Chapter 4

Orthogonality

Orthogonality is the mathematical formalization of the geometrical property of perpendicularity, as adapted to general inner product spaces. In linear algebra, bases consisting of mutually orthogonal elements play an essential role in theoretical developments, in a broad range of applications, and in the design of practical numerical algorithms. Computations become dramatically simpler and less prone to numerical instabilities when performed in orthogonal coordinate systems. Indeed, many large-scale modern applications would be impractical, if not completely infeasible, were it not for the dramatic simplifying power of orthogonality.

The duly famous Gram–Schmidt process will convert an arbitrary basis of an inner product space into an orthogonal basis. In Euclidean space, the Gram–Schmidt process can be reinterpreted as a new kind of matrix factorization, in which a nonsingular matrix $A = Q\,R$ is written as the product of an orthogonal matrix Q and an upper triangular matrix R. The $Q\,R$ factorization and its generalizations are used in statistical data analysis as well as the design of numerical algorithms for computing eigenvalues and eigenvectors. In function space, the Gram–Schmidt algorithm is employed to construct orthogonal polynomials and other useful systems of orthogonal functions.

Orthogonality is motivated by geometry, and orthogonal matrices, meaning those whose columns form an orthonormal system, are of fundamental importance in the mathematics of symmetry, in image processing, and in computer graphics, animation, and cinema, [**5**, **12**, **72**, **73**]. The orthogonal projection of a point onto a subspace turns out to be the closest point or least squares minimizer, as we discuss in Chapter 5. Yet another important fact is that the four fundamental subspaces of a matrix that were introduced in Chapter 2 come in mutually orthogonal pairs. This observation leads directly to a new characterization of the compatibility conditions for linear algebraic systems known as the Fredholm alternative, whose extensions are used in the analysis of linear boundary value problems, differential equations, and integral equations, [**16**, **61**]. The orthogonality of eigenvector and eigenfunction bases for symmetric matrices and self-adjoint operators provides the key to understanding the dynamics of discrete and continuous mechanical, thermodynamical, electrical, and quantum mechanical systems.

One of the most fertile applications of orthogonal bases is in signal processing. Fourier analysis decomposes a signal into its simple periodic components — sines and cosines — which form an orthogonal system of functions, [**61**, **77**]. Modern digital media, such as CD's, DVD's and MP3's, are based on discrete data obtained by sampling a physical signal. The Discrete Fourier Transform (DFT) uses orthogonality to decompose the sampled signal vector into a linear combination of sampled trigonometric functions (or, more accurately, complex exponentials). Basic data compression and noise removal algorithms are applied to the discrete Fourier coefficients, acting on the observation that noise tends to accumulate in the high-frequency Fourier modes. More sophisticated signal and image processing techniques, including smoothing and compression algorithms, are based on orthogonal wavelet bases, which are discussed in Section 9.7.

P. J. Olver, C. Shakiban, *Applied Linear Algebra*, Undergraduate Texts in Mathematics,
https://doi.org/10.1007/978-3-319-91041-3_4

Figure 4.1. Orthonormal Bases in $\mathbb{R}^2$ and $\mathbb{R}^3$.

4.1 Orthogonal and Orthonormal Bases

Let V be a real[†] inner product space. Recall that two elements $\mathbf{v}, \mathbf{w} \in V$ are called *orthogonal* if their inner product vanishes: $\langle \mathbf{v}, \mathbf{w} \rangle = 0$. In the case of vectors in Euclidean space, orthogonality under the dot product means that they meet at a right angle.

A particularly important configuration arises when V admits a basis consisting of mutually orthogonal elements.

Definition 4.1. A basis $\mathbf{u}_1, \ldots, \mathbf{u}_n$ of an n-dimensional inner product space V is called *orthogonal* if $\langle \mathbf{u}_i, \mathbf{u}_j \rangle = 0$ for all $i \neq j$. The basis is called *orthonormal* if, in addition, each vector has unit length: $\| \mathbf{u}_i \| = 1$, for all $i = 1, \ldots, n$.

For the Euclidean space $\mathbb{R}^n$ equipped with the standard dot product, the simplest example of an orthonormal basis is the standard basis

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \qquad \ldots \qquad \mathbf{e}_n = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}.$$

Orthogonality follows because $\mathbf{e}_i \cdot \mathbf{e}_j = 0$, for $i \neq j$, while $\| \mathbf{e}_i \| = 1$ implies normality.

Since a basis cannot contain the zero vector, there is an easy way to convert an orthogonal basis to an orthonormal basis. Namely, we replace each basis vector with a unit vector pointing in the same direction, as in Lemma 3.14.

Lemma 4.2. If $\mathbf{v}_1, \ldots, \mathbf{v}_n$ is an orthogonal basis of a vector space V, then the normalized vectors $\mathbf{u}_i = \mathbf{v}_i / \| \mathbf{v}_i \|$, $i = 1, \ldots, n$, form an orthonormal basis.

[†] The methods can be adapted more or less straightforwardly to the complex realm. The main complication, as noted in Section 3.6, is that we need to be careful with the order of vectors appearing in the conjugate symmetric complex inner products. In this chapter, we will be careful to write the inner product formulas in the proper order so that they retain their validity in complex vector spaces.

Example 4.3. The vectors

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 2 \\ -1 \end{pmatrix}, \qquad \mathbf{v}_2 = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}, \qquad \mathbf{v}_3 = \begin{pmatrix} 5 \\ -2 \\ 1 \end{pmatrix},$$

are easily seen to form a basis of $\mathbb{R}^3$. Moreover, they are mutually perpendicular, $\mathbf{v}_1 \cdot \mathbf{v}_2 = \mathbf{v}_1 \cdot \mathbf{v}_3 = \mathbf{v}_2 \cdot \mathbf{v}_3 = 0$, and so form an orthogonal basis with respect to the standard dot product on $\mathbb{R}^3$. When we divide each orthogonal basis vector by its length, the result is the orthonormal basis

$$\mathbf{u}_1 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ 2 \\ -1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \end{pmatrix}, \quad \mathbf{u}_2 = \frac{1}{\sqrt{5}}\begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} \end{pmatrix}, \quad \mathbf{u}_3 = \frac{1}{\sqrt{30}}\begin{pmatrix} 5 \\ -2 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{5}{\sqrt{30}} \\ -\frac{2}{\sqrt{30}} \\ \frac{1}{\sqrt{30}} \end{pmatrix},$$

satisfying $\mathbf{u}_1 \cdot \mathbf{u}_2 = \mathbf{u}_1 \cdot \mathbf{u}_3 = \mathbf{u}_2 \cdot \mathbf{u}_3 = 0$ and $\| \mathbf{u}_1 \| = \| \mathbf{u}_2 \| = \| \mathbf{u}_3 \| = 1$. The appearance of square roots in the elements of an orthonormal basis is fairly typical.

A useful observation is that every orthogonal collection of nonzero vectors is automatically linearly independent.

Proposition 4.4. Let $\mathbf{v}_1, \ldots, \mathbf{v}_k \in V$ be nonzero, mutually orthogonal elements, so $\mathbf{v}_i \neq \mathbf{0}$ and $\langle \mathbf{v}_i , \mathbf{v}_j \rangle = 0$ for all $i \neq j$. Then $\mathbf{v}_1, \ldots, \mathbf{v}_k$ are linearly independent.

Proof: Suppose

$$c_1 \mathbf{v}_1 + \cdots + c_k \mathbf{v}_k = \mathbf{0}.$$

Let us take the inner product of this equation with any $\mathbf{v}_i$. Using linearity of the inner product and orthogonality, we compute

$$0 = \langle c_1 \mathbf{v}_1 + \cdots + c_k \mathbf{v}_k , \mathbf{v}_i \rangle = c_1 \langle \mathbf{v}_1 , \mathbf{v}_i \rangle + \cdots + c_k \langle \mathbf{v}_k , \mathbf{v}_i \rangle = c_i \langle \mathbf{v}_i , \mathbf{v}_i \rangle = c_i \| \mathbf{v}_i \|^2.$$

Therefore, given that $\mathbf{v}_i \neq \mathbf{0}$, we conclude that $c_i = 0$. Since this holds for all $i = 1, \ldots, k$, the linear independence of $\mathbf{v}_1, \ldots, \mathbf{v}_k$ follows. *Q.E.D.*

As a direct corollary, we infer that every collection of nonzero orthogonal vectors forms a basis for its span.

Theorem 4.5. Suppose $\mathbf{v}_1, \ldots, \mathbf{v}_n \in V$ are nonzero, mutually orthogonal elements of an inner product space V. Then $\mathbf{v}_1, \ldots, \mathbf{v}_n$ form an orthogonal basis for their span $W = \operatorname{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subset V$, which is therefore a subspace of dimension $n = \dim W$. In particular, if $\dim V = n$, then $\mathbf{v}_1, \ldots, \mathbf{v}_n$ form a orthogonal basis for V.

Orthogonality is also of profound significance for function spaces. Here is a relatively simple example.

Example 4.6. Consider the vector space $\mathcal{P}^{(2)}$ consisting of all quadratic polynomials $p(x) = \alpha + \beta x + \gamma x^2$, equipped with the L^2 inner product and norm

$$\langle p , q \rangle = \int_0^1 p(x)\, q(x)\, dx, \qquad \| p \| = \sqrt{\langle p , p \rangle} = \sqrt{\int_0^1 p(x)^2\, dx}\ .$$

The standard monomials $1, x, x^2$ do *not* form an orthogonal basis. Indeed,

$$\langle\, 1\,, x\,\rangle = \tfrac{1}{2}\,, \qquad \langle\, 1\,, x^2\,\rangle = \tfrac{1}{3}\,, \qquad \langle\, x\,, x^2\,\rangle = \tfrac{1}{4}\,.$$

One orthogonal basis of $\mathcal{P}^{(2)}$ is provided by following polynomials:

$$p_1(x) = 1, \qquad p_2(x) = x - \tfrac{1}{2}\,, \qquad p_3(x) = x^2 - x + \tfrac{1}{6}\,. \tag{4.1}$$

Indeed, one easily verifies that $\langle\, p_1\,, p_2\,\rangle = \langle\, p_1\,, p_3\,\rangle = \langle\, p_2\,, p_3\,\rangle = 0$, while

$$\|\, p_1 \,\| = 1, \qquad \|\, p_2 \,\| = \frac{1}{\sqrt{12}} = \frac{1}{2\,\sqrt{3}}\,, \qquad \|\, p_3 \,\| = \frac{1}{\sqrt{180}} = \frac{1}{6\,\sqrt{5}}\,.$$

The corresponding orthonormal basis is found by dividing each orthogonal basis element by its norm:

$$u_1(x) = 1, \qquad u_2(x) = \sqrt{3}\,\left(\, 2x - 1\,\right), \qquad u_3(x) = \sqrt{5}\,\left(\, 6x^2 - 6x + 1\,\right).$$

In Section 4.5 below, we will learn how to systematically construct such orthogonal systems of polynomials.

Exercises

4.1.1. Let $\mathbb{R}^2$ have the standard dot product. Classify the following pairs of vectors as (i) basis, (ii) orthogonal basis, and/or (iii) orthonormal basis:
(a) $\mathbf{v}_1 = \begin{pmatrix} -1 \\ 2 \end{pmatrix}$, $\mathbf{v}_2 = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$; (b) $\mathbf{v}_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$, $\mathbf{v}_2 = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$; (c) $\mathbf{v}_1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$, $\mathbf{v}_2 = \begin{pmatrix} 2 \\ 2 \end{pmatrix}$;
(d) $\mathbf{v}_1 = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$, $\mathbf{v}_2 = \begin{pmatrix} 1 \\ -6 \end{pmatrix}$; (e) $\mathbf{v}_1 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$, $\mathbf{v}_2 = \begin{pmatrix} 0 \\ 3 \end{pmatrix}$; (f) $\mathbf{v}_1 = \begin{pmatrix} \frac{3}{5} \\ \frac{4}{5} \end{pmatrix}$, $\mathbf{v}_2 = \begin{pmatrix} -\frac{4}{5} \\ \frac{3}{5} \end{pmatrix}$.

4.1.2. Let $\mathbb{R}^3$ have the standard dot product. Classify the following sets of vectors as (i) basis, (ii) orthogonal basis, and/or (iii) orthonormal basis:
(a) $\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$; (b) $\begin{pmatrix} -\frac{4}{13} \\ \frac{3}{5} \\ -\frac{48}{65} \end{pmatrix}, \begin{pmatrix} \frac{12}{13} \\ 0 \\ -\frac{5}{13} \end{pmatrix}, \begin{pmatrix} \frac{3}{13} \\ \frac{4}{5} \\ \frac{36}{65} \end{pmatrix}$; (c) $\begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}, \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$.

4.1.3. Repeat Exercise 4.1.1, but use the weighted inner product $\langle\, \mathbf{v}\,, \mathbf{w}\,\rangle = v_1 w_1 + \frac{1}{9} v_2 w_2$ instead of the dot product.

4.1.4. Show that the standard basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ form an orthogonal basis with respect to the weighted inner product $\langle\, \mathbf{v}\,, \mathbf{w}\,\rangle = v_1 w_1 + 2 v_2 w_2 + 3 v_3 w_3$ on $\mathbb{R}^3$. Find an orthonormal basis for this inner product space.

4.1.5. Find all values of a such that the vectors $\begin{pmatrix} a \\ 1 \end{pmatrix}, \begin{pmatrix} -a \\ 1 \end{pmatrix}$ form an orthogonal basis of $\mathbb{R}^2$ under (a) the dot product; (b) the weighted inner product $\langle\, \mathbf{v}\,, \mathbf{w}\,\rangle = 3 v_1 w_1 + 2 v_2 w_2$; (c) the inner product prescribed by the positive definite matrix $K = \begin{pmatrix} 2 & -1 \\ -1 & 3 \end{pmatrix}$.

4.1.6. Find all possible values of a and b in the inner product $\langle\, \mathbf{v}\,, \mathbf{w}\,\rangle = a\, v_1 w_1 + b\, v_2 w_2$ that make the vectors $(\,1, 2\,)^T$, $(\,-1, 1\,)^T$, an orthogonal basis in $\mathbb{R}^2$.

4.1.7. Answer Exercise 4.1.6 for the vectors (a) $(\,2, 3\,)^T$, $(\,-2, 2\,)^T$; (b) $(\,1, 4\,)^T$, $(\,2, 1\,)^T$.

4.1.8. Find an inner product such that the vectors $(-1,2)^T$ and $(1,2)^T$ form an orthonormal basis of $\mathbb{R}^2$.

4.1.9. *True or false*: If $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ are a basis for $\mathbb{R}^3$, then they form an orthogonal basis under some appropriately weighted inner product $\langle \mathbf{v}, \mathbf{w} \rangle = a\, v_1 w_1 + b\, v_2 w_2 + c\, v_3 w_3$.

♡ 4.1.10. The *cross product* between two vectors in $\mathbb{R}^3$ is the vector defined by the formula

$$\mathbf{v} \times \mathbf{w} = \begin{pmatrix} v_2 w_3 - v_3 w_2 \\ v_3 w_1 - v_1 w_3 \\ v_1 w_2 - v_2 w_1 \end{pmatrix}, \qquad \text{where} \qquad \mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}, \quad \mathbf{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}. \tag{4.2}$$

(*a*) Show that $\mathbf{u} = \mathbf{v} \times \mathbf{w}$ is orthogonal, under the dot product, to both $\mathbf{v}$ and $\mathbf{w}$. (*b*) Show that $\mathbf{v} \times \mathbf{w} = \mathbf{0}$ if and only if $\mathbf{v}$ and $\mathbf{w}$ are parallel. (*c*) Prove that if $\mathbf{v}, \mathbf{w} \in \mathbb{R}^3$ are orthogonal nonzero vectors, then $\mathbf{u} = \mathbf{v} \times \mathbf{w}, \mathbf{v}, \mathbf{w}$ form an orthogonal basis of $\mathbb{R}^3$. (*d*) *True or false*: If $\mathbf{v}, \mathbf{w} \in \mathbb{R}^3$ are orthogonal unit vectors, then $\mathbf{v}, \mathbf{w}$ and $\mathbf{u} = \mathbf{v} \times \mathbf{w}$ form an orthonormal basis of $\mathbb{R}^3$.

♢ 4.1.11. Prove that every orthonormal basis of $\mathbb{R}^2$ under the standard dot product has the form $\mathbf{u}_1 = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$ and $\mathbf{u}_2 = \pm \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}$ for some $0 \le \theta < 2\pi$ and some choice of $\pm$ sign.

♢ 4.1.12. Given angles θ, φ, ψ, prove that the vectors $\mathbf{u}_1 = \begin{pmatrix} \cos\psi\cos\varphi - \cos\theta\sin\varphi\sin\psi \\ -\sin\psi\cos\varphi - \cos\theta\sin\varphi\cos\psi \\ \sin\theta\sin\varphi \end{pmatrix}$,

$\mathbf{u}_2 = \begin{pmatrix} \cos\psi\sin\varphi + \cos\theta\cos\varphi\sin\psi \\ -\sin\psi\sin\varphi + \cos\theta\cos\varphi\cos\psi \\ -\sin\theta\cos\varphi \end{pmatrix}$, $\mathbf{u}_3 = \begin{pmatrix} \sin\theta\sin\varphi \\ \sin\theta\cos\varphi \\ \cos\theta \end{pmatrix}$, form an orthonormal basis of $\mathbb{R}^3$ under the standard dot product. **Remark.** It can be proved, [**31**; p. 147], that *every* orthonormal basis of $\mathbb{R}^3$ has the form $\mathbf{u}_1, \mathbf{u}_2, \pm\mathbf{u}_3$ for some choice of angles θ, φ, ψ.

♡ 4.1.13. (a) Show that $\mathbf{v}_1, \ldots, \mathbf{v}_n$ form an orthonormal basis of $\mathbb{R}^n$ for the inner product $\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^T K \mathbf{w}$ for $K > 0$ if and only if $A^T K A = \mathrm{I}$, where $A = (\, \mathbf{v}_1 \ \mathbf{v}_2 \ \ldots \ \mathbf{v}_n \,)$. (*b*) Prove that every basis of $\mathbb{R}^n$ is an orthonormal basis with respect to some inner product. Is the inner product uniquely determined? (*c*) Find the inner product on $\mathbb{R}^2$ that makes $\mathbf{v}_1 = (1,1)^T$, $\mathbf{v}_2 = (2,3)^T$ into an orthonormal basis. (*d*) Find the inner product on $\mathbb{R}^3$ that makes $\mathbf{v}_1 = (1,1,1)^T$, $\mathbf{v}_2 = (1,1,2)^T$, $\mathbf{v}_3 = (1,2,3)^T$ an orthonormal basis.

4.1.14. Describe all orthonormal bases of $\mathbb{R}^2$ for the inner products

$$(a)\ \langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^T \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \mathbf{w}; \qquad (b)\ \langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^T \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix} \mathbf{w}.$$

4.1.15. Let $\mathbf{v}$ and $\mathbf{w}$ be elements of an inner product space. Prove that $\| \mathbf{v} + \mathbf{w} \|^2 = \| \mathbf{v} \|^2 + \| \mathbf{w} \|^2$ if and only if $\mathbf{v}, \mathbf{w}$ are orthogonal. Explain why this formula can be viewed as the generalization of the Pythagorean Theorem.

4.1.16. Prove that if $\mathbf{v}_1, \mathbf{v}_2$ form a basis of an inner product space V and $\| \mathbf{v}_1 \| = \| \mathbf{v}_2 \|$, then $\mathbf{v}_1 + \mathbf{v}_2$ and $\mathbf{v}_1 - \mathbf{v}_2$ form an orthogonal basis of V.

4.1.17. Suppose $\mathbf{v}_1, \ldots, \mathbf{v}_k$ are nonzero mutually orthogonal elements of an inner product space V. Write down their Gram matrix. Why is it nonsingular?

4.1.18. Let $V = \mathcal{P}^{(1)}$ be the vector space consisting of linear polynomials $p(t) = a\,t + b$. (*a*) Carefully explain why $\langle p, q \rangle = \displaystyle\int_0^1 t\, p(t)\, q(t)\, dt$ defines an inner product on V. (*b*) Find all polynomials $p(t) = a\,t + b \in V$ that are orthogonal to $p_1(t) = 1$ based on this inner product. (*c*) Use part (*b*) to construct an orthonormal basis of V for this inner product. (*d*) Find an orthonormal basis of the space $\mathcal{P}^{(2)}$ of quadratic polynomials for the same inner product. *Hint*: First find a quadratic polynomial that is orthogonal to the basis you constructed in part (*c*).

4.1.19. Explain why the functions $\cos x, \sin x$ form an orthogonal basis for the space of solutions to the differential equation $y'' + y = 0$ under the L^2 inner product on $[-\pi, \pi]$.

4.1.20. Do the functions $e^{x/2}, e^{-x/2}$ form an orthogonal basis for the space of solutions to the differential equation $4y'' - y = 0$ under the L^2 inner product on $[0,1]$? If not, can you find an orthogonal basis of the solution space?

Computations in Orthogonal Bases

What are the advantages of orthogonal and orthonormal bases? Once one has a basis of a vector space, a key issue is how to express other elements as linear combinations of the basis elements — that is, to find their *coordinates* in the prescribed basis. In general, this is not so easy, since it requires solving a system of linear equations, as described in (2.23). In high-dimensional situations arising in applications, computing the solution may require a considerable, if not infeasible, amount of time and effort.

However, if the basis is orthogonal, or, even better, orthonormal, then the change of basis computation requires almost no work. This is the crucial insight underlying the efficacy of both discrete and continuous Fourier analysis in signal, image, and video processing, least squares approximations, the statistical analysis of large data sets, and a multitude of other applications, both classical and modern.

Theorem 4.7. Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be an orthonormal basis for an inner product space V. Then one can write any element $\mathbf{v} \in V$ as a linear combination

$$\mathbf{v} = c_1 \mathbf{u}_1 + \cdots + c_n \mathbf{u}_n, \tag{4.3}$$

in which its *coordinates*

$$c_i = \langle \mathbf{v}, \mathbf{u}_i \rangle, \qquad i = 1, \ldots, n, \tag{4.4}$$

are explicitly given as inner products. Moreover, its norm is given by the *Pythagorean formula*

$$\| \mathbf{v} \| = \sqrt{c_1^2 + \cdots + c_n^2} = \sqrt{\sum_{i=1}^{n} \langle \mathbf{v}, \mathbf{u}_i \rangle^2}, \tag{4.5}$$

namely, the square root of the sum of the squares of its orthonormal basis coordinates.

Proof: Let us compute the inner product of the element (4.3) with one of the basis vectors. Using the orthonormality conditions

$$\langle \mathbf{u}_i, \mathbf{u}_j \rangle = \begin{cases} 0 & i \neq j, \\ 1 & i = j, \end{cases} \tag{4.6}$$

and bilinearity of the inner product, we obtain

$$\langle \mathbf{v}, \mathbf{u}_i \rangle = \left\langle \sum_{j=1}^{n} c_j \mathbf{u}_j, \mathbf{u}_i \right\rangle = \sum_{j=1}^{n} c_j \langle \mathbf{u}_j, \mathbf{u}_i \rangle = c_i \| \mathbf{u}_i \|^2 = c_i.$$

To prove formula (4.5), we similarly expand

$$\| \mathbf{v} \|^2 = \langle \mathbf{v}, \mathbf{v} \rangle = \left\langle \sum_{j=1}^{n} c_i \mathbf{u}_i, \sum_{j=1}^{n} c_j \mathbf{u}_j \right\rangle = \sum_{i,j=1}^{n} c_i c_j \langle \mathbf{u}_i, \mathbf{u}_j \rangle = \sum_{i=1}^{n} c_i^2,$$

again making use of the orthonormality of the basis elements. *Q.E.D.*

It is worth emphasizing that the Pythagorean-type formula (4.5) is valid for *all* inner products.

Example 4.8. Let us rewrite the vector $\mathbf{v} = (1,1,1)^T$ in terms of the orthonormal basis

$$\mathbf{u}_1 = \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \end{pmatrix}, \qquad \mathbf{u}_2 = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} \end{pmatrix}, \qquad \mathbf{u}_3 = \begin{pmatrix} \frac{5}{\sqrt{30}} \\ -\frac{2}{\sqrt{30}} \\ \frac{1}{\sqrt{30}} \end{pmatrix},$$

constructed in Example 4.3. Computing the dot products

$$\mathbf{v} \cdot \mathbf{u}_1 = \frac{2}{\sqrt{6}}, \qquad \mathbf{v} \cdot \mathbf{u}_2 = \frac{3}{\sqrt{5}}, \qquad \mathbf{v} \cdot \mathbf{u}_3 = \frac{4}{\sqrt{30}},$$

we immediately conclude that

$$\mathbf{v} = \frac{2}{\sqrt{6}}\,\mathbf{u}_1 + \frac{3}{\sqrt{5}}\,\mathbf{u}_2 + \frac{4}{\sqrt{30}}\,\mathbf{u}_3.$$

Needless to say, a direct computation based on solving the associated linear system, as in Chapter 2, is more tedious.

While passage from an orthogonal basis to its orthonormal version is elementary — one simply divides each basis element by its norm — we shall often find it more convenient to work directly with the unnormalized version. The next result provides the corresponding formula expressing a vector in terms of an orthogonal, but not necessarily orthonormal basis. The proof proceeds exactly as in the orthonormal case, and details are left to the reader.

Theorem 4.9. If $\mathbf{v}_1, \ldots, \mathbf{v}_n$ form an orthogonal basis, then the corresponding coordinates of a vector

$$\mathbf{v} = a_1 \mathbf{v}_1 + \cdots + a_n \mathbf{v}_n \qquad \text{are given by} \qquad a_i = \frac{\langle \mathbf{v}, \mathbf{v}_i \rangle}{\| \mathbf{v}_i \|^2}. \tag{4.7}$$

In this case, its norm can be computed using the formula

$$\| \mathbf{v} \|^2 = \sum_{i=1}^{n} a_i^2 \, \| \mathbf{v}_i \|^2 = \sum_{i=1}^{n} \left(\frac{\langle \mathbf{v}, \mathbf{v}_i \rangle}{\| \mathbf{v}_i \|} \right)^2. \tag{4.8}$$

Equation (4.7), along with its orthonormal simplification (4.4), is one of the most useful formulas we shall establish, and applications will appear repeatedly throughout this text and beyond.

