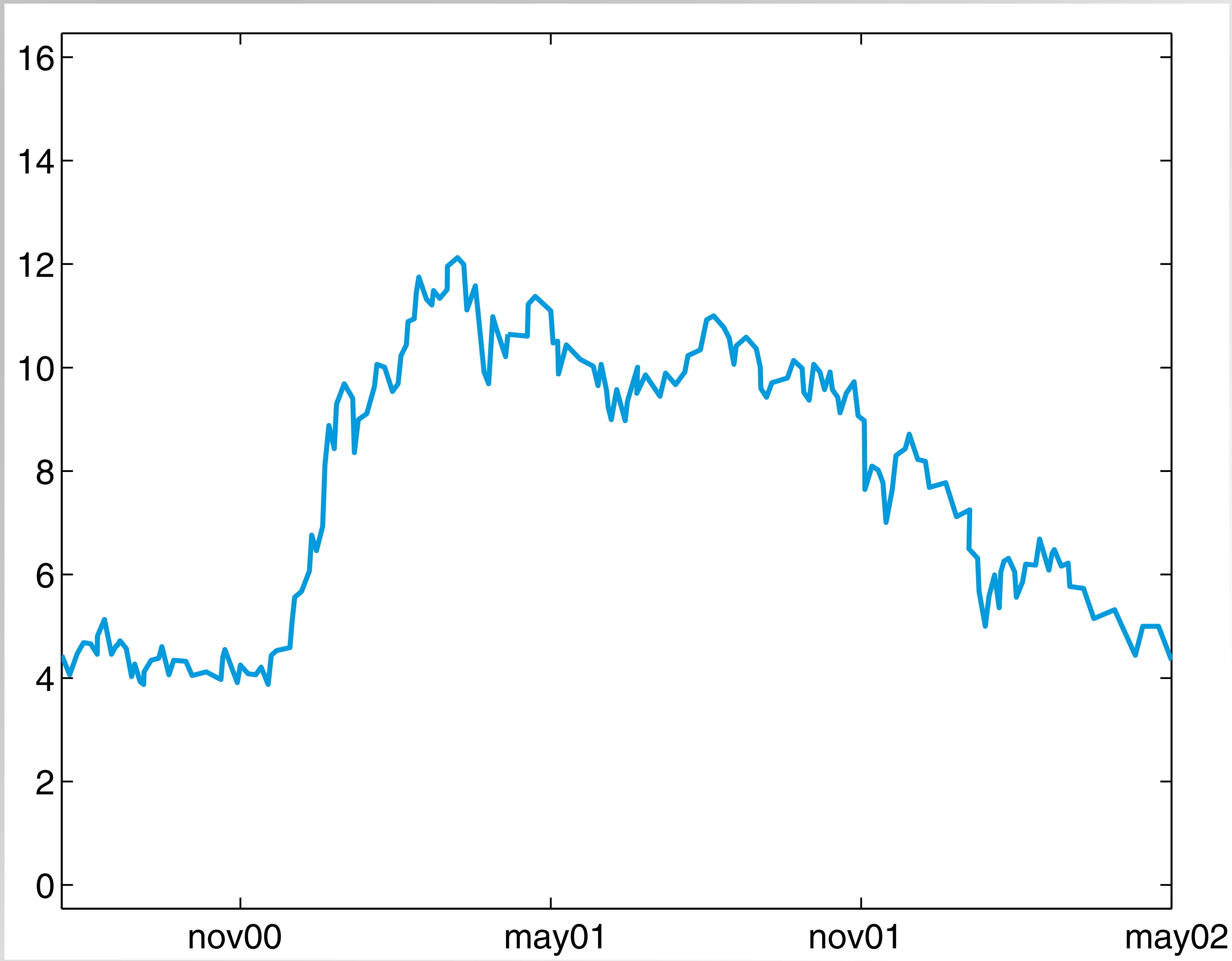


Fig. 3.1. Price variation of a stock over two years

Example #3: Biomechanics

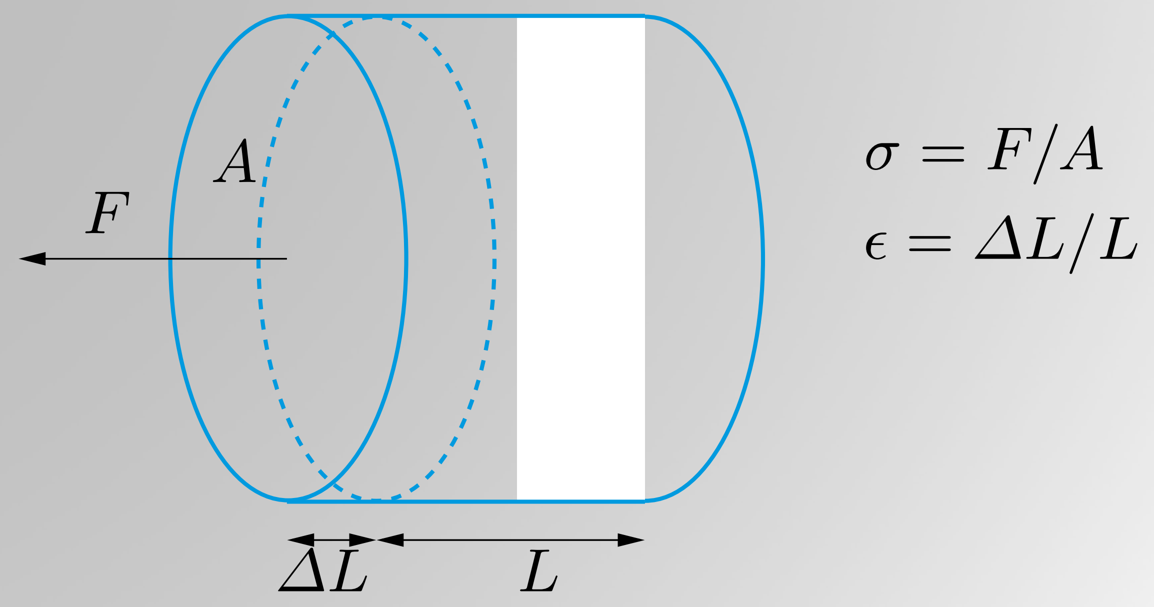


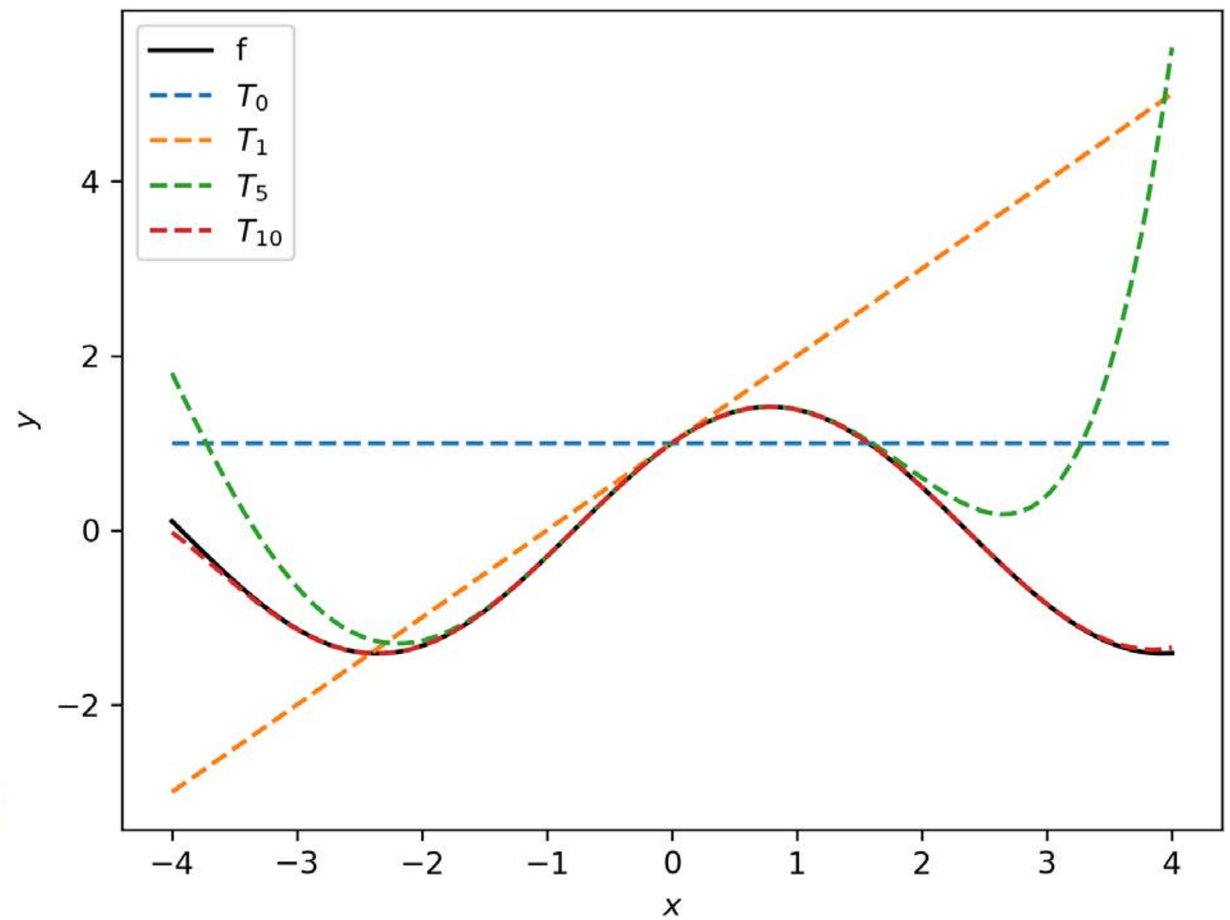
Fig. 3.2. A schematic representation of an intervertebral disc

test	stress σ	stress ϵ	test	stress σ	stress ϵ
1	0.00	0.00	5	0.31	0.23
2	0.06	0.08	6	0.47	0.25
3	0.14	0.14	7	0.60	0.28
4	0.25	0.20	8	0.70	0.29

Table 3.2. Values of the deformation for different values of a stress applied on an intervertebral disc

Local approximation with Taylor series

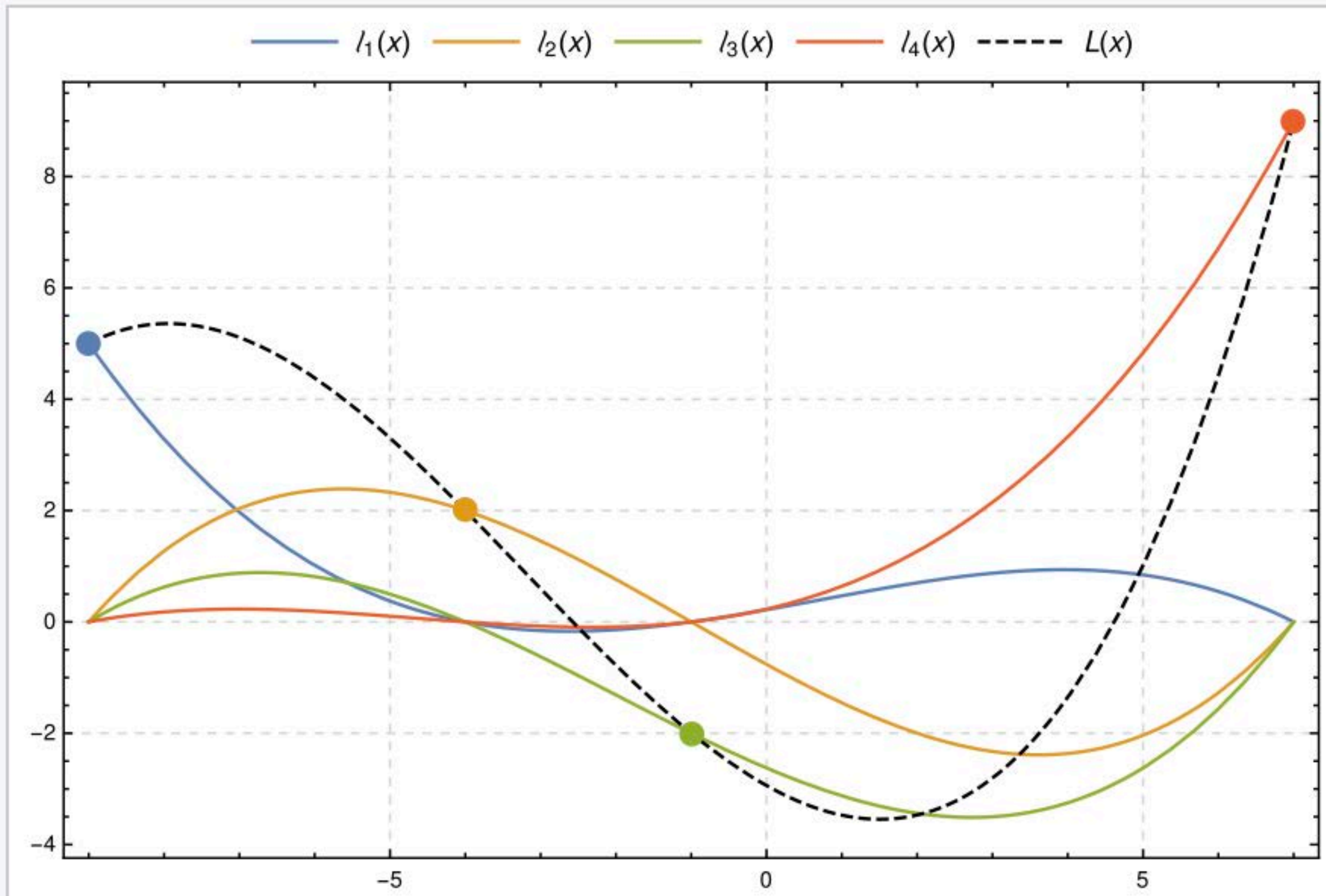
```python
#!/usr/bin/env python3
# -*- coding: utf-8 -*-
"""
Created on Tue Aug 28 12:27:37 2018

@author: paris
"""

import autograd.numpy as np
from autograd import grad
from scipy.special import factorial
import matplotlib.pyplot as plt

if __name__ == '__main__':

    def f(x):
        return np.sin(x) + np.cos(x)

    def TaylorSeries(f, x, x0, n = 2):
        T = f(x0)*np.ones_like(x)
        grad_f = grad(f)
        for i in range(0, n):
            T += grad_f(x0)*(x-x0)**(i+1) / factorial(i+1)
            grad_f = grad(grad_f)
        return T


    N = 100
    x = np.linspace(-4.0,4.0,N)
    y = f(x)

    x0 = 0.0

    n = [0, 1, 5, 10]
    plt.figure(1)
    plt.plot(x, y, 'k-', label = 'f')
    for i in range(0, len(n)):
        T = TaylorSeries(f, x, x0, n[i])
        plt.plot(x, T, '--', label = '$T_{%d}$' % (n[i]))
    plt.xlabel('$x$')
    plt.ylabel('$y$')
    plt.legend()
```



