Chapter 9
A General Framework for
Linear Partial Differential Equations

Before pressing on to the higher-dimensional manifestations of the heat, wave, and Laplace/ Poisson equations, it is worth pausing to develop a general, abstract, linear-algebraic framework that underlies many of the linear partial differential equations arising throughout the subject and its applications. The power of mathematical abstraction is that concentrating on the essential features and not being distracted by the at times messy particular details enables one to establish, relatively painlessly, very general results that can be applied throughout the subject and beyond. Each abstract concept has, as its source, an elementary finite-dimensional version valid for linear algebraic systems and matrices, which is then generalized and extended to include linear boundary value problems and then initial-boundary value problems governed by differential equations. All of the abstract definitions and results contained here will be immediately applicable to the boundary and initial value problems of physical interest, and serve to deepen our understanding of the underlying commonalities among systems and solution techniques. Nevertheless, a more applications-oriented reader may prefer to skip ahead to the more concrete developments contained in the following chapters, referring to the background material presented here as necessary.

Most equilibrium systems are modeled as boundary value problems involving a linear differential operator that satisfies the two key conditions of being "self-adjoint" and either "positive definite" or, slightly more generally, "positive semi-definite". So, our first task is to introduce the adjoint of a linear function in general, and, for our specific purposes, a linear differential operator. The adjoint is a far-reaching generalization of the elementary matrix transpose. Its formulation relies on the specification of inner products on both the domain and target spaces of the operator, and, when one is dealing with linear differential operators, the imposition of suitable homogeneous boundary conditions on the spaces of allowable functions. In applications, the relevant inner products are typically dictated by the underlying physics. One immediate application of the adjoint is the Fredholm Alternative, which delineates the constraints required for the existence of solutions to linear systems, including linear boundary value problems.

A linear operator that equals its own adjoint is called self-adjoint. The simplest example is the linear function defined by a symmetric matrix. The most important subclasses are the positive definite and positive semi-definite operators, which are the natural analogues of positive (semi-)definite matrices. We will learn how to construct self-adjoint positive (semi-)definite operators in a canonical manner. Almost all of the linear differential operators studied in this text, including the Laplacian, are, when subject to suitable

boundary conditions, self-adjoint and either positive definite or positive semi-definite. The key distinction is that positive definite linear systems and boundary value problems admit unique solutions, whereas in the positive semi-definite case, the solution either does not exist, since the Fredholm constraints are not satisfied, or, when it exists, is not unique. In their dynamical manifestations, positive definite operators induce stable vibrational systems, whereas the positive semi-definite cases contain unstable modes that can lead to disastrous physical consequences.

A critically important fact is that the solution to a positive definite linear system can be characterized by a minimization principle, provided by a certain quadratic function or, in the infinite-dimensional function-space version, quadratic functional. In physical contexts, the function(al) often represents the potential energy of the system, and the solution minimizes said energy among all possible configurations satisfying the prescribed boundary conditions, thereby quantifying the maxim that Nature is inherently conservative and seeks to minimize energy. In mathematics, minimization principles underlie advanced functional-analytic methods used to establish existence theorems, as well as the finite element numerical schemes to be presented in Chapter 10.

For linear dynamical systems like the heat and wave equations, separation of variables leads to an eigenvalue problem for the linear differential operator governing the corresponding equilibrium system. In the simple one-dimensional cases discussed in Chapter 4, the eigenfunctions are trigonometric, producing the classical Fourier expansions for the solutions. The effectuality of the Fourier method relies on the eigenfunctions' orthogonality, and we already hinted that this is no accident. Rather, it is a consequence of their status as the eigenfunctions of a self-adjoint linear operator. Not only are such eigenfunctions automatically mutually orthogonal with respect to the underlying inner product, the eigenvalues are necessarily real and, when the operator is positive definite, also positive.