Example 4.10. The wavelet basis

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \qquad \mathbf{v}_2 = \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, \qquad \mathbf{v}_3 = \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{v}_4 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}, \tag{4.9}$$

introduced in Example 2.35 is, in fact, an orthogonal basis of $\mathbb{R}^4$. The norms are

$$\| \mathbf{v}_1 \| = 2, \qquad \| \mathbf{v}_2 \| = 2, \qquad \| \mathbf{v}_3 \| = \sqrt{2}, \qquad \| \mathbf{v}_4 \| = \sqrt{2}.$$

Therefore, using (4.7), we can readily express any vector as a linear combination of the wavelet basis vectors. For example,

$$\mathbf{v} = \begin{pmatrix} 4 \\ -2 \\ 1 \\ 5 \end{pmatrix} = 2\,\mathbf{v}_1 - \mathbf{v}_2 + 3\,\mathbf{v}_3 - 2\,\mathbf{v}_4,$$

where the wavelet coordinates are computed directly by

$$\frac{\langle\, \mathbf{v}\,,\mathbf{v}_1 \,\rangle}{\|\,\mathbf{v}_1\,\|^2} = \frac{8}{4} = 2, \qquad \frac{\langle\, \mathbf{v}\,,\mathbf{v}_2 \,\rangle}{\|\,\mathbf{v}_2\,\|^2} = \frac{-4}{4} = -1, \qquad \frac{\langle\, \mathbf{v}\,,\mathbf{v}_3 \,\rangle}{\|\,\mathbf{v}_3\,\|^2} = \frac{6}{2} = 3, \qquad \frac{\langle\, \mathbf{v}\,,\mathbf{v}_4 \,\rangle}{\|\,\mathbf{v}_4\,\|^2} = \frac{-4}{2} = -2.$$

This is clearly quicker than solving the linear system, as we did earlier in Example 2.35. Finally, we note that

$$46 = \|\,\mathbf{v}\,\|^2 = 2^2\,\|\,\mathbf{v}_1\,\|^2 + (-1)^2\,\|\,\mathbf{v}_2\,\|^2 + 3^2\,\|\,\mathbf{v}_3\,\|^2 + (-2)^2\,\|\,\mathbf{v}_4\,\|^2 = 4\cdot 4 + 1\cdot 4 + 9\cdot 2 + 4\cdot 2,$$

in conformity with (4.8).

Example 4.11. The same formulas are equally valid for orthogonal bases in function spaces. For example, to express a quadratic polynomial

$$p(x) = c_1\,p_1(x) + c_2\,p_2(x) + c_3\,p_3(x) = c_1 + c_2\left(x - \tfrac{1}{2}\right) + c_3\left(x^2 - x + \tfrac{1}{6}\right)$$

in terms of the orthogonal basis (4.1), we merely compute the L^2 inner product integrals

$$c_1 = \frac{\langle\, p\,,p_1 \,\rangle}{\|\,p_1\,\|^2} = \int_0^1 p(x)\,dx, \qquad c_2 = \frac{\langle\, p\,,p_2 \,\rangle}{\|\,p_2\,\|^2} = 12\int_0^1 p(x)\left(x - \tfrac{1}{2}\right)dx,$$

$$c_3 = \frac{\langle\, p\,,p_3 \,\rangle}{\|\,p_3\,\|^2} = 180\int_0^1 p(x)\left(x^2 - x + \tfrac{1}{6}\right)dx.$$

Thus, for example, the coefficients for $p(x) = x^2 + x + 1$ are

$$c_1 = \int_0^1 (x^2 + x + 1)\,dx = \tfrac{11}{6}, \qquad c_2 = 12\int_0^1 (x^2 + x + 1)\left(x - \tfrac{1}{2}\right)dx = 2,$$

$$c_3 = 180\int_0^1 (x^2 + x + 1)\left(x^2 - x + \tfrac{1}{6}\right)dx = 1,$$

and so

$$p(x) = x^2 + x + 1 = \tfrac{11}{6} + 2\left(x - \tfrac{1}{2}\right) + \left(x^2 - x + \tfrac{1}{6}\right).$$

Example 4.12. Perhaps the most important example of an orthogonal basis is provided by the basic trigonometric functions. Let $\mathcal{T}^{(n)}$ denote the vector space consisting of all *trigonometric polynomials*

$$T(x) = \sum_{0\le j+k\le n} a_{jk}\,(\sin x)^j\,(\cos x)^k \tag{4.10}$$

of *degree* $\le n$. The individual monomials $(\sin x)^j\,(\cos x)^k$ span $\mathcal{T}^{(n)}$, but, as we saw in Example 2.20, they do not form a basis, owing to identities stemming from the basic trigonometric formula $\cos^2 x + \sin^2 x = 1$. Exercise 3.6.21 introduced a more convenient spanning set consisting of the $2n+1$ functions

$$1, \qquad \cos x, \qquad \sin x, \qquad \cos 2x, \qquad \sin 2x, \qquad \ldots \qquad \cos nx, \qquad \sin nx. \tag{4.11}$$

Let us prove that these functions form an orthogonal basis of $\mathcal{T}^{(n)}$ with respect to the L^2 inner product and norm:

$$\langle f, g \rangle = \int_{-\pi}^{\pi} f(x)\, g(x)\, dx, \qquad\qquad \| f \|^2 = \int_{-\pi}^{\pi} f(x)^2\, dx. \tag{4.12}$$

The elementary integration formulas

$$\int_{-\pi}^{\pi} \cos kx \, \cos lx \, dx = \begin{cases} 0, & k \neq l, \\ 2\pi, & k = l = 0, \\ \pi, & k = l \neq 0, \end{cases} \qquad \int_{-\pi}^{\pi} \sin kx \, \sin lx \, dx = \begin{cases} 0, & k \neq l, \\ \pi, & k = l \neq 0, \end{cases}$$
$$\int_{-\pi}^{\pi} \cos kx \, \sin lx \, dx = 0, \tag{4.13}$$

which are valid for all nonnegative integers $k, l \geq 0$, imply the orthogonality relations

$$\begin{aligned} \langle \cos kx, \cos lx \rangle = \langle \sin kx, \sin lx \rangle = 0, \qquad & k \neq l, \qquad \langle \cos kx, \sin lx \rangle = 0, \\ \| \cos kx \| = \| \sin kx \| = \sqrt{\pi}, \qquad & k \neq 0, \qquad\qquad \| 1 \| = \sqrt{2\pi}. \end{aligned} \tag{4.14}$$

Theorem 4.5 now assures us that the functions (4.11) form a basis for $\mathcal{T}^{(n)}$. One consequence is that $\dim \mathcal{T}^{(n)} = 2n+1$ — a fact that is not so easy to establish directly.

Orthogonality of the trigonometric functions (4.11) means that we can compute the coefficients $a_0, \ldots, a_n, b_1, \ldots, b_n$ of any trigonometric polynomial

$$p(x) = a_0 + \sum_{k=1}^{n} \left(a_k \cos kx + b_k \sin kx \right) \tag{4.15}$$

by an explicit integration formula. Namely,

$$\begin{aligned} a_0 &= \frac{\langle f, 1 \rangle}{\| 1 \|^2} = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x)\, dx, \qquad a_k = \frac{\langle f, \cos kx \rangle}{\| \cos kx \|^2} = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos kx \, dx, \\ b_k &= \frac{\langle f, \sin kx \rangle}{\| \sin kx \|^2} = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin kx \, dx, \qquad k \geq 1. \end{aligned} \tag{4.16}$$

These fundamental formulas play an essential role in the theory and applications of Fourier series, [**61**, **79**, **77**].

Exercises

♡ 4.1.21. (a) Prove that the vectors $\mathbf{v}_1 = (1, 1, 1)^T$, $\mathbf{v}_2 = (1, 1, -2)^T$, $\mathbf{v}_3 = (-1, 1, 0)^T$, form an orthogonal basis of $\mathbb{R}^3$ with the dot product. (*b*) Use orthogonality to write the vector $\mathbf{v} = (1, 2, 3)^T$ as a linear combination of $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$. (*c*) Verify the formula (4.8) for $\| \mathbf{v} \|$. (*d*) Construct an orthonormal basis, using the given vectors. (*e*) Write $\mathbf{v}$ as a linear combination of the orthonormal basis, and verify (4.5).

4.1.22. (a) Prove that $\mathbf{v}_1 = \left(\frac{3}{5}, 0, \frac{4}{5} \right)^T$, $\mathbf{v}_2 = \left(-\frac{4}{13}, \frac{12}{13}, \frac{3}{13} \right)^T$, $\mathbf{v}_3 = \left(-\frac{48}{65}, -\frac{5}{13}, \frac{36}{65} \right)^T$, form an orthonormal basis for $\mathbb{R}^3$ for the usual dot product. (*b*) Find the coordinates of $\mathbf{v} = (1, 1, 1)^T$ relative to this basis. (*c*) Verify formula (4.5) in this particular case.

4.1.23. Let $\mathbb{R}^2$ have the inner product defined by the positive definite matrix $K = \begin{pmatrix} 2 & -1 \\ -1 & 3 \end{pmatrix}$.
(a) Show that $\mathbf{v}_1 = (1,1)^T$, $\mathbf{v}_2 = (-2,1)^T$ form an orthogonal basis. (b) Write the vector $\mathbf{v} = (3,2)^T$ as a linear combination of $\mathbf{v}_1, \mathbf{v}_2$ using the orthogonality formula (4.7). (c) Verify the formula (4.8) for $\|\mathbf{v}\|$. (d) Find an orthonormal basis $\mathbf{u}_1, \mathbf{u}_2$ for this inner product. (e) Write $\mathbf{v}$ as a linear combination of the orthonormal basis, and verify (4.5).

♢ 4.1.24. (a) Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be an orthonormal basis of a finite-dimensional inner product space V. Let $\mathbf{v} = c_1\mathbf{u}_1 + \cdots + c_n\mathbf{u}_n$ and $\mathbf{w} = d_1\mathbf{u}_1 + \cdots + d_n\mathbf{u}_n$ be any two elements of V. Prove that $\langle \mathbf{v}, \mathbf{w} \rangle = c_1 d_1 + \cdots + c_n d_n$.
(b) Write down the corresponding inner product formula for an orthogonal basis.

4.1.25. Find an example that demonstrates why equation (4.5) is not valid for a non-orthonormal basis.

4.1.26. Use orthogonality to write the polynomials $1, x$ and x^2 as linear combinations of the orthogonal basis (4.1).

4.1.27. (a) Prove that the polynomials $P_0(t) = 1$, $P_1(t) = t$, $P_2(t) = t^2 - \frac{1}{3}$, $P_3(t) = t^3 - \frac{3}{5}t$, form an orthogonal basis for the vector space $\mathcal{P}^{(3)}$ of cubic polynomials for the L^2 inner product $\langle f, g \rangle = \int_{-1}^{1} f(t)\, g(t)\, dt$. (b) Find an orthonormal basis of $\mathcal{P}^{(3)}$. (c) Write t^3 as a linear combination of P_0, P_1, P_2, P_3 using the orthogonal basis formula (4.7).

4.1.28. (a) Prove that the polynomials $P_0(t) = 1$, $P_1(t) = t - \frac{2}{3}$, $P_2(t) = t^2 - \frac{6}{5}t + \frac{3}{10}$, form an orthogonal basis for $\mathcal{P}^{(2)}$ with respect to the weighted inner product
$\langle f, g \rangle = \int_{0}^{1} f(t)\, g(t)\, t\, dt$. (b) Find the corresponding orthonormal basis.
(c) Write t^2 as a linear combination of P_0, P_1, P_2 using the orthogonal basis formula (4.7).

4.1.29. Write the following trigonometric polynomials in terms of the basis functions (4.11):
(a) $\cos^2 x$, (b) $\cos x \sin x$, (c) $\sin^3 x$, (d) $\cos^2 x \sin^3 x$, (e) $\cos^4 x$.
Hint: You can use complex exponentials to simplify the inner product integrals.

4.1.30. Write down an orthonormal basis of the space of trigonometric polynomials $\mathcal{T}^{(n)}$ with respect to the L^2 inner product $\langle f, g \rangle = \int_{-\pi}^{\pi} f(x)\, g(x)\, dx$.

♢ 4.1.31. Show that the $2n+1$ complex exponentials $e^{\,\mathrm{i}\,k x}$ for $k = -n, -n+1, \ldots, -1, 0, 1, \ldots, n$, form an orthonormal basis for the space of complex-valued trigonometric polynomials under the Hermitian inner product $\langle f, g \rangle = \dfrac{1}{2\pi} \int_{-\pi}^{\pi} f(x)\, \overline{g(x)}\, dx$.

♢ 4.1.32. Prove the trigonometric integral identities (4.13). *Hint*: You can either use a trigonometric summation identity, or, if you can't remember the right one, use Euler's formula (3.94) to rewrite sine and cosine as combinations of complex exponentials.

♢ 4.1.33. Fill in the complete details of the proof of Theorem 4.9.

4.2 The Gram–Schmidt Process

Once we become convinced of the utility of orthogonal and orthonormal bases, a natural question arises: How can we construct them? A practical algorithm was first discovered by the French mathematician Pierre–Simon Laplace in the eighteenth century. Today the algorithm is known as the *Gram–Schmidt process*, after its rediscovery by Gram, whom we already met in Chapter 3, and the twentieth-century German mathematician Erhard

Schmidt. The Gram–Schmidt process is one of the premier algorithms of applied and computational linear algebra.

Let W denote a finite-dimensional inner product space. (To begin with, you might wish to think of W as a subspace of $\mathbb{R}^m$, equipped with the standard Euclidean dot product, although the algorithm will be formulated in complete generality.) We assume that we already know some basis $\mathbf{w}_1, \ldots, \mathbf{w}_n$ of W, where $n = \dim W$. Our goal is to use this information to construct an orthogonal basis $\mathbf{v}_1, \ldots, \mathbf{v}_n$.

We will construct the orthogonal basis elements one by one. Since initially we are not worrying about normality, there are no conditions on the first orthogonal basis element $\mathbf{v}_1$, and so there is no harm in choosing

$$\mathbf{v}_1 = \mathbf{w}_1.$$

Note that $\mathbf{v}_1 \neq \mathbf{0}$, since $\mathbf{w}_1$ appears in the original basis. Starting with $\mathbf{w}_2$, the second basis vector $\mathbf{v}_2$ must be orthogonal to the first: $\langle \mathbf{v}_2 , \mathbf{v}_1 \rangle = 0$. Let us try to arrange this by subtracting a suitable multiple of $\mathbf{v}_1$, and set

$$\mathbf{v}_2 = \mathbf{w}_2 - c\,\mathbf{v}_1,$$

where c is a scalar to be determined. The orthogonality condition

$$0 = \langle \mathbf{v}_2 , \mathbf{v}_1 \rangle = \langle \mathbf{w}_2 , \mathbf{v}_1 \rangle - c \langle \mathbf{v}_1 , \mathbf{v}_1 \rangle = \langle \mathbf{w}_2 , \mathbf{v}_1 \rangle - c \, \| \mathbf{v}_1 \|^2$$

requires that $c = \langle \mathbf{w}_2 , \mathbf{v}_1 \rangle / \| \mathbf{v}_1 \|^2$, and therefore

$$\mathbf{v}_2 = \mathbf{w}_2 - \frac{\langle \mathbf{w}_2 , \mathbf{v}_1 \rangle}{\| \mathbf{v}_1 \|^2}\, \mathbf{v}_1. \tag{4.17}$$

Linear independence of $\mathbf{v}_1 = \mathbf{w}_1$ and $\mathbf{w}_2$ ensures that $\mathbf{v}_2 \neq \mathbf{0}$. (Check!)

Next, we construct

$$\mathbf{v}_3 = \mathbf{w}_3 - c_1 \mathbf{v}_1 - c_2 \mathbf{v}_2$$

by subtracting suitable multiples of the first two orthogonal basis elements from $\mathbf{w}_3$. We want $\mathbf{v}_3$ to be orthogonal to both $\mathbf{v}_1$ and $\mathbf{v}_2$. Since we already arranged that $\langle \mathbf{v}_1 , \mathbf{v}_2 \rangle = 0$, this requires

$$0 = \langle \mathbf{v}_3 , \mathbf{v}_1 \rangle = \langle \mathbf{w}_3 , \mathbf{v}_1 \rangle - c_1 \langle \mathbf{v}_1 , \mathbf{v}_1 \rangle, \qquad 0 = \langle \mathbf{v}_3 , \mathbf{v}_2 \rangle = \langle \mathbf{w}_3 , \mathbf{v}_2 \rangle - c_2 \langle \mathbf{v}_2 , \mathbf{v}_2 \rangle,$$

and hence

$$c_1 = \frac{\langle \mathbf{w}_3 , \mathbf{v}_1 \rangle}{\| \mathbf{v}_1 \|^2}\,, \qquad c_2 = \frac{\langle \mathbf{w}_3 , \mathbf{v}_2 \rangle}{\| \mathbf{v}_2 \|^2}\,.$$

Therefore, the next orthogonal basis vector is given by the formula

$$\mathbf{v}_3 = \mathbf{w}_3 - \frac{\langle \mathbf{w}_3 , \mathbf{v}_1 \rangle}{\| \mathbf{v}_1 \|^2}\, \mathbf{v}_1 - \frac{\langle \mathbf{w}_3 , \mathbf{v}_2 \rangle}{\| \mathbf{v}_2 \|^2}\, \mathbf{v}_2.$$

Since $\mathbf{v}_1$ and $\mathbf{v}_2$ are linear combinations of $\mathbf{w}_1$ and $\mathbf{w}_2$, we must have $\mathbf{v}_3 \neq \mathbf{0}$, since otherwise, this would imply that $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$ are linearly dependent, and hence could not come from a basis.

Continuing in the same manner, suppose we have already constructed the mutually orthogonal vectors $\mathbf{v}_1, \ldots, \mathbf{v}_{k-1}$ as linear combinations of $\mathbf{w}_1, \ldots, \mathbf{w}_{k-1}$. The next orthogonal basis element $\mathbf{v}_k$ will be obtained from $\mathbf{w}_k$ by subtracting off a suitable linear combination of the previous orthogonal basis elements:

$$\mathbf{v}_k = \mathbf{w}_k - c_1 \mathbf{v}_1 - \cdots - c_{k-1} \mathbf{v}_{k-1}.$$

Since $\mathbf{v}_1, \ldots, \mathbf{v}_{k-1}$ are already orthogonal, the orthogonality constraint

$$0 = \langle \mathbf{v}_k , \mathbf{v}_j \rangle = \langle \mathbf{w}_k , \mathbf{v}_j \rangle - c_j \langle \mathbf{v}_j , \mathbf{v}_j \rangle$$

requires

$$c_j = \frac{\langle \mathbf{w}_k , \mathbf{v}_j \rangle}{\| \mathbf{v}_j \|^2} \qquad \text{for} \qquad j = 1, \ldots, k-1. \tag{4.18}$$

In this fashion, we establish the general *Gram–Schmidt formula*

$$\mathbf{v}_k = \mathbf{w}_k - \sum_{j=1}^{k-1} \frac{\langle \mathbf{w}_k , \mathbf{v}_j \rangle}{\| \mathbf{v}_j \|^2} \mathbf{v}_j, \qquad k = 1, \ldots, n. \tag{4.19}$$

The iterative Gram–Schmidt process (4.19), where we start with $\mathbf{v}_1 = \mathbf{w}_1$ and successively construct $\mathbf{v}_2, \ldots, \mathbf{v}_n$, defines an explicit, recursive procedure for constructing the desired orthogonal basis vectors. If we are actually after an orthonormal basis $\mathbf{u}_1, \ldots, \mathbf{u}_n$, we merely normalize the resulting orthogonal basis vectors, setting $\mathbf{u}_k = \mathbf{v}_k / \| \mathbf{v}_k \|$ for each $k = 1, \ldots, n$.

Example 4.13. The vectors

$$\mathbf{w}_1 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, \qquad \mathbf{w}_2 = \begin{pmatrix} 1 \\ 0 \\ 2 \end{pmatrix}, \qquad \mathbf{w}_3 = \begin{pmatrix} 2 \\ -2 \\ 3 \end{pmatrix}, \tag{4.20}$$

are readily seen to form a basis[†] of $\mathbb{R}^3$. To construct an orthogonal basis (with respect to the standard dot product) using the Gram–Schmidt process, we begin by setting

$$\mathbf{v}_1 = \mathbf{w}_1 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}.$$

The next basis vector is

$$\mathbf{v}_2 = \mathbf{w}_2 - \frac{\mathbf{w}_2 \cdot \mathbf{v}_1}{\| \mathbf{v}_1 \|^2} \mathbf{v}_1 = \begin{pmatrix} 1 \\ 0 \\ 2 \end{pmatrix} - \frac{-1}{3} \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} = \begin{pmatrix} \frac{4}{3} \\ \frac{1}{3} \\ \frac{5}{3} \end{pmatrix}.$$

The last orthogonal basis vector is

$$\mathbf{v}_3 = \mathbf{w}_3 - \frac{\mathbf{w}_3 \cdot \mathbf{v}_1}{\| \mathbf{v}_1 \|^2} \mathbf{v}_1 - \frac{\mathbf{w}_3 \cdot \mathbf{v}_2}{\| \mathbf{v}_2 \|^2} \mathbf{v}_2 = \begin{pmatrix} 2 \\ -2 \\ 3 \end{pmatrix} - \frac{-3}{3} \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} - \frac{7}{\frac{14}{3}} \begin{pmatrix} \frac{4}{3} \\ \frac{1}{3} \\ \frac{5}{3} \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{3}{2} \\ -\frac{1}{2} \end{pmatrix}.$$

The reader can easily validate the orthogonality of $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$.

An orthonormal basis is obtained by dividing each vector by its length. Since

$$\| \mathbf{v}_1 \| = \sqrt{3}, \qquad \| \mathbf{v}_2 \| = \sqrt{\frac{14}{3}}, \qquad \| \mathbf{v}_3 \| = \sqrt{\frac{7}{2}}.$$

[†] This will, in fact, be a consequence of the successful completion of the Gram–Schmidt process and does not need to be checked in advance. If the given vectors were not linearly independent, then eventually one of the Gram–Schmidt vectors would vanish, $\mathbf{v}_k = \mathbf{0}$, and the iterative algorithm would break down.

we produce the corresponding orthonormal basis vectors

$$\mathbf{u}_1 = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \end{pmatrix}, \qquad \mathbf{u}_2 = \begin{pmatrix} \frac{4}{\sqrt{42}} \\ \frac{1}{\sqrt{42}} \\ \frac{5}{\sqrt{42}} \end{pmatrix}, \qquad \mathbf{u}_3 = \begin{pmatrix} \frac{2}{\sqrt{14}} \\ -\frac{3}{\sqrt{14}} \\ -\frac{1}{\sqrt{14}} \end{pmatrix}. \tag{4.21}$$

Example 4.14. Here is a typical problem: find an orthonormal basis, with respect to the dot product, for the subspace $W \subset \mathbb{R}^4$ consisting of all vectors that are orthogonal to the given vector $\mathbf{a} = (1, 2, -1, -3)^T$. The first task is to find a basis for the subspace. Now, a vector $\mathbf{x} = (x_1, x_2, x_3, x_4)^T$ is orthogonal to $\mathbf{a}$ if and only if

$$\mathbf{x} \cdot \mathbf{a} = x_1 + 2x_2 - x_3 - 3x_4 = 0.$$

Solving this homogeneous linear system by the usual method, we observe that the free variables are x_2, x_3, x_4, and so a (non-orthogonal) basis for the subspace is

$$\mathbf{w}_1 = \begin{pmatrix} -2 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{w}_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \mathbf{w}_3 = \begin{pmatrix} 3 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

To obtain an orthogonal basis, we apply the Gram–Schmidt process. First,

$$\mathbf{v}_1 = \mathbf{w}_1 = \begin{pmatrix} -2 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

The next element is

$$\mathbf{v}_2 = \mathbf{w}_2 - \frac{\mathbf{w}_2 \cdot \mathbf{v}_1}{\|\mathbf{v}_1\|^2}\,\mathbf{v}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} - \frac{-2}{5}\begin{pmatrix} -2 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{5} \\ \frac{2}{5} \\ 1 \\ 0 \end{pmatrix}.$$

The last element of our orthogonal basis is

$$\mathbf{v}_3 = \mathbf{w}_3 - \frac{\mathbf{w}_3 \cdot \mathbf{v}_1}{\|\mathbf{v}_1\|^2}\,\mathbf{v}_1 - \frac{\mathbf{w}_3 \cdot \mathbf{v}_2}{\|\mathbf{v}_2\|^2}\,\mathbf{v}_2 = \begin{pmatrix} 3 \\ 0 \\ 0 \\ 1 \end{pmatrix} - \frac{-6}{5}\begin{pmatrix} -2 \\ 1 \\ 0 \\ 0 \end{pmatrix} - \frac{\frac{3}{5}}{\frac{6}{5}}\begin{pmatrix} \frac{1}{5} \\ \frac{2}{5} \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 1 \\ -\frac{1}{2} \\ 1 \end{pmatrix}.$$

An orthonormal basis can then be obtained by dividing each $\mathbf{v}_i$ by its length:

$$\mathbf{u}_1 = \begin{pmatrix} -\frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{u}_2 = \begin{pmatrix} \frac{1}{\sqrt{30}} \\ \frac{2}{\sqrt{30}} \\ \frac{5}{\sqrt{30}} \\ 0 \end{pmatrix}, \qquad \mathbf{u}_3 = \begin{pmatrix} \frac{1}{\sqrt{10}} \\ \frac{2}{\sqrt{10}} \\ -\frac{1}{\sqrt{10}} \\ \frac{2}{\sqrt{10}} \end{pmatrix}. \tag{4.22}$$

Remark. The orthonormal basis produced by the Gram–Schmidt process depends on the order of the vectors in the original basis. Different orderings produce different orthonormal bases.