$$T_n(x) := \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k$$

Interpolation with Lagrange polynomials

$$f(x) = \sum_{k=1}^{n} y_k \phi_k(x), \quad \phi_k(x) = \prod_{\substack{0 \le k \le n \\ k \ne j}} \frac{x - x_j}{x_k - x_j}$$



This image shows, for four points ((−9, 5), (−4, 2), (−1, −2), (7, 9)), the (cubic) interpolation polynomial $L(x)$ (dashed, black), which is the sum of the *scaled* basis polynomials $y_0\ell_0(x)$, $y_1\ell_1(x)$, $y_2\ell_2(x)$ and $y_3\ell_3(x)$. The interpolation polynomial passes through all four control points, and each *scaled* basis polynomial passes through its respective control point and is 0 where x corresponds to the other three control points.

Runge's phenomenon

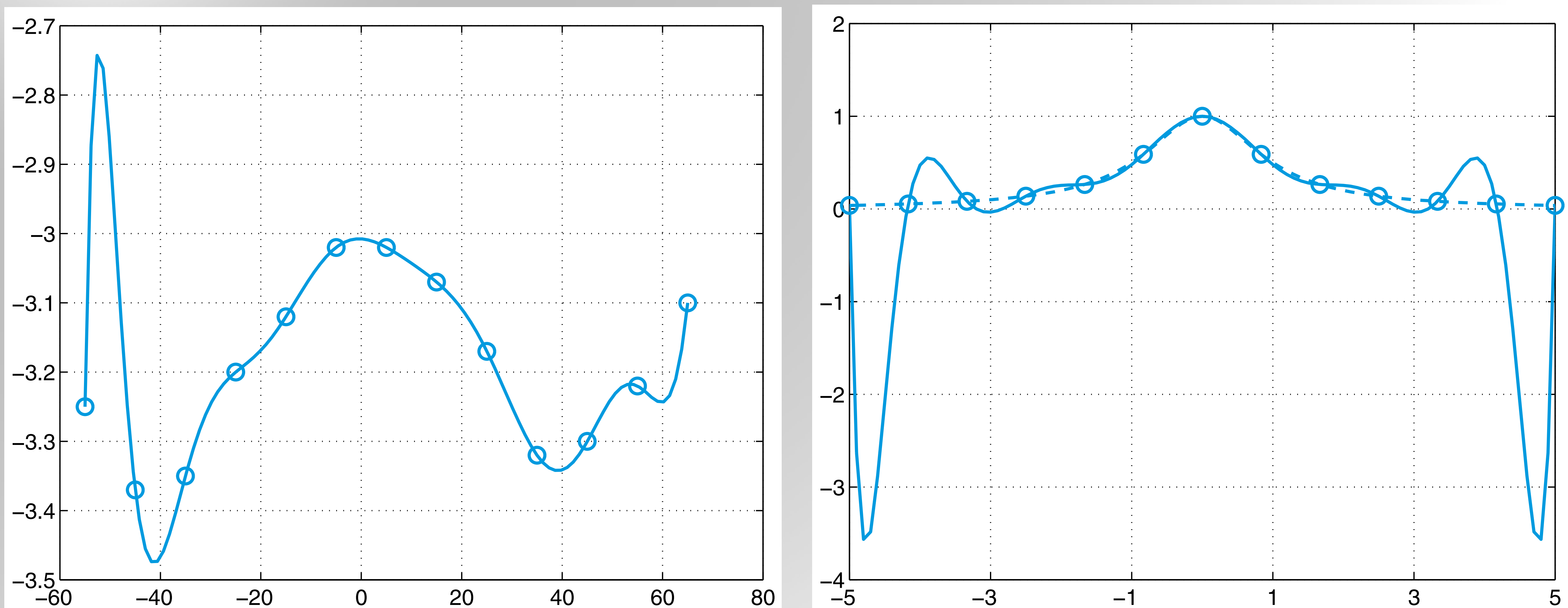
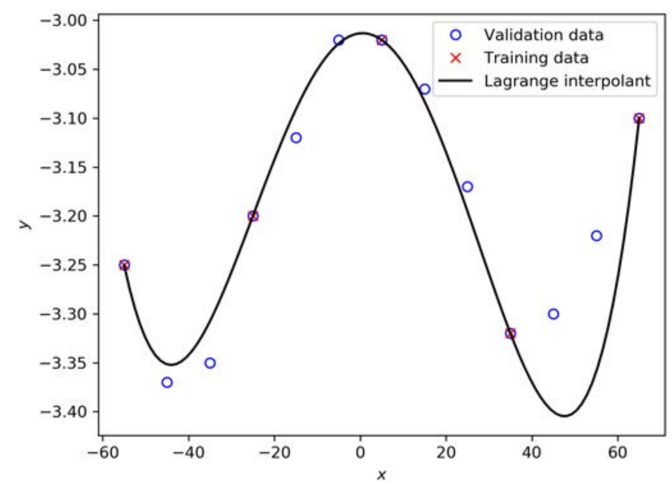