Orthogonality underlies the Fourier-like expansion of quite general functions as series in the eigenfunctions, whose convergence, in general, requires that the eigenfunctions form a complete system. For positive definite boundary value problems on bounded domains, we will establish completeness by combining the eigenfunction expansion for the associated Green's function with a basic minimization principle for the eigenvalues based on the Rayleigh quotient. On the other hand, problems on unbounded domains do not typically admit complete systems of eigenfunctions and require the more advanced analytical concepts of continuous spectrum and generalized Fourier transforms that lie beyond the scope of this text.

The chapter concludes by describing a general framework for dynamics that produces time-dependent series solutions, in terms of the eigenfunctions of the underlying equilibrium operator, for diffusion equations, vibration equations, and quantum-mechanical systems. The final two chapters will then specialize these general theories and constructions to analyze initial-boundary value problems for the two- and three-dimensional heat, wave, and Schrödinger equations in simple geometries. More advanced developments and further applications can be found in higher-level texts, including [**35**, **38**, **44**, **61**, **99**].

9.1 Adjoints

Our starting point is a linear operator

$$L : U \; \longrightarrow \; V \tag{9.1}$$

that maps a vector space U to another vector space V. For most of the development, we deal with real vector spaces, although the final discussion of the Schrödinger equation requires us to venture into the complex realm. For our purposes, L represents a linear differential operator, and the elements of the domain space U and the target space V are suitable scalar- or vector-valued functions. In elastomechanics, the elements of U are displacements of a deformable body, while the elements of V are the associated strains. In electromagnetism and gravitation, elements of U represent potentials, and elements of V are electric or magnetic or gravitational fields. In thermodynamics, U contains temperature distributions, while V contains temperature gradients. In fluid mechanics, U is the space of potential functions, while V is the space of fluid velocities. And so on.

The abstract definition of the adjoint of a linear operator relies on an inner product structure on both its domain and target spaces. We distinguish the inner products on U and V (which may be different even when U and V happen to be the same vector space) by using a single angle bracket

$$\langle\, u\,,\widetilde{u}\,\rangle \quad \text{to denote the inner product between } u,\widetilde{u} \in U,$$

and a double angle bracket

$$\langle\!\langle\, v\,,\widetilde{v}\,\rangle\!\rangle \quad \text{to denote the inner product between } v,\widetilde{v} \in V.$$

In applications, the appropriate inner products are often based on the underlying physics.

Definition 9.1. Let U, V be inner product spaces, and let $L: U \to V$ be a linear operator. The *adjoint* of L is the unique linear operator $L^*: V \to U$ that satisfies

$$\langle\!\langle\, L[u]\,,v\,\rangle\!\rangle = \langle\, u\,,L^*[v]\,\rangle \qquad \text{for all} \qquad u \in U, \quad v \in V. \tag{9.2}$$

Observe that the adjoint goes in the *reverse* direction, that is, from V back to U. To master the definition, let us first look at the finite-dimensional case.

Example 9.2. According to Theorem B.33, every linear function $L: \mathbb{R}^n \to \mathbb{R}^m$ is given by matrix multiplication, so that $L[\mathbf{u}] = A\mathbf{u}$ for $\mathbf{u} \in \mathbb{R}^n$, where A is an $m \times n$ matrix. The adjoint function $L^*: \mathbb{R}^m \to \mathbb{R}^n$ is also linear, so it is also represented by matrix multiplication, $L^*[\mathbf{v}] = A^*\mathbf{v}$ for $\mathbf{v} \in \mathbb{R}^m$, by an $n \times m$ matrix A^*.