The Gram–Schmidt process has one final important consequence. According to Theorem 2.29, every finite-dimensional vector space — except $\{\mathbf{0}\}$ — admits a basis. Given an inner product, the Gram–Schmidt process enables one to construct an orthogonal and even orthonormal basis of the space. Therefore, we have, in fact, implemented a constructive proof of the existence of orthogonal and orthonormal bases of an arbitrary finite-dimensional inner product space.

Theorem 4.15. Every non-zero finite-dimensional inner product space has an orthonormal basis.

In fact, if its dimension is > 1, then the inner product space has infinitely many orthonormal bases.

Exercises

Note: For Exercises #1–7 use the Euclidean dot product on $\mathbb{R}^n$.

4.2.1. Use the Gram–Schmidt process to determine an orthonormal basis for $\mathbb{R}^3$ starting with the following sets of vectors:

$$(a)\ \begin{pmatrix}1\\0\\1\end{pmatrix}, \begin{pmatrix}1\\1\\1\end{pmatrix}, \begin{pmatrix}-1\\2\\1\end{pmatrix}; \quad (b)\ \begin{pmatrix}1\\1\\0\end{pmatrix}, \begin{pmatrix}0\\1\\-1\end{pmatrix}, \begin{pmatrix}1\\0\\-1\end{pmatrix}; \quad (c)\ \begin{pmatrix}1\\2\\3\end{pmatrix}, \begin{pmatrix}4\\5\\0\end{pmatrix}, \begin{pmatrix}2\\3\\-1\end{pmatrix}.$$

4.2.2. Use the Gram–Schmidt process to construct an orthonormal basis for $\mathbb{R}^4$ starting with the following sets of vectors: (a) $(1,0,1,0)^T, (0,1,0,-1)^T, (1,0,0,1)^T, (1,1,1,1)^T$; (b) $(1,0,0,1)^T, (4,1,0,0)^T, (1,0,2,1)^T, (0,2,0,1)^T$.

4.2.3. Try the Gram–Schmidt procedure on the vectors $\begin{pmatrix}1\\-1\\0\\1\end{pmatrix}, \begin{pmatrix}0\\-1\\1\\2\end{pmatrix}, \begin{pmatrix}2\\-1\\-1\\0\end{pmatrix}, \begin{pmatrix}2\\2\\-2\\1\end{pmatrix}$.

What happens? Can you explain why you are unable to complete the algorithm?

4.2.4. Use the Gram–Schmidt process to construct an orthonormal basis for the following subspaces of $\mathbb{R}^3$: (a) the plane spanned by $(0,2,1)^T, (1,-2,-1)^T$; (b) the plane defined by the equation $2x - y + 3z = 0$; (c) the set of all vectors orthogonal to $(1,-1,-2)^T$.

4.2.5. Find an orthogonal basis of the subspace spanned by the vectors $\mathbf{w}_1 = (1,-1,-1,1,1)^T$, $\mathbf{w}_2 = (2,1,4,-4,2)^T$, and $\mathbf{w}_3 = (5,-4,-3,7,1)^T$.

4.2.6. Find an orthonormal basis for the following subspaces of $\mathbb{R}^4$: (a) the span of the vectors $\begin{pmatrix}1\\1\\-1\\0\end{pmatrix}, \begin{pmatrix}-1\\0\\1\\1\end{pmatrix}, \begin{pmatrix}2\\-1\\2\\1\end{pmatrix}$; (b) the kernel of the matrix $\begin{pmatrix}2 & 1 & 0 & -1\\ 3 & 2 & -1 & -1\end{pmatrix}$; (c) the coimage of the preceding matrix; (d) the image of the matrix $\begin{pmatrix}1 & -2 & 2\\ 2 & -4 & 1\\ 0 & 0 & -1\\ -2 & 4 & 5\end{pmatrix}$; (e) the cokernel of the preceding matrix; (f) the set of all vectors orthogonal to $(1,1,-1,-1)^T$.

4.2.7. Find orthonormal bases for the four fundamental subspaces associated with the following matrices:

$$(a)\ \begin{pmatrix}1 & -1\\ -3 & 3\end{pmatrix}, \quad (b)\ \begin{pmatrix}-1 & 0 & 2\\ 1 & 1 & -1\\ 0 & 1 & 1\end{pmatrix}, \quad (c)\ \begin{pmatrix}1 & 0 & 1 & 0\\ 1 & 1 & 1 & 1\\ -1 & 2 & 0 & 1\end{pmatrix}, \quad (d)\ \begin{pmatrix}1 & 2 & 1\\ 0 & -2 & 1\\ -1 & 0 & -2\\ 1 & -2 & 3\end{pmatrix}.$$

4.2.8. Construct an orthonormal basis of $\mathbb{R}^2$ for the nonstandard inner products
(a) $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \begin{pmatrix} 3 & 0 \\ 0 & 5 \end{pmatrix} \mathbf{y}$, (b) $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \begin{pmatrix} 4 & -1 \\ -1 & 1 \end{pmatrix} \mathbf{y}$, (c) $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} \mathbf{y}$.

4.2.9. Construct an orthonormal basis for $\mathbb{R}^3$ with respect to the inner products defined by the following positive definite matrices: (a) $\begin{pmatrix} 4 & -2 & 0 \\ -2 & 3 & -1 \\ 0 & -1 & 2 \end{pmatrix}$, (b) $\begin{pmatrix} 3 & -1 & 1 \\ -1 & 4 & -2 \\ 1 & -2 & 4 \end{pmatrix}$.

4.2.10. Redo Exercise 4.2.1 using
(i) the weighted inner product $\langle \mathbf{v}, \mathbf{w} \rangle = 3 v_1 w_1 + 2 v_2 w_2 + v_3 w_3$;
(ii) the inner product induced by the positive definite matrix $K = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$.

♢ 4.2.11. (a) How many orthonormal bases does $\mathbb{R}$ have? (b) What about $\mathbb{R}^2$? (c) Does your answer change if you use a different inner product? Justify your answers.

4.2.12. *True or false*: Reordering the original basis before starting the Gram–Schmidt process leads to the same orthogonal basis.

♢ 4.2.13. Suppose that $W \subsetneq \mathbb{R}^n$ is a proper subspace, and $\mathbf{u}_1, \ldots, \mathbf{u}_m$ forms an orthonormal basis of W. Prove that there exist vectors $\mathbf{u}_{m+1}, \ldots, \mathbf{u}_n \in \mathbb{R}^n \setminus W$ such that the complete collection $\mathbf{u}_1, \ldots, \mathbf{u}_n$ forms an orthonormal basis for $\mathbb{R}^n$. *Hint*: Begin with Exercise 2.4.20.

♢ 4.2.14. Verify that the Gram–Schmidt formula (4.19) also produce an orthogonal basis of a complex vector space under a Hermitian inner product.

4.2.15. (a) Apply the complex Gram–Schmidt algorithm from Exercise 4.2.14 to produce an orthonormal basis starting with the vectors $(1 + \mathrm{i}, 1 - \mathrm{i})^T, (1 - 2\mathrm{i}, 5\mathrm{i})^T \in \mathbb{C}^2$.
(b) Do the same for $(1 + \mathrm{i}, 1 - \mathrm{i}, 2 - \mathrm{i})^T, (1 + 2\mathrm{i}, -2\mathrm{i}, 2 - \mathrm{i})^T, (1, 1 - 2\mathrm{i}, \mathrm{i})^T \in \mathbb{C}^3$.

4.2.16. Use the complex Gram–Schmidt algorithm from Exercise 4.2.14 to construct orthonormal bases for (a) the subspace spanned by $(1 - \mathrm{i}, 1, 0)^T, (0, 3 - \mathrm{i}, 2\mathrm{i})^T$;
(b) the set of solutions to $(2 - \mathrm{i})x - 2\mathrm{i}\,y + (1 - 2\mathrm{i})z = 0$;
(c) the subspace spanned by $(-\mathrm{i}, 1, -1, \mathrm{i})^T, (0, 2\mathrm{i}, 1 - \mathrm{i}, -1 + \mathrm{i})^T, (1, \mathrm{i}, -\mathrm{i}, 1 - 2\mathrm{i})^T$.

Modifications of the Gram–Schmidt Process

With the basic Gram–Schmidt algorithm now in hand, it is worth looking at a couple of reformulations that have both practical and theoretical advantages. The first can be used to construct the orthonormal basis vectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$ directly from the basis $\mathbf{w}_1, \ldots, \mathbf{w}_n$.

We begin by replacing each orthogonal basis vector in the basic Gram–Schmidt formula (4.19) by its normalized version $\mathbf{u}_j = \mathbf{v}_j / \| \mathbf{v}_j \|$. The original basis vectors can be expressed in terms of the orthonormal basis via a "triangular" system

$$\begin{aligned} \mathbf{w}_1 &= r_{11}\,\mathbf{u}_1, \\ \mathbf{w}_2 &= r_{12}\,\mathbf{u}_1 + r_{22}\,\mathbf{u}_2, \\ \mathbf{w}_3 &= r_{13}\,\mathbf{u}_1 + r_{23}\,\mathbf{u}_2 + r_{33}\,\mathbf{u}_3, \\ &\ \ \vdots \qquad\quad \vdots \qquad\quad \vdots \qquad\qquad \ddots \\ \mathbf{w}_n &= r_{1n}\,\mathbf{u}_1 + r_{2n}\,\mathbf{u}_2 + \cdots + r_{nn}\,\mathbf{u}_n. \end{aligned} \tag{4.23}$$

The coefficients r_{ij} can, in fact, be computed directly from these formulas. Indeed, taking the inner product of the equation for $\mathbf{w}_j$ with the orthonormal basis vector $\mathbf{u}_i$ for $i \leq j$, we obtain, in view of the orthonormality constraints (4.6),

$$\langle \mathbf{w}_j , \mathbf{u}_i \rangle = \langle r_{1j} \mathbf{u}_1 + \cdots + r_{jj} \mathbf{u}_j , \mathbf{u}_i \rangle = r_{1j} \langle \mathbf{u}_1 , \mathbf{u}_i \rangle + \cdots + r_{jj} \langle \mathbf{u}_n , \mathbf{u}_i \rangle = r_{ij},$$

and hence

$$r_{ij} = \langle \mathbf{w}_j , \mathbf{u}_i \rangle. \tag{4.24}$$

On the other hand, according to (4.5),

$$\| \mathbf{w}_j \|^2 = \| r_{1j} \mathbf{u}_1 + \cdots + r_{jj} \mathbf{u}_j \|^2 = r_{1j}^2 + \cdots + r_{j-1,j}^2 + r_{jj}^2. \tag{4.25}$$

The pair of equations (4.24–25) can be rearranged to devise a recursive procedure to compute the orthonormal basis. We begin by setting $r_{11} = \| \mathbf{w}_1 \|$ and so $\mathbf{u}_1 = \mathbf{w}_1 / r_{11}$. At each subsequent stage $j \geq 2$, we assume that we have already constructed $\mathbf{u}_1, \ldots, \mathbf{u}_{j-1}$. We then compute

$$r_{ij} = \langle \mathbf{w}_j , \mathbf{u}_i \rangle, \qquad \text{for each} \qquad i = 1, \ldots, j-1. \tag{4.26}$$

We obtain the next orthonormal basis vector $\mathbf{u}_j$ by computing

$$r_{jj} = \sqrt{\| \mathbf{w}_j \|^2 - r_{1j}^2 - \cdots - r_{j-1,j}^2}\,, \qquad \mathbf{u}_j = \frac{\mathbf{w}_j - r_{1j} \mathbf{u}_1 - \cdots - r_{j-1,j} \mathbf{u}_{j-1}}{r_{jj}}. \tag{4.27}$$

Running through the formulas (4.26–27) for $j = 1, \ldots, n$ leads to the *same* orthonormal basis $\mathbf{u}_1, \ldots, \mathbf{u}_n$ produced by the previous version of the Gram–Schmidt procedure.

Example 4.16. Let us apply the revised algorithm to the vectors

$$\mathbf{w}_1 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, \qquad \mathbf{w}_2 = \begin{pmatrix} 1 \\ 0 \\ 2 \end{pmatrix}, \qquad \mathbf{w}_3 = \begin{pmatrix} 2 \\ -2 \\ 3 \end{pmatrix},$$

of Example 4.13. To begin, we set

$$r_{11} = \| \mathbf{w}_1 \| = \sqrt{3}, \qquad \mathbf{u}_1 = \frac{\mathbf{w}_1}{r_{11}} = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \end{pmatrix}.$$

The next step is to compute

$$r_{12} = \langle \mathbf{w}_2 , \mathbf{u}_1 \rangle = -\frac{1}{\sqrt{3}}, \; r_{22} = \sqrt{\| \mathbf{w}_2 \|^2 - r_{12}^2} = \sqrt{\frac{14}{3}}, \; \mathbf{u}_2 = \frac{\mathbf{w}_2 - r_{12}\mathbf{u}_1}{r_{22}} = \begin{pmatrix} \frac{4}{\sqrt{42}} \\ \frac{1}{\sqrt{42}} \\ \frac{5}{\sqrt{42}} \end{pmatrix}.$$

The final step yields

$$r_{13} = \langle \mathbf{w}_3 , \mathbf{u}_1 \rangle = -\sqrt{3}, \qquad r_{23} = \langle \mathbf{w}_3 , \mathbf{u}_2 \rangle = \sqrt{\frac{21}{2}},$$

$$r_{33} = \sqrt{\| \mathbf{w}_3 \|^2 - r_{13}^2 - r_{23}^2} = \sqrt{\frac{7}{2}}, \qquad \mathbf{u}_3 = \frac{\mathbf{w}_3 - r_{13} \mathbf{u}_1 - r_{23} \mathbf{u}_2}{r_{33}} = \begin{pmatrix} \frac{2}{\sqrt{14}} \\ -\frac{3}{\sqrt{14}} \\ -\frac{1}{\sqrt{14}} \end{pmatrix}.$$

As advertised, the result is the same orthonormal basis vectors that we previously found in Example 4.13.

For hand computations, the original version (4.19) of the Gram–Schmidt process is slightly easier — even if one does ultimately want an orthonormal basis — since it avoids the square roots that are ubiquitous in the orthonormal version (4.26–27). On the other hand, for numerical implementation on a computer, the orthonormal version is a bit faster, since it involves fewer arithmetic operations.

However, in practical, large-scale computations, both versions of the Gram–Schmidt process suffer from a serious flaw. They are subject to numerical instabilities, and so accumulating round-off errors may seriously corrupt the computations, leading to inaccurate, non-orthogonal vectors. Fortunately, there is a simple rearrangement of the calculation that ameliorates this difficulty and leads to the numerically robust algorithm that is most often used in practice, [**21**, **40**, **66**]. The idea is to treat the vectors simultaneously rather than sequentially, making full use of the orthonormal basis vectors as they arise. More specifically, the algorithm begins as before — we take $\mathbf{u}_1 = \mathbf{w}_1 / \| \mathbf{w}_1 \|$. We then subtract off the appropriate multiples of $\mathbf{u}_1$ from *all* of the remaining basis vectors so as to arrange their orthogonality to $\mathbf{u}_1$. This is accomplished by setting

$$\mathbf{w}_k^{(2)} = \mathbf{w}_k - \langle \mathbf{w}_k , \mathbf{u}_1 \rangle \, \mathbf{u}_1 \qquad \text{for} \qquad k = 2, \ldots, n.$$

The second orthonormal basis vector $\mathbf{u}_2 = \mathbf{w}_2^{(2)} / \| \mathbf{w}_2^{(2)} \|$ is then obtained by normalizing. We next modify the remaining $\mathbf{w}_3^{(2)}, \ldots, \mathbf{w}_n^{(2)}$ to produce vectors

$$\mathbf{w}_k^{(3)} = \mathbf{w}_k^{(2)} - \langle \mathbf{w}_k^{(2)} , \mathbf{u}_2 \rangle \, \mathbf{u}_2, \qquad k = 3, \ldots, n,$$

that are orthogonal to both $\mathbf{u}_1$ and $\mathbf{u}_2$. Then $\mathbf{u}_3 = \mathbf{w}_3^{(3)} / \| \mathbf{w}_3^{(3)} \|$ is the next orthonormal basis element, and the process continues. The full algorithm starts with the initial basis vectors $\mathbf{w}_j = \mathbf{w}_j^{(1)}$, $j = 1, \ldots, n$, and then recursively computes

$$\mathbf{u}_j = \frac{\mathbf{w}_j^{(j)}}{\| \mathbf{w}_j^{(j)} \|}, \qquad \mathbf{w}_k^{(j+1)} = \mathbf{w}_k^{(j)} - \langle \mathbf{w}_k^{(j)} , \mathbf{u}_j \rangle \, \mathbf{u}_j, \qquad \begin{array}{l} j = 1, \ldots, n, \\ k = j+1, \ldots, n. \end{array} \tag{4.28}$$

(In the final phase, when $j = n$, the second formula is no longer needed.) The result is a numerically stable computation of the *same* orthonormal basis vectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$.

Example 4.17. Let us apply the stable Gram–Schmidt process to the basis vectors

$$\mathbf{w}_1^{(1)} = \mathbf{w}_1 = \begin{pmatrix} 2 \\ 2 \\ -1 \end{pmatrix}, \qquad \mathbf{w}_2^{(1)} = \mathbf{w}_2 = \begin{pmatrix} 0 \\ 4 \\ -1 \end{pmatrix}, \qquad \mathbf{w}_3^{(1)} = \mathbf{w}_3 = \begin{pmatrix} 1 \\ 2 \\ -3 \end{pmatrix}.$$

The first orthonormal basis vector is $\mathbf{u}_1 = \dfrac{\mathbf{w}_1^{(1)}}{\| \mathbf{w}_1^{(1)} \|} = \begin{pmatrix} \frac{2}{3} \\ \frac{2}{3} \\ -\frac{1}{3} \end{pmatrix}$. Next, we compute

$$\mathbf{w}_2^{(2)} = \mathbf{w}_2^{(1)} - \langle \mathbf{w}_2^{(1)} , \mathbf{u}_1 \rangle \, \mathbf{u}_1 = \begin{pmatrix} -2 \\ 2 \\ 0 \end{pmatrix}, \qquad \mathbf{w}_3^{(2)} = \mathbf{w}_3^{(1)} - \langle \mathbf{w}_3^{(1)} , \mathbf{u}_1 \rangle \, \mathbf{u}_1 = \begin{pmatrix} -1 \\ 0 \\ -2 \end{pmatrix}.$$

The second orthonormal basis vector is $\mathbf{u}_2 = \dfrac{\mathbf{w}_2^{(2)}}{\| \mathbf{w}_2^{(2)} \|} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$. Finally,

$$\mathbf{w}_3^{(3)} = \mathbf{w}_3^{(2)} - \langle \mathbf{w}_3^{(2)} , \mathbf{u}_2 \rangle \, \mathbf{u}_2 = \begin{pmatrix} -\frac{1}{2} \\ -\frac{1}{2} \\ -2 \end{pmatrix}, \qquad \mathbf{u}_3 = \frac{\mathbf{w}_3^{(3)}}{\| \mathbf{w}_3^{(3)} \|} = \begin{pmatrix} -\frac{\sqrt{2}}{6} \\ -\frac{\sqrt{2}}{6} \\ -\frac{2\sqrt{2}}{3} \end{pmatrix}.$$

The resulting vectors $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ form the desired orthonormal basis.

Exercises

4.2.17. Use the modified Gram-Schmidt process (4.26–27) to produce orthonormal bases for the spaces spanned by the following vectors: (a) $\begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}, \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 3 \end{pmatrix}$, (b) $\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix}$, (c) $\begin{pmatrix} 1 \\ 1 \\ -1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ -1 \\ 2 \\ 1 \end{pmatrix}$, (d) $\begin{pmatrix} 2 \\ 1 \\ 3 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \\ 2 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \\ -1 \\ 0 \\ 1 \end{pmatrix}$, (e) $\begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 0 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 1 \end{pmatrix}$.

4.2.18. Repeat Exercise 4.2.17 using the numerically stable algorithm (4.28) and check that you get the same result. Which of the two algorithms was easier for you to implement?

4.2.19. Redo each of the exercises in the preceding subsection by implementing the numerically stable Gram–Schmidt process (4.28) instead, and verify that you end up with the same orthonormal basis.

♢ 4.2.20. Prove that (4.28) does indeed produce an orthonormal basis. Explain why the result is the same orthonormal basis as the ordinary Gram–Schmidt method.

4.2.21. Let $\mathbf{w}_j^{(j)}$ be the vectors in the stable Gram–Schmidt algorithm (4.28). Prove that the coefficients in (4.23) are given by $r_{ii} = \| \mathbf{w}_i^{(i)} \|$, and $r_{ij} = \langle \mathbf{w}_j^{(i)}, \mathbf{u}_i \rangle$ for $i < j$.

4.3 Orthogonal Matrices

Matrices whose columns form an orthonormal basis of $\mathbb{R}^n$ relative to the standard Euclidean dot product play a distinguished role. Such "orthogonal matrices" appear in a wide range of applications in geometry, physics, quantum mechanics, crystallography, partial differential equations, [**61**], symmetry theory, [**60**], and special functions, [**59**]. Rotational motions of bodies in three-dimensional space are described by orthogonal matrices, and hence they lie at the foundations of rigid body mechanics, [**31**], including satellites, airplanes, drones, and underwater vehicles, as well as three-dimensional computer graphics and animation for video games and movies, [**5**]. Furthermore, orthogonal matrices are an essential ingredient in one of the most important methods of numerical linear algebra: the QR algorithm for computing eigenvalues of matrices, to be presented in Section 9.5.

Definition 4.18. A square matrix Q is called *orthogonal* if it satisfies

$$Q^T Q = Q\,Q^T = \mathrm{I}. \tag{4.29}$$

The orthogonality condition implies that one can easily invert an orthogonal matrix:

$$Q^{-1} = Q^T. \tag{4.30}$$

In fact, the two conditions are equivalent, and hence a matrix is orthogonal if and only if its inverse is equal to its transpose. In particular, the identity matrix I is orthogonal. Also note that if Q is orthogonal, so is Q^T. The second important characterization of orthogonal matrices relates them directly to orthonormal bases.

Proposition 4.19. A matrix Q is orthogonal if and only if its columns form an orthonormal basis with respect to the Euclidean dot product on $\mathbb{R}^n$.

Proof: Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be the columns of Q. Then $\mathbf{u}_1^T, \ldots, \mathbf{u}_n^T$ are the rows of the transposed matrix Q^T. The (i,j) entry of the product $Q^T Q$ is given as the product of the i^{th} row of Q^T and the j^{th} column of Q. Thus, the orthogonality requirement (4.29) implies $\mathbf{u}_i \cdot \mathbf{u}_j = \mathbf{u}_i^T \mathbf{u}_j = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases}$ which are precisely the conditions (4.6) for $\mathbf{u}_1, \ldots, \mathbf{u}_n$ to form an orthonormal basis. *Q.E.D.*

In particular, the columns of the identity matrix produce the standard basis $\mathbf{e}_1, \ldots, \mathbf{e}_n$ of $\mathbb{R}^n$. Also, the rows of an orthogonal matrix Q also produce an (in general different) orthonormal basis.

Warning. Technically, we should be referring to an "orthonormal" matrix, not an "orthogonal" matrix. But the terminology is so standard throughout mathematics and physics that we have no choice but to adopt it here. There is no commonly accepted name for a matrix whose columns form an orthogonal but not orthonormal basis.

Example 4.20. A 2×2 matrix $Q = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is orthogonal if and only if its columns $\mathbf{u}_1 = \begin{pmatrix} a \\ c \end{pmatrix}$, $\mathbf{u}_2 = \begin{pmatrix} b \\ d \end{pmatrix}$, form an orthonormal basis of $\mathbb{R}^2$. Equivalently, the requirement

$$Q^T Q = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a^2 + c^2 & a\,b + c\,d \\ a\,b + c\,d & b^2 + d^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

implies that its entries must satisfy the algebraic equations

$$a^2 + c^2 = 1, \qquad a\,b + c\,d = 0, \qquad b^2 + d^2 = 1.$$

The first and last equations say that the points $(a, c)^T$ and $(b, d)^T$ lie on the unit circle in $\mathbb{R}^2$, and so

$$a = \cos\theta, \qquad c = \sin\theta, \qquad b = \cos\psi, \qquad d = \sin\psi,$$

for some choice of angles θ, ψ. The remaining orthogonality condition is

$$0 = a\,b + c\,d = \cos\theta\ \cos\psi + \sin\theta\ \sin\psi = \cos(\theta - \psi),$$

which implies that θ and ψ differ by a right angle: $\psi = \theta \pm \frac{1}{2}\pi$. The $\pm$ sign leads to two cases:

$$b = -\sin\theta, \qquad d = \cos\theta, \qquad \text{or} \qquad b = \sin\theta, \qquad d = -\cos\theta.$$

As a result, every 2×2 orthogonal matrix has one of two possible forms

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \qquad \text{or} \qquad \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}, \qquad \text{where} \qquad 0 \le \theta < 2\pi. \tag{4.31}$$

The corresponding orthonormal bases are illustrated in Figure 4.2. The former is a right-handed basis, as defined in Exercise 2.4.7, and can be obtained from the standard basis $\mathbf{e}_1, \mathbf{e}_2$ by a rotation through angle θ, while the latter has the opposite, reflected orientation.

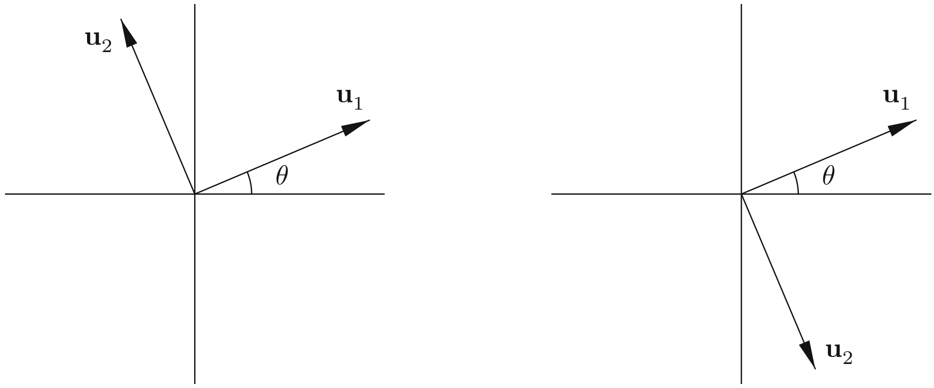

Figure 4.2. Orthonormal Bases in $\mathbb{R}^2$.