Fig. 3.6. Two examples of Runge's phenomenon: to the left, Π_{12} computed for the data of Table 3.1, column $K = 0.67$; to the right, $\Pi_{12}f$ (*solid line*) computed on 13 equispaced nodes for the function $f(x) = 1/(1 + x^2)$ (*dashed line*)

Deterministic vs probabilistic modeling

$\boldsymbol{x}$

Inputs
(deterministic)



$\boldsymbol{y} = f_\theta(\boldsymbol{x})$

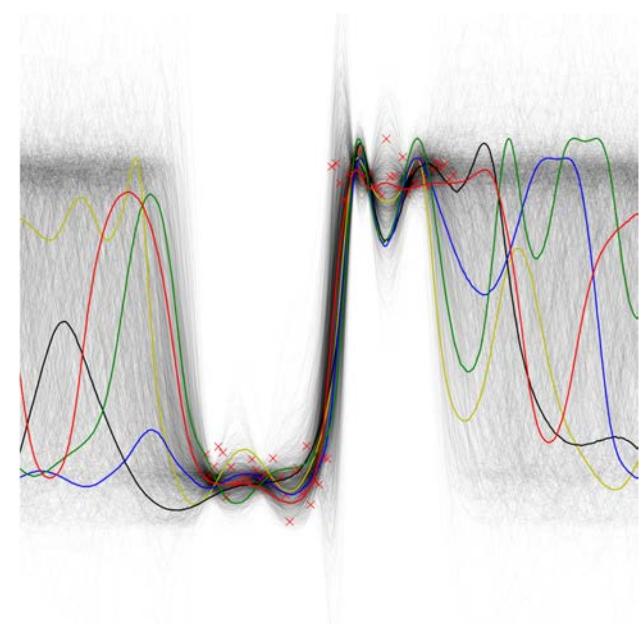
Outputs

Inputs
(random)

$\boldsymbol{z} \sim p(\boldsymbol{z})$

$\boldsymbol{x}$

Inputs
(deterministic)



$p_\theta(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{z})$

Outputs

Supervised learning

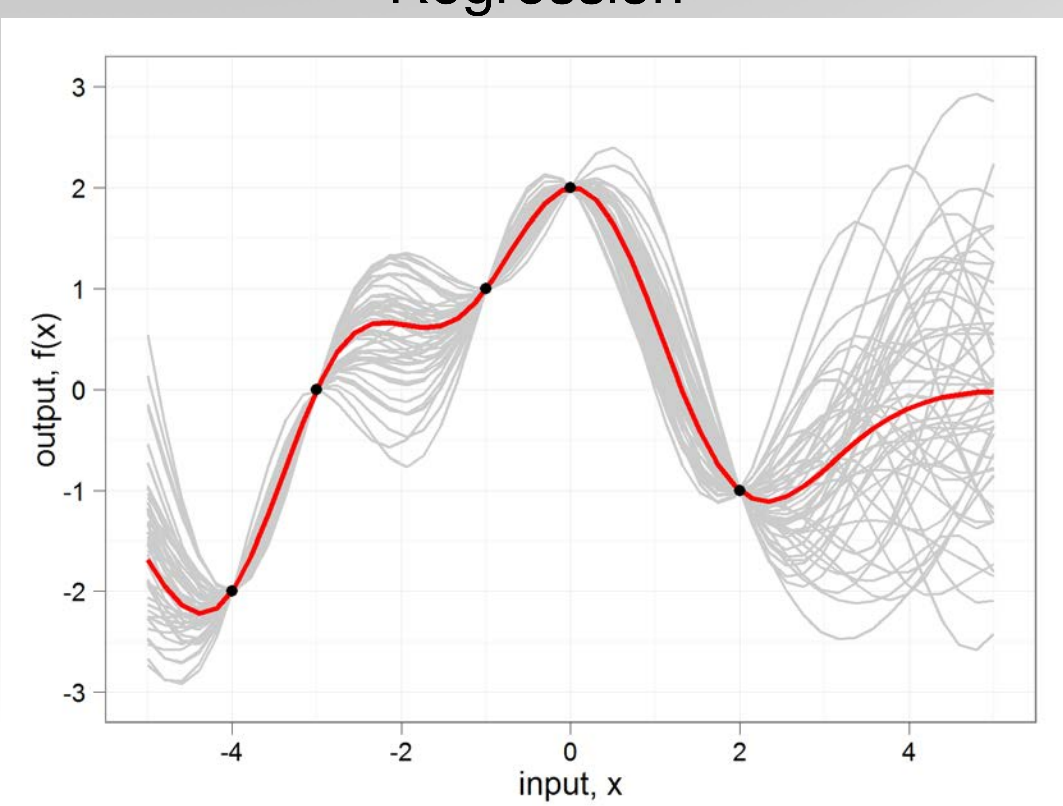
$$f : \mathcal{X} \rightarrow \mathcal{Y}$$

$$\mathcal{D} = \{\boldsymbol{x}, \boldsymbol{y}\},\ \boldsymbol{x} \in \mathcal{X},\ \boldsymbol{y} \in \mathcal{Y}$$

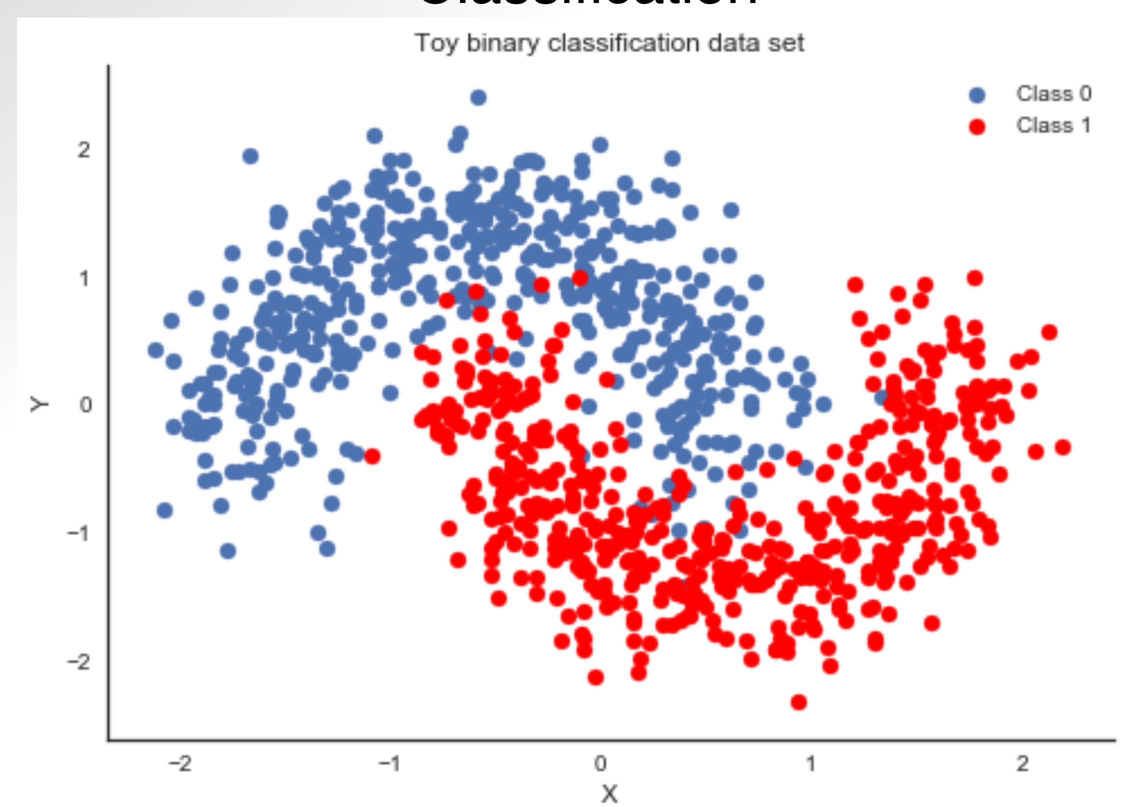
$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon$$

