ENM 360: Introduction to Data-driven Modeling

Lecture #2: Primer on Linear Algebra and Scientific Computing

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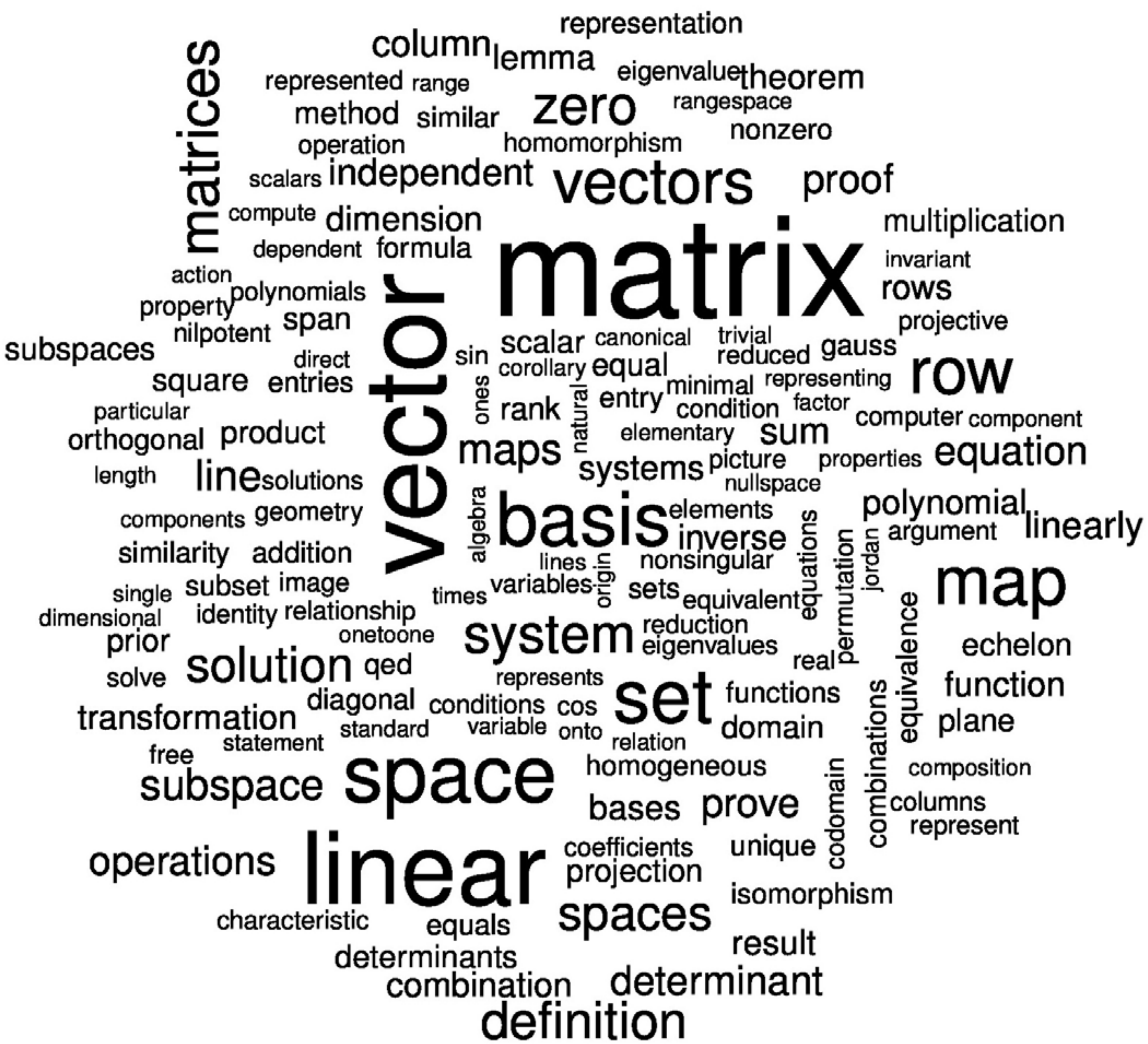
Lecture outline