Example 4.21. A 3×3 orthogonal matrix $Q = (\mathbf{u}_1\ \mathbf{u}_2\ \mathbf{u}_3)$ is prescribed by 3 mutually perpendicular vectors of unit length in $\mathbb{R}^3$. For instance, the orthonormal basis constructed in (4.21) corresponds to the orthogonal matrix $Q = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{4}{\sqrt{42}} & \frac{2}{\sqrt{14}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{42}} & -\frac{3}{\sqrt{14}} \\ -\frac{1}{\sqrt{3}} & \frac{5}{\sqrt{42}} & -\frac{1}{\sqrt{14}} \end{pmatrix}$. A complete list of 3×3 orthogonal matrices can be found in Exercises 4.3.4 and 4.3.5.

Lemma 4.22. An orthogonal matrix Q has determinant $\det Q = \pm 1$.

Proof: Taking the determinant of (4.29), and using the determinantal formulas (1.85), (1.89), shows that

$$1 = \det \mathrm{I} = \det(Q^T Q) = \det Q^T \det Q = (\det Q)^2,$$

which immediately proves the lemma. *Q.E.D.*

An orthogonal matrix is called *proper* or *special* if it has determinant $+1$. Geometrically, the columns of a proper orthogonal matrix form a right-handed basis of $\mathbb{R}^n$, as defined in Exercise 2.4.7. An *improper* orthogonal matrix, with determinant -1, corresponds to a left handed basis that lives in a mirror-image world.

Proposition 4.23. The product of two orthogonal matrices is also orthogonal.

Proof: If

$$Q_1^T Q_1 = \mathrm{I} = Q_2^T Q_2, \qquad \text{then} \qquad (Q_1 Q_2)^T (Q_1 Q_2) = Q_2^T Q_1^T Q_1 Q_2 = Q_2^T Q_2 = \mathrm{I},$$

and so the product matrix $Q_1 Q_2$ is also orthogonal. *Q.E.D.*

This multiplicative property combined with the fact that the inverse of an orthogonal matrix is also orthogonal says that the set of all orthogonal matrices forms a *group*†. The

† The precise mathematical definition of a group can be found in Exercise 4.3.24. Although they will not play a significant role in this text, groups underlie the mathematical formalization of symmetry and, as such, form one of the most fundamental concepts in advanced mathematics and its applications, particularly quantum mechanics and modern theoretical physics, [**54**]. Indeed, according to the mathematician Felix Klein, cf. [**92**], all geometry is based on group theory.

orthogonal group lies at the foundation of everyday Euclidean geometry, as well as rigid body mechanics, atomic structure and chemistry, computer graphics and animation, and many other areas.

Exercises

4.3.1. Determine which of the following matrices are (i) orthogonal; (ii) proper orthogonal.

$$(a)\ \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix},\quad (b)\ \begin{pmatrix} \frac{12}{13} & \frac{5}{13} \\ -\frac{5}{13} & \frac{12}{13} \end{pmatrix},\quad (c)\ \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},\quad (d)\ \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{pmatrix},$$

$$(e)\ \begin{pmatrix} \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \end{pmatrix},\quad (f)\ \begin{pmatrix} \frac{3}{5} & 0 & \frac{4}{5} \\ -\frac{4}{13} & \frac{12}{13} & \frac{3}{13} \\ -\frac{48}{65} & -\frac{5}{13} & \frac{36}{65} \end{pmatrix},\quad (g)\ \begin{pmatrix} \frac{2}{3} & -\frac{\sqrt{2}}{6} & \frac{\sqrt{2}}{2} \\ -\frac{2}{3} & \frac{\sqrt{2}}{6} & \frac{\sqrt{2}}{2} \\ \frac{1}{3} & \frac{2\sqrt{2}}{3} & 0 \end{pmatrix}.$$

4.3.2. (a) Show that $R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$, a reflection matrix, and $Q = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$, representing a rotation by the angle θ around the z-axis, are both orthogonal. (b) Verify that the products RQ and QR are also orthogonal. (c) Which of the preceding matrices, R, Q, RQ, QR, are proper orthogonal?

4.3.3. *True or false*: (a) If Q is an improper 2×2 orthogonal matrix, then $Q^2 = \mathrm{I}$. (b) If Q is an improper 3×3 orthogonal matrix, then $Q^2 = \mathrm{I}$.

♡ 4.3.4. (a) Prove that, for all θ, φ, ψ,

$$Q = \begin{pmatrix} \cos\varphi\,\cos\psi - \cos\theta\,\sin\varphi\,\sin\psi & \sin\varphi\,\cos\psi + \cos\theta\,\cos\varphi\,\sin\psi & \sin\theta\,\sin\psi \\ -\cos\varphi\,\sin\psi - \cos\theta\,\sin\varphi\,\cos\psi & -\sin\varphi\,\sin\psi + \cos\theta\,\cos\varphi\,\cos\psi & \sin\theta\,\cos\psi \\ \sin\theta\,\sin\varphi & -\sin\theta\,\cos\varphi & \cos\theta \end{pmatrix}$$

is a proper orthogonal matrix. (b) Write down a formula for Q^{-1}.

Remark. It can be shown that every proper orthogonal matrix can be parameterized in this manner; θ, φ, ψ are known as the *Euler angles*, and play an important role in applications in mechanics and geometry, [**31**; p. 147].

♡ 4.3.5. (a) Show that if $y_1^2 + y_2^2 + y_3^2 + y_4^2 = 1$, then the matrix

$$Q = \begin{pmatrix} y_1^2 + y_2^2 - y_3^2 - y_4^2 & 2\,(y_2\,y_3 + y_1\,y_4) & 2\,(y_2\,y_4 - y_1\,y_3) \\ 2\,(y_2\,y_3 - y_1\,y_4) & y_1^2 - y_2^2 + y_3^2 - y_4^2 & 2\,(y_3\,y_4 + y_1\,y_2) \\ 2\,(y_2\,y_4 + y_1\,y_3) & 2\,(y_3\,y_4 - y_1\,y_2) & y_1^2 - y_2^2 - y_3^2 + y_4^2 \end{pmatrix}$$

is a proper orthogonal matrix. The numbers y_1, y_2, y_3, y_4 are known as *Cayley–Klein parameters*. (b) Write down a formula for Q^{-1}. (c) Prove the formulas

$$y_1 = \cos\frac{\varphi+\psi}{2}\,\cos\frac{\theta}{2},\quad y_2 = \cos\frac{\varphi-\psi}{2}\,\sin\frac{\theta}{2},\quad y_3 = \sin\frac{\varphi-\psi}{2}\,\sin\frac{\theta}{2},\quad y_4 = \sin\frac{\varphi+\psi}{2}\,\cos\frac{\theta}{2},$$

relating the Cayley–Klein parameters and the Euler angles of Exercise 4.3.4, cf. [**31**; §§4–5].

◇ 4.3.6. (a) Prove that the transpose of an orthogonal matrix is also orthogonal. (b) Explain why the rows of an $n\times n$ orthogonal matrix also form an orthonormal basis of $\mathbb{R}^n$.

4.3.7. Prove that the inverse of an orthogonal matrix is orthogonal.

4.3.8. Show that if Q is a proper orthogonal matrix, and R is obtained from Q by interchanging two rows, then R is an improper orthogonal matrix.

4.3.9. Show that the product of two proper orthogonal matrices is also proper orthogonal. What can you say about the product of two improper orthogonal matrices? What about an improper times a proper orthogonal matrix?

4.3.10. *True or false*: (*a*) A matrix whose columns form an orthogonal basis of $\mathbb{R}^n$ is an orthogonal matrix. (*b*) A matrix whose rows form an orthonormal basis of $\mathbb{R}^n$ is an orthogonal matrix. (*c*) An orthogonal matrix is symmetric if and only if it is a diagonal matrix.

4.3.11. Write down all diagonal $n \times n$ orthogonal matrices.

♢ 4.3.12. Prove that an upper triangular matrix U is orthogonal if and only if U is a diagonal matrix. What are its diagonal entries?

4.3.13. (*a*) Show that the elementary row operation matrix corresponding to the interchange of two rows is an improper orthogonal matrix. (*b*) Are there any other orthogonal elementary matrices?

4.3.14. *True or false*: Applying an elementary row operation to an orthogonal matrix produces an orthogonal matrix.

4.3.15. (*a*) Prove that every permutation matrix is orthogonal. (*b*) How many permutation matrices of a given size are proper orthogonal?

♢ 4.3.16. (*a*) Prove that if Q is an orthogonal matrix, then $\| Q\mathbf{x} \| = \| \mathbf{x} \|$ for every vector $\mathbf{x} \in \mathbb{R}^n$, where $\| \cdot \|$ denotes the standard Euclidean norm. (*b*) Prove the converse: if $\| Q\mathbf{x} \| = \| \mathbf{x} \|$ for all $\mathbf{x} \in \mathbb{R}^n$, then Q is an orthogonal matrix.

♢ 4.3.17. Show that if $A^T = -A$ is any skew-symmetric matrix, then its *Cayley Transform* $Q = (\mathrm{I} - A)^{-1}(\mathrm{I} + A)$ is an orthogonal matrix. Can you prove that $\mathrm{I} - A$ is always invertible?

4.3.18. Suppose S is an $n \times n$ matrix whose columns form an orthogonal, but not orthonormal, basis of $\mathbb{R}^n$. (*a*) Find a formula for S^{-1} mimicking the formula $Q^{-1} = Q^T$ for an orthogonal matrix. (*b*) Use your formula to determine the inverse of the wavelet matrix W whose columns form the orthogonal wavelet basis (4.9) of $\mathbb{R}^4$.

♢ 4.3.19. Let $\mathbf{v}_1, \ldots, \mathbf{v}_n$ and $\mathbf{w}_1, \ldots, \mathbf{w}_n$ be two sets of linearly independent vectors in $\mathbb{R}^n$. Show that all their dot products are the same, so $\mathbf{v}_i \cdot \mathbf{v}_j = \mathbf{w}_i \cdot \mathbf{w}_j$ for all $i, j = 1, \ldots, n$, if and only if there is an orthogonal matrix Q such that $\mathbf{w}_i = Q\mathbf{v}_i$ for all $i = 1, \ldots, n$.

4.3.20. Suppose $\mathbf{u}_1, \ldots, \mathbf{u}_k$ form an orthonormal set of vectors in $\mathbb{R}^n$ with $k < n$. Let $Q = (\, \mathbf{u}_1 \; \mathbf{u}_2 \; \ldots \; \mathbf{u}_k \,)$ denote the $n \times k$ matrix whose columns are the orthonormal vectors. (*a*) Prove that $Q^T Q = \mathrm{I}_k$. (*b*) Is $Q Q^T = \mathrm{I}_n$?

♢ 4.3.21. Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ and $\widehat{\mathbf{u}}_1, \ldots, \widehat{\mathbf{u}}_n$ be orthonormal bases of an inner product space V. Prove that $\widehat{\mathbf{u}}_i = \sum_{j=1}^{n} q_{ij} \mathbf{u}_j$ for $i = 1, \ldots, n$, where $Q = (q_{ij})$ is an orthogonal matrix.

4.3.22. Let A be an $m \times n$ matrix whose columns are nonzero, mutually orthogonal vectors in $\mathbb{R}^m$. (*a*) Explain why $m \geq n$. (*b*) Prove that $A^T A$ is a diagonal matrix. What are the diagonal entries? (*c*) Is $A A^T$ diagonal?

♢ 4.3.23. Let $K > 0$ be a positive definite $n \times n$ matrix. Prove that an $n \times n$ matrix S satisfies $S^T K S = \mathrm{I}$ if and only if the columns of S form an orthonormal basis of $\mathbb{R}^n$ with respect to the inner product $\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^T K \mathbf{w}$.

♡ 4.3.24. *Groups*: A set of $n \times n$ matrices $G \subset \mathcal{M}_{n \times n}$ is said to form a *group* if
(1) whenever $A, B \in G$, so is the product $AB \in G$, and
(2) whenever $A \in G$, then A is nonsingular, and $A^{-1} \in G$.

(a) Show that $\mathrm{I} \in G$. (b) Prove that the following sets of $n \times n$ matrices form a group: (i) all nonsingular matrices; (ii) all nonsingular upper triangular matrices; (iii) all matrices of determinant 1; (iv) all orthogonal matrices; (v) all proper orthogonal matrices; (vi) all permutation matrices; (vii) all 2×2 matrices with integer entries and determinant equal to 1. (c) Explain why the set of all nonsingular 2×2 matrices with integer entries does not form a group. (d) Does the set of positive definite matrices form a group?

♡ 4.3.25. *Unitary matrices*: A complex, square matrix U is called *unitary* if it satisfies $U^\dagger U = \mathrm{I}$, where $U^\dagger = \overline{U^T}$ denotes the *Hermitian adjoint* in which one first transposes and then takes complex conjugates of all entries. (a) Show that U is a unitary matrix if and only if $U^{-1} = U^\dagger$. (b) Show that the following matrices are unitary and compute their inverses:

$$(i)\ \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{\mathrm{i}}{\sqrt{2}} \\ \frac{\mathrm{i}}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}, \quad (ii)\ \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{2\sqrt{3}} + \frac{\mathrm{i}}{2} & -\frac{1}{2\sqrt{3}} - \frac{\mathrm{i}}{2} \\ \frac{1}{\sqrt{3}} & -\frac{1}{2\sqrt{3}} - \frac{\mathrm{i}}{2} & -\frac{1}{2\sqrt{3}} + \frac{\mathrm{i}}{2} \end{pmatrix}, \quad (iii)\ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{\mathrm{i}}{2} & -\frac{1}{2} & -\frac{\mathrm{i}}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{\mathrm{i}}{2} & -\frac{1}{2} & \frac{\mathrm{i}}{2} \end{pmatrix}.$$

(c) Are the following matrices unitary?

$$(i)\ \begin{pmatrix} 2 & 1+2\,\mathrm{i} \\ 1-2\,\mathrm{i} & 3 \end{pmatrix}, \qquad (ii)\ \frac{1}{5}\begin{pmatrix} -1+2\,\mathrm{i} & -4-2\,\mathrm{i} \\ 2-4\,\mathrm{i} & -2-\mathrm{i} \end{pmatrix}, \qquad (iii)\ \begin{pmatrix} \frac{12}{13} & \frac{5}{13} \\ \frac{5}{13} & -\frac{12}{13} \end{pmatrix}.$$

(d) Show that U is a unitary matrix if and only if its columns form an orthonormal basis of $\mathbb{C}^n$ with respect to the Hermitian dot product. (e) Prove that the set of unitary matrices forms a group, as defined in Exercise 4.3.24.

The QR Factorization

The Gram–Schmidt procedure for orthonormalizing bases of $\mathbb{R}^n$ can be reinterpreted as a matrix factorization. This is more subtle than the LU factorization that resulted from Gaussian Elimination, but is of comparable significance, and is used in a broad range of applications in mathematics, statistics, physics, engineering, and numerical analysis.

Let $\mathbf{w}_1, \ldots, \mathbf{w}_n$ be a basis of $\mathbb{R}^n$, and let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be the corresponding orthonormal basis that results from any one of the three implementations of the Gram–Schmidt process. We assemble both sets of column vectors to form nonsingular $n \times n$ matrices

$$A = (\,\mathbf{w}_1 \ \ \mathbf{w}_2 \ \ \ldots \ \ \mathbf{w}_n\,), \qquad Q = (\,\mathbf{u}_1 \ \ \mathbf{u}_2 \ \ \ldots \ \ \mathbf{u}_n\,).$$

Since the $\mathbf{u}_i$ form an orthonormal basis, Q is an orthogonal matrix. In view of the matrix multiplication formula (2.13), the Gram–Schmidt equations (4.23) can be recast into an equivalent matrix form:

$$A = QR, \qquad \text{where} \qquad R = \begin{pmatrix} r_{11} & r_{12} & \ldots & r_{1n} \\ 0 & r_{22} & \ldots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & r_{nn} \end{pmatrix} \tag{4.32}$$

is an upper triangular matrix whose entries are the coefficients in (4.26–27). Since the Gram–Schmidt process works on any basis, the only requirement on the matrix A is that its columns form a basis of $\mathbb{R}^n$, and hence A can be any nonsingular matrix. We have therefore established the celebrated QR *factorization* of nonsingular matrices.

Theorem 4.24. Every nonsingular matrix can be factored, $A = QR$, into the product of an orthogonal matrix Q and an upper triangular matrix R. The factorization is unique if R is *positive upper triangular*, meaning that all its diagonal entries of are positive.

QR Factorization of a Matrix A

```
start
    for j = 1 to n
        set r_jj = sqrt(a_1j^2 + ··· + a_nj^2)
        if r_jj = 0, stop; print "A has linearly dependent columns"
            else for i = 1 to n
                set a_ij = a_ij / r_jj
            next i
        for k = j + 1 to n
            set r_jk = a_1j a_1k + ··· + a_nj a_nk
            for i = 1 to n
                set a_ik = a_ik − a_ij r_jk
            next i
        next k
    next j
end
```

The proof of uniqueness is relegated to Exercise 4.3.30.

Example 4.25. The columns of the matrix $A = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 0 & -2 \\ -1 & 2 & 3 \end{pmatrix}$ are the same basis vectors considered in Example 4.16. The orthonormal basis (4.21) constructed using the Gram–Schmidt algorithm leads to the orthogonal and upper triangular matrices

$$Q = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{4}{\sqrt{42}} & \frac{2}{\sqrt{14}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{42}} & -\frac{3}{\sqrt{14}} \\ -\frac{1}{\sqrt{3}} & \frac{5}{\sqrt{42}} & -\frac{1}{\sqrt{14}} \end{pmatrix}, \qquad R = \begin{pmatrix} \sqrt{3} & -\frac{1}{\sqrt{3}} & -\sqrt{3} \\ 0 & \frac{\sqrt{14}}{\sqrt{3}} & \frac{\sqrt{21}}{\sqrt{2}} \\ 0 & 0 & \frac{\sqrt{7}}{\sqrt{2}} \end{pmatrix}. \tag{4.33}$$

The reader may wish to verify that, indeed, $A = QR$.

While any of the three implementations of the Gram–Schmidt algorithm will produce the QR factorization of a given matrix $A = (\, \mathbf{w}_1\ \mathbf{w}_2\ \ldots\ \mathbf{w}_n \,)$, the stable version, as encoded in equations (4.28), is the one to use in practical computations, since it is the least likely to fail due to numerical artifacts produced by round-off errors. The accompanying pseudocode program reformulates the algorithm purely in terms of the matrix entries a_{ij} of A. During the course of the algorithm, the entries of the matrix A are successively overwritten; the final result is the orthogonal matrix Q appearing in place of A. The entries r_{ij} of R must be stored separately.

Example 4.26. Let us factor the matrix $A = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix}$ using the numerically stable QR algorithm. As in the program, we work directly on the matrix A, gradually changing it into orthogonal form. In the first loop, we set $r_{11} = \sqrt{5}$ to be the norm of the first column vector of A. We then normalize the first column by dividing by r_{11}; the resulting matrix is $\begin{pmatrix} \frac{2}{\sqrt{5}} & 1 & 0 & 0 \\ \frac{1}{\sqrt{5}} & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix}$. The next entries $r_{12} = \frac{4}{\sqrt{5}}$, $r_{13} = \frac{1}{\sqrt{5}}$, $r_{14} = 0$, are obtained by taking the dot products of the first column with the other three columns. For $j = 1, 2, 3$, we subtract r_{1j} times the first column from the j^{th} column; the result $\begin{pmatrix} \frac{2}{\sqrt{5}} & -\frac{3}{5} & -\frac{2}{5} & 0 \\ \frac{1}{\sqrt{5}} & \frac{6}{5} & \frac{4}{5} & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix}$ is a matrix whose first column is normalized to have unit length, and whose second, third and fourth columns are orthogonal to it. In the next loop, we normalize the second column by dividing by its norm $r_{22} = \sqrt{\frac{14}{5}}$, and so obtain the matrix $\begin{pmatrix} \frac{2}{\sqrt{5}} & -\frac{3}{\sqrt{70}} & -\frac{2}{5} & 0 \\ \frac{1}{\sqrt{5}} & \frac{6}{\sqrt{70}} & \frac{4}{5} & 0 \\ 0 & \frac{5}{\sqrt{70}} & 2 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix}$. We then take dot products of the second column with the remaining two columns to produce $r_{23} = \frac{16}{\sqrt{70}}$, $r_{24} = \frac{5}{\sqrt{70}}$. Subtracting these multiples of the second column from the third and fourth columns, we obtain $\begin{pmatrix} \frac{2}{\sqrt{5}} & -\frac{3}{\sqrt{70}} & \frac{2}{7} & \frac{3}{14} \\ \frac{1}{\sqrt{5}} & \frac{6}{\sqrt{70}} & -\frac{4}{7} & -\frac{3}{7} \\ 0 & \frac{5}{\sqrt{70}} & \frac{6}{7} & \frac{9}{14} \\ 0 & 0 & 1 & 2 \end{pmatrix}$, which now has its first two columns orthonormalized, and orthogonal to the last two columns. We then normalize the third column by dividing by $r_{33} = \sqrt{\frac{15}{7}}$, yielding $\begin{pmatrix} \frac{2}{\sqrt{5}} & -\frac{3}{\sqrt{70}} & \frac{2}{\sqrt{105}} & \frac{3}{14} \\ \frac{1}{\sqrt{5}} & \frac{6}{\sqrt{70}} & -\frac{4}{\sqrt{105}} & -\frac{3}{7} \\ 0 & \frac{5}{\sqrt{70}} & \frac{6}{\sqrt{105}} & \frac{9}{14} \\ 0 & 0 & \frac{7}{\sqrt{105}} & 2 \end{pmatrix}$. Finally, we subtract $r_{34} = \frac{20}{\sqrt{105}}$ times the third column from the fourth column. Dividing the resulting fourth column by its norm $r_{44} = \sqrt{\frac{5}{6}}$ results in the final formulas,

$$Q = \begin{pmatrix} \frac{2}{\sqrt{5}} & -\frac{3}{\sqrt{70}} & \frac{2}{\sqrt{105}} & -\frac{1}{\sqrt{30}} \\ \frac{1}{\sqrt{5}} & \frac{6}{\sqrt{70}} & -\frac{4}{\sqrt{105}} & \frac{2}{\sqrt{30}} \\ 0 & \frac{5}{\sqrt{70}} & \frac{6}{\sqrt{105}} & -\frac{3}{\sqrt{30}} \\ 0 & 0 & \frac{7}{\sqrt{105}} & \frac{4}{\sqrt{30}} \end{pmatrix}, \qquad R = \begin{pmatrix} \sqrt{5} & \frac{4}{\sqrt{5}} & \frac{1}{\sqrt{5}} & 0 \\ 0 & \frac{\sqrt{14}}{\sqrt{5}} & \frac{16}{\sqrt{70}} & \frac{5}{\sqrt{70}} \\ 0 & 0 & \frac{\sqrt{15}}{\sqrt{7}} & \frac{20}{\sqrt{105}} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{\sqrt{6}} \end{pmatrix},$$

for the $A = Q\,R$ factorization.

Ill-Conditioned Systems and Householder's Method

The $Q\,R$ factorization can be employed as an alternative to Gaussian Elimination to solve linear systems. Indeed, the system

$$A\,\mathbf{x} = \mathbf{b} \qquad \text{becomes} \qquad Q\,R\,\mathbf{x} = \mathbf{b}, \qquad \text{and hence} \qquad R\,\mathbf{x} = Q^T\mathbf{b}, \tag{4.34}$$

because $Q^{-1} = Q^T$ is an orthogonal matrix. Since R is upper triangular, the latter system can be solved for $\mathbf{x}$ by Back Substitution. The resulting algorithm, while more expensive to compute, offers some numerical advantages over traditional Gaussian Elimination, since it is less prone to inaccuracies resulting from ill-conditioning.

Example 4.27. Let us apply the $A = Q\,R$ factorization

$$\begin{pmatrix} 1 & 1 & 2 \\ 1 & 0 & -2 \\ -1 & 2 & 3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{4}{\sqrt{42}} & \frac{2}{\sqrt{14}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{42}} & -\frac{3}{\sqrt{14}} \\ -\frac{1}{\sqrt{3}} & \frac{5}{\sqrt{42}} & -\frac{1}{\sqrt{14}} \end{pmatrix} \begin{pmatrix} \sqrt{3} & -\frac{1}{\sqrt{3}} & -\sqrt{3} \\ 0 & \frac{\sqrt{14}}{\sqrt{3}} & \frac{\sqrt{21}}{\sqrt{2}} \\ 0 & 0 & \frac{\sqrt{7}}{\sqrt{2}} \end{pmatrix}$$

that we found in Example 4.25 to solve the linear system $A\,\mathbf{x} = (\,0, -4, 5\,)^T$. We first compute

$$Q^T\mathbf{b} = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ \frac{4}{\sqrt{42}} & \frac{1}{\sqrt{42}} & \frac{5}{\sqrt{42}} \\ \frac{2}{\sqrt{14}} & -\frac{3}{\sqrt{14}} & -\frac{1}{\sqrt{14}} \end{pmatrix} \begin{pmatrix} 0 \\ -4 \\ 5 \end{pmatrix} = \begin{pmatrix} -3\sqrt{3} \\ \frac{\sqrt{21}}{\sqrt{2}} \\ \frac{\sqrt{7}}{\sqrt{2}} \end{pmatrix}.$$

We then solve the upper triangular system

$$R\,\mathbf{x} = \begin{pmatrix} \sqrt{3} & -\frac{1}{\sqrt{3}} & -\sqrt{3} \\ 0 & \frac{\sqrt{14}}{\sqrt{3}} & \frac{\sqrt{21}}{\sqrt{2}} \\ 0 & 0 & \frac{\sqrt{7}}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -3\sqrt{3} \\ \frac{\sqrt{21}}{\sqrt{2}} \\ \frac{\sqrt{7}}{\sqrt{2}} \end{pmatrix}$$

by Back Substitution, leading to the solution $\mathbf{x} = (\,-2, 0, 1\,)^T$.

