Chapter 1

A few motivating examples

Computational physics relies fundamentally on the mathematical framework of linear algebra to solve complex physical systems. In this chapter, we explore how diverse physical problems can be reformulated into two fundamental types of linear algebra problems: linear systems and eigenvalue problems. Before examining specific applications, let us establish precise mathematical definitions and notation.

1.1 Mathematical Foundations

1.1.1 Linear Systems

A linear system in n variables can be expressed as a matrix equation:

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{1.1.1}$$

where:

- $\mathbf{A} \in \mathbb{R}^{m\times n}$ is the coefficient matrix
- $\mathbf{x} \in \mathbb{R}^n$ is the column vector of unknowns
- $\mathbf{b} \in \mathbb{R}^m$ is the column vector of constants

More explicitly, Equation (1.1.1) represents the system:

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix} \tag{1.1.2}$$

A vector $\mathbf{x}^* \in \mathbb{R}^n$ is a solution to the linear system (1.1.1) if and only if $\mathbf{A}\mathbf{x}^* = \mathbf{b}$.

Theorem 1.1.1. *For a square matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$, the linear system (1.1.1) has a unique solution if and only if $\mathbf{A}$ is nonsingular (i.e., $\det(\mathbf{A}) \neq 0$).*

1.1.2 Eigenvalue Problems

The second fundamental problem type we encounter is the eigenvalue problem:

$$\mathbf{A}\mathbf{x}_n = \lambda_n \mathbf{x}_n \tag{1.1.3}$$

where:

- $\mathbf{A} \in \mathbb{R}^{n\times n}$ is a square matrix
- $\lambda_n \in \mathbb{C}$ is called an eigenvalue of $\mathbf{A}$
- $\mathbf{x}_n \in \mathbb{C}^n \setminus \{\mathbf{0}\}$ is the corresponding eigenvector

A scalar λ_n and a nonzero vector $\mathbf{x}_n$ form an **eigenvalue-eigenvector pair** of matrix $\mathbf{A}$ if they satisfy Equation (1.1.3). The eigenvalue problem can be rewritten as:

$$(\mathbf{A} - \lambda_n \mathbf{I})\mathbf{x}_n = \mathbf{0} \tag{1.1.4}$$

where $\mathbf{I}$ is the $n \times n$ identity matrix. This leads to the characteristic equation:

$$\det(\mathbf{A} - \lambda \mathbf{I}) = 0 \tag{1.1.5}$$

Theorem 1.1.2. *Every square matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ has at least one complex eigenvalue. If $\mathbf{A}$ is real and symmetric, all its eigenvalues are real.*

1.2 Linear Systems: Circuits

Electrical circuits are classic examples where linear algebra is applied to solve practical physical problems. By applying Kirchhoff's laws (voltage and current laws), we can set up systems of linear equations that describe the behavior of circuits.

Kirchhoff's Voltage Law (KVL) states that the directed sum of the electrical potential differences (voltage) around any closed network is zero. For instance, in a loop containing a voltage source and several resistors where different currents may flow through different parts of the circuit:

$$V = I_1 R_1 + I_2 R_2 + \cdots + I_n R_n \tag{1.2.1}$$

where V is the voltage supplied by the source, I_k are the currents flowing through each part of the circuit, and R_k are the corresponding resistances. The sign of each term depends on the chosen direction of current flow relative to the direction in which we traverse the loop.

Kirchhoff's Current Law (KCL) states that the total current entering a junction must equal the total current leaving the junction. This law is used to set up equations where the sum of currents entering and exiting a node is zero:

$$\sum_{k=1}^{n} I_k = 0 \tag{1.2.2}$$

where I_k represents the current through the k-th component connected to the junction, with appropriate signs (+ for entering, - for leaving).

For complex circuits with multiple loops and junctions, we combine both KVL and KCL equations into a single matrix equation:

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{11} & b_{12} & \cdots & b_{1n} \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \\ \vdots \\ I_n \end{pmatrix} = \begin{pmatrix} V_1 \\ V_2 \\ \vdots \\ 0 \end{pmatrix} \tag{1.2.3}$$

or more compactly as:

$$\mathbf{AI} = \mathbf{b} \tag{1.2.4}$$

where $\mathbf{A}$ is the coefficient matrix containing terms from both resistance laws and current laws, $\mathbf{I}$ is the vector of unknown currents, and $\mathbf{b}$ is the right-hand side vector containing both voltage values (from KVL equations) and zeros (from KCL equations). The elements a_{ij} in the upper part of matrix $\mathbf{A}$ come from voltage laws and contain resistance values with appropriate signs, while the elements b_{ij} in the lower part come from current laws and contain only 1's and -1's depending on current direction conventions.