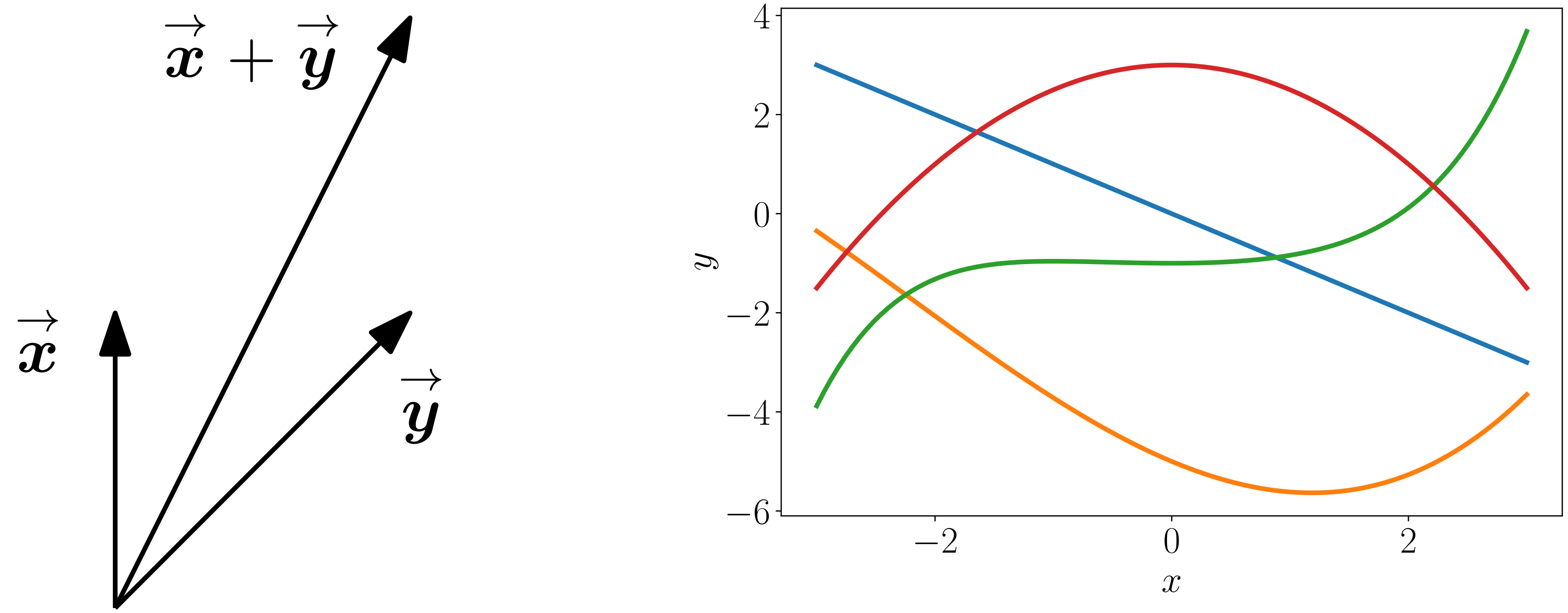
Scientific computing

Linear algebra

Matrix/vector calculus/operations

Vectors

- Basic definitions
- Vector operations (e.g. addition, subtraction, multiplication, etc.)
- Linear combinations
- Dot products
- Norms
- Vector/Linear spaces
- Linear (in)dependance
- Bases



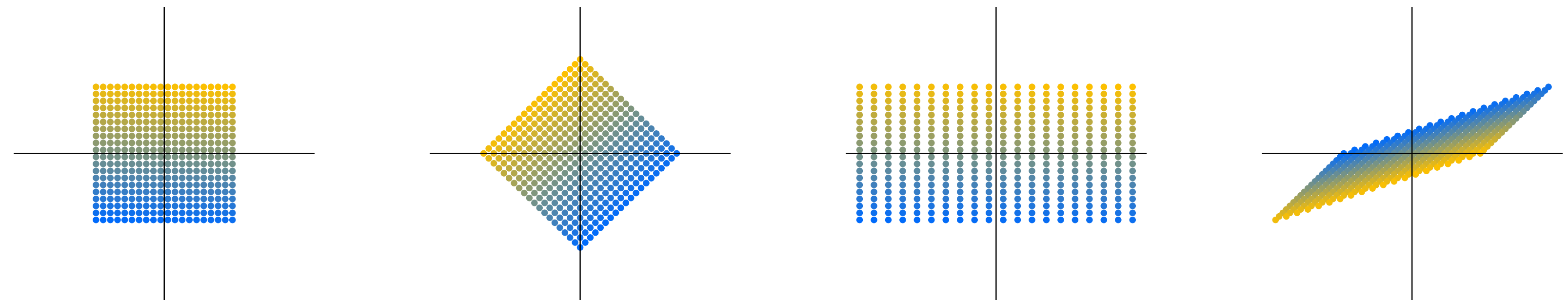
(a) Geometric vectors. (b) Polynomials.