In computing the $Q\,R$ factorization of a mildly ill-conditioned matrix, one should employ the stable version (4.28) of the Gram–Schmidt process. However, yet more recalcitrant matrices require a completely different approach to the factorization, as formulated by the mid-twentieth-century American mathematician Alston Householder. His idea was to use a sequence of certain simple orthogonal matrices to gradually convert the matrix into upper triangular form.

Consider the *Householder* or *elementary reflection matrix*

$$H = \mathrm{I} - 2\,\mathbf{u}\,\mathbf{u}^T, \tag{4.35}$$

in which $\mathbf{u}$ is a unit vector (in the Euclidean norm). Geometrically, the matrix H represents a reflection of vectors through the subspace

$$\mathbf{u}^{\perp} = \{\,\mathbf{v} \mid \mathbf{v}\cdot\mathbf{u} = 0\,\} \tag{4.36}$$

consisting of all vectors orthogonal to $\mathbf{u}$, as illustrated in Figure 4.3. It is a symmetric orthogonal matrix, and so

$$H^T = H, \qquad H^2 = \mathrm{I}, \qquad H^{-1} = H. \tag{4.37}$$

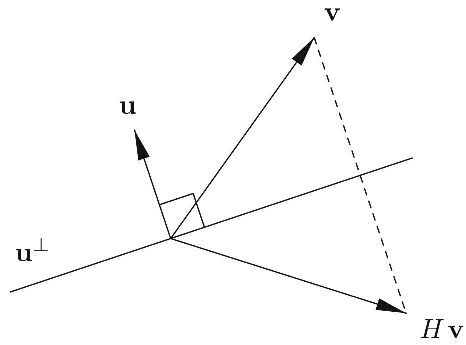

Figure 4.3. Elementary Reflection Matrix.

The proof is straightforward: symmetry is immediate, while

$$H H^T = H^2 = (\mathrm{I} - 2\,\mathbf{u}\,\mathbf{u}^T)\,(\mathrm{I} - 2\,\mathbf{u}\,\mathbf{u}^T) = \mathrm{I} - 4\,\mathbf{u}\,\mathbf{u}^T + 4\,\mathbf{u}\,(\mathbf{u}^T\mathbf{u})\,\mathbf{u}^T = \mathrm{I}\,,$$

since, by assumption, $\mathbf{u}^T\mathbf{u} = \|\,\mathbf{u}\,\|^2 = 1$. Thus, by suitably forming the unit vector $\mathbf{u}$, we can construct a Householder matrix that interchanges any two vectors of the same length.

Lemma 4.28. Let $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$ with $\|\,\mathbf{v}\,\| = \|\,\mathbf{w}\,\|$. Set $\mathbf{u} = (\mathbf{v} - \mathbf{w})/\|\,\mathbf{v} - \mathbf{w}\,\|$. Let $H = \mathrm{I} - 2\,\mathbf{u}\,\mathbf{u}^T$ be the corresponding elementary reflection matrix. Then $H\,\mathbf{v} = \mathbf{w}$ and $H\,\mathbf{w} = \mathbf{v}$.

Proof: Keeping in mind that $\mathbf{v}$ and $\mathbf{w}$ have the same Euclidean norm, we compute

$$\begin{aligned} H\,\mathbf{v} = (\mathrm{I} - 2\,\mathbf{u}\,\mathbf{u}^T)\,\mathbf{v} = \mathbf{v} \;-\; 2\,\frac{(\mathbf{v}-\mathbf{w})(\mathbf{v}-\mathbf{w})^T\mathbf{v}}{\|\,\mathbf{v}-\mathbf{w}\,\|^2} \\ = \mathbf{v} \;-\; 2\,\frac{\|\,\mathbf{v}\,\|^2 - \mathbf{w}\cdot\mathbf{v}}{2\,\|\,\mathbf{v}\,\|^2 - 2\,\mathbf{v}\cdot\mathbf{w}}\,(\mathbf{v}-\mathbf{w}) = \mathbf{v} - (\mathbf{v}-\mathbf{w}) = \mathbf{w}. \end{aligned}$$

The proof of the second equation is similar. *Q.E.D.*

In the first phase of Householder's method, we introduce the elementary reflection matrix that maps the first column $\mathbf{v}_1$ of the matrix A to a multiple of the first standard basis vector, namely $\mathbf{w}_1 = \|\,\mathbf{v}_1\,\|\,\mathbf{e}_1$, noting that $\|\,\mathbf{v}_1\,\| = \|\,\mathbf{w}_1\,\|$. Assuming $\mathbf{v}_1 \neq c\,\mathbf{e}_1$, we define the first unit vector and corresponding elementary reflection matrix as

$$\mathbf{u}_1 = \frac{\mathbf{v}_1 - \|\,\mathbf{v}_1\,\|\,\mathbf{e}_1}{\|\,\mathbf{v}_1 - \|\,\mathbf{v}_1\,\|\,\mathbf{e}_1\,\|}\,, \qquad H_1 = \mathrm{I} - 2\,\mathbf{u}_1\mathbf{u}_1^T.$$

On the other hand, if $\mathbf{v}_1 = c\,\mathbf{e}_1$ is already in the desired form, then we set $\mathbf{u}_1 = \mathbf{0}$ and $H_1 = \mathrm{I}$. Since, by the lemma, $H_1\mathbf{v}_1 = \mathbf{w}_1$, when we multiply A on the left by H_1, we obtain a matrix

$$A_2 = H_1\,A = \begin{pmatrix} r_{11} & \widetilde{a}_{12} & \widetilde{a}_{13} & \dots & \widetilde{a}_{1n} \\ 0 & \widetilde{a}_{22} & \widetilde{a}_{23} & \dots & \widetilde{a}_{2n} \\ 0 & \widetilde{a}_{32} & \widetilde{a}_{33} & \dots & \widetilde{a}_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \widetilde{a}_{n2} & \widetilde{a}_{n3} & \dots & \widetilde{a}_{nn} \end{pmatrix}$$

whose first column is in the desired upper triangular form.

In the next phase, we construct a second elementary reflection matrix to make all the entries below the diagonal in the second column of A_2 zero, keeping in mind that, at the same time, we should not mess up the first column. The latter requirement tells us that the vector used for the reflection should have a zero in its first entry. The correct choice is to set

$$\widetilde{\mathbf{v}}_2 = (0, \widetilde{a}_{22}, \widetilde{a}_{32}, \ldots, \widetilde{a}_{n2})^T, \qquad \mathbf{u}_2 = \frac{\widetilde{\mathbf{v}}_2 - \|\widetilde{\mathbf{v}}_2\|\,\mathbf{e}_2}{\|\widetilde{\mathbf{v}}_2 - \|\widetilde{\mathbf{v}}_2\|\,\mathbf{e}_2\|}, \qquad H_2 = \mathrm{I} - 2\,\mathbf{u}_2\,\mathbf{u}_2^T.$$

As before, if $\widetilde{\mathbf{v}}_2 = c\,\mathbf{e}_2$, then $\mathbf{u}_2 = \mathbf{0}$ and $H_2 = \mathrm{I}$. The net effect is

$$A_3 = H_2\,A_2 = \begin{pmatrix} r_{11} & r_{12} & \widehat{a}_{13} & \ldots & \widehat{a}_{1n} \\ 0 & r_{22} & \widehat{a}_{23} & \ldots & \widehat{a}_{2n} \\ 0 & 0 & \widehat{a}_{33} & \ldots & \widehat{a}_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \widehat{a}_{n3} & \ldots & \widehat{a}_{nn} \end{pmatrix},$$

and now the first two columns are in upper triangular form.

The process continues; at the k^{th} stage, we are dealing with a matrix A_k whose first $k-1$ columns coincide with the first k columns of the eventual upper triangular matrix R. Let $\widehat{\mathbf{v}}_k$ denote the vector obtained from the k^{th} column of A_k by setting its initial $k-1$ entries equal to 0. We define the k^{th} Householder vector and corresponding elementary reflection matrix by

$$\begin{aligned} \mathbf{w}_k &= \widehat{\mathbf{v}}_k - \|\widehat{\mathbf{v}}_k\|\,\mathbf{e}_k, \qquad & \mathbf{u}_k &= \begin{cases} \mathbf{w}_k/\|\mathbf{w}_k\|, & \text{if} \quad \mathbf{w}_k \neq \mathbf{0}, \\ \mathbf{0}, & \text{if} \quad \mathbf{w}_k = \mathbf{0}, \end{cases} \\ H_k &= \mathrm{I} - 2\,\mathbf{u}_k\,\mathbf{u}_k^T, & A_{k+1} &= H_k\,A_k. \end{aligned} \tag{4.38}$$

The process is completed after $n-1$ steps, and the final result is

$$R = H_{n-1}A_{n-1} = H_{n-1}H_{n-2}\,\cdots\,H_1 A = Q^T A, \qquad \text{where} \qquad Q = H_1 H_2\,\cdots\,H_{n-1}$$

is an orthogonal matrix, since it is the product of orthogonal matrices, cf. Proposition 4.23. In this manner, we have reproduced a[†] $Q\,R$ factorization of

$$A = Q\,R = H_1 H_2\,\cdots\,H_{n-1} R. \tag{4.39}$$

Example 4.29. Let us implement Householder's Method on the particular matrix

$$A = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 0 & -2 \\ -1 & 2 & 3 \end{pmatrix}$$

considered earlier in Example 4.25. The first Householder vector

$$\widehat{\mathbf{v}}_1 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} - \sqrt{3}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -.7321 \\ 1 \\ -1 \end{pmatrix}$$

leads to the elementary reflection matrix

$$H_1 = \begin{pmatrix} .5774 & .5774 & -.5774 \\ .5774 & .2113 & .7887 \\ -.5774 & .7887 & .2113 \end{pmatrix}, \text{ whereby } A_2 = H_1 A = \begin{pmatrix} 1.7321 & -.5774 & -1.7321 \\ 0 & 2.1547 & 3.0981 \\ 0 & -.1547 & -2.0981 \end{pmatrix}.$$

[†] The upper triangular matrix R may not have positive diagonal entries; if desired, this can be easily fixed by changing the signs of the appropriate columns of Q.

To construct the second and final Householder matrix, we start with the second column of A_2 and then set the first entry to 0; the resulting Householder vector is

$$\widehat{\mathbf{v}}_2 = \begin{pmatrix} 0 \\ 2.1547 \\ -.1547 \end{pmatrix} - 2.1603 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -.0055 \\ -.1547 \end{pmatrix}.$$

Therefore,

$$H_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & .9974 & -.0716 \\ 0 & -.0716 & -.9974 \end{pmatrix}, \quad \text{and so} \quad R = H_2 A_2 = \begin{pmatrix} 1.7321 & -.5774 & -1.7321 \\ 0 & 2.1603 & 3.2404 \\ 0 & 0 & 1.8708 \end{pmatrix}$$

is the upper triangular matrix in the QR decomposition of A. The orthogonal matrix Q is obtained by multiplying the reflection matrices:

$$Q = H_1 H_2 = \begin{pmatrix} .5774 & .6172 & .5345 \\ .5774 & .1543 & -.8018 \\ -.5774 & .7715 & -.2673 \end{pmatrix},$$

which numerically reconfirms the previous factorization (4.33).

Remark. If the purpose of the QR factorization is to solve a linear system via (4.34), it is not necessary to explicitly multiply out the Householder matrices to form Q; we merely need to store the corresponding unit Householder vectors $\mathbf{u}_1, \ldots, \mathbf{u}_{n-1}$. The solution to

$$A\mathbf{x} = QR\mathbf{x} = \mathbf{b} \qquad \text{can be found by solving} \qquad R\mathbf{x} = H_{n-1} H_{n-2} \cdots H_1 \mathbf{b} \tag{4.40}$$

by Back Substitution. This is the method of choice for moderately ill-conditioned systems. Severe ill-conditioning will defeat even this ingenious approach, and accurately solving such systems can be an extreme challenge.

Exercises

4.3.26. Write down the QR matrix factorization corresponding to the vectors in Example 4.17.

4.3.27. Find the QR factorization of the following matrices: (*a*) $\begin{pmatrix} 1 & -3 \\ 2 & 1 \end{pmatrix}$, (*b*) $\begin{pmatrix} 4 & 3 \\ 3 & 2 \end{pmatrix}$, (*c*) $\begin{pmatrix} 2 & 1 & -1 \\ 0 & 1 & 3 \\ -1 & -1 & 1 \end{pmatrix}$, (*d*) $\begin{pmatrix} 0 & 1 & 2 \\ -1 & 1 & 1 \\ -1 & 1 & 3 \end{pmatrix}$, (*e*) $\begin{pmatrix} 0 & 0 & 2 \\ 0 & 4 & 1 \\ -1 & 0 & 1 \end{pmatrix}$, (*f*) $\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & 0 \\ 1 & 1 & 2 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}$.

4.3.28. For each of the following linear systems, find the QR factorization of the coefficient matrix, and then use your factorization to solve the system: (*i*) $\begin{pmatrix} 1 & 2 \\ -1 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \end{pmatrix}$, (*ii*) $\begin{pmatrix} 2 & 1 & -1 \\ 1 & 0 & 2 \\ 2 & -1 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix}$, (*iii*) $\begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$.

♠ 4.3.29. Use the numerically stable version of the Gram–Schmidt process to find the QR factorizations of the 3×3, 4×4 and 5×5 versions of the tridiagonal matrix that has 4's along the diagonal and 1's on the sub- and super-diagonals, as in Example 1.37.

♢ 4.3.30. Prove that the QR factorization of a matrix is unique if all the diagonal entries of R are assumed to be positive. *Hint*: Use Exercise 4.3.12.

♡ 4.3.31. (a) How many arithmetic operations are required to compute the QR factorization of an $n \times n$ matrix? (b) How many additional operations are needed to utilize the factorization to solve a linear system $A\mathbf{x} = \mathbf{b}$ via (4.34)? (c) Compare the amount of computational effort with standard Gaussian Elimination.

♡ 4.3.32. Suppose A is an $m \times n$ matrix with $\operatorname{rank} A = n$. (a) Show that applying the Gram–Schmidt algorithm to the columns of A produces an orthonormal basis for $\operatorname{img} A$. (b) Prove that this is equivalent to the matrix factorization $A = QR$, where Q is an $m \times n$ matrix with orthonormal columns, while R is a nonsingular $n \times n$ upper triangular matrix. (c) Show that the QR program in the text also works for rectangular, $m \times n$, matrices as stated, the only modification being that the row indices i run from 1 to m. (d) Apply this method to factor

$$(i)\ \begin{pmatrix} 1 & -1 \\ 2 & 3 \\ 0 & 2 \end{pmatrix},\quad (ii)\ \begin{pmatrix} -3 & 2 \\ 1 & -1 \\ 4 & 1 \end{pmatrix},\quad (iii)\ \begin{pmatrix} -1 & 1 \\ 1 & -2 \\ -1 & -3 \\ 0 & 5 \end{pmatrix},\quad (iv)\ \begin{pmatrix} 0 & 1 & 2 \\ -3 & 1 & -1 \\ -1 & 0 & -2 \\ 1 & 1 & -2 \end{pmatrix}.$$

(e) Explain what happens if $\operatorname{rank} A < n$.

♡ 4.3.33. (a) According to Exercise 4.2.14, the Gram–Schmidt process can also be applied to produce orthonormal bases of complex vector spaces. In the case of $\mathbb{C}^n$, explain how this is equivalent to the factorization of a nonsingular complex matrix $A = UR$ into the product of a unitary matrix U (see Exercise 4.3.25) and a nonsingular upper triangular matrix R. (b) Factor the following complex matrices into unitary times upper triangular:

$$(i)\ \begin{pmatrix} \mathrm{i} & 1 \\ -1 & 2\,\mathrm{i} \end{pmatrix},\quad (ii)\ \begin{pmatrix} 1+\mathrm{i} & 2-\mathrm{i} \\ 1-\mathrm{i} & -\mathrm{i} \end{pmatrix},\quad (iii)\ \begin{pmatrix} \mathrm{i} & 1 & 0 \\ 1 & \mathrm{i} & 1 \\ 0 & 1 & \mathrm{i} \end{pmatrix},\quad (iv)\ \begin{pmatrix} \mathrm{i} & 1 & -\mathrm{i} \\ 1-\mathrm{i} & 0 & 1+\mathrm{i} \\ -1 & 2+3\,\mathrm{i} & 1 \end{pmatrix}.$$

(c) What can you say about uniqueness of the factorization?

4.3.34. (a) Write down the Householder matrices corresponding to the following unit vectors: (i) $(1, 0)^T$, (ii) $\left(\frac{3}{5}, \frac{4}{5}\right)^T$, (iii) $(0, 1, 0)^T$, (iv) $\left(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right)^T$. (b) Find all vectors fixed by a Householder matrix, i.e., $H\mathbf{v} = \mathbf{v}$ — first for the matrices in part (a), and then in general. (c) Is a Householder matrix a proper or improper orthogonal matrix?

4.3.35. Use Householder's Method to solve Exercises 4.3.27 and 4.3.29.

♣ 4.3.36. Let $H_n = Q_n R_n$ be the QR factorization of the $n \times n$ Hilbert matrix (1.72). (a) Find Q_n and R_n for $n = 2, 3, 4$. (b) Use a computer to find Q_n and R_n for $n = 10$ and 20. (c) Let $\mathbf{x}^\star \in \mathbb{R}^n$ denote the vector whose i^{th} entry is $x_i^\star = (-1)^i\, i/(i+1)$. For the values of n in parts (a) and (b), compute $\mathbf{y}^\star = H_n \mathbf{x}^\star$. Then solve the system $H_n \mathbf{x} = \mathbf{y}^\star$ (i) directly using Gaussian Elimination; (ii) using the QR factorization based on(4.34); (iii) using Householder's Method. Compare the results to the correct solution $\mathbf{x}^\star$ and discuss the pros and cons of each method.

4.3.37. Write out a pseudocode program to implement Householder's Method. The input should be an $n \times n$ matrix A and the output should be the Householder unit vectors $\mathbf{u}_1, \ldots, \mathbf{u}_{n-1}$ and the upper triangular matrix R. Test your code on one of the examples in Exercises 4.3.26–28.

4.4 Orthogonal Projections and Orthogonal Subspaces

Orthogonality is important, not just for individual vectors, but also for subspaces. In this section, we develop two concepts. First, we investigate the orthogonal projection of a vector onto a subspace, an operation that plays a key role in least squares minimization and data

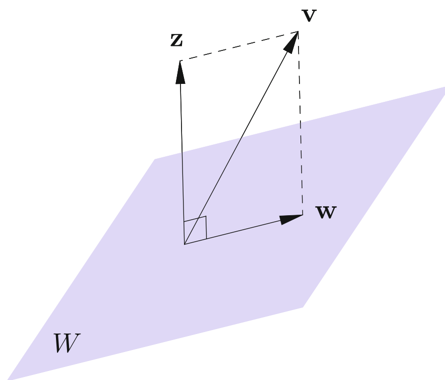

Figure 4.4. The Orthogonal Projection of a Vector onto a Subspace.

fitting, as we shall discuss in Chapter 5. Second, we develop the concept of orthogonality for a pair of subspaces, culminating with a proof of the orthogonality of the fundamental subspaces associated with an $m \times n$ matrix that at last reveals the striking geometry that underlies linear systems of equations and matrix multiplication.

Orthogonal Projection

Throughout this section, $W \subset V$ will be a finite-dimensional subspace of a real inner product space. The inner product space V is allowed to be infinite-dimensional. But, to facilitate your geometric intuition, you may initially want to view W as a subspace of Euclidean space $V = \mathbb{R}^m$ equipped with the ordinary dot product.

Definition 4.30. A vector $\mathbf{z} \in V$ is said to be *orthogonal* to the subspace $W \subset V$ if it is orthogonal to every vector in W, so $\langle \mathbf{z}, \mathbf{w} \rangle = 0$ for all $\mathbf{w} \in W$.

Given a basis $\mathbf{w}_1, \ldots, \mathbf{w}_n$ of the subspace W, we note that $\mathbf{z}$ is orthogonal to W if and only if it is orthogonal to every basis vector: $\langle \mathbf{z}, \mathbf{w}_i \rangle = 0$ for $i = 1, \ldots, n$. Indeed, any other vector in W has the form $\mathbf{w} = c_1 \mathbf{w}_1 + \cdots + c_n \mathbf{w}_n$, and hence, by linearity, $\langle \mathbf{z}, \mathbf{w} \rangle = c_1 \langle \mathbf{z}, \mathbf{w}_1 \rangle + \cdots + c_n \langle \mathbf{z}, \mathbf{w}_n \rangle = 0$, as required.

Definition 4.31. The *orthogonal projection* of $\mathbf{v}$ onto the subspace W is the element $\mathbf{w} \in W$ that makes the difference $\mathbf{z} = \mathbf{v} - \mathbf{w}$ orthogonal to W.

The geometric configuration underlying orthogonal projection is sketched in Figure 4.4. As we shall see, the orthogonal projection is unique. Note that $\mathbf{v} = \mathbf{w} + \mathbf{z}$ is the sum of its orthogonal projection $\mathbf{w} \in V$ and the perpendicular vector $\mathbf{z} \perp W$.

The explicit construction is greatly simplified by taking an orthonormal basis of the subspace, which, if necessary, can be arranged by applying the Gram–Schmidt process to a known basis. (The direct construction of the orthogonal projection in terms of a non-orthogonal basis appears in Exercise 4.4.10.)

Theorem 4.32. Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be an orthonormal basis for the subspace $W \subset V$. Then the orthogonal projection of $\mathbf{v} \in V$ onto $\mathbf{w} \in W$ is given by

$$\mathbf{w} = c_1 \mathbf{u}_1 + \cdots + c_n \mathbf{u}_n \qquad \text{where} \qquad c_i = \langle \mathbf{v}, \mathbf{u}_i \rangle, \qquad i = 1, \ldots, n. \tag{4.41}$$

Proof: First, since $\mathbf{u}_1, \ldots, \mathbf{u}_n$ form a basis of the subspace, the orthogonal projection element must be some linear combination thereof: $\mathbf{w} = c_1 \mathbf{u}_1 + \cdots + c_n \mathbf{u}_n$. Definition 4.31 requires that the difference $\mathbf{z} = \mathbf{v} - \mathbf{w}$ be orthogonal to W, and, as noted above, it suffices to check orthogonality to the basis vectors. By our orthonormality assumption,

$$\begin{aligned} 0 = \langle \mathbf{z}, \mathbf{u}_i \rangle = \langle \mathbf{v} - \mathbf{w}, \mathbf{u}_i \rangle &= \langle \mathbf{v} - c_1 \mathbf{u}_1 - \cdots - c_n \mathbf{u}_n, \mathbf{u}_i \rangle \\ &= \langle \mathbf{v}, \mathbf{u}_i \rangle - c_1 \langle \mathbf{u}_1, \mathbf{u}_i \rangle - \cdots - c_n \langle \mathbf{u}_n, \mathbf{u}_i \rangle = \langle \mathbf{v}, \mathbf{u}_i \rangle - c_i. \end{aligned}$$

The coefficients $c_i = \langle \mathbf{v}, \mathbf{u}_i \rangle$ of the orthogonal projection $\mathbf{w}$ are thus uniquely prescribed by the orthogonality requirement, which thereby proves its uniqueness. *Q.E.D.*

More generally, if we employ an orthogonal basis $\mathbf{v}_1, \ldots, \mathbf{v}_n$ for the subspace W, then the same argument demonstrates that the orthogonal projection of $\mathbf{v}$ onto W is given by

$$\mathbf{w} = a_1 \mathbf{v}_1 + \cdots + a_n \mathbf{v}_n, \qquad \text{where} \qquad a_i = \frac{\langle \mathbf{v}, \mathbf{v}_i \rangle}{\| \mathbf{v}_i \|^2}, \qquad i = 1, \ldots, n. \tag{4.42}$$

We could equally well replace the orthogonal basis by the orthonormal basis obtained by dividing each vector by its length: $\mathbf{u}_i = \mathbf{v}_i / \| \mathbf{v}_i \|$. The reader should be able to prove that the two formulas (4.41, 42) for the orthogonal projection yield the same vector $\mathbf{w}$.

Example 4.33. Consider the plane $W \subset \mathbb{R}^3$ spanned by the orthogonal vectors

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}, \qquad \mathbf{v}_2 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

According to formula (4.42), the orthogonal projection of $\mathbf{v} = (1, 0, 0)^T$ onto W is

$$\mathbf{w} = \frac{\langle \mathbf{v}, \mathbf{v}_1 \rangle}{\| \mathbf{v}_1 \|^2} \mathbf{v}_1 + \frac{\langle \mathbf{v}, \mathbf{v}_2 \rangle}{\| \mathbf{v}_2 \|^2} \mathbf{v}_2 = \frac{1}{6} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} + \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}.$$

Alternatively, we can replace $\mathbf{v}_1, \mathbf{v}_2$ by the orthonormal basis

$$\mathbf{u}_1 = \frac{\mathbf{v}_1}{\| \mathbf{v}_1 \|} = \begin{pmatrix} \frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}, \qquad \mathbf{u}_2 = \frac{\mathbf{v}_2}{\| \mathbf{v}_2 \|} = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}.$$

Then, using the orthonormal version (4.41),

$$\mathbf{w} = \langle \mathbf{v}, \mathbf{u}_1 \rangle \mathbf{u}_1 + \langle \mathbf{v}, \mathbf{u}_2 \rangle \mathbf{u}_2 = \frac{1}{\sqrt{6}} \begin{pmatrix} \frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix} + \frac{1}{\sqrt{3}} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}.$$

The answer is, of course, the same. As the reader may notice, while the theoretical formula is simpler when written in an orthonormal basis, for hand computations the orthogonal basis version avoids having to deal with square roots. (Of course, when the numerical computation is performed on a computer, this is not a significant issue.)