$$p(f(\boldsymbol{x}^*)|\boldsymbol{x}^*, \mathcal{D})$$

Regression



Classification



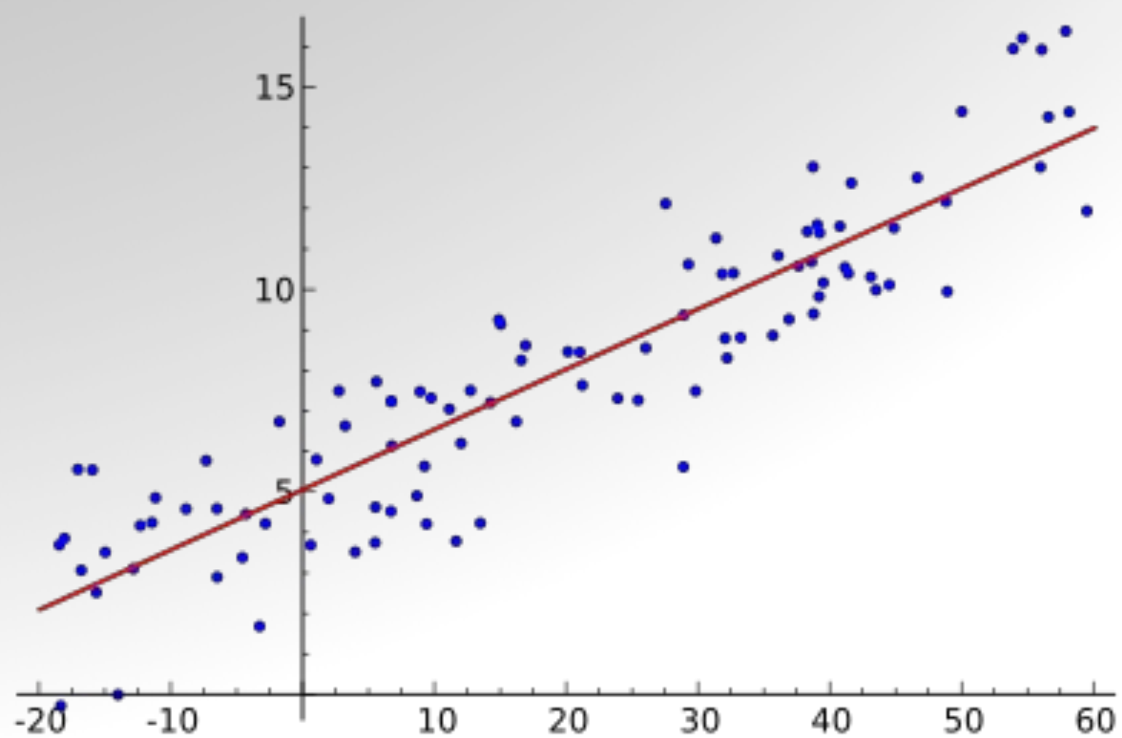
Linear regression

$$f : \mathcal{X} \rightarrow \mathcal{Y}$$

$$\mathcal{D} = \{\boldsymbol{x}, \boldsymbol{y}\},\ \boldsymbol{x} \in \mathcal{X},\ \boldsymbol{y} \in \mathcal{Y}$$

$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon$$

$$f(\boldsymbol{x}) = w^T \boldsymbol{x}$$



"It's <u>not</u> just about lines and planes!"

Linear regression

Nonlinear functions can be approximating using basis functions (or features)