1.2.1 Example: A Parallel-Series Circuit

Consider the following circuit with parallel resistors:

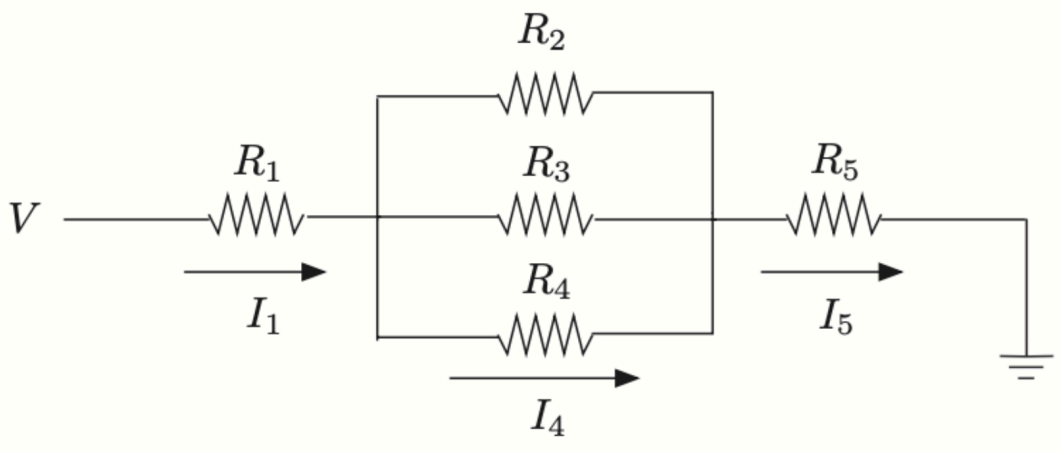

Figure 1.2.1: A simple circuit with parallel resistors

In this circuit:

- One voltage source V

- Five resistors R_1 through R_5
- R_2, R_3, and R_4 form a parallel network
- R_1 and R_5 are in series with the parallel network
- Five currents I_1 through I_5 to be determined

Applying Kirchhoff's voltage law to the three possible paths from voltage source to ground yields:

$$V - I_1R_1 - I_2R_2 - I_5R_5 = 0 \tag{1.2.5}$$
$$V - I_1R_1 - I_3R_3 - I_5R_5 = 0 \tag{1.2.6}$$
$$V - I_1R_1 - I_4R_4 - I_5R_5 = 0 \tag{1.2.7}$$

From the conservation of current, we know that all current that leaves the voltage source must eventually flow into ground:

$$I_5 = I_1 \tag{1.2.8}$$

Additionally, the current leaving the voltage source must split between the three parallel paths:

$$I_1 = I_2 + I_3 + I_4 \tag{1.2.9}$$

Substituting $I_5 = I_1$ and rearranging the equations, we obtain:

$$I_1(R_1 + R_5) + I_2R_2 = V \tag{1.2.10}$$
$$I_1(R_1 + R_5) + I_3R_3 = V \tag{1.2.11}$$
$$I_1(R_1 + R_5) + I_4R_4 = V \tag{1.2.12}$$
$$I_1 - I_2 - I_3 - I_4 = 0 \tag{1.2.13}$$

This system can be written in matrix form $\mathbf{Ax} = \mathbf{b}$:

$$\begin{pmatrix} R_1 + R_5 & R_2 & 0 & 0 \\ R_1 + R_5 & 0 & R_3 & 0 \\ R_1 + R_5 & 0 & 0 & R_4 \\ 1 & -1 & -1 & -1 \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_4 \end{pmatrix} = \begin{pmatrix} V \\ V \\ V \\ 0 \end{pmatrix} \tag{1.2.14}$$

1.3 Linear Systems: Data Fitting

Data fitting is an indispensable tool in both theoretical and experimental physics. It involves modeling the relationship between variables in a dataset to extrapolate or interpolate information. Consider a set of experimental data points (x_i, y_i) for $i = 1, 2, ..., m$. We want to model the relationship using a linear combination of basis functions:

$$y \simeq \sum_{j=1}^{n} \beta_j \phi_j(x) \tag{1.3.1}$$

Here, $\phi_j(x)$ are the chosen basis functions, and β_j are the coefficients to be determined. The choice of basis functions depends on the context, we will see some examples later.