An intriguing observation is that the coefficients in the orthogonal projection formulas (4.41–42) coincide with the formulas (4.4, 7) for writing a vector in terms of an orthonormal or orthogonal basis. Indeed, if $\mathbf{v}$ were an element of W, then it would coincide with its orthogonal projection, $\mathbf{w} = \mathbf{v}$. (Why?) As a result, the orthogonal projection formula include the orthogonal basis formula as a special case.

It is also worth noting that the *same* formulae occur in the Gram–Schmidt algorithm, cf. (4.19). This observation leads to a useful geometric interpretation of the Gram–Schmidt construction. For each $k = 1, \ldots, n$, let

$$W_k = \operatorname{span}\{\mathbf{w}_1, \ldots, \mathbf{w}_k\} = \operatorname{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_k\} = \operatorname{span}\{\mathbf{u}_1, \ldots, \mathbf{u}_k\} \tag{4.43}$$

denote the k-dimensional subspace spanned by the first k basis elements, which is the same as that spanned by their orthogonalized and orthonormalized counterparts. In view of (4.41), the basic Gram–Schmidt formula (4.19) can be re-expressed in the form $\mathbf{v}_k = \mathbf{w}_k - \mathbf{p}_k$, where $\mathbf{p}_k$ is the orthogonal projection of $\mathbf{w}_k$ onto the subspace W_{k-1}. The resulting vector $\mathbf{v}_k$ is, by construction, orthogonal to the subspace, and hence orthogonal to all of the previous basis elements, which serves to rejustify the Gram–Schmidt construction.

Exercises

Note: Use the dot product and Euclidean norm unless otherwise specified.

4.4.1. Determine which of the vectors $\mathbf{v}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \mathbf{v}_2 = \begin{pmatrix} -2 \\ 2 \\ 2 \end{pmatrix}, \mathbf{v}_3 = \begin{pmatrix} 2 \\ -1 \\ -3 \end{pmatrix}, \mathbf{v}_4 = \begin{pmatrix} -1 \\ 3 \\ 4 \end{pmatrix}$, is orthogonal to (*a*) the line spanned by $\begin{pmatrix} 1 \\ 3 \\ -2 \end{pmatrix}$; (*b*) the plane spanned by $\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix}$; (*c*) the plane defined by $x - y - z = 0$; (*d*) the kernel of the matrix $\begin{pmatrix} 1 & -1 & -1 \\ 3 & -2 & -4 \end{pmatrix}$; (*e*) the image of the matrix $\begin{pmatrix} -3 & 1 \\ 3 & -1 \\ -1 & 0 \end{pmatrix}$; (*f*) the cokernel of the matrix $\begin{pmatrix} -1 & 0 & 3 \\ 2 & 1 & -2 \\ 3 & 1 & -5 \end{pmatrix}$.

4.4.2. Find the orthogonal projection of the vector $\mathbf{v} = (1,1,1)^T$ onto the following subspaces, using the indicated orthonormal/orthogonal bases: (a) the line in the direction $\left(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)^T$; (*b*) the line spanned by $(2,-1,3)^T$; (*c*) the plane spanned by $(1,1,0)^T, (-2,2,1)^T$; (*d*) the plane spanned by $\left(-\frac{3}{5}, \frac{4}{5}, 0\right)^T, \left(\frac{4}{13}, \frac{3}{13}, -\frac{12}{13}\right)^T$.

4.4.3. Find the orthogonal projection of $\mathbf{v} = (1,2,-1,2)^T$ onto the following subspaces: (a) the span of $\begin{pmatrix} 1 \\ -1 \\ 2 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 1 \\ 0 \\ -1 \end{pmatrix}$; (*b*) the image of the matrix $\begin{pmatrix} 1 & 2 \\ -1 & 1 \\ 0 & 3 \\ -1 & 1 \end{pmatrix}$; (*c*) the kernel of the matrix $\begin{pmatrix} 1 & -1 & 0 & 1 \\ -2 & 1 & 1 & 0 \end{pmatrix}$; (*d*) the subspace orthogonal to $\mathbf{a} = (1,-1,0,1)^T$.

Warning. Make sure you have an orthogonal basis before applying formula (4.42)!

4.4.4. Find the orthogonal projection of the vector $\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$ onto the image of $\begin{pmatrix} 3 & 2 \\ 2 & -2 \\ 1 & -2 \end{pmatrix}$.

4.4.5. Find the orthogonal projection of the vector $\mathbf{v} = (1,3,-1)^T$ onto the plane spanned by $(-1,2,1)^T, (2,1,-3)^T$ by first using the Gram–Schmidt process to construct an orthogonal basis.

4.4.6. Find the orthogonal projection of $\mathbf{v} = (1,2,-1,2)^T$ onto the span of $(1,-1,2,5)^T$ and $(2,1,0,-1)^T$ using the weighted inner product $\langle \mathbf{v}, \mathbf{w} \rangle = 4v_1 w_1 + 3v_2 w_2 + 2v_3 w_3 + v_4 w_4$.

4.4.7. Redo Exercise 4.4.2 using

(i) the weighted inner product $\langle \mathbf{v}, \mathbf{w} \rangle = 2v_1 w_1 + 2v_2 w_2 + v_3 w_3$;

(ii) the inner product induced by the positive definite matrix $K = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$.

4.4.8. (a) Prove that the set of all vectors orthogonal to a given subspace $V \subset \mathbb{R}^m$ forms a subspace. (b) Find a basis for the set of all vectors in $\mathbb{R}^4$ that are orthogonal to the subspace spanned by $(1,2,0,-1)^T$, $(2,0,3,1)^T$.

♡ 4.4.9. Let $\mathbf{u}_1, \ldots, \mathbf{u}_k$ be an orthonormal basis for the subspace $W \subset \mathbb{R}^m$. Let $A = (\mathbf{u}_1\ \mathbf{u}_2\ \ldots\ \mathbf{u}_k)$ be the $m \times k$ matrix whose columns are the orthonormal basis vectors, and define $P = A A^T$ to be the corresponding *projection matrix*. (a) Given $\mathbf{v} \in \mathbb{R}^n$, prove that its orthogonal projection $\mathbf{w} \in W$ is given by matrix multiplication: $\mathbf{w} = P\mathbf{v}$. (b) Prove that $P = P^T$ is symmetric. (c) Prove that P is idempotent: $P^2 = P$. Give a geometrical explanation of this fact. (d) Prove that $\operatorname{rank} P = k$. (e) Write out the projection matrix corresponding to the subspaces spanned by

$$(i)\ \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \quad (ii)\ \begin{pmatrix} \frac{2}{3} \\ -\frac{2}{3} \\ \frac{1}{3} \end{pmatrix}, \quad (iii)\ \begin{pmatrix} \frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}, \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \quad (iv)\ \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \end{pmatrix}.$$

♡ 4.4.10. Let $\mathbf{w}_1, \ldots, \mathbf{w}_n$ be an arbitrary basis of the subspace $W \subset \mathbb{R}^m$. Let $A = (\mathbf{w}_1, \ldots, \mathbf{w}_n)$ be the $m \times n$ matrix whose columns are the basis vectors, so that $W = \operatorname{img} A$ and $\operatorname{rank} A = n$. (a) Prove that the corresponding *projection matrix* $P = A(A^T A)^{-1} A^T$ is idempotent: $P^2 = P$. (b) Prove that P is symmetric. (c) Prove that $\operatorname{img} P = W$. (d) (e) Prove that the orthogonal projection of $\mathbf{v} \in \mathbb{R}^n$ onto $\mathbf{w} \in W$ is obtained by multiplying by the projection matrix: $\mathbf{w} = P\mathbf{v}$. (f) Show that if A is nonsingular, then $P = \mathrm{I}$. How do you interpret this in light of part (e)? (g) Explain why Exercise 4.4.9 is a special case of this result. (h) Show that if $A = QR$ is the factorization of A given in Exercise 4.3.32, then $P = QQ^T$. Why is $P \neq \mathrm{I}$?

4.4.11. Use the projection matrix method of Exercise 4.4.10 to find the orthogonal projection of $\mathbf{v} = (1,0,0,0)^T$ onto the image of the following matrices:

$$(a)\ \begin{pmatrix} 5 \\ -5 \\ -7 \\ 1 \end{pmatrix}, \quad (b)\ \begin{pmatrix} 1 & 0 \\ -1 & 2 \\ 0 & -1 \\ 1 & 2 \end{pmatrix}, \quad (c)\ \begin{pmatrix} 2 & -1 \\ -3 & 1 \\ 1 & -2 \\ 1 & 2 \end{pmatrix}, \quad (d)\ \begin{pmatrix} 0 & 1 & -1 \\ 0 & -1 & 2 \\ 1 & 1 & 1 \\ -2 & -1 & 0 \end{pmatrix}.$$

Orthogonal Subspaces

We now extend the notion of orthogonality from individual elements to entire subspaces of an inner product space V.

Definition 4.34. Two subspaces $W, Z \subset V$ are called *orthogonal* if every vector in W is orthogonal to every vector in Z.

In other words, W and Z are orthogonal subspaces if and only if $\langle \mathbf{w}, \mathbf{z} \rangle = 0$ for every $\mathbf{w} \in W$ and $\mathbf{z} \in Z$. In practice, one only needs to check orthogonality of basis elements,

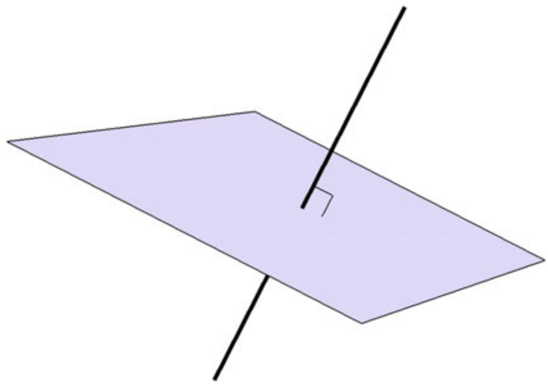

Figure 4.5. Orthogonal Complement to a Line.

or, more generally, spanning sets.

Lemma 4.35. If $\mathbf{w}_1, \ldots, \mathbf{w}_k$ span W and $\mathbf{z}_1, \ldots, \mathbf{z}_l$ span Z, then W and Z are orthogonal subspaces if and only if $\langle \mathbf{w}_i , \mathbf{z}_j \rangle = 0$ for all $i = 1, \ldots, k$ and $j = 1, \ldots, l$.

The proof of this lemma is left to the reader; see Exercise 4.4.26.

Example 4.36. Let $V = \mathbb{R}^3$ have the ordinary dot product. Then the plane $W \subset \mathbb{R}^3$ defined by the equation $2x - y + 3z = 0$ is orthogonal to the line Z spanned by its normal vector $\mathbf{n} = (2, -1, 3)^T$. Indeed, every $\mathbf{w} = (x, y, z)^T \in W$ satisfies the orthogonality condition $\mathbf{w} \cdot \mathbf{n} = 2x - y + 3z = 0$, which is simply the equation for the plane.

Example 4.37. Let W be the span of $\mathbf{w}_1 = (1, -2, 0, 1)^T$, $\mathbf{w}_2 = (3, -5, 2, 1)^T$, and let Z be the span of the vectors $\mathbf{z}_1 = (3, 2, 0, 1)^T$, $\mathbf{z}_2 = (1, 0, -1, -1)^T$. We find that $\mathbf{w}_1 \cdot \mathbf{z}_1 = \mathbf{w}_1 \cdot \mathbf{z}_2 = \mathbf{w}_2 \cdot \mathbf{z}_1 = \mathbf{w}_2 \cdot \mathbf{z}_2 = 0$, and so W and Z are orthogonal two-dimensional subspaces of $\mathbb{R}^4$ under the Euclidean dot product.

Definition 4.38. The *orthogonal complement* of a subspace $W \subset V$, denoted† $W^\perp$, is defined as the set of all vectors that are orthogonal to W:

$$W^\perp = \{ \mathbf{v} \in V \mid \langle \mathbf{v} , \mathbf{w} \rangle = 0 \text{ for all } \mathbf{w} \in W \}. \tag{4.44}$$

If W is the one-dimensional subspace (line) spanned by a single vector $\mathbf{w} \neq \mathbf{0}$ then we also denote $W^\perp$ by $\mathbf{w}^\perp$, as in (4.36). One easily checks that the orthogonal complement $W^\perp$ is also a subspace. Moreover, $W \cap W^\perp = \{\mathbf{0}\}$. (Why?) Keep in mind that the orthogonal complement will depend upon which inner product is being used.

Example 4.39. Let $W = \{ (t, 2t, 3t)^T \mid t \in \mathbb{R} \}$ be the line (one-dimensional subspace) in the direction of the vector $\mathbf{w}_1 = (1, 2, 3)^T \in \mathbb{R}^3$. Under the dot product, its orthogonal

† And usually pronounced "W perp"

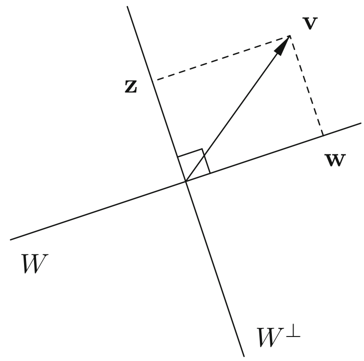

Figure 4.6. Orthogonal Decomposition of a Vector.

complement $W^\perp = \mathbf{w}_1^\perp$ is the plane passing through the origin having normal vector $\mathbf{w}_1$, as sketched in Figure 4.5. In other words, $\mathbf{z} = (\,x, y, z\,)^T \in W^\perp$ if and only if

$$\mathbf{z} \cdot \mathbf{w}_1 = x + 2\,y + 3\,z = 0. \tag{4.45}$$

Thus, $W^\perp$ is characterized as the solution space of the homogeneous linear equation (4.45), or, equivalently, the kernel of the 1×3 matrix $A = \mathbf{w}_1^T = (\,1 \;\; 2 \;\; 3\,)$. We can write the general solution in the form

$$\mathbf{z} = \begin{pmatrix} -2\,y - 3\,z \\ y \\ z \end{pmatrix} = y \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix} + z \begin{pmatrix} -3 \\ 0 \\ 1 \end{pmatrix} = y\,\mathbf{z}_1 + z\,\mathbf{z}_2,$$

where y, z are the free variables. The indicated vectors $\mathbf{z}_1 = (\,-2, 1, 0\,)^T$, $\mathbf{z}_2 = (\,-3, 0, 1\,)^T$, form a (non-orthogonal) basis for the orthogonal complement $W^\perp$.

Proposition 4.40. Suppose that $W \subset V$ is a finite-dimensional subspace of an inner product space. Then every vector $\mathbf{v} \in V$ can be uniquely decomposed into $\mathbf{v} = \mathbf{w} + \mathbf{z}$, where $\mathbf{w} \in W$ and $\mathbf{z} \in W^\perp$.

Proof: We let $\mathbf{w} \in W$ be the orthogonal projection of $\mathbf{v}$ onto W. Then $\mathbf{z} = \mathbf{v} - \mathbf{w}$ is, by definition, orthogonal to W and hence belongs to $W^\perp$. Note that $\mathbf{z}$ can be viewed as the orthogonal projection of $\mathbf{v}$ onto the complementary subspace $W^\perp$ (provided it is finite-dimensional). If we are given two such decompositions, $\mathbf{v} = \mathbf{w} + \mathbf{z} = \widetilde{\mathbf{w}} + \widetilde{\mathbf{z}}$, then $\mathbf{w} - \widetilde{\mathbf{w}} = \widetilde{\mathbf{z}} - \mathbf{z}$. The left-hand side of this equation lies in W, while the right-hand side belongs to $W^\perp$. But, as we already noted, the only vector that belongs to both W and $W^\perp$ is the zero vector. Thus, $\mathbf{w} - \widetilde{\mathbf{w}} = \mathbf{0} = \widetilde{\mathbf{z}} - \mathbf{z}$, so $\mathbf{w} = \widetilde{\mathbf{w}}$ and $\mathbf{z} = \widetilde{\mathbf{z}}$, which proves uniqueness. *Q.E.D.*

As a direct consequence of Exercise 2.4.26, in a finite-dimensional inner product space, a subspace and its orthogonal complement have complementary dimensions:

Proposition 4.41. If $W \subset V$ is a subspace with $\dim W = n$ and $\dim V = m$, then $\dim W^\perp = m - n$.

Example 4.42. Return to the situation described in Example 4.39. Let us decompose the vector $\mathbf{v} = (\,1, 0, 0\,)^T \in \mathbb{R}^3$ into a sum $\mathbf{v} = \mathbf{w} + \mathbf{z}$ of a vector $\mathbf{w}$ lying on the line W

and a vector $\mathbf{z}$ belonging to its orthogonal plane $W^\perp$, defined by (4.45). Each is obtained by an orthogonal projection onto the subspace in question, but we only need to compute one of the two directly, since the second can be obtained by subtracting the first from $\mathbf{v}$.

Orthogonal projection onto a one-dimensional subspace is easy, since every basis is, trivially, an orthogonal basis. Thus, the projection of $\mathbf{v}$ onto the line spanned by

$$\mathbf{w}_1 = (\,1,2,3\,)^T \qquad \text{is} \qquad \mathbf{w} = \frac{\langle\, \mathbf{v}\,,\mathbf{w}_1\,\rangle}{\|\,\mathbf{w}_1\,\|^2}\,\mathbf{w}_1 = \left(\,\tfrac{1}{14}, \tfrac{2}{14}, \tfrac{3}{14}\,\right)^T.$$

The component in $W^\perp$ is then obtained by subtraction:

$$\mathbf{z} = \mathbf{v} - \mathbf{w} = \left(\,\tfrac{13}{14}, -\tfrac{2}{14}, -\tfrac{3}{14}\,\right)^T.$$

Alternatively, one can obtain $\mathbf{z}$ directly by orthogonal projection onto the plane $W^\perp$. But you need to be careful: the basis found in Example 4.39 is not orthogonal, and so you will need to either first convert to an orthogonal basis and then use the orthogonal projection formula (4.42), or apply the more direct result in Exercise 4.4.10.

Example 4.43. Let $W \subset \mathbb{R}^4$ be the two-dimensional subspace spanned by the orthogonal vectors $\mathbf{w}_1 = (\,1,1,0,1\,)^T$ and $\mathbf{w}_2 = (\,1,1,1,-2\,)^T$. Its orthogonal complement $W^\perp$ (with respect to the Euclidean dot product) is the set of all vectors $\mathbf{v} = (\,x,y,z,w\,)^T$ that satisfy the linear system

$$\mathbf{v}\cdot\mathbf{w}_1 = x + y + w = 0, \qquad \mathbf{v}\cdot\mathbf{w}_2 = x + y + z - 2w = 0.$$

Applying the usual algorithm — the free variables are y and w — we find that the solution space is spanned by

$$\mathbf{z}_1 = (\,-1,1,0,0\,)^T, \qquad \mathbf{z}_2 = (\,-1,0,3,1\,)^T,$$

which form a non-orthogonal basis for $W^\perp$. An orthogonal basis

$$\mathbf{y}_1 = \mathbf{z}_1 = (\,-1,1,0,0\,)^T, \qquad \mathbf{y}_2 = \mathbf{z}_2 - \tfrac{1}{2}\mathbf{z}_1 = \left(\,-\tfrac{1}{2}, -\tfrac{1}{2}, 3, 1\,\right)^T,$$

for $W^\perp$ is obtained by a single Gram–Schmidt step. To decompose the vector $\mathbf{v} = (\,1,0,0,0\,)^T = \mathbf{w} + \mathbf{z}$, say, we compute the two orthogonal projections:

$$\begin{aligned} \mathbf{w} &= \tfrac{1}{3}\mathbf{w}_1 + \tfrac{1}{7}\mathbf{w}_2 = \left(\,\tfrac{10}{21}, \tfrac{10}{21}, \tfrac{1}{7}, \tfrac{1}{21}\,\right)^T \in W, \\ \mathbf{z} = \mathbf{v} - \mathbf{w} &= -\tfrac{1}{2}\mathbf{y}_1 - \tfrac{1}{21}\mathbf{y}_2 = \left(\,\tfrac{11}{21}, -\tfrac{10}{21}, -\tfrac{1}{7}, -\tfrac{1}{21}\,\right)^T \in W^\perp. \end{aligned}$$

Proposition 4.44. If W is a finite-dimensional subspace of an inner product space, then $(W^\perp)^\perp = W$.

This result is a corollary of the orthogonal decomposition derived in Proposition 4.40.

Warning. Propositions 4.40 and 4.44 are *not* necessarily true for infinite-dimensional subspaces. If $\dim W = \infty$, one can assert only that $W \subseteq (W^\perp)^\perp$. For example, it can be shown, [**19**; Exercise 10.2.D], that on every bounded interval $[a,b]$ the orthogonal complement of the subspace of all polynomials $\mathcal{P}^{(\infty)} \subset \mathrm{C}^0[a,b]$ with respect to the L^2 inner product is trivial: $(\mathcal{P}^{(\infty)})^\perp = \{0\}$. This means that the only continuous function that satisfies

$$\langle\, x^n\,, f(x)\,\rangle = \int_a^b x^n f(x)\,dx = 0 \qquad \text{for all} \qquad n = 0,1,2,\ldots$$

is the zero function $f(x) \equiv 0$. But the orthogonal complement of $\{0\}$ is the entire space, and so $((\mathcal{P}^{(\infty)})^\perp)^\perp = \mathrm{C}^0[a,b] \neq \mathcal{P}^{(\infty)}$.

The difference is that, in infinite-dimensional function space, a proper subspace $W \subsetneq V$ can be *dense*†, whereas in finite dimensions, every proper subspace is a "thin" subset that occupies only an infinitesimal fraction of the entire vector space. However, this seeming paradox is, interestingly, the reason behind the success of numerical approximation schemes in function space, such as the finite element method, [**81**].

Exercises

Note: In Exercises 4.4.12–15, use the dot product.

4.4.12. Find the orthogonal complement $W^\perp$ of the subspaces $W \subset \mathbb{R}^3$ spanned by the indicated vectors. What is the dimension of $W^\perp$ in each case?

(a) $\begin{pmatrix} 3 \\ -1 \\ 1 \end{pmatrix}$, (b) $\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}, \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix}$, (c) $\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}, \begin{pmatrix} 2 \\ 4 \\ 6 \end{pmatrix}$, (d) $\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} -2 \\ 3 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 2 \\ 0 \end{pmatrix}$, (e) $\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$.

4.4.13. Find a basis for the orthogonal complement of the following subspaces of $\mathbb{R}^3$: (a) the plane $3x + 4y - 5z = 0$; (b) the line in the direction $(-2, 1, 3)^T$; (c) the image of the matrix $\begin{pmatrix} 1 & 2 & -1 & 3 \\ -2 & 0 & 2 & 1 \\ -1 & 2 & 1 & 4 \end{pmatrix}$; (d) the cokernel of the same matrix.

4.4.14. Find a basis for the orthogonal complement of the following subspaces of $\mathbb{R}^4$: (a) the set of solutions to $-x + 3y - 2z + w = 0$; (b) the subspace spanned by $(1, 2, -1, 3)^T$, $(-2, 0, 1, -2)^T$, $(-1, 2, 0, 1)^T$; (c) the kernel of the matrix in Exercise 4.4.13c; (d) the coimage of the same matrix.

4.4.15. Decompose each of the following vectors with respect to the indicated subspace as $\mathbf{v} = \mathbf{w} + \mathbf{z}$, where $\mathbf{w} \in W, \mathbf{z} \in W^\perp$. (a) $\mathbf{v} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$, $W = \operatorname{span}\left\{ \begin{pmatrix} -3 \\ 1 \end{pmatrix} \right\}$;

(b) $\mathbf{v} = \begin{pmatrix} 1 \\ 2 \\ -1 \end{pmatrix}$, $W = \operatorname{span}\left\{ \begin{pmatrix} -3 \\ 2 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 5 \end{pmatrix} \right\}$; (c) $\mathbf{v} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $W = \ker \begin{pmatrix} 1 & 2 & -1 \\ 2 & 0 & 2 \end{pmatrix}$;

(d) $\mathbf{v} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $W = \operatorname{img} \begin{pmatrix} 1 & 0 & 1 \\ -2 & -1 & 0 \\ 1 & 3 & -5 \end{pmatrix}$; (e) $\mathbf{v} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$, $W = \ker \begin{pmatrix} 1 & 0 & 0 & 2 \\ -2 & -1 & 1 & -3 \end{pmatrix}$.

4.4.16. Redo Exercise 4.4.12 using the weighted inner product $\langle \mathbf{v}, \mathbf{w} \rangle = v_1 w_1 + 2 v_2 w_2 + 3 v_3 w_3$ instead of the dot product.

4.4.17. Redo Example 4.43 with the dot product replaced by the weighted inner product

$$\langle \mathbf{v}, \mathbf{w} \rangle = v_1 w_1 + 2 v_2 w_2 + 3 v_3 w_3 + 4 v_4 w_4.$$

♢ 4.4.18. Prove that the orthogonal complement $W^\perp$ of a subspace $W \subset V$ is itself a subspace.

† In general, a subset $W \subset V$ of a normed vector space is *dense* if, for every $\mathbf{v} \in V$, and every $\varepsilon > 0$, one can find $\mathbf{w} \in W$ with $\| \mathbf{v} - \mathbf{w} \| < \varepsilon$. The Weierstrass Approximation Theorem, [**19**; Theorem 10.2.2], tells us that the polynomials form a dense subspace of the space of continuous functions, and underlies the proof of the result mentioned in the preceding paragraph.

4.4.19. Let $V = \mathcal{P}^{(4)}$ denote the space of quartic polynomials, with the L^2 inner product $\langle\, p\,, q\,\rangle = \int_{-1}^{1} p(x)\, q(x)\, dx$. Let $W = \mathcal{P}^{(2)}$ be the subspace of quadratic polynomials.
(*a*) Write down the conditions that a polynomial $p \in \mathcal{P}^{(4)}$ must satisfy in order to belong to the orthogonal complement $W^\perp$. (*b*) Find a basis for and the dimension of $W^\perp$.
(*c*) Find an orthogonal basis for $W^\perp$.