Useful resources:

- *Gilbert Strang's lectures at MIT OCW: https://ocw.mit.edu/courses/mathematics/18-06-linear-algebra-spring-2010/video-lectures/*
- *Pavel Grinfeld's series on linear algebra: https://www.youtube.com/playlist?list=PLlXfTHzgMRUKXD88IdzS14F4NxAZudSmv*

Matrices

- Basic definitions
- Matrix operations (e.g. addition, subtraction, multiplication, etc.)
- Unit matrices, transposes, inverses
- Basic properties
- Norms
- Linear transformation of vectors
- Eigenvalues and eigenvectors
- Linear systems



(a) Original data. (b) Rotation by 45°. (c) Stretch along the horizontal axis. (d) General linear mapping.

$$\underbrace{\boldsymbol{A}}_{n\times k}\underbrace{\boldsymbol{B}}_{k\times m} = \underbrace{\boldsymbol{C}}_{n\times m}$$

For $\boldsymbol{A} = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{bmatrix} \in \mathbb{R}^{2\times 3}$, $\boldsymbol{B} = \begin{bmatrix} 0 & 2 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \in \mathbb{R}^{3\times 2}$, we obtain

$$\boldsymbol{AB} = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} 0 & 2 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 3 \\ 2 & 5 \end{bmatrix} \in \mathbb{R}^{2\times 2},$$

$$\begin{aligned} 2x_1 + 3x_2 + 5x_3 &= 1 \\ 4x_1 - 2x_2 - 7x_3 &= 8 \\ 9x_1 + 5x_2 - 3x_3 &= 2 \end{aligned}$$

$$\begin{bmatrix} 2 & 3 & 5 \\ 4 & -2 & -7 \\ 9 & 5 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 8 \\ 2 \end{bmatrix}$$

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Linear systems

- Direct solvers:
  - Gauss elimination/LU decomposition
  - Cholesky decomposition (SPD matrices)
  - QR decomposition
  - SVD
- Iterative solvers:
  - Jacobi iterations
  - Gauss-Seidel
  - Successive over-relaxation (SOR)
  - Krylov subspace methods (conjugate gradients, etc.)

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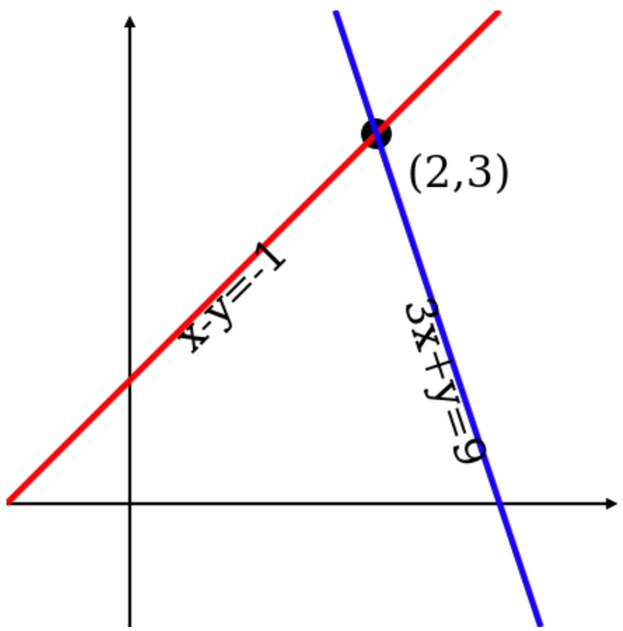
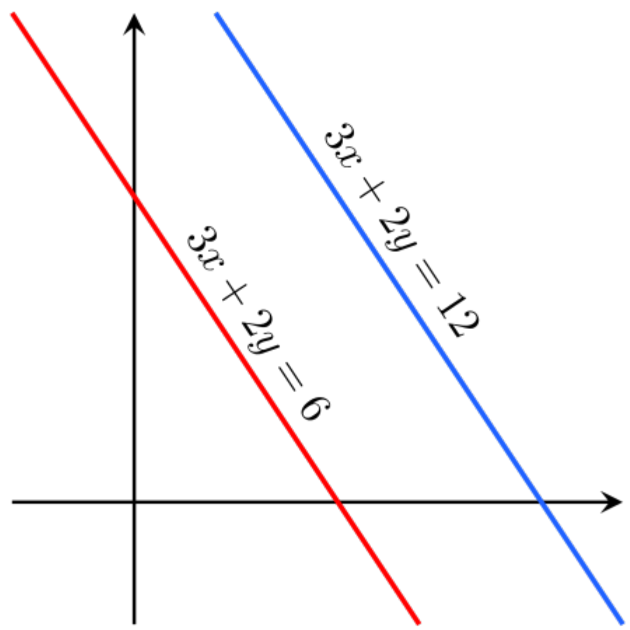
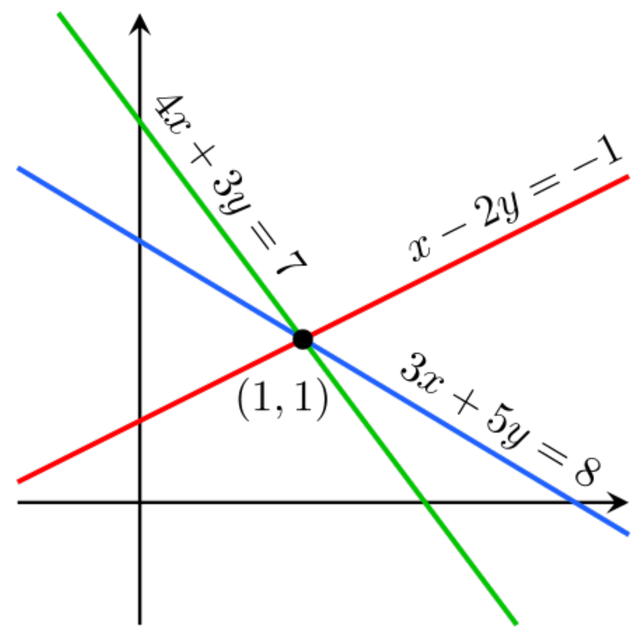
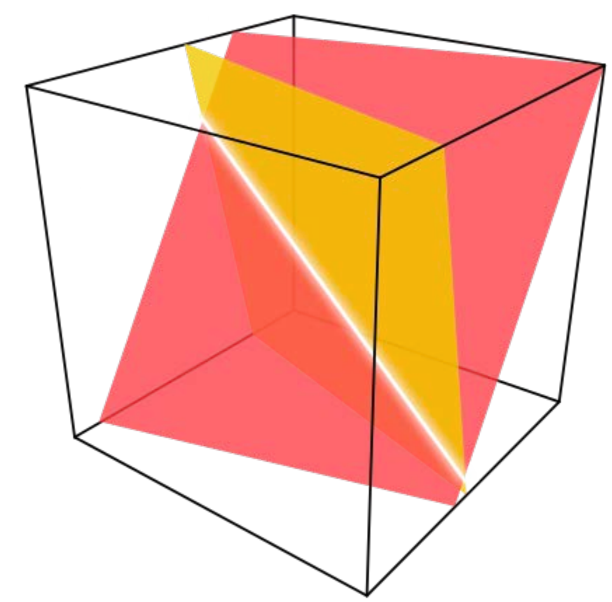
$$\begin{bmatrix} 2 & 3 & 5 \\ 4 & -2 & -7 \\ 9 & 5 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 8 \\ 2 \end{bmatrix}$$