Suppose first that we impose the ordinary Euclidean dot products

$$\langle\, \mathbf{u}\,,\widetilde{\mathbf{u}}\,\rangle = \mathbf{u} \cdot \widetilde{\mathbf{u}} = \mathbf{u}^T\,\widetilde{\mathbf{u}}, \qquad \mathbf{u},\widetilde{\mathbf{u}} \in \mathbb{R}^n, \qquad\qquad \langle\!\langle\, \mathbf{v}\,,\widetilde{\mathbf{v}}\,\rangle\!\rangle = \mathbf{v} \cdot \widetilde{\mathbf{v}} = \mathbf{v}^T\,\widetilde{\mathbf{v}}, \qquad \mathbf{v},\widetilde{\mathbf{v}} \in \mathbb{R}^m,$$

as our inner products on both $\mathbb{R}^n$ and $\mathbb{R}^m$. Evaluation of both sides of the adjoint identity (9.2) yields

$$\begin{aligned} \langle\!\langle\, L[\mathbf{u}]\,,\mathbf{v}\,\rangle\!\rangle &= \langle\!\langle\, A\mathbf{u}\,,\mathbf{v}\,\rangle\!\rangle = (A\mathbf{u})^T\mathbf{v} = \mathbf{u}^T A^T\,\mathbf{v}, \\ \langle\, \mathbf{u}\,,L^*[\mathbf{v}]\,\rangle &= \langle\, \mathbf{u}\,,A^*\,\mathbf{v}\,\rangle = \mathbf{u}^T A^*\,\mathbf{v}. \end{aligned} \tag{9.3}$$

Since these expressions must agree for all $\mathbf{u}, \mathbf{v}$, we conclude (see Exercise 9.1.6) that the matrix A^* representing L^* is equal to the transposed matrix A^T. Therefore, *the adjoint of a matrix with respect to the Euclidean dot product is its transpose*: $A^* = A^T$. So one can regard the adjoint as a vast generalization of the elementary operation of transposing a matrix.

More generally, suppose we take weighted inner products on the domain and target spaces:

$$\langle\, \mathbf{u}\,,\widetilde{\mathbf{u}}\,\rangle = \mathbf{u}^T M\,\widetilde{\mathbf{u}}, \qquad \mathbf{u},\widetilde{\mathbf{u}} \in \mathbb{R}^n, \qquad \langle\!\langle\, \mathbf{v}\,,\widetilde{\mathbf{v}}\,\rangle\!\rangle = \mathbf{v}^T C\,\widetilde{\mathbf{v}}, \qquad \mathbf{v},\widetilde{\mathbf{v}} \in \mathbb{R}^m, \tag{9.4}$$

where M and C are symmetric, positive definite matrices of respective sizes $n \times n$ and $m \times m$, cf. Proposition B.13. Then, repeating the previous calculation (9.3), we find

$$\langle\!\langle\, L[\mathbf{u}]\,,\mathbf{v}\,\rangle\!\rangle = \langle\!\langle\, A\,\mathbf{u}\,,\mathbf{v}\,\rangle\!\rangle = (A\,\mathbf{u})^T C\,\mathbf{v} = \mathbf{u}^T A^T C\,\mathbf{v},$$
$$\langle\,\mathbf{u}\,,L^*[\mathbf{v}]\,\rangle = \langle\,\mathbf{u}\,,A^*\,\mathbf{v}\,\rangle = \mathbf{u}^T M A^*\,\mathbf{v}. \tag{9.5}$$

Comparing these expressions, we conclude that the *weighted adjoint matrix* is

$$A^* = M^{-1} A^T C. \tag{9.6}$$

Therefore, the adjoint does indeed depend on which inner products are being used on both the domain and target spaces.

Differential Operators

For applications to linear differential equations, our attention is focused on adjoints of differential operators defined on infinite-dimensional function spaces. Let us begin with the simplest example.

Example 9.3. Consider the derivative $v = D[u] = du/dx$, which defines a linear operator $D: U \to V$ mapping a vector space U of differentiable functions $u(x)$ to a vector space containing their derivatives $v(x) = u'(x)$. We assume that the functions in question are defined on a fixed bounded interval $a \le x \le b$.