4.4.20. Let $W \subset V$. Prove that (*a*) $W \cap W^\perp = \{0\}$, (*b*) $W \subseteq (W^\perp)^\perp$.

4.4.21. Let V be an inner product space. Prove that (*a*) $V^\perp = \{\mathbf{0}\}$, (*b*) $\{\mathbf{0}\}^\perp = V$.

4.4.22. Prove that if $W_1 \subset W_2$ are finite-dimensional subspaces of an inner product space, then $W_1^\perp \supset W_2^\perp$.

4.4.23. (*a*) Show that if $W, Z \subset \mathbb{R}^n$ are complementary subspaces, then $W^\perp$ and $Z^\perp$ are also complementary subspaces. (*b*) Sketch a picture illustrating this result when W and Z are lines in $\mathbb{R}^2$.

4.4.24. Prove that if W, Z are subspaces of an inner product space, then $(W+Z)^\perp = W^\perp \cap Z^\perp$. (See Exercise 2.2.22(*b*) for the definition of the sum of two subspaces.)

♢ 4.4.25. Fill in the details of the proof of Proposition 4.44.

♢ 4.4.26. Prove Lemma 4.35.

♢ 4.4.27. Let $W \subset V$ with $\dim V = n$. Suppose $\mathbf{w}_1, \ldots, \mathbf{w}_m$ is an orthogonal basis for W and $\mathbf{w}_{m+1}, \ldots, \mathbf{w}_n$ is an orthogonal basis for $W^\perp$. (*a*) Prove that the combination $\mathbf{w}_1, \ldots, \mathbf{w}_n$ forms an orthogonal basis of V. (*b*) Show that if $\mathbf{v} = c_1 \mathbf{w}_1 + \cdots + c_n \mathbf{w}_n$ is any vector in V, then its orthogonal decomposition $\mathbf{v} = \mathbf{w} + \mathbf{z}$ is given by $\mathbf{w} = c_1 \mathbf{w}_1 + \cdots + c_m \mathbf{w}_m \in W$ and $\mathbf{z} = c_{m+1} \mathbf{w}_{m+1} + \cdots + c_n \mathbf{w}_n \in W^\perp$.

♡ 4.4.28. Consider the subspace $W = \{\, u(a) = 0 = u(b)\,\}$ of the vector space $\mathrm{C}^0[a, b]$ with the usual L^2 inner product. (*a*) Show that W has a complementary subspace of dimension 2. (*b*) Prove that there does not exist an orthogonal complement of W. Thus, an infinite-dimensional subspace may not admit an orthogonal complement!

Orthogonality of the Fundamental Matrix Subspaces and the Fredholm Alternative

In Chapter 2, we introduced the four fundamental subspaces associated with an $m \times n$ matrix A. According to the Fundamental Theorem 2.49, the first two, the kernel (null space) and the coimage (row space), are subspaces of $\mathbb{R}^n$ having complementary dimensions. The second two, the cokernel (left null space) and the image (column space), are subspaces of $\mathbb{R}^m$, also of complementary dimensions. In fact, more than this is true — the paired subspaces are orthogonal complements with respect to the standard Euclidean dot product!

Theorem 4.45. Let A be a real $m \times n$ matrix. Then its kernel and coimage are orthogonal complements as subspaces of $\mathbb{R}^n$ under the dot product, while its cokernel and image are orthogonal complements in $\mathbb{R}^m$, also under the dot product:

$$\ker A = (\operatorname{coimg} A)^\perp \subset \mathbb{R}^n, \qquad \operatorname{coker} A = (\operatorname{img} A)^\perp \subset \mathbb{R}^m. \tag{4.46}$$

Proof: A vector $\mathbf{x} \in \mathbb{R}^n$ lies in $\ker A$ if and only if $A\mathbf{x} = \mathbf{0}$. According to the rules of matrix multiplication, the i^{th} entry of $A\mathbf{x}$ equals the vector product of the i^{th} row $\mathbf{r}_i^T$ of

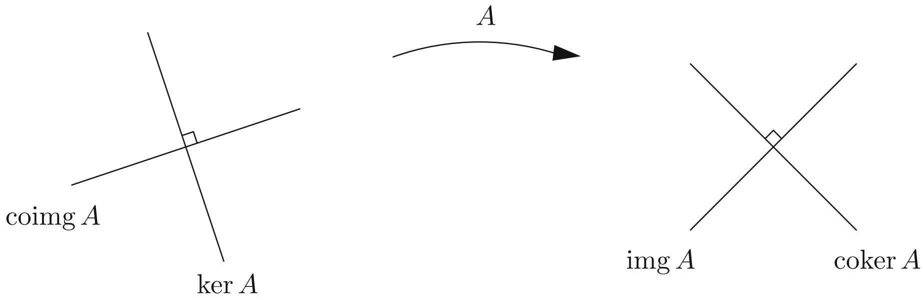

Figure 4.7. The Fundamental Matrix Subspaces.

A and $\mathbf{x}$. But this product vanishes, $\mathbf{r}_i^T \mathbf{x} = \mathbf{r}_i \cdot \mathbf{x} = 0$, if and only if $\mathbf{x}$ is orthogonal to $\mathbf{r}_i$. Therefore, $\mathbf{x} \in \ker A$ if and only if $\mathbf{x}$ is orthogonal to all the rows of A. Since the rows span $\operatorname{coimg} A$, this is equivalent to $\mathbf{x}$ lying in its orthogonal complement $(\operatorname{coimg} A)^\perp$, which proves the first statement. Orthogonality of the image and cokernel follows by the same argument applied to the transposed matrix A^T. *Q.E.D.*

Combining Theorems 2.49 and 4.45, we deduce the following important characterization of compatible linear systems.

Theorem 4.46. A linear system $A\mathbf{x} = \mathbf{b}$ has a solution if and only if $\mathbf{b}$ is orthogonal to the cokernel of A.

Indeed, the system has a solution if and only if the right-hand side belongs to the image of the coefficient matrix, $\mathbf{b} \in \operatorname{img} A$, which, by (4.46), requires that $\mathbf{b}$ be orthogonal to its cokernel. Thus, the compatibility conditions for the linear system $A\mathbf{x} = \mathbf{b}$ can be written in the form

$$\mathbf{y} \cdot \mathbf{b} = 0 \qquad \text{for every } \mathbf{y} \text{ satisfying} \qquad A^T \mathbf{y} = \mathbf{0}. \tag{4.47}$$

In practice, one only needs to check orthogonality of $\mathbf{b}$ with respect to a basis $\mathbf{y}_1, \ldots, \mathbf{y}_{m-r}$ of the cokernel, leading to a system of $m - r$ compatibility constraints

$$\mathbf{y}_i \cdot \mathbf{b} = 0, \qquad i = 1, \ldots, m - r. \tag{4.48}$$

Here $r = \operatorname{rank} A$ denotes the rank of the coefficient matrix, and so $m - r$ is also the number of all zero rows in the row echelon form of A. Hence, (4.48) contains precisely the same number of constraints as would be derived using Gaussian Elimination.

Theorem 4.46 is known as the *Fredholm alternative*, named after the Swedish mathematician Ivar Fredholm. His primary motivation was to solve linear integral equations, but his compatibility criterion was recognized to be a general property of linear systems, including linear algebraic systems, linear differential equations, linear boundary value problems, and so on.

Example 4.47. In Example 2.40, we analyzed the linear system $A\mathbf{x} = \mathbf{b}$ with coefficient matrix $A = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -2 \\ 1 & -2 & 3 \end{pmatrix}$. Using direct Gaussian Elimination, we were led to a single compatibility condition, namely $-b_1 + 2b_2 + b_3 = 0$, required for the system to have a solution. We now understand the meaning behind this equation: it is telling us that the right-hand side $\mathbf{b}$ must be orthogonal to the cokernel of A. The cokernel is determined by solving the homogeneous adjoint system $A^T \mathbf{y} = \mathbf{0}$, and is the line spanned by the vector $\mathbf{y}_1 = (-1, 2, 1)^T$. Thus, the compatibility condition requires that $\mathbf{b}$ be orthogonal to $\mathbf{y}_1$, in accordance with the Fredholm alternative (4.48).

Example 4.48. Let us determine the compatibility conditions for the linear system

$$x_1 - x_2 + 3x_3 = b_1, \quad -x_1 + 2x_2 - 4x_3 = b_2, \quad 2x_1 + 3x_2 + x_3 = b_3, \quad x_1 + 2x_3 = b_4,$$

by computing the cokernel of its coefficient matrix

$$A = \begin{pmatrix} 1 & -1 & 3 \\ -1 & 2 & -4 \\ 2 & 3 & 1 \\ 1 & 0 & 2 \end{pmatrix}.$$

We need to solve the homogeneous adjoint system $A^T \mathbf{y} = \mathbf{0}$, namely

$$y_1 - y_2 + 2y_3 + y_4 = 0, \qquad -y_1 + 2y_2 + 3y_3 = 0, \qquad 3y_1 - 4y_2 + y_3 + 2y_4 = 0.$$

Applying Gaussian Elimination, we deduce that the general solution

$$\mathbf{y} = y_3 \,(-7, -5, 1, 0\,)^T + y_4 \,(-2, -1, 0, 1\,)^T$$

is a linear combination (whose coefficients are the free variables) of the two basis vectors for $\operatorname{coker} A$. Thus, the Fredholm compatibility conditions (4.48) are obtained by taking their dot products with the right-hand side of the original system:

$$-7b_1 - 5b_2 + b_3 = 0, \qquad -2b_1 - b_2 + b_4 = 0.$$

The reader can check that these are indeed the same compatibility conditions that result from a direct Gaussian Elimination on the augmented matrix $\left(A \mid \mathbf{b} \right)$.

Remark. Conversely, rather than solving the homogeneous adjoint system, we can use Gaussian Elimination on the augmented matrix $\left(A \mid \mathbf{b} \right)$ to determine the $m - r$ basis vectors $\mathbf{y}_1, \ldots, \mathbf{y}_{m-r}$ for $\operatorname{coker} A$. They are formed from the coefficients of $b_1, \ldots, b_m$ in the $m - r$ consistency conditions $\mathbf{y}_i \cdot \mathbf{b} = 0$ for $i = 1, \ldots, m - r$, arising from the all zero rows in the reduced row echelon form.

We are now very close to a full understanding of the fascinating geometry that lurks behind the simple algebraic operation of multiplying a vector $\mathbf{x} \in \mathbb{R}^n$ by an $m \times n$ matrix, resulting in a vector $\mathbf{b} = A\mathbf{x} \in \mathbb{R}^m$. Since the kernel and coimage of A are orthogonal complements in the domain space $\mathbb{R}^n$, Proposition 4.41 tells us that we can uniquely decompose $\mathbf{x} = \mathbf{w} + \mathbf{z}$, where $\mathbf{w} \in \operatorname{coimg} A$, while $\mathbf{z} \in \ker A$. Since $A\mathbf{z} = \mathbf{0}$, we have

$$\mathbf{b} = A\mathbf{x} = A(\mathbf{w} + \mathbf{z}) = A\mathbf{w}.$$

Therefore, we can regard multiplication by A as a combination of two operations:

(i) The first is an orthogonal projection onto the coimage of A taking $\mathbf{x}$ to $\mathbf{w}$.

(ii) The second maps a vector in $\operatorname{coimg} A \subset \mathbb{R}^n$ to a vector in $\operatorname{img} A \subset \mathbb{R}^m$, taking the orthogonal projection $\mathbf{w}$ to the image vector $\mathbf{b} = A\mathbf{w} = A\mathbf{x}$.

Moreover, if A has rank r, then both $\operatorname{img} A$ and $\operatorname{coimg} A$ are r-dimensional subspaces, albeit of different vector spaces. Each vector $\mathbf{b} \in \operatorname{img} A$ corresponds to a *unique* vector $\mathbf{w} \in \operatorname{coimg} A$. Indeed, if $\mathbf{w}, \widetilde{\mathbf{w}} \in \operatorname{coimg} A$ satisfy $\mathbf{b} = A\mathbf{w} = A\widetilde{\mathbf{w}}$, then $A(\mathbf{w} - \widetilde{\mathbf{w}}) = \mathbf{0}$, and hence $\mathbf{w} - \widetilde{\mathbf{w}} \in \ker A$. But, since the kernel and the coimage are orthogonal complements, the only vector that belongs to both is the zero vector, and hence $\mathbf{w} = \widetilde{\mathbf{w}}$. In this manner, we have proved the first part of the following result; the second is left as Exercise 4.4.38.

Theorem 4.49. Multiplication by an $m \times n$ matrix A of rank r defines a one-to-one correspondence between the r-dimensional subspaces $\operatorname{coimg} A \subset \mathbb{R}^n$ and $\operatorname{img} A \subset \mathbb{R}^m$. Moreover, if $\mathbf{v}_1, \ldots, \mathbf{v}_r$ forms a basis of $\operatorname{coimg} A$ then their images $A\mathbf{v}_1, \ldots, A\mathbf{v}_r$ form a basis for $\operatorname{img} A$.

In summary, the linear system $A\mathbf{x} = \mathbf{b}$ has a solution if and only if $\mathbf{b} \in \operatorname{img} A$, or, equivalently, is orthogonal to every vector $\mathbf{y} \in \operatorname{coker} A$. If the compatibility conditions hold, then the system has a *unique* solution $\mathbf{w} \in \operatorname{coimg} A$ that, by the definition of the coimage, is a linear combination of the *rows* of A. The general solution to the system is $\mathbf{x} = \mathbf{w} + \mathbf{z}$, where $\mathbf{w}$ is the particular solution belonging to the coimage, while $\mathbf{z} \in \ker A$ is an arbitrary element of the kernel.

Theorem 4.50. A compatible linear system $A\mathbf{x} = \mathbf{b}$ with $\mathbf{b} \in \operatorname{img} A = (\operatorname{coker} A)^\perp$ has a unique solution $\mathbf{w} \in \operatorname{coimg} A$ satisfying $A\mathbf{w} = \mathbf{b}$. The general solution is $\mathbf{x} = \mathbf{w} + \mathbf{z}$, where $\mathbf{z} \in \ker A$. The particular solution $\mathbf{w} \in \operatorname{coimg} A$ is distinguished by the fact that it has the smallest Euclidean norm of all possible solutions: $\|\mathbf{w}\| \le \|\mathbf{x}\|$ whenever $A\mathbf{x} = \mathbf{b}$.

Proof: We have already established all but the last statement. Since the coimage and kernel are orthogonal subspaces, the norm of a general solution $\mathbf{x} = \mathbf{w} + \mathbf{z}$ is

$$\|\mathbf{x}\|^2 = \|\mathbf{w} + \mathbf{z}\|^2 = \|\mathbf{w}\|^2 + 2\,\mathbf{w}\cdot\mathbf{z} + \|\mathbf{z}\|^2 = \|\mathbf{w}\|^2 + \|\mathbf{z}\|^2 \ge \|\mathbf{w}\|^2,$$

with equality if and only if $\mathbf{z} = \mathbf{0}$. *Q.E.D.*

In practice, to determine the unique minimum-norm solution to a compatible linear system, we invoke the orthogonality of the coimage and kernel of the coefficient matrix. Thus, if $\mathbf{z}_1, \ldots, \mathbf{z}_{n-r}$ form a basis for $\ker A$, then the minimum-norm solution $\mathbf{x} = \mathbf{w} \in \operatorname{coimg} A$ is obtained by solving the enlarged system

$$A\mathbf{x} = \mathbf{b}, \qquad \mathbf{z}_1^T\mathbf{x} = 0, \qquad \ldots \qquad \mathbf{z}_{n-r}^T\mathbf{x} = 0. \tag{4.49}$$

The associated $(m + n - r) \times n$ coefficient matrix is simply obtained by appending the (transposed) kernel vectors to the original matrix A. The resulting matrix is guaranteed to have maximum rank n, and so, assuming $\mathbf{b} \in \operatorname{img} A$, the enlarged system has a unique solution, which is the minimum-norm solution to the original system $A\mathbf{x} = \mathbf{b}$.

Example 4.51. Consider the linear system

$$\begin{pmatrix} 1 & -1 & 2 & -2 \\ 0 & 1 & -2 & 1 \\ 1 & 3 & -5 & 2 \\ 5 & -1 & 9 & -6 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ 4 \\ 6 \end{pmatrix}. \tag{4.50}$$

Applying the usual Gaussian Elimination algorithm, we discover that the coefficient matrix has rank 3, and its kernel is spanned by the single vector $\mathbf{z}_1 = (1, -1, 0, 1)^T$. The system itself is compatible; indeed, the right-hand side is orthogonal to the basis cokernel vector $(2, 24, -7, 1)^T$, and so satisfies the Fredholm condition (4.48). The general solution to the linear system is $\mathbf{x} = (t, 3 - t, 1, t)^T$, where $t = w$ is the free variable.

To find the solution of minimum Euclidean norm, we can apply the algorithm described in the previous paragraph.† Thus, we supplement the original system by the constraint

$$\begin{pmatrix} 1 & -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix} = x - y + w = 0 \qquad (4.51)$$

that the solution be orthogonal to the kernel basis vector. Solving the combined linear system (4.50–51) leads to the unique solution $\mathbf{x} = \mathbf{w} = (1, 2, 1, 1)^T$, obtained by setting the free variable t equal to 1. Let us check that its norm is indeed the smallest among all solutions to the original system:

$$\| \mathbf{w} \| = \sqrt{7} \le \| \mathbf{x} \| = \| (t, 3 - t, 1, t)^T \| = \sqrt{3t^2 - 6t + 10},$$

where the quadratic function inside the square root achieves its minimum value of $\sqrt{7}$ at $t = 1$. It is further distinguished as the only solution that can be expressed as a linear combination of the rows of the coefficient matrix:

$$\begin{aligned} \mathbf{w}^T &= (1,\ 2,\ 1,\ 1) \\ &= -4\,(1,\ -1,\ 2,\ -2) - 17\,(0,\ 1,\ -2,\ 1) + 5\,(1,\ 3,\ -5,\ 2), \end{aligned}$$

meaning that $\mathbf{w}$ lies in the coimage of the coefficient matrix.

Exercises

4.4.29. For each of the following matrices A, (i) find a basis for each of the four fundamental subspaces; (ii) verify that the image and cokernel are orthogonal complements; (iii) verify that the coimage and kernel are orthogonal complements:

(a) $\begin{pmatrix} 1 & -2 \\ 2 & -4 \end{pmatrix}$, (b) $\begin{pmatrix} 5 & 0 \\ 1 & 2 \\ 0 & 2 \end{pmatrix}$, (c) $\begin{pmatrix} 0 & 1 & 2 \\ -1 & 0 & -3 \\ -2 & 3 & 0 \end{pmatrix}$, (d) $\begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 3 & 1 \\ 0 & 3 & 3 & 2 \end{pmatrix}$,

(e) $\begin{pmatrix} 3 & 1 & 4 & 2 & 7 \\ 1 & 1 & 2 & 0 & 3 \\ 5 & 2 & 7 & 3 & 12 \end{pmatrix}$, (f) $\begin{pmatrix} 1 & 3 & 0 & -2 \\ -2 & 1 & 2 & 3 \\ -3 & 5 & 4 & 4 \\ 1 & -4 & -2 & -1 \end{pmatrix}$, (g) $\begin{pmatrix} -1 & 2 & 2 & -1 \\ 2 & -4 & -5 & 2 \\ -3 & 6 & 2 & -3 \\ 1 & -2 & -3 & 1 \\ -2 & 4 & -5 & -2 \end{pmatrix}$.

4.4.30. For each of the following matrices, use Gaussian elimination on the augmented matrix $\left(A \mid \mathbf{b} \right)$ to determine a basis for its cokernel:

(a) $\begin{pmatrix} 9 & -6 \\ 6 & -4 \end{pmatrix}$, (b) $\begin{pmatrix} 1 & 3 \\ 2 & 6 \\ -3 & -9 \end{pmatrix}$, (c) $\begin{pmatrix} 1 & 1 & 3 \\ -1 & 1 & -2 \\ -1 & 3 & 6 \end{pmatrix}$, (d) $\begin{pmatrix} 1 & -2 & -2 \\ 0 & -1 & 3 \\ 2 & -5 & -1 \\ -2 & 2 & 10 \end{pmatrix}$.

4.4.31. Let $A = \begin{pmatrix} 1 & -2 & 2 & -1 \\ -2 & 4 & -3 & 5 \\ -1 & 2 & 0 & 7 \end{pmatrix}$. (a) Find a basis for coimg A. (b) Use Theorem 4.49 to find a basis of img A. (c) Write each column of A as a linear combination of the basis vectors you found in part (b).

† An alternative is to orthogonally project the general solution onto the coimage. The result is the same.

4.4.32. Write down the compatibility conditions on the following systems of linear equations by first computing a basis for the cokernel of the coefficient matrix. (*a*) $2x+y=a$, $x+4y=b$, $-3x+2y=c$; (*b*) $x+2y+3z=a$, $-x+5y-2z=b$, $2x-3y+5z=c$; (*c*) $x_1+2x_2+3x_3=b_1$, $x_2+2x_3=b_2$, $3x_1+5x_2+7x_3=b_3$, $-2x_1+x_2+4x_3=b_4$; (*d*) $x-3y+2z+w=a$, $4x-2y+2z+3w=b$, $5x-5y+4z+4w=c$, $2x+4y-2z+w=d$.

4.4.33. For each of the following $m \times n$ matrices, decompose the first standard basis vector $\mathbf{e}_1 = \mathbf{w} + \mathbf{z} \in \mathbb{R}^n$, where $\mathbf{w} \in \operatorname{coimg} A$ and $\mathbf{z} \in \ker A$. Verify your answer by expressing $\mathbf{w}$ as a linear combination of the rows of A.

(a) $\begin{pmatrix} 1 & -2 & 1 \\ 2 & -3 & 2 \end{pmatrix}$, (*b*) $\begin{pmatrix} 1 & 1 & 2 \\ -1 & 0 & -1 \\ -2 & -1 & -3 \end{pmatrix}$, (*c*) $\begin{pmatrix} 1 & -1 & 0 & 3 \\ 2 & 1 & 3 & 3 \\ 1 & 2 & 3 & 0 \end{pmatrix}$, (*d*) $\begin{pmatrix} -1 & 1 & 1 & -1 & 2 \\ -3 & 2 & -1 & -2 & 0 \end{pmatrix}$.

4.4.34. For each of the following linear systems, (*i*) verify compatibility using the Fredholm alternative, (*ii*) find the general solution, and (*iii*) find the solution of minimum Euclidean norm:

(*a*) $\begin{aligned} 2x-4y&=-6, \\ -x+2y&=3, \end{aligned}$ (*b*) $\begin{aligned} 2x+3y&=-1, \\ 3x+7y&=1, \\ -3x+2y&=8, \end{aligned}$ (*c*) $\begin{aligned} 6x-3y+9z&=12, \\ 2x-y+3z&=4, \end{aligned}$

(*d*) $\begin{aligned} x+3y+5z&=3, \\ -x+4y+9z&=11, \\ 2x+3y+4z&=0, \end{aligned}$ (*e*) $\begin{aligned} x_1-3x_2+7x_3&=-8, \\ 2x_1+x_2&=5, \\ 4x_1-3x_2+10x_3&=-5, \\ -2x_1+2x_2-6x_3&=4. \end{aligned}$ (*f*) $\begin{aligned} x-y+2z+3w&=5, \\ 3x-3y+5z+7w&=13, \\ -2x+2y+z+4w&=0. \end{aligned}$

4.4.35. Show that if $A = A^T$ is a symmetric matrix, then $A\mathbf{x} = \mathbf{b}$ has a solution if and only if $\mathbf{b}$ is orthogonal to $\ker A$.

♢ 4.4.36. Suppose $\mathbf{v}_1, \ldots, \mathbf{v}_n$ span a subspace $V \subset \mathbb{R}^m$. Prove that $\mathbf{w}$ is orthogonal to V if and only if $\mathbf{w} \in \operatorname{coker} A$, where $A = (\,\mathbf{v}_1\ \mathbf{v}_2\ \ldots\ \mathbf{v}_n\,)$ is the matrix with the indicated columns.

4.4.37. Let $A = \begin{pmatrix} 1 & -1 & 0 & 2 \\ 2 & -2 & 0 & 4 \\ -1 & 1 & 1 & -1 \\ 0 & 0 & 2 & 2 \end{pmatrix}$. (a) Find an orthogonal basis for $\operatorname{coimg} A$. (*b*) Find an orthogonal basis for $\ker A$. (*c*) If you combine your bases from parts (a) and (*b*), do you get an orthogonal basis of $\mathbb{R}^4$? Why or why not?

♢ 4.4.38. Prove that if $\mathbf{v}_1, \ldots, \mathbf{v}_r$ are a basis of $\operatorname{coimg} A$, then their images $A\mathbf{v}_1, \ldots, A\mathbf{v}_r$ are a basis for $\operatorname{img} A$.

4.4.39. *True or false*: The standard algorithm for finding a basis for $\ker A$ will always produce an orthogonal basis.

♢ 4.4.40. Is Theorem 4.45 true as stated for complex matrices? If not, can you formulate a similar theorem that is true? What is the Fredholm alternative for complex matrices?

4.5 Orthogonal Polynomials

Orthogonal and orthonormal bases play, if anything, an even more essential role in function spaces. Unlike the Euclidean space $\mathbb{R}^n$, most of the obvious bases of a typical (finite-dimensional) function space are not orthogonal with respect to any natural inner product. Thus, the computation of an orthonormal basis of functions is a critical step towards simplification of the analysis. The Gram–Schmidt algorithm, in any of the above formulations, can be successfully applied to construct suitably orthogonal functions. The most important examples are the classical orthogonal polynomials that arise in approximation and interpolation theory. Other orthogonal systems of functions play starring roles in Fourier analysis and its generalizations, including wavelets, in quantum mechanics, in the solution of partial differential equations by separation of variables, and a host of further applications in mathematics, physics, engineering, numerical analysis, etc., [**43**, **54**, **62**, **61**, **77**, **79**, **88**].