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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

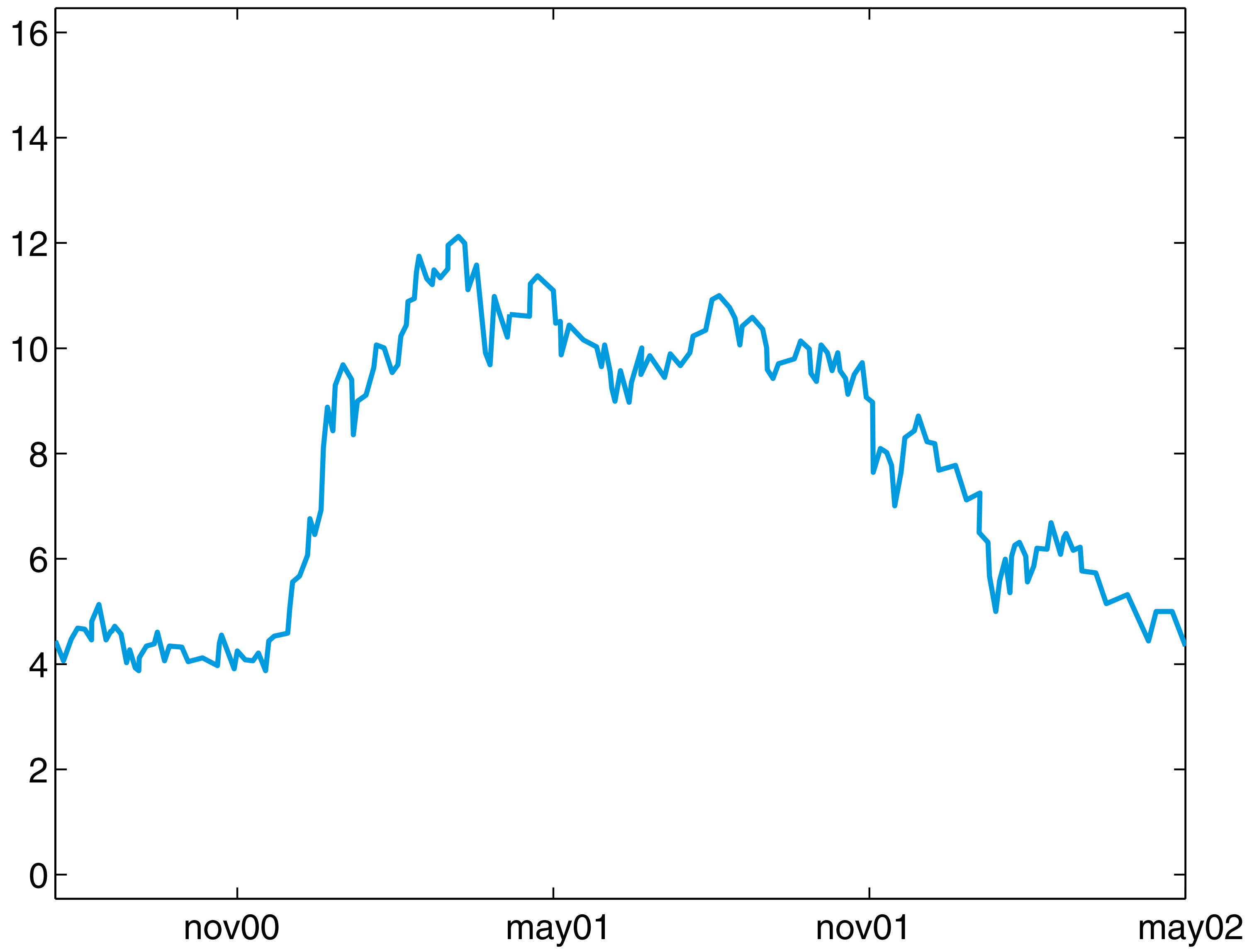


Fig. 3.1. Price variation of a stock over two years