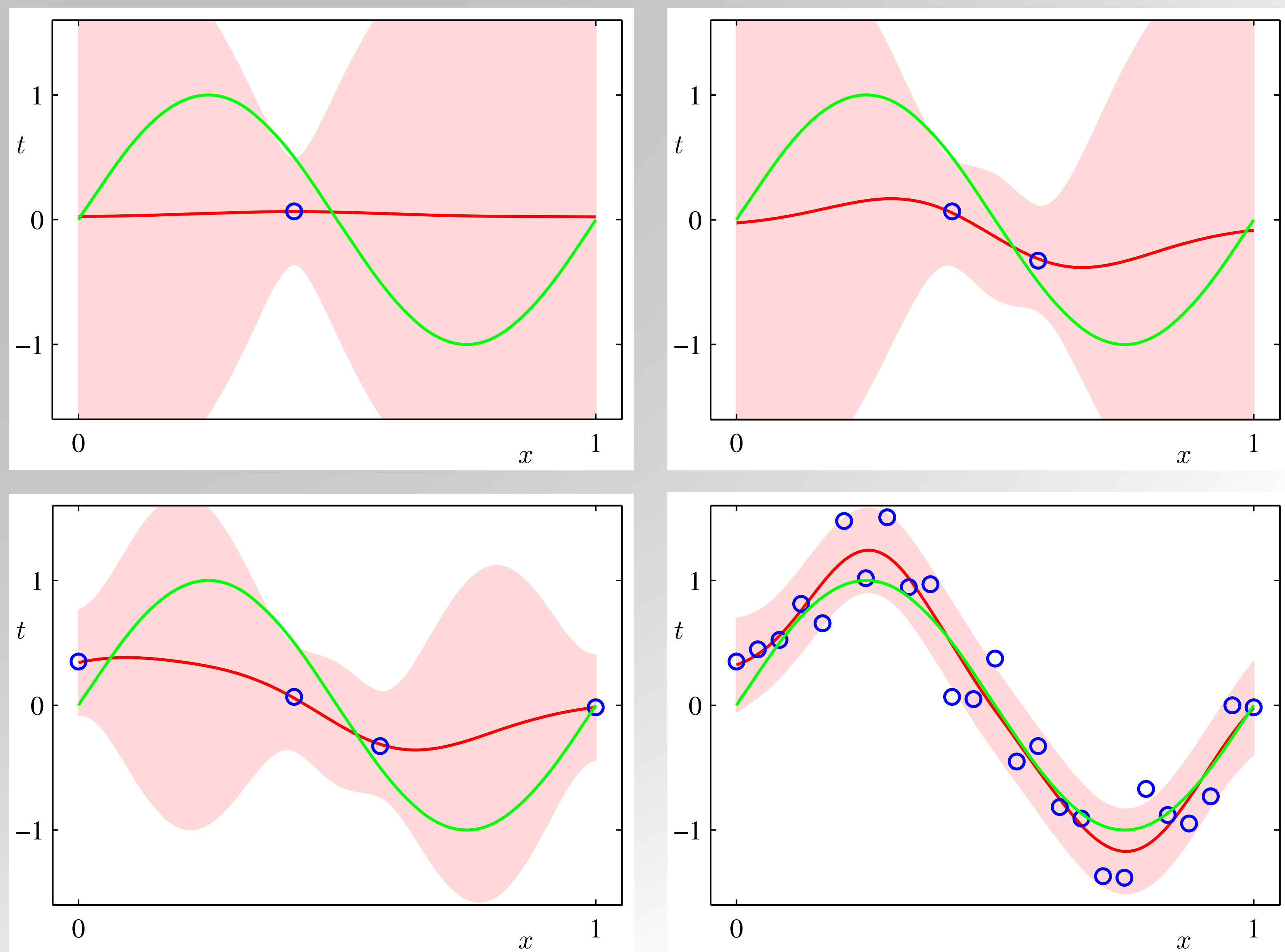


Figure 3.8 Examples of the predictive distribution (3.58) for a model consisting of 9 Gaussian basis functions of the form (3.4) using the synthetic sinusoidal data set of Section 1.1. See the text for a detailed discussion.

$$\boldsymbol{y} = w^T \phi(\boldsymbol{x}) + \epsilon$$

Linear regression with basis functions

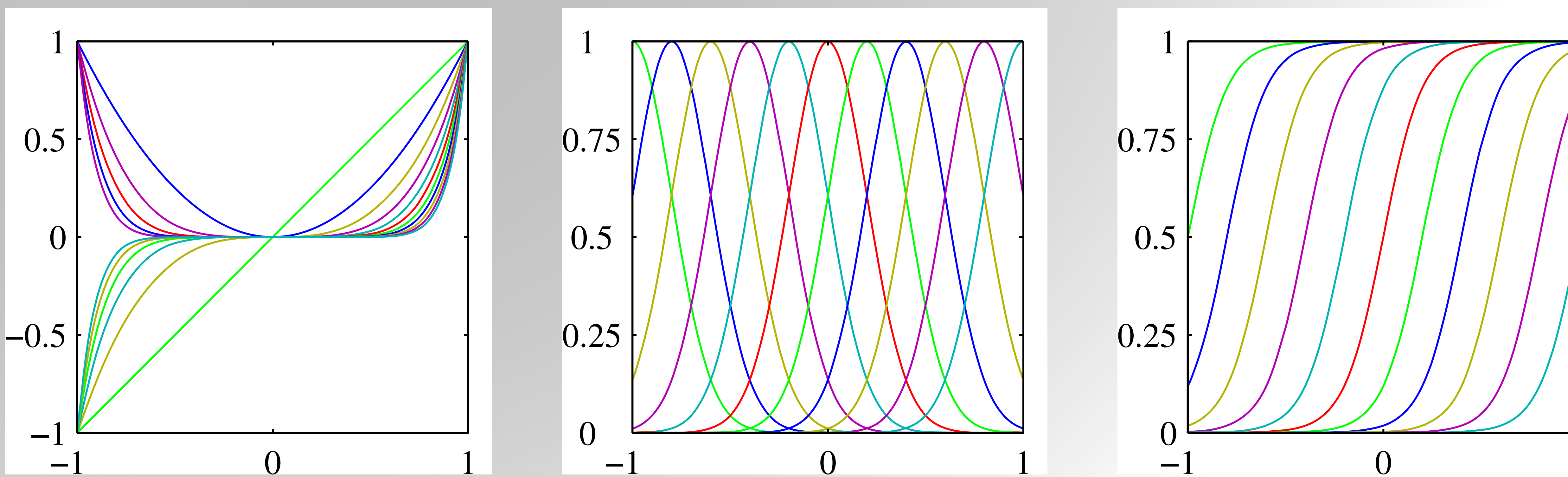
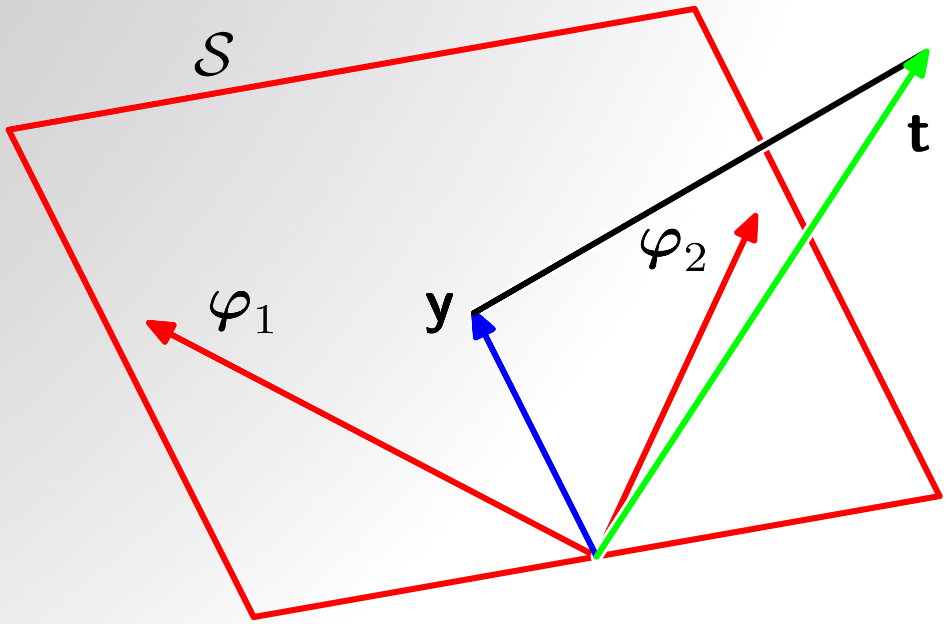