The general fitting problem can be expressed in matrix form:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \tag{1.3.2}$$

where $\mathbf{y}$ is the $m \times 1$ vector of observed values, $\boldsymbol{\beta}$ is the $n \times 1$ vector of coefficients, and $\boldsymbol{\epsilon}$ is the $m \times 1$ vector of residuals.

The so-called "design matrix" $\mathbf{X}$ is constructed using our chosen basis functions evaluated on the dataset:

$$\mathbf{X} = \begin{pmatrix} \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_n(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \cdots & \phi_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_m) & \phi_2(x_m) & \cdots & \phi_n(x_m) \end{pmatrix}, \tag{1.3.3}$$

thus

$$X_{ij} \;=\; \phi_j(x_i)$$

1.3.1 Solving the Generalized Least Squares Problem

Our objective is to minimize the sum of squared residuals:

$$S = \|\boldsymbol{\epsilon}\|^2 = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 = \sum_{i=1}^{m} \left(y_i - \sum_{j=1}^{n} \beta_j \phi_j(x_i) \right)^2 \tag{1.3.4}$$

By taking the partial derivatives of S with respect to each β_j and setting them to zero:

$$\frac{\partial S}{\partial \beta_k} = -2 \sum_{i=1}^{m} \left(y_i - \sum_{j=1}^{n} \beta_j \phi_j(x_i) \right) \phi_k(x_i) = 0, \tag{1.3.5}$$

we arrive at the normal equations

$$\sum_{ij} \beta_j \phi_j(x_i) \phi_k(x_i) \;=\; \sum_{i} y_i \phi_k(x_i) \tag{1.3.6}$$

$$\sum_{ij} \phi_k(x_i) \phi_j(x_i) \beta_j \;=\; \sum_{i} \phi_k(x_i) y_i \tag{1.3.7}$$

$$\sum_{ij} X_{ik} X_{ij} \beta_j \;=\; \sum_{i} X_{ik} y_i, \tag{1.3.8}$$

which can be written in compact form as:

$$\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} = \mathbf{X}^T\mathbf{y} \tag{1.3.9}$$

The solution, assuming $\mathbf{X}^T\mathbf{X}$ is non-singular, is given by the solution of the following linear system:

$$\boldsymbol{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \tag{1.3.10}$$

1.3.2 Common Basis Function Applications

Polynomial Fitting: For a quadratic model $y = \beta_1 + \beta_2 x + \beta_3 x^2$, the basis functions are $\phi_1(x) = 1$, $\phi_2(x) = x$, and $\phi_3(x) = x^2$.
The design matrix becomes:

$$\mathbf{X} = \begin{pmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_m & x_m^2 \end{pmatrix}. \tag{1.3.11}$$

Fourier Series: For periodic data, we might use $\phi_1(x) = 1$, $\phi_{2k}(x) = \sin(kx)$, and $\phi_{2k+1}(x) = \cos(kx)$ for $k = 1, 2, \ldots$.
This is particularly useful for analyzing oscillatory phenomena in physics.

Damped Oscillation: For a damped oscillation, we might use a model:

$$y = \alpha_0 + \alpha_1 e^{-\alpha_2 x}\sin(\alpha_3 x) \tag{1.3.12}$$

This is non-linear in α_2 and α_3, but we can linearize it by choosing:

$$\phi_1(x) = 1, \quad \phi_2(x) = e^{-\lambda x}\sin(\omega x), \quad \phi_3(x) = e^{-\lambda x}\cos(\omega x) \tag{1.3.13}$$

for fixed λ and ω. We can then solve the linear least squares problem for β_1, β_2, and β_3, and iterate over different values of λ and ω to find the best fit.

1.4 Eigenvalue Problem: Harmonic Oscillations

Harmonic oscillations are crucial in understanding the dynamics of many physical systems. They offer a fundamental insight into how systems revert to equilibrium when displaced. Let's explore the dynamics of such systems in the context of springs and masses, commonly used as models in physics to illustrate basic and complex concepts in mechanics.