In order to compute its adjoint, we need to impose inner products on both the domain space U and the target space V. The simplest context is to adopt the standard L^2 inner product on both:

$$\langle\,u\,,\widetilde{u}\,\rangle = \int_a^b u(x)\,\widetilde{u}(x)\,dx, \qquad\qquad \langle\!\langle\, v\,,\widetilde{v}\,\rangle\!\rangle = \int_a^b v(x)\,\widetilde{v}(x)\,dx. \tag{9.7}$$

According to the defining equation (9.2), the adjoint operator $D^*: V \to U$ must satisfy the inner product identity

$$\langle\!\langle\, D[u]\,,v\,\rangle\!\rangle = \langle\,u\,,D^*[v]\,\rangle \qquad \text{for all} \qquad u \in U, \quad v \in V. \tag{9.8}$$

First, we compute the left-hand side:

$$\langle\!\langle\, D[u]\,,v\,\rangle\!\rangle = \left\langle\!\!\left\langle\, \frac{du}{dx}\,,\,v\,\right\rangle\!\!\right\rangle = \int_a^b \frac{du}{dx}\,v\,dx. \tag{9.9}$$

On the other hand, the right-hand side should equal

$$\langle\,u\,,D^*[v]\,\rangle = \int_a^b u\,D^*[v]\,dx. \tag{9.10}$$

Now, in the latter integral, we see u multiplying the result of applying the linear operator D^* to v. To identify this integrand with that in (9.9), we need to somehow remove the derivative from u. The secret is *integration by parts*, which allows us to rewrite the first integral in the form

$$\int_a^b \frac{du}{dx}\,v\,dx = \big[\,u(b)\,v(b) - u(a)\,v(a)\,\big] - \int_a^b u\,\frac{dv}{dx}\,dx. \tag{9.11}$$

Ignoring the two boundary terms for a moment, we observe that the remaining integral has the form of an inner product

$$-\int_a^b u \, \frac{dv}{dx} \, dx = \int_a^b u \left[-\frac{dv}{dx} \right] dx = \left\langle \, u \, , \, -\frac{dv}{dx} \, \right\rangle = \langle \, u \, , -D[v] \, \rangle. \qquad (9.12)$$

Equating (9.9) and (9.12), we deduce that

$$\langle\!\langle \, D[u] \, , v \, \rangle\!\rangle = \left\langle\!\left\langle \, \frac{du}{dx} \, , v \, \right\rangle\!\right\rangle = \left\langle \, u \, , \, -\frac{dv}{dx} \, \right\rangle = \langle \, u \, , -D[v] \, \rangle.$$

Thus, to satisfy the adjoint equation (9.8), we must have

$$\langle \, u \, , D^*[v] \, \rangle = \langle \, u \, , -D[v] \, \rangle \qquad \text{for all} \qquad u \in U, \quad v \in V,$$

and so the adjoint of the derivative operator is its negative:

$$D^* = -D. \qquad (9.13)$$

However, the preceding argument is valid *only* if the boundary terms in the integration by parts formula (9.11) vanish:

$$u(b) \, v(b) - u(a) \, v(a) = 0, \qquad (9.14)$$

which necessitates imposing suitable boundary conditions on the functions u and v. For example, imposing Dirichlet boundary conditions

$$u(a) = 0, \qquad\qquad u(b) = 0, \qquad (9.15)$$

will ensure that (9.14) holds, and therefore validates (9.13). In this case, the domain space of $D : U \to V$ is the vector space

$$U = \{ \, u(x) \mid \, u(a) = u(b) = 0 \, \},$$

while no boundary conditions need be imposed on the functions $v(x)$ in the target space V. An evident alternative is to require that $v(a) = v(b) = 0$. In this case, the target space

$$V = \{ \, v(x) \mid \, v(a) = v(b) = 0 \, \}$$

consists of all functions that vanish at the endpoints. Since the derivative $D : U \to V$ is required to map a function $u(x) \in U$ to an *allowable* function $v(x) \in V$, the domain space now consists of functions satisfying the Neumann boundary conditions:

$$U = \{ \, u(x) \mid \, u'(a) = u'(b) = 0 \, \}.$$

These are evidently not the only two possibilities. Let us list the most important combinations of boundary conditions that imply the vanishing of the boundary terms (9.14), and so ensure the validity of the adjoint equation (9.13):