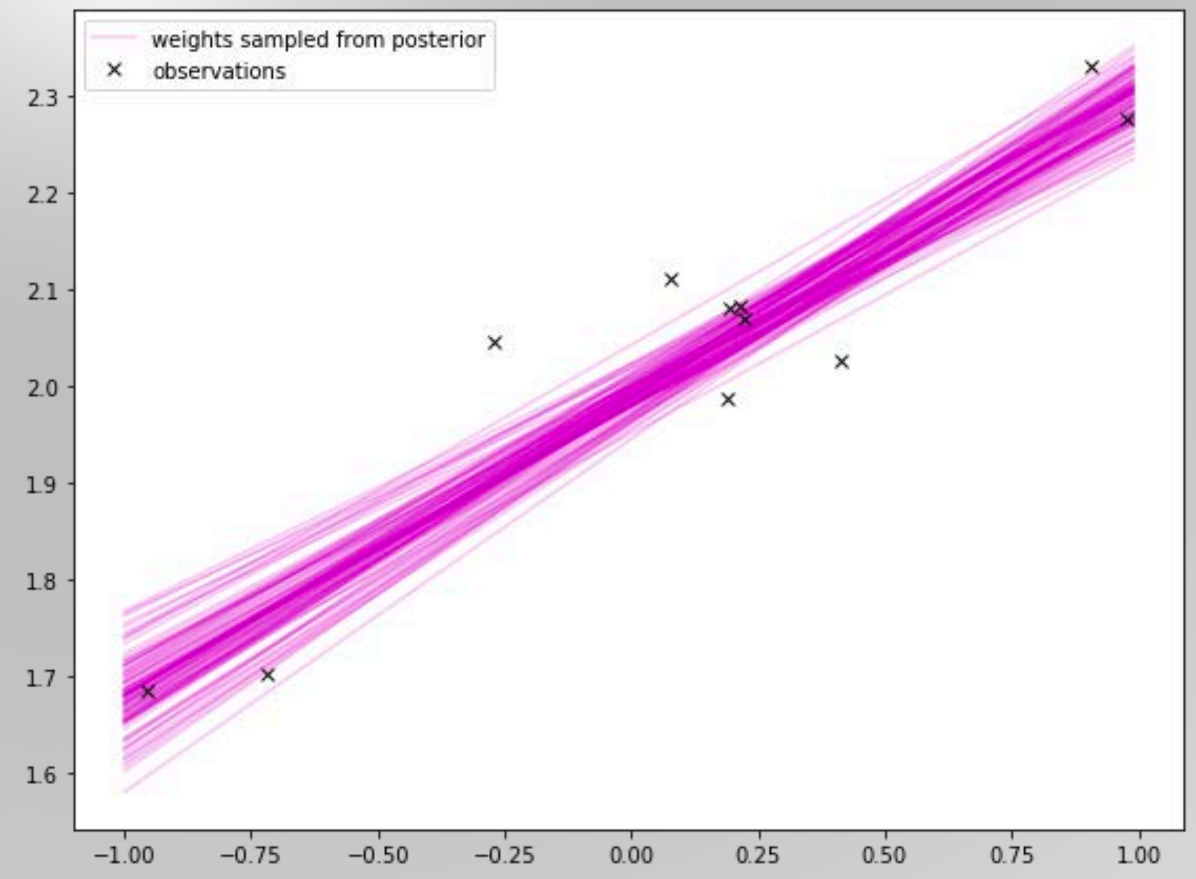
Figure 3.1 Examples of basis functions, showing polynomials on the left, Gaussians of the form (3.4) in the centre, and sigmoidal of the form (3.5) on the right.