Example #3: Biomechanics

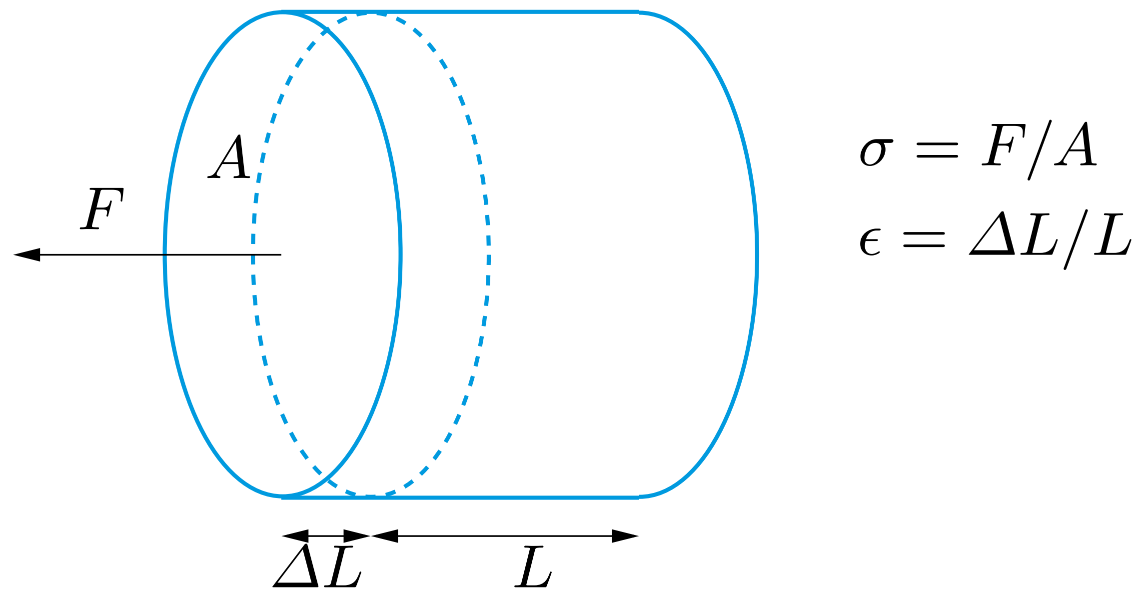


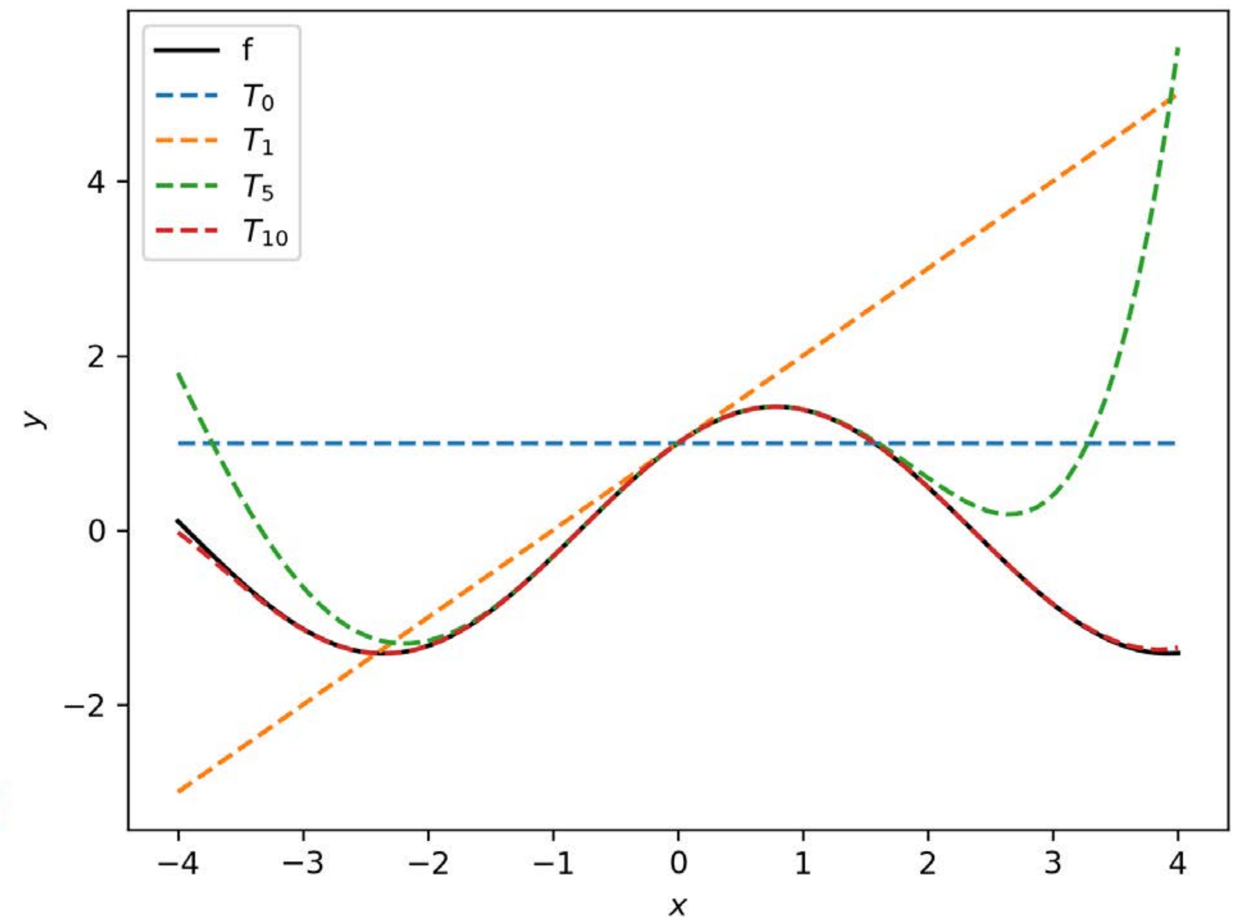
Fig. 3.2. A schematic representation of an intervertebral disc