The Legendre Polynomials

We shall construct an orthonormal basis for the vector space $\mathcal{P}^{(n)}$ of polynomials of degree $\leq n$. For definiteness, the construction will be based on the L^2 inner product

$$\langle\, p\,, q\,\rangle = \int_{-1}^{1} p(t)\, q(t)\, dt \tag{4.52}$$

on the interval $[-1,1]$. The underlying method will work on any other bounded interval, as well as for weighted inner products, but (4.52) is of particular importance. We shall apply the Gram–Schmidt orthogonalization process to the elementary, but non-orthogonal monomial basis $1,\ t,\ t^2,\ \ldots\ t^n$. Because

$$\langle\, t^k\,, t^l\,\rangle = \int_{-1}^{1} t^{k+l}\, dt = \begin{cases} \dfrac{2}{k+l+1}, & k+l \text{ even},\\ 0, & k+l \text{ odd}, \end{cases} \tag{4.53}$$

odd-degree monomials are orthogonal to those of even degree, but that is all. We will use $q_0(t), q_1(t), \ldots, q_n(t)$ to denote the resulting orthogonal polynomials. We begin by setting

$$q_0(t) = 1, \qquad \text{with} \qquad \|\, q_0 \|^2 = \int_{-1}^{1} q_0(t)^2\, dt = 2.$$

According to formula (4.17), the next orthogonal basis polynomial is

$$q_1(t) = t \;-\; \frac{\langle\, t\,, q_0\,\rangle}{\|\, q_0 \|^2}\, q_0(t) = t, \qquad \text{with} \qquad \|\, q_1 \|^2 = \tfrac{2}{3}\,.$$

In general, the Gram–Schmidt formula (4.19) says we should define

$$q_k(t) \;=\; t^k \;-\; \sum_{j=0}^{k-1} \frac{\langle\, t^k\,, q_j\,\rangle}{\|\, q_j \|^2}\, q_j(t) \qquad \text{for} \qquad k = 1, 2, \ldots\,.$$

We can thus recursively compute the next few orthogonal polynomials:

$$\begin{aligned} q_2(t) &= t^2 - \tfrac{1}{3}, & \|\, q_2 \|^2 &= \tfrac{8}{45}\,,\\ q_3(t) &= t^3 - \tfrac{3}{5}\, t, & \|\, q_3 \|^2 &= \tfrac{8}{175}\,,\\ q_4(t) &= t^4 - \tfrac{6}{7}\, t^2 + \tfrac{3}{35}\,, & \|\, q_4 \|^2 &= \tfrac{128}{11025}\,,\\ q_5(t) &= t^5 - \tfrac{10}{9}\, t^3 + \tfrac{5}{21}\, t & \|\, q_6 \|^2 &= \tfrac{128}{43659}\,, \end{aligned} \tag{4.54}$$

and so on. The reader can verify that they satisfy the orthogonality conditions

$$\langle\, q_i\,, q_j\,\rangle = \int_{-1}^{1} q_i(t)\, q_j(t)\, dt = 0, \qquad i \neq j.$$

The resulting polynomials $q_0, q_1, q_2, \ldots$ are known as the *monic*† *Legendre polynomials*, in honor of the eighteenth-century French mathematician Adrien-Marie Legendre, who first

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† A polynomial is called *monic* if its leading coefficient is equal to 1.

used them for studying Newtonian gravitation. Since the first n Legendre polynomials, namely $q_0, \ldots, q_{n-1}$ span the subspace $\mathcal{P}^{(n-1)}$ of polynomials of degree $\leq n-1$, the next one, q_n, can be characterized as the unique monic polynomial that is orthogonal to every polynomial of degree $\leq n-1$:

$$\langle t^k , q_n \rangle = 0, \qquad\qquad k = 0, \ldots, n-1. \tag{4.55}$$

Since the monic Legendre polynomials form a basis for the space of polynomials, we can uniquely rewrite any polynomial of degree n as a linear combination:

$$p(t) = c_0\, q_0(t) + c_1\, q_1(t) + \;\cdots\; + c_n\, q_n(t). \tag{4.56}$$

In view of the general orthogonality formula (4.7), the coefficients are simply given by inner products

$$c_k = \frac{\langle p , q_k \rangle}{\| q_k \|^2} = \frac{1}{\| q_k \|^2} \int_{-1}^{1} p(t)\, q_k(t)\, dt, \qquad\qquad k = 0, \ldots, n. \tag{4.57}$$

For example,

$$t^4 = q_4(t) + \tfrac{6}{7}\, q_2(t) + \tfrac{1}{5}\, q_0(t) = \bigl(t^4 - \tfrac{6}{7}\, t^2 + \tfrac{3}{35} \bigr) + \tfrac{6}{7} \bigl(t^2 - \tfrac{1}{3} \bigr) + \tfrac{1}{5},$$

where the coefficients can be obtained either directly or via (4.57):

$$c_4 = \frac{11025}{128} \int_{-1}^{1} t^4\, q_4(t)\, dt = 1, \qquad c_3 = \frac{175}{8} \int_{-1}^{1} t^4\, q_3(t)\, dt = 0, \qquad \text{and so on.}$$

The classical *Legendre polynomials*, [**59**], are certain scalar multiples, namely

$$P_k(t) = \frac{(2\,k)\,!}{2^k\,(k\,!)^2}\, q_k(t), \qquad\qquad k = 0, 1, 2, \ldots, \tag{4.58}$$

and so also define a system of orthogonal polynomials. The multiple is fixed by the requirement that

$$P_k(1) = 1, \tag{4.59}$$

which is not so important here, but does play a role in other applications. The first few classical Legendre polynomials are

$$\begin{aligned}
&P_0(t) = 1, && \| P_0 \|^2 = 2,\\
&P_1(t) = t, && \| P_1 \|^2 = \tfrac{2}{3},\\
&P_2(t) = \tfrac{3}{2}\, t^2 - \tfrac{1}{2}, && \| P_2 \|^2 = \tfrac{2}{5},\\
&P_3(t) = \tfrac{5}{2}\, t^3 - \tfrac{3}{2}\, t, && \| P_3 \|^2 = \tfrac{2}{7},\\
&P_4(t) = \tfrac{35}{8}\, t^4 - \tfrac{15}{4}\, t^2 + \tfrac{3}{8}, && \| P_4 \|^2 = \tfrac{2}{9},\\
&P_5(t) = \tfrac{63}{8}\, t^5 - \tfrac{35}{4}\, t^3 + \tfrac{15}{8}\, t, && \| P_5 \|^2 = \tfrac{2}{11},
\end{aligned} \tag{4.60}$$

and are graphed in Figure 4.8. There is, in fact, an explicit formula for the Legendre polynomials, due to the early nineteenth-century mathematician, banker, and social reformer Olinde Rodrigues.

Theorem 4.52. The *Rodrigues formula* for the classical Legendre polynomials is

$$P_k(t) = \frac{1}{2^k\, k\,!}\, \frac{d^k}{dt^k}\, (t^2 - 1)^k, \qquad \| P_k \| = \sqrt{\frac{2}{2\,k+1}}\,, \qquad k = 0, 1, 2, \ldots\,. \tag{4.61}$$

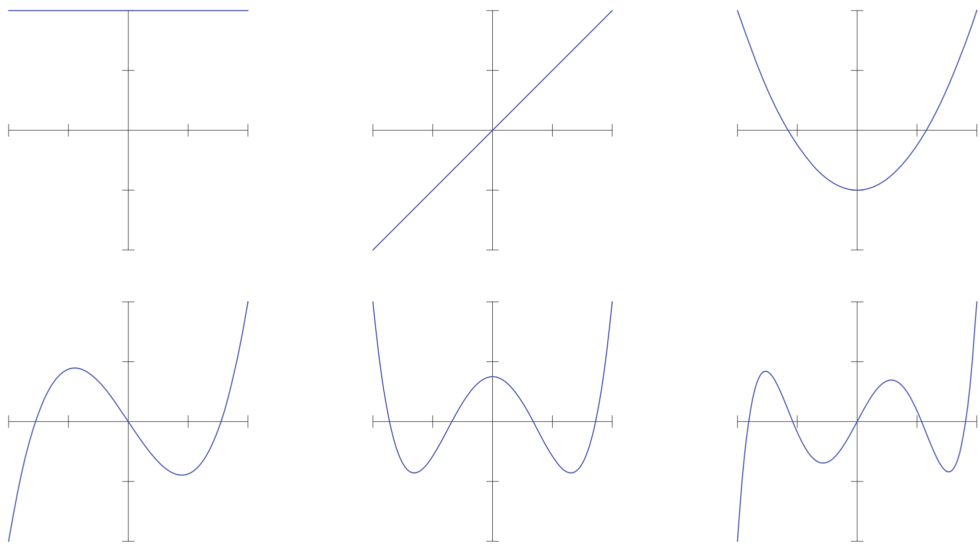

Figure 4.8. The Legendre Polynomials $P_0(t), \ldots, P_5(t)$.

Thus, for example,

$$P_4(t) = \frac{1}{16 \cdot 4!} \frac{d^4}{dt^4} (t^2 - 1)^4 = \frac{1}{384} \frac{d^4}{dt^4} (t^2 - 1)^4 = \tfrac{35}{8} t^4 - \tfrac{15}{4} t^2 + \tfrac{3}{8}.$$

Proof of Theorem 4.52: Let

$$R_{j,k}(t) = \frac{d^j}{dt^j} (t^2 - 1)^k, \tag{4.62}$$

which is evidently a polynomial of degree $2k-j$. In particular, the Rodrigues formula (4.61) claims that $P_k(t)$ is a multiple of $R_{k,k}(t)$. Note that

$$\frac{d}{dt} R_{j,k}(t) = R_{j+1,k}(t). \tag{4.63}$$

Moreover,

$$R_{j,k}(1) = 0 = R_{j,k}(-1) \qquad \text{whenever} \qquad j < k, \tag{4.64}$$

since, by the product rule, differentiating $(t^2 - 1)^k$ a total of $j < k$ times still leaves at least one factor of $t^2 - 1$ in each summand, which therefore vanishes at $t = \pm 1$. In order to complete the proof of the first formula, let us establish the following result:

Lemma 4.53. If $j \le k$, then the polynomial $R_{j,k}(t)$ is orthogonal to all polynomials of degree $\le j - 1$.

Proof: In other words,

$$\langle t^i, R_{j,k} \rangle = \int_{-1}^{1} t^i R_{j,k}(t)\, dt = 0, \qquad \text{for all} \qquad 0 \le i < j \le k. \tag{4.65}$$

Since $j > 0$, we use (4.63) to write $R_{j,k}(t) = R'_{j-1,k}(t)$. Integrating by parts,

$$\begin{aligned} \langle\, t^i \,, R_{j,k} \,\rangle &= \int_{-1}^{1} t^i\, R'_{j-1,k}(t)\, dt \\ &= i\, t^i\, R_{j-1,k}(t)\, \Big|_{t=-1}^{1} - i \int_{-1}^{1} t^{i-1}\, R_{j-1,k}(t)\, dt = -\, i\, \langle\, t^{i-1} \,, R_{j-1,k} \,\rangle, \end{aligned}$$

where the boundary terms vanish owing to (4.64). In particular, setting $i = 0$ proves $\langle\, 1 \,, R_{j,k} \,\rangle = 0$ for all $j > 0$. We then repeat the process, and, eventually, for any $j > i$,

$$\begin{aligned} \langle\, t^i \,, R_{j,k} \,\rangle &= -\, i\, \langle\, t^{i-1} \,, R_{j-1,k} \,\rangle \\ &= i(i-1)\, \langle\, t^{i-2} \,, R_{j-2,k} \,\rangle = \;\cdots\; = (-1)^i\, i\,(i-1) \;\cdots\; 3 \cdot 2\, \langle\, 1 \,, R_{j-i,k} \,\rangle = 0, \end{aligned}$$

completing the proof. *Q.E.D.*

In particular, $R_{k,k}(t)$ is a polynomial of degree k that is orthogonal to every polynomial of degree $\leq k-1$. By our earlier remarks, this implies that it must be a constant multiple,

$$R_{k,k}(t) = c_k\, P_k(t),$$

of the k^{th} Legendre polynomial. To determine c_k, we need only compare the leading terms:

$$R_{k,k}(t) = \frac{d^k}{dt^k}\,(t^2 - 1)^k = \frac{d^k}{dt^k}\,(t^{2k} + \cdots) = \frac{(2k)!}{k!}\, t^k + \cdots\,, \quad \text{while} \quad P_k(t) = \frac{(2k)!}{2^k\,(k!)^2}\, t^{2k} + \cdots\,.$$

We conclude that $c_k = 2^k\, k!$, which proves the first formula in (4.61). The proof of the formula for $\|\, P_k \,\|$ can be found in Exercise 4.5.9. *Q.E.D.*

The Legendre polynomials play an important role in many aspects of applied mathematics, including numerical analysis, least squares approximation of functions, and the solution of partial differential equations, [**61**].

Exercises

4.5.1. Write the following polynomials as linear combinations of monic Legendre polynomials. Use orthogonality to compute the coefficients: (*a*) t^3, (*b*) $t^4 + t^2$, (*c*) $7t^4 + 2t^3 - t$.

4.5.2. (*a*) Find the monic Legendre polynomial of degree 5 using the Gram–Schmidt process. Check your answer using the Rodrigues formula. (*b*) Use orthogonality to write t^5 as a linear combination of Legendre polynomials. (*c*) Repeat the exercise for degree 6.

♢ 4.5.3. (*a*) Explain why q_n is the unique monic polynomial that satisfies (4.55). (*b*) Use this characterization to directly construct $q_5(t)$.

4.5.4. Prove that the even (odd) degree Legendre polynomials are even (odd) functions of t.

4.5.5. Prove that if $p(t) = p(-t)$ is an even polynomial, then all the odd-order coefficients $c_{2j+1} = 0$ in its Legendre expansion (4.56) vanish.

4.5.6. Write out an explicit Rodrigues-type formula for the monic Legendre polynomial $q_k(t)$ and its norm.

4.5.7. Write out an explicit Rodrigues-type formula for an *orthonormal basis* $Q_0(t), \ldots, Q_n(t)$ for the space of polynomials of degree $\leq n$ under the inner product (4.52).

♢ 4.5.8. Use the Rodrigues formula to prove (4.59). *Hint*: Write $(t^2 - 1)^k = (t-1)^k\,(t+1)^k$.

♡ 4.5.9. A proof of the formula in (4.61) for the norms of the Legendre polynomials is based on the following steps. (a) First, prove that $\| R_{k,k} \|^2 = (-1)^k (2k)! \int_{-1}^{1} (t^2-1)^k \, dt$ by a repeated integration by parts. (b) Second, prove that $\int_{-1}^{1} (t^2-1)^k \, dt = (-1)^k \dfrac{2^{2k+1} (k!)^2}{(2k+1)!}$ by using the change of variables $t = \cos\theta$ in the integral. The resulting trigonometric integral can be done by another repeated integration by parts. (c) Finally, use the Rodrigues formula to complete the proof.

♡ 4.5.10. (a) Find the roots, $P_n(t) = 0$, of the Legendre polynomials P_2, P_3 and P_4. (b) Prove that for $0 \le j \le k$, the polynomial $R_{j,k}(t)$ defined in (4.62) has roots of order $k-j$ at $t = \pm 1$, and j additional simple roots lying between -1 and 1. *Hint*: Use induction on j and Rolle's Theorem from calculus, [**2**, **78**]. (c) Conclude that all k roots of the Legendre polynomial $P_k(t)$ are real and simple, and that they lie in the interval $-1 < t < 1$.

Other Systems of Orthogonal Polynomials

The standard Legendre polynomials form an orthogonal system with respect to the L^2 inner product on the interval $[-1,1]$. Dealing with any other interval, or, more generally, a weighted inner product, leads to a different, suitably adapted collection of orthogonal polynomials. In all cases, applying the Gram–Schmidt process to the standard monomials $1, t, t^2, t^3, \ldots$ will produce the desired orthogonal system.

Example 4.54. In this example, we construct orthogonal polynomials for the weighted inner product†

$$\langle f, g \rangle = \int_0^\infty f(t)\, g(t)\, e^{-t}\, dt \tag{4.66}$$

on the interval $[0,\infty)$. A straightforward integration by parts proves that

$$\int_0^\infty t^k e^{-t}\, dt = k!, \qquad \text{and hence} \qquad \langle t^i, t^j \rangle = (i+j)!, \qquad \| t^i \|^2 = (2i)!. \tag{4.67}$$

We apply the Gram–Schmidt process to construct a system of orthogonal polynomials for this inner product. The first few are

$$\begin{aligned}
q_0(t) &= 1, && \| q_0 \|^2 = 1,\\
q_1(t) &= t - \frac{\langle t, q_0 \rangle}{\| q_0 \|^2}\, q_0(t) = t - 1, && \| q_1 \|^2 = 1,\\
q_2(t) &= t^2 - \frac{\langle t^2, q_0 \rangle}{\| q_0 \|^2}\, q_0(t) - \frac{\langle t^2, q_1 \rangle}{\| q_1 \|^2}\, q_1(t) = t^2 - 4t + 2, && \| q_2 \|^2 = 4,\\
q_3(t) &= t^3 - 9t^2 + 18t - 6, && \| q_3 \|^2 = 36.
\end{aligned} \tag{4.68}$$

The resulting orthogonal polynomials are known as the (monic) *Laguerre polynomials*, named after the nineteenth-century French mathematician Edmond Laguerre, [**59**].

† The functions f, g must not grow too rapidly as $t \to \infty$ in order that the inner product be defined. For example, polynomial growth, meaning $|f(t)|, |g(t)| \le C t^N$ for $t \gg 0$ and some $C > 0$, $0 \le N < \infty$, suffices.

In some cases, a change of variables may be used to relate systems of orthogonal polynomials and thereby circumvent the Gram–Schmidt computation. Suppose, for instance, that our goal is to construct an orthogonal system of polynomials for the L^2 inner product

$$\langle\!\langle f, g \rangle\!\rangle = \int_a^b f(t)\, g(t)\, dt$$

on the interval $[a,b]$. The key remark is that we can map the interval $[-1,1]$ to $[a,b]$ by a simple change of variables of the form $s = \alpha + \beta t$. Specifically,

$$s = \frac{2t-b-a}{b-a} \qquad \text{will change} \qquad a \le t \le b \quad \text{to} \quad -1 \le s \le 1. \tag{4.69}$$

It therefore changes functions $F(s), G(s)$, defined for $-1 \le s \le 1$, into functions

$$f(t) = F\left(\frac{2t-b-a}{b-a}\right), \qquad g(t) = G\left(\frac{2t-b-a}{b-a}\right), \tag{4.70}$$

defined for $a \le t \le b$. Moreover, when integrating, we have $ds = \dfrac{2}{b-a}\, dt$, and so the inner products are related by

$$\begin{aligned} \langle f, g \rangle = \int_a^b f(t)\, g(t)\, dt &= \int_a^b F\left(\frac{2t-b-a}{b-a}\right) G\left(\frac{2t-b-a}{b-a}\right) dt \\ &= \int_{-1}^1 F(s)\, G(s)\, \frac{b-a}{2}\, ds = \frac{b-a}{2}\, \langle F, G \rangle, \end{aligned} \tag{4.71}$$

where the final L^2 inner product is over the interval $[-1,1]$. In particular, the change of variables maintains orthogonality, while rescaling the norms; explicitly,

$$\langle f, g \rangle = 0 \quad \text{if and only if} \quad \langle F, G \rangle = 0, \quad \text{while} \quad \| f \| = \sqrt{\frac{b-a}{2}}\ \| F \|. \tag{4.72}$$

Moreover, if $F(s)$ is a polynomial of degree n in s, then $f(t)$ is a polynomial of degree n in t and conversely. Let us apply these observations to the Legendre polynomials:

Proposition 4.55. The transformed Legendre polynomials

$$\widetilde{P}_k(t) = P_k\left(\frac{2t-b-a}{b-a}\right), \qquad \| \widetilde{P}_k \| = \sqrt{\frac{b-a}{2k+1}}, \qquad k = 0,1,2,\ldots, \tag{4.73}$$

form an orthogonal system of polynomials with respect to the L^2 inner product on the interval $[a,b]$.

Example 4.56. Consider the L^2 inner product $\langle\!\langle f, g \rangle\!\rangle = \int_0^1 f(t)\, g(t)\, dt$. The map $s = 2t - 1$ will change $0 \le t \le 1$ to $-1 \le s \le 1$. According to Proposition 4.55, this change of variables will convert the Legendre polynomials $P_k(s)$ into an orthogonal system of polynomials on $[0,1]$, namely

$$\widetilde{P}_k(t) = P_k(2t-1), \qquad \text{with corresponding } L^2 \text{ norms} \qquad \| \widetilde{P}_k \| = \sqrt{\frac{1}{2k+1}}.$$

The first few are

$$\begin{aligned} &\widetilde{P}_0(t) = 1, &&\widetilde{P}_3(t) = 20t^3 - 30t^2 + 12t - 1, \\ &\widetilde{P}_1(t) = 2t - 1, &&\widetilde{P}_4(t) = 70t^4 - 140t^3 + 90t^2 - 20t + 1, \\ &\widetilde{P}_2(t) = 6t^2 - 6t + 1, &&\widetilde{P}_5(t) = 252t^5 - 630t^4 + 560t^3 - 210t^2 + 30t - 1. \end{aligned} \tag{4.74}$$

Alternatively, one can derive these formulas through a direct application of the Gram–Schmidt process.

Exercises

4.5.11. Construct polynomials P_0, P_1, P_2, and P_3 of degree $0, 1, 2$, and 3, respectively, that are orthogonal with respect to the inner products (a) $\langle f, g \rangle = \int_1^2 f(t)\, g(t)\, dt$, (b) $\langle f, g \rangle = \int_0^1 f(t)\, g(t)\, t\, dt$, (c) $\langle f, g \rangle = \int_{-1}^1 f(t)\, g(t)\, t^2\, dt$, (d) $\langle f, g \rangle = \int_{-\infty}^{\infty} f(t)\, g(t)\, e^{-|t|}\, dt$..

4.5.12. Find the first four orthogonal polynomials on the interval $[0,1]$ for the weighted L^2 inner product with weight $w(t) = t^2$.

4.5.13. Write down an orthogonal basis for vector space $\mathcal{P}^{(5)}$ of quintic polynomials under the inner product $\langle f, g \rangle = \int_{-2}^2 f(t)\, g(t)\, dt$.

4.5.14. Use the Gram–Schmidt process based on the L^2 inner product on $[0,1]$ to construct a system of orthogonal polynomials of degree ≤ 4. Verify that your polynomials are multiples of the modified Legendre polynomials found in Example 4.56.

4.5.15. Find the first four orthogonal polynomials under the Sobolev H^1 inner product

$$\langle f, g \rangle = \int_{-1}^1 \left[\, f(t)\, g(t) + f'(t)\, g'(t) \,\right] dt; \quad \text{cf. Exercise 3.1.27.}$$

♢ 4.5.16. Prove the formula for $\| \widetilde{P}_k \|$ in (4.73) .

4.5.17. Find the monic Laguerre polynomials of degrees 4 and 5 and their norms.

♢ 4.5.18. Prove the integration formula (4.67).

♢ 4.5.19. (a) The physicists' *Hermite polynomials* are orthogonal with respect to the inner product $\langle f, g \rangle = \int_{-\infty}^{\infty} f(t)\, g(t)\, e^{-t^2}\, dt$. Find the first five monic Hermite polynomials. *Hint*: $\int_{-\infty}^{\infty} e^{-t^2}\, dt = \sqrt{\pi}$. (b) The probabilists prefer to use the inner product $\langle f, g \rangle = \int_{-\infty}^{\infty} f(t)\, g(t)\, e^{-t^2/2}\, dt$. Find the first five of their monic Hermite polynomials.
(c) Can you find a change of variables that transforms the physicists' versions to the probabilists' versions?

♡ 4.5.20. The *Chebyshev polynomials*: (a) Prove that $T_n(t) = \cos(n \arccos t)$, $n = 0, 1, 2, \ldots,$ form a system of orthogonal polynomials under the weighted inner product

$$\langle f, g \rangle = \int_{-1}^1 \frac{f(t)\, g(t)\, dt}{\sqrt{1 - t^2}}\,. \tag{4.75}$$

(b) What is $\| T_n \|$? (c) Write out the formulas for $T_0(t), \ldots, T_6(t)$ and plot their graphs.

4.5.21. Does the Gram–Schmidt process for the inner product (4.75) lead to the Chebyshev polynomials $T_n(t)$ defined in the preceding exercise? Explain why or why not.

4.5.22. Find two functions that form an orthogonal basis for the space of the solutions to the differential equation $y'' - 3y' + 2y = 0$ under the L^2 inner product on $[0,1]$.

4.5.23. Find an orthogonal basis for the space of solutions to the differential equation $y''' - y'' + y' - y = 0$ for the L^2 inner product on $[-\pi, \pi]$.

♡ 4.5.24. In this exercise, we investigate the effect of more general changes of variables on orthogonal polynomials. (*a*) Prove that $t = 2s^2 - 1$ defines a one-to-one map from the interval $0 \le s \le 1$ to the interval $-1 \le t \le 1$. (*b*) Let $p_k(t)$ denote the monic Legendre polynomials, which are orthogonal on $-1 \le t \le 1$. Show that $q_k(s) = p_k(2s^2 - 1)$ defines a polynomial. Write out the cases $k = 0, 1, 2, 3$ explicitly. (*c*) Are the polynomials $q_k(s)$ orthogonal under the L^2 inner product on $[0, 1]$? If not, do they retain any sort of orthogonality property? *Hint*: What happens to the L^2 inner product on $[-1, 1]$ under the change of variables?

4.5.25. (*a*) Show that the change of variables $s = e^{-t}$ maps the Laguerre inner product (4.66) to the standard L^2 inner product on $[0, 1]$. However, explain why this does *not* allow you to change Legendre polynomials into Laguerre polynomials. (*b*) Describe the functions resulting from applying the change of variables to the modified Legendre polynomials (4.74) and their orthogonality properties. (*c*) Describe the functions that result from applying the inverse change of variables to the Laguerre polynomials (4.68) and their orthogonality properties.

4.5.26. Explain how to adapt the numerically stable Gram–Schmidt method in (4.28) to construct a system of orthogonal polynomials. Test your algorithm on one of the preceding exercises.