(a) Dirichlet boundary conditions: $\qquad u(a) = u(b) = 0.$

(b) Mixed boundary conditions: $\qquad u(a) = u'(b) = 0, \quad$ or $\quad u'(a) = u(b) = 0.$

(c) Neumann boundary conditions: $\qquad u'(a) = u'(b) = 0.$

(d) Periodic boundary conditions: $\qquad u(a) = u(b) \quad$ and $\quad u'(a) = u'(b).$

In all cases, the boundary conditions impose restrictions on the domain space U and, in cases (b–d) when we are identifying $v(x) = u'(x)$, the target space V also.

Remark: In the preceding discussion, we were purposely vague about the required differentiability of the functions. In finite dimensions, every linear function $L: \mathbb{R}^n \to \mathbb{R}^m$ is given by matrix multiplication $L[u] = A\mathbf{u}$, and hence is defined on all of the underlying vector space $\mathbb{R}^n$. Linear operators on infinite-dimensional function spaces are typically not defined on all possible functions. For example, the derivative operator $L = D: U \to V$ requires the function $u \in U$ to be differentiable. However, the target function $v = D[u] = u'$ is not necessarily as smooth, and so may belong to a different function space; for instance if $u \in \mathrm{C}^1[a,b]$, then $v = u' \in \mathrm{C}^0[a,b]$. On the other hand, the adjoint $D^* = -D$ is defined only on differentiable functions v, so if $v \in \mathrm{C}^1[a,b]$, then $u = -v' \in \mathrm{C}^0[a,b]$. Keeping a detailed account of the various smoothness requirements quickly becomes distracting.

To circumvent this technical annoyance, we will always deal with a fixed class of functions, e.g., continuous functions or, more generally, L^2 functions, that are constrained only by the imposed boundary conditions. When we write $L: U \to V$, we allow the possibility that the linear operator L may be defined only on a "dense" subspace of the domain space U. For instance, we will write $D: U \to V$ with $U = V = \mathrm{C}^0[a,b]$, even though $D[u] = u' \in V$ only if u belongs to the dense subspace $\mathrm{C}^1[a,b] \subset U = \mathrm{C}^0[a,b]$. Similarly, $D^*: V \to U$ is also defined only on the dense subspace $\mathrm{C}^1[a,b] \subset V = \mathrm{C}^0[a,b]$. The term *dense* refers to the fact that any continuous function in the full space $U = \mathrm{C}^0[a,b]$ can be arbitrarily closely approximated in norm by a continuously differentiable function in the subspace $\mathrm{C}^1[a,b]$. Or, to put it another way, given a continuous function $u \in \mathrm{C}^0[a,b]$, there exists a sequence of continuously differentiable functions $u_1, u_2, u_3, \ldots \in \mathrm{C}^1[a,b]$ such that $\| u_k - u \| \to 0$ as $k \to \infty$. A similar density result can be proved for $U = \mathrm{L}^2[a,b]$; see [**37**, **96**, **98**] for details.

Warning: In more advanced treatments, our notion of adjoint is usually called the *formal adjoint*. A true adjoint requires more subtle technical hypotheses on the operator and its domain, cf. [**95**].