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

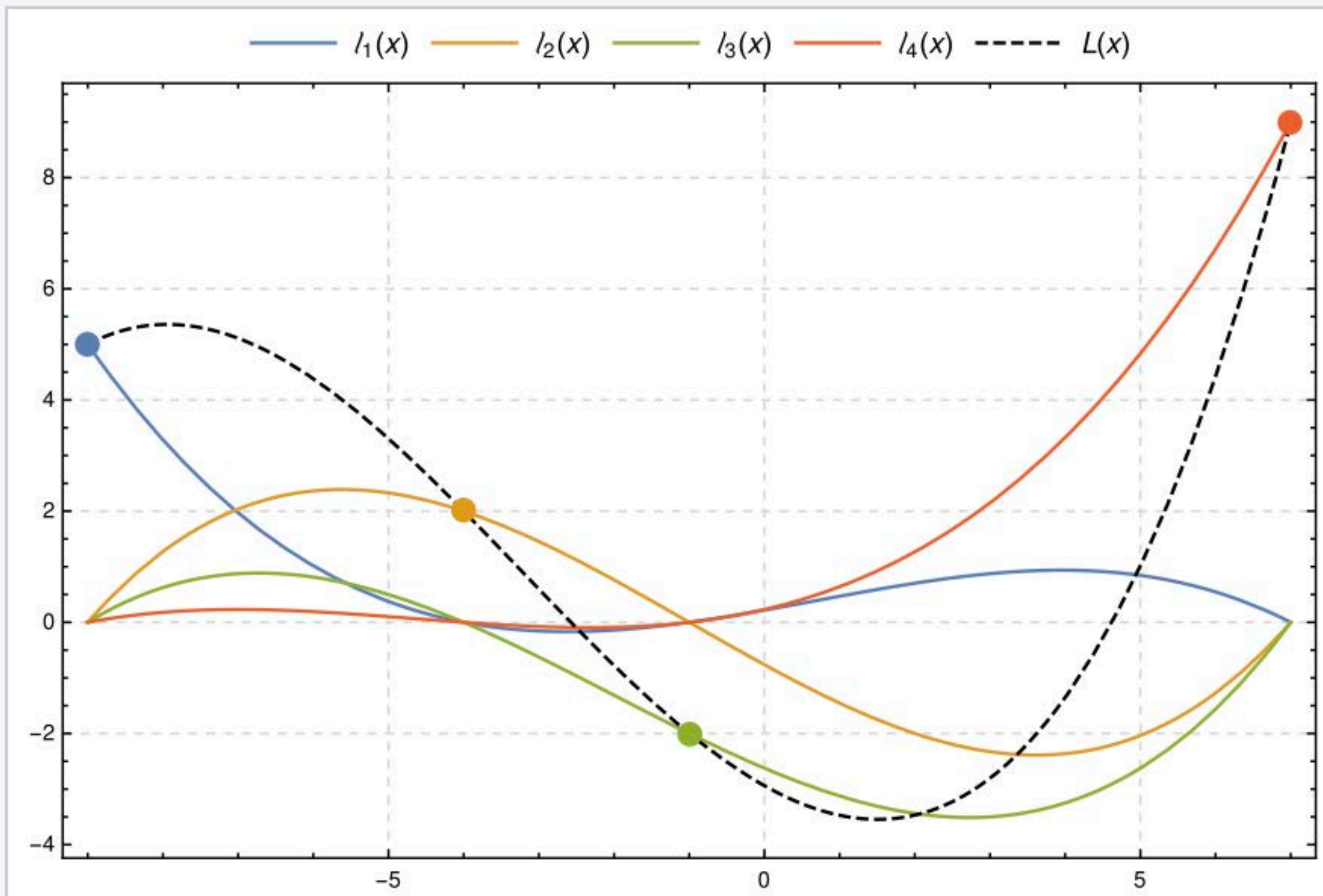
```python
#!/usr/bin/env python3
# -*- coding: utf-8 -*-
"""
Created on Tue Aug 28 12:27:37 2018

@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

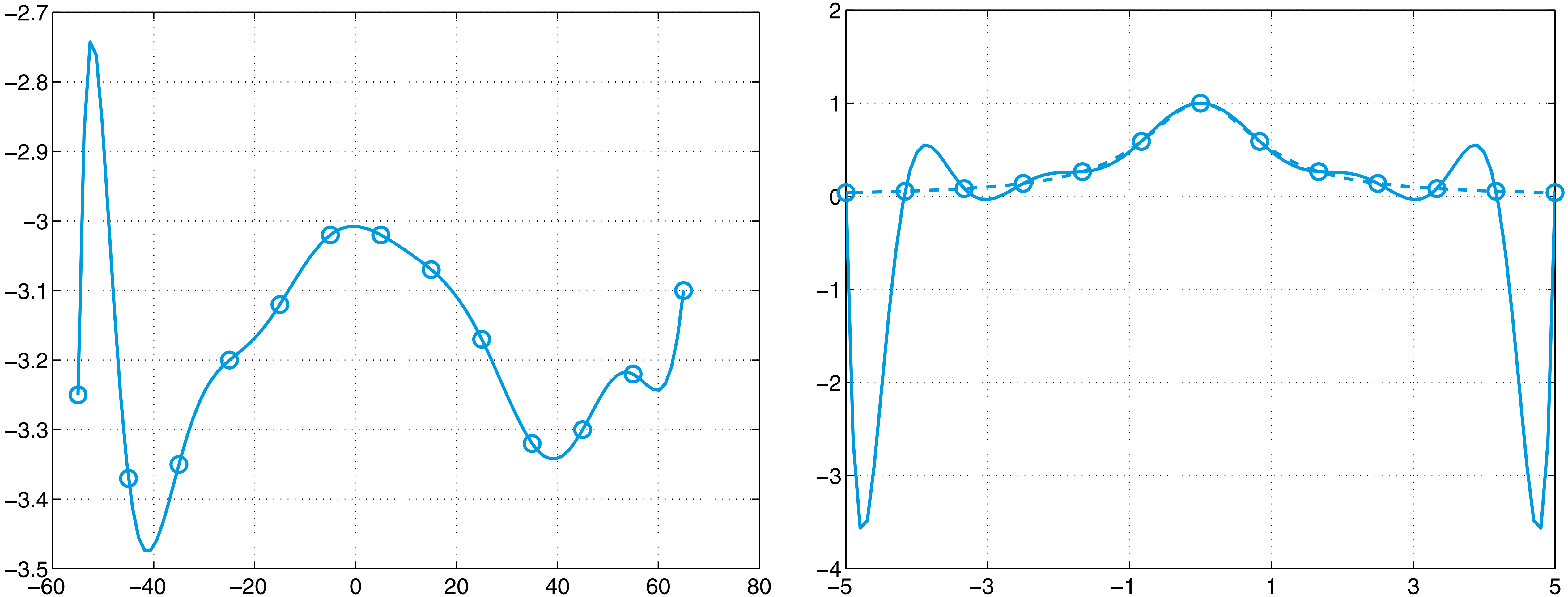


Fig. 3.6. Two examples of Runge's phenomenon: to the left, Π_{12} computed for the data of Table 3.1, column $K = 0.67$; to the right, $\Pi_{12}f$ (*solid line*) computed on 13 equispaced nodes for the function $f(x) = 1/(1 + x^2)$ (*dashed line*)

Interpolation with trigonometric polynomials

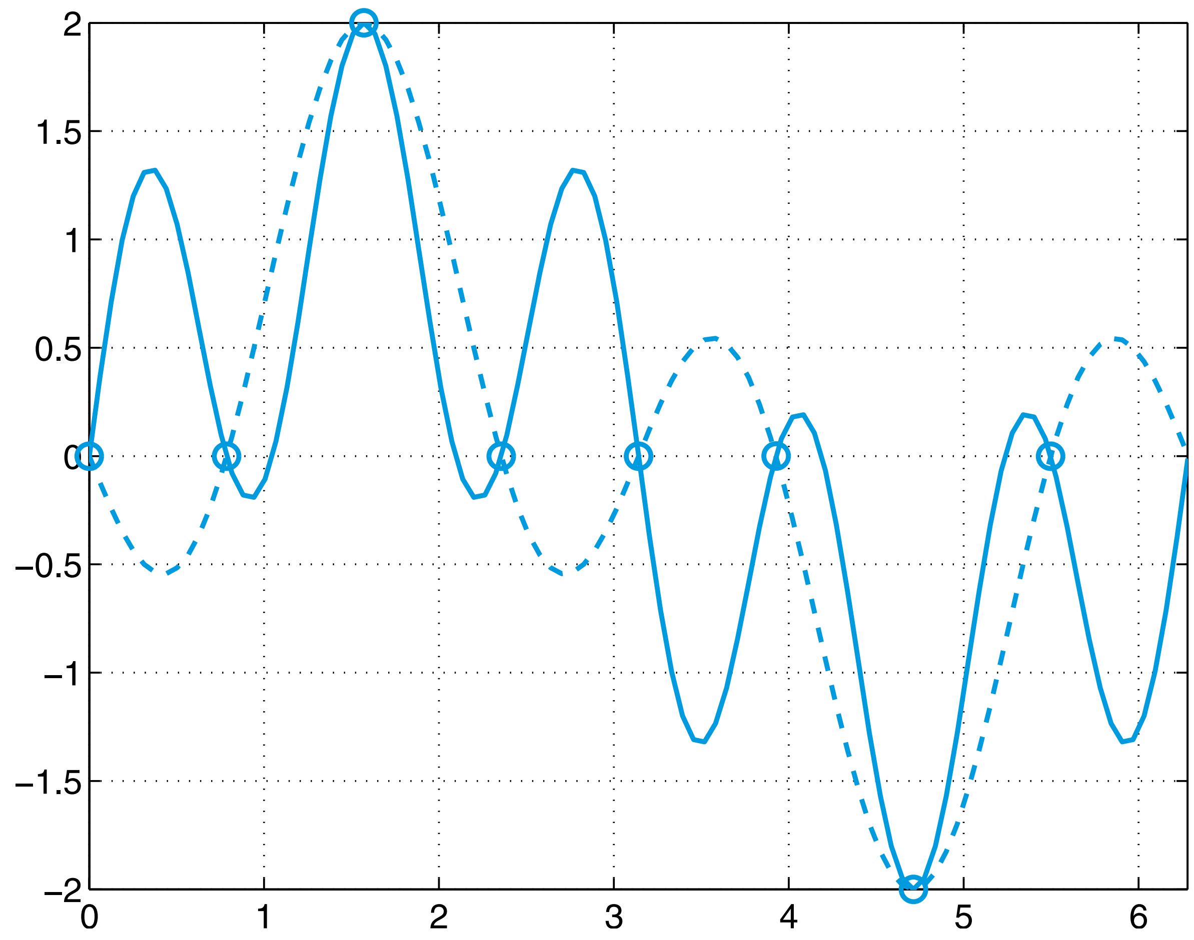


Fig. 3.9. The effects of aliasing: comparison between the function $f(x) = \sin(x)+\sin(5x)$ (*solid line*) and its trigonometric interpolant (3.11) with $M = 3$ (*dashed line*)

Nyquist–Shannon sampling theorem

From Wikipedia, the free encyclopedia

In the field of digital signal processing, the **sampling theorem** is a fundamental bridge between continuous-time signals (often called "analog signals") and discrete-time signals (often called "digital signals"). It establishes a sufficient condition for a sample rate that permits a discrete sequence of *samples* to capture all the information from a continuous-time signal of finite bandwidth.