Consider a simple system composed of several masses connected by springs in a one-dimensional array. Each mass is connected to its neighbors by springs, and possibly to fixed points at the boundary, depending on the system configuration (e.g., fixed-fixed, free-free, fixed-free).

The system can be described using Newton's second law. For a mass m_i connected to two neighbors by springs with spring constant k, the equation of motion is given by Hooke's law:

$$m_i \ddot{x}_i = k(x_{i+1} - x_i) + k(x_{i-1} - x_i), \tag{1.4.1}$$

where $\ddot{x}_i$ is the acceleration of mass i, and x_i, x_{i+1}, and x_{i-1} are the displacements of mass i and its immediate neighbors from their equilibrium positions.

These equations for an array of masses can be compactly represented in matrix form. For simplicity, let us assume that all masses are identical, thus $m_i = m$. Now, defining $\mathbf{x} = (x_1, x_2, \ldots, x_N)^T$ as the displacement vector, the system of equations can be written as:

$$m\ddot{\mathbf{x}} = -\mathbf{K}\mathbf{x}, \tag{1.4.2}$$

where $\mathbf{K}$ is also called the stiffness matrix.

For a system with N masses and fixed ends, the stiffness matrix $\mathbf{K}$ takes the form:

$$\mathbf{K} = k \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix} \tag{1.4.3}$$

This tridiagonal matrix encodes the coupling between adjacent masses. The diagonal elements (2k) represent the restoring force on each mass due to its displacement, while the off-diagonal elements (-k) represent the coupling forces between neighboring masses.

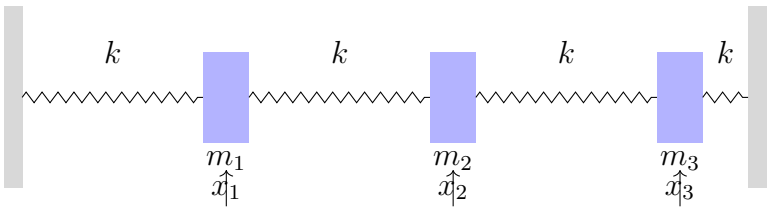

Figure 1.4.1: A system of three masses connected by springs with fixed ends. Each mass can move horizontally, and its displacement is measured relative to its equilibrium position.

The system shown in Figure 1.4.1 illustrates the physical setup of our mathematical model. Each mass can move horizontally along the x-axis, and the springs provide restoring forces according to Hooke's law. The displacements x_1, x_2, and x_3 are measured relative to the equilibrium positions of the masses.

1.4.1 Natural Frequencies and Modes

The solution to the motion of this system involves finding the natural frequencies and mode shapes, which are characterized by the eigenvalues and eigenvectors of the system matrix. Transforming the system into a standard eigenvalue problem, we consider harmonic solutions of the form

$$\mathbf{x}_n(t) = \mathbf{v}_n e^{i\omega_n t}, \tag{1.4.4}$$

leading to:

$$(\mathbf{K} - \omega_n^2 m)\mathbf{v}_n = 0. \tag{1.4.5}$$

We therefore see that all eigenvectors $\mathbf{v}_n$ of the stiffness matrix $\mathbf{K}$ are a valid solution, since the equation above is completely equivalent to an eigenvalue problem with eigenvalues $\lambda_n = \omega_n^2 m$:

$$\mathbf{K}\mathbf{v}_n \quad = \quad \left(\omega_n^2 m\right)\mathbf{v}_n. \tag{1.4.6}$$

For the fixed-ends case, the eigenvalues and eigenvectors have analytical expressions:

$$\omega_n^2 = \frac{4k}{m}\sin^2\left(\frac{n\pi}{2(N+1)}\right), \quad n = 1, 2, \ldots, N \tag{1.4.7}$$

$$v_n(j) = \sin\left(\frac{nj\pi}{N+1}\right), \quad j = 1, 2, \ldots, N \tag{1.4.8}$$

These normal modes form a complete orthogonal basis for describing any motion of the system. The general solution for the motion can be written as a superposition of these modes:

$$\mathbf{x}(t) = \sum_{n=1}^{N} \mathbf{v}_n(a_n \cos(\omega_n t) + b_n \sin(\omega_n t)) \tag{1.4.9}$$

where A_n and ϕ_n are determined by the initial conditions. Each mode represents a particular pattern of oscillation where all masses move with the same frequency but with different amplitudes given by the components of the eigenvector $\mathbf{v}_n$.