Example 9.4. Let us recompute the adjoint of the derivative operator $D: U \to V$, this time with respect to the weighted L^2 inner products

$$\langle\, u\,, \widetilde{u}\,\rangle = \int_a^b u(x)\,\widetilde{u}(x)\,\rho(x)\,dx, \qquad\qquad \langle\!\langle\, v\,, \widetilde{v}\,\rangle\!\rangle = \int_a^b v(x)\,\widetilde{v}(x)\,\kappa(x)\,dx, \qquad (9.16)$$

where $\rho(x) > 0$ and $\kappa(x) > 0$ are strictly positive functions that, physically, might represent the density and stiffness of a nonuniform bar. Now we need to compare

$$\langle\!\langle\, D[u]\,, v\,\rangle\!\rangle = \int_a^b \frac{du}{dx}\, v(x)\,\kappa(x)\,dx, \qquad \text{with} \qquad \langle\, u\,, D^*[v]\,\rangle = \int_a^b u(x)\,D^*[v]\,\rho(x)\,dx.$$

Integrating the first expression by parts, we obtain

$$\begin{aligned}
\int_a^b \frac{du}{dx}\, v\,\kappa\,dx &= \bigl[\, u(b)\,v(b)\,\kappa(b) - u(a)\,v(a)\,\kappa(a)\,\bigr] - \int_a^b u\,\frac{d(\kappa\,v)}{dx}\,dx \\
&= \int_a^b u\left(-\frac{1}{\rho}\,\frac{d(\kappa\,v)}{dx}\right)\rho\,dx,
\end{aligned} \qquad (9.17)$$

provided that we select our boundary conditions so that

$$u(b)\,v(b)\,\kappa(b) - u(a)\,v(a)\,\kappa(a) = 0. \qquad (9.18)$$

As you can check, this follows from any of the listed boundary conditions: Dirichlet, Neumann, or mixed, as well as periodic, provided $\kappa(a) = \kappa(b)$. We conclude that, in such situations, the weighted adjoint of the derivative operator D is the differential operator

$$D^*[v(x)] = -\frac{1}{\rho(x)}\frac{d}{dx}\big[\,\kappa(x)\,v(x)\,\big] = -\frac{\kappa(x)}{\rho(x)}\frac{dv}{dx} - \frac{\kappa'(x)}{\rho(x)}\,v(x). \tag{9.19}$$

As with matrices, the adjoint of a differential operator depends crucially on the specification of inner products.

The following basic results are left as exercises for the reader. The first generalizes the fact that transposing a transposed matrix reverts to the original.

Proposition 9.5. *The adjoint of the adjoint is the original operator:* $L = (L^*)^*$.

The second generalizes the fact that the transpose of the product of two matrices is the product of the transposes, but in the reverse order.

Proposition 9.6. *If* $L\!: U \to V$ *and* $M\!: V \to W$ *are linear operators on inner product spaces, with* $L^*\!: V \to U$ *and* $M^*\!: W \to V$ *their respective adjoints, then the composite linear operator* $M \circ L\!: U \to W$ *has adjoint* $(M \circ L)^* = L^* \circ M^*\!: W \to U$.

Example 9.7. Let us compute the adjoint of the second derivative operator $D^2 = D \circ D$ with respect to the standard L^2 inner products on both the domain and target spaces. According to Proposition 9.6 and equation (9.13), at least on a formal level,

$$(D^2)^* = D^* \circ D^* = (-D) \circ (-D) = D^2, \tag{9.20}$$

and hence D^2 equals its own adjoint. However, the validity of (9.13) required that the functions in the domain and target spaces of both D's satisfy appropriate boundary conditions. For example, the domain of the first $D\!: U \to V$ could be $U = \{\,u(x)\,|\,u(a) = u(b) = 0\,\}$, while its target space V is unconstrained; the second D could then map V to $W = \{\,w(x)\,|\,w(a) = w(b) = 0\,\}$, which will thus also require that $u''(a) = u''(b) = 0$ in order that $D^2 = D \circ D$ map U to W. Another option would be to impose Neumann conditions on the first D, with $U = \{\,u'(a) = u'(b) = 0\,\}$ and thus $V = \{\,v(a) = v(b) = 0\,\}$, while W remains unconstrained. Under either these or other suitably compatible constraints, both adjoint identifications $D^* = -D$ are valid, thus justifying (9.20). Keep in mind that, according to our earlier remark, the differentiation operators are, in fact, defined only on the dense subspaces containing sufficiently smooth functions.