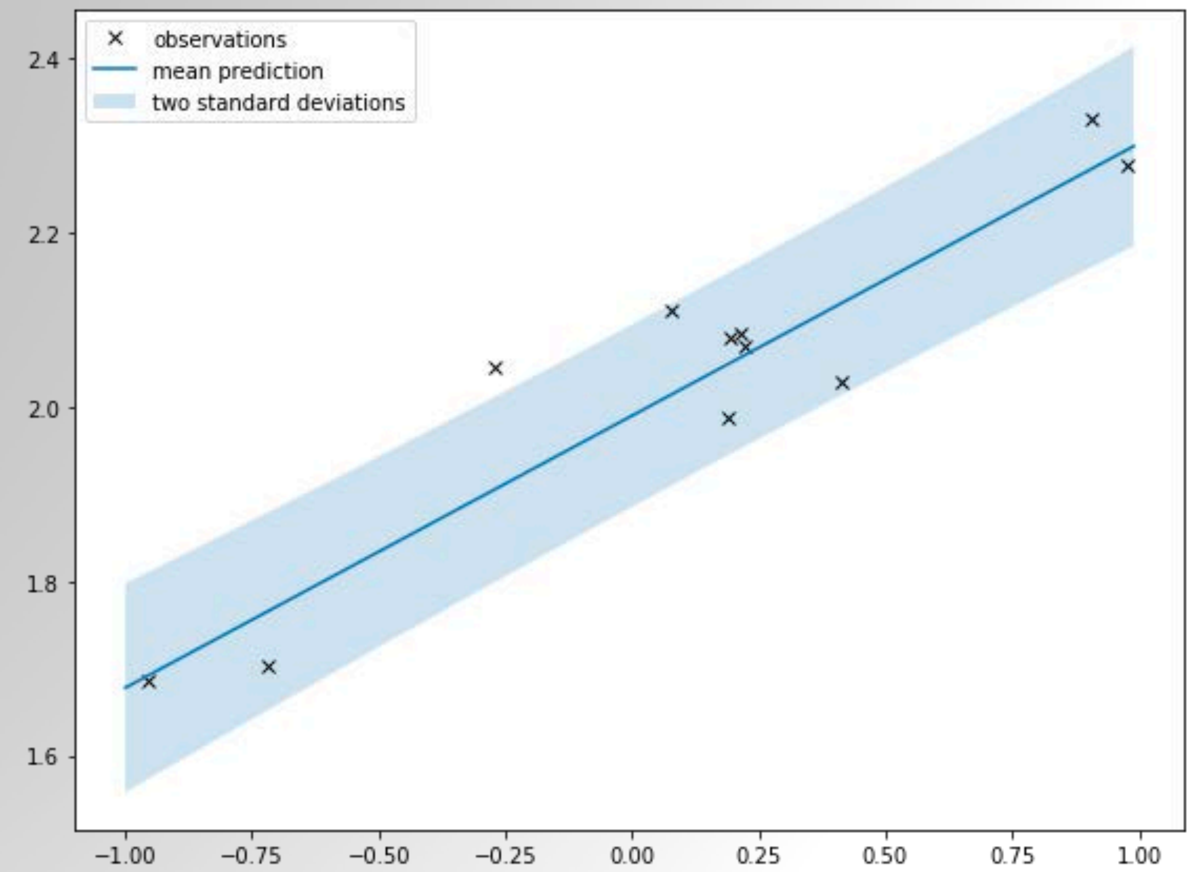
Geometrical interpretation

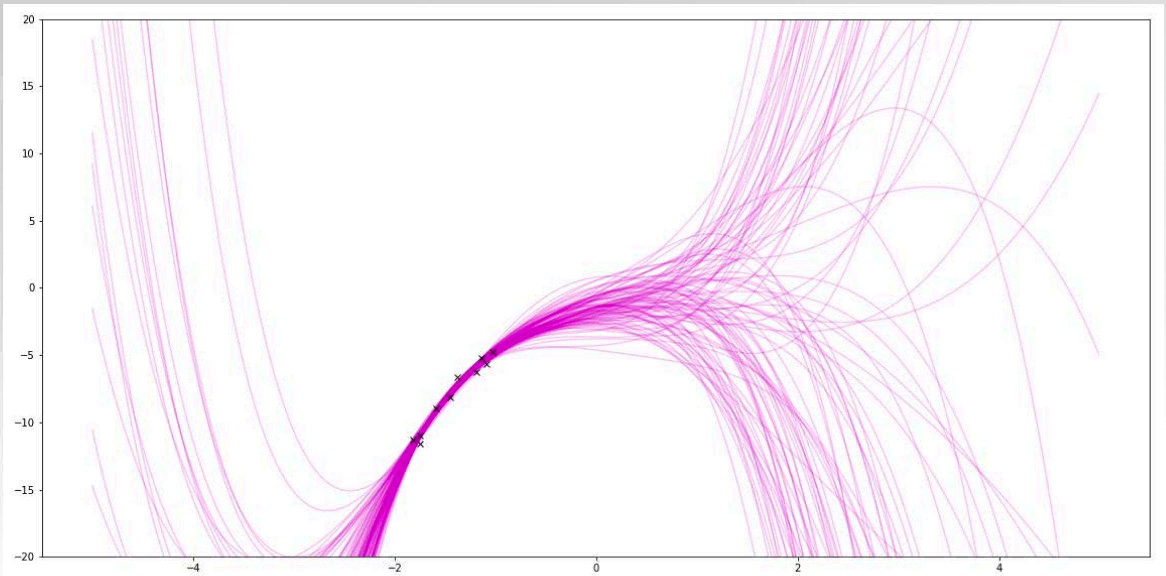
Figure 3.2 Geometrical interpretation of the least-squares solution, in an N-dimensional space whose axes are the values of $t_1, \ldots, t_N$. The least-squares regression function is obtained by finding the orthogonal projection of the data vector **t** onto the subspace spanned by the basis functions $\phi_j(\mathbf{x})$ in which each basis function is viewed as a vector $\boldsymbol{\varphi}_j$ of length N with elements $\phi_j(\mathbf{x}_n)$.

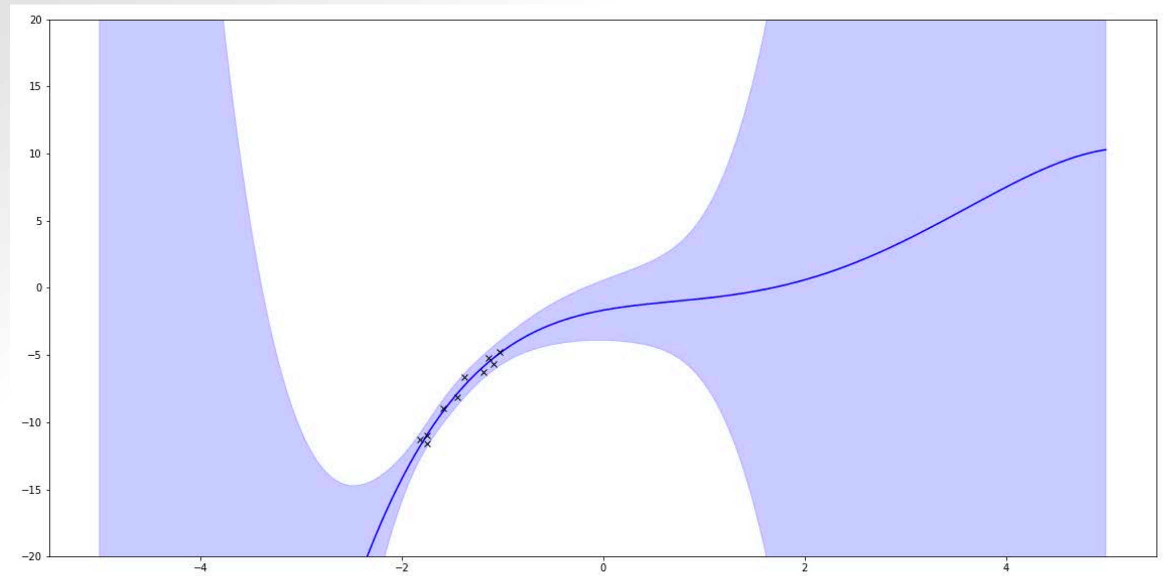


Bayesian linear regression









Bayesian linear regression

```python
class BayesianLinearRegression:
  """
    Linear regression model: y = (w.T)*x + \epsilon
    w ~ N(0,beta^(-1)I)
    P(y|x,w) ~ N(y|(w.T)*x,alpha^(-1)I)
  """
  def __init__(self, X, y, alpha = 1.0, beta = 1.0):

      self.X = X
      self.y = y

      self.alpha = alpha
      self.beta = beta

      self.jitter = 1e-8


  def fit_MLE(self):
      xTx_inv = np.linalg.inv(np.matmul(self.X.T,self.X) + self.jitter)
      xTy = np.matmul(self.X.T, self.y)
      w_MLE = np.matmul(xTx_inv, xTy)

      self.w_MLE = w_MLE

      return w_MLE

  def fit_MAP(self):
      Lambda = np.matmul(self.X.T,self.X) + \
               (self.beta/self.alpha)*np.eye(self.X.shape[1])
      Lambda_inv = np.linalg.inv(Lambda)
      xTy = np.matmul(self.X.T, self.y)
      mu = np.matmul(Lambda_inv, xTy)

      self.w_MAP = mu
      self.Lambda_inv = Lambda_inv

      return mu, Lambda_inv

  def predictive_distribution(self, X_star):
      mean_star = np.matmul(X_star, self.w_MAP)
      var_star = 1.0/self.alpha + \
                 np.matmul(X_star, np.matmul(self.Lambda_inv, X_star.T))
      return mean_star, var_star
```