1.4.2 Proof of General Solution

Let's derive the general solution of our system. We'll see that while it naturally arises in terms of both sines and cosines, it can be rewritten in a more compact form using just cosines with phase shifts.

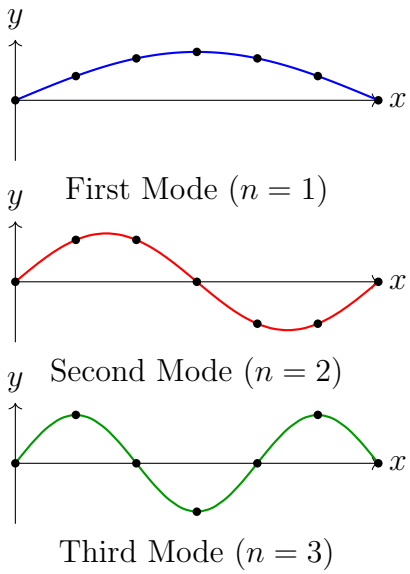

Figure 1.4.2: First three normal modes of the string with fixed ends. Black dots represent the masses, and the continuous curves show the mode shapes.

First, let's write the most general form of the solution:

$$\mathbf{x}(t) = \sum_{n=1}^{N} \mathbf{v}_n (a_n \cos(\omega_n t) + b_n \sin(\omega_n t)) \tag{1.4.10}$$

This can be rewritten using the trigonometric identity for the cosine of a sum:

$$a\cos(t) + b\sin(t) = A\cos(t + \phi) \tag{1.4.11}$$

where

$$A = \sqrt{a^2 + b^2}, \quad \phi = \arctan(b/a) \tag{1.4.12}$$

Therefore, our solution can be expressed as:

$$\mathbf{x}(t) = \sum_{n=1}^{N} A_n \mathbf{v}_n \cos(\omega_n t + \phi_n) \tag{1.4.13}$$

Let's prove this is indeed the general solution. First, recall that for a system with N degrees of freedom, the symmetric matrix $\mathbf{K}$ has N linearly independent eigenvectors $\{\mathbf{v}_n\}$ that form a complete basis. Due to this completeness property, any initial displacement $\mathbf{x}(0)$ and velocity $\dot{\mathbf{x}}(0)$ can be expressed as linear combinations of these eigenvectors:

$$\mathbf{x}(0) = \sum_{n=1}^{N} c_n \mathbf{v}_n \tag{1.4.14}$$

$$\dot{\mathbf{x}}(0) = \sum_{n=1}^{N} d_n \mathbf{v}_n \tag{1.4.15}$$

For each eigenvector $\mathbf{v}_n$, we have:

$$\mathbf{K}\mathbf{v}_n = \omega_n^2 \mathbf{M}\mathbf{v}_n \tag{1.4.16}$$

Given these properties, we can propose a general solution of the form:

$$\mathbf{x}(t) = \sum_{n=1}^{N} \mathbf{v}_n (a_n \cos(\omega_n t) + b_n \sin(\omega_n t)) \tag{1.4.17}$$

This solution satisfies the original differential equation because each term individually satisfies it:

$$\mathbf{M}\ddot{\mathbf{x}} + \mathbf{K}\mathbf{x} = \sum_{n=1}^{N} [-\omega_n^2 \mathbf{M}\mathbf{v}_n (a_n \cos(\omega_n t) + b_n \sin(\omega_n t)) + \mathbf{K}\mathbf{v}_n (a_n \cos(\omega_n t) + b_n \sin(\omega_n t))] = 0 \tag{1.4.18}$$

The coefficients a_n and b_n can be determined from the initial conditions. For a given set of initial conditions $\mathbf{x}(0)$ and $\dot{\mathbf{x}}(0)$, we have:

$$a_n = \frac{\mathbf{v}_n^T \mathbf{M}\mathbf{x}(0)}{\mathbf{v}_n^T \mathbf{M}\mathbf{v}_n}, \quad b_n = \frac{\mathbf{v}_n^T \mathbf{M}\dot{\mathbf{x}}(0)}{\omega_n \mathbf{v}_n^T \mathbf{M}\mathbf{v}_n} \tag{1.4.19}$$