Higher–Dimensional Operators

The most natural multi-dimensional analogue of the derivative is the *gradient* operator, which, on a two-dimensional space, is given by

$$\nabla u = \operatorname{grad} u = \begin{pmatrix} \partial u/\partial x \\ \partial u/\partial y \end{pmatrix}.$$

The gradient ∇ defines a linear operator that takes a scalar-valued function $u(x,y)$ to the vector-valued function consisting of its two first-order partial derivatives. Thus, the domain space U consists of scalar-valued functions $u(x,y)$, or *scalar fields*, defined for $(x,y) \in \Omega$, where the domain $\Omega \subset \mathbb{R}^2$ is assumed to be both bounded and connected,

and with a nice boundary $\partial\Omega$. (Similar considerations apply to three- and even higher-dimensional problems.) The target space V consists of vector-valued functions, or *vector fields*, $\mathbf{v}(x,y) = (\,v_1(x,y), v_2(x,y)\,)^T$ defined on Ω. As in the preceding subsection, the gradient operator $\nabla: U \to V$ is well defined only on the dense subspace $\mathrm{C}^1(\Omega) \subset U$ consisting of continuously differentiable scalar fields.

In accordance with the general Definition 9.1, the adjoint of the gradient must go in the reverse direction,

$$\nabla^*: V \longrightarrow U,$$

mapping a vector field $\mathbf{v}(x,y)$ to a scalar field $w(x,y) = \nabla^*\mathbf{v}$. The defining equation (9.2) for the adjoint, namely

$$\langle\!\langle\, \nabla u\,,\mathbf{v}\,\rangle\!\rangle = \langle\, u\,,\nabla^*\mathbf{v}\,\rangle, \tag{9.21}$$

relies on the choice of inner products on the two vector spaces. Let us start with the L^2 *inner product* between scalar fields:

$$\langle\, u\,,\widetilde{u}\,\rangle = \iint_\Omega u(x,y)\,\widetilde{u}(x,y)\,dx\,dy. \tag{9.22}$$

Similarly, the L^2 inner product between vector fields defined on Ω is obtained by integrating their usual dot product:

$$\langle\!\langle\, \mathbf{v}\,,\widetilde{\mathbf{v}}\,\rangle\!\rangle = \iint_\Omega \mathbf{v}(x,y)\cdot\widetilde{\mathbf{v}}(x,y)\,dx\,dy = \iint_\Omega \left[\, v_1(x,y)\,\widetilde{v}_1(x,y) + v_2(x,y)\,\widetilde{v}_2(x,y)\,\right] dx\,dy. \tag{9.23}$$

The adjoint identity (9.21) is supposed to hold for all appropriate scalar fields u and vector fields $\mathbf{v}$. For the L^2 inner products (9.22, 23), the two sides of the identity read

$$\langle\!\langle\, \nabla u\,,\mathbf{v}\,\rangle\!\rangle = \iint_\Omega \nabla u\cdot\mathbf{v}\,dx\,dy = \iint_\Omega \left(\frac{\partial u}{\partial x}\,v_1 + \frac{\partial u}{\partial y}\,v_2\right) dx\,dy,$$

$$\langle\, u\,,\nabla^*\mathbf{v}\,\rangle = \iint_\Omega u\,\nabla^*\mathbf{v}\,dx\,dy.$$

Thus, to compare these two double integrals, we must somehow remove the derivatives from the scalar field u. As in the one-dimensional computation (9.8), the mechanism is an *integration by parts* formula for double integrals:

$$\iint_\Omega \nabla u\cdot\mathbf{v}\,dx\,dy = \oint_{\partial\Omega} u\,(\mathbf{v}\cdot\mathbf{n})\,ds \;-\; \iint_\Omega u\,(\nabla\cdot\mathbf{v})\,dx\,dy, \tag{9.24}$$

which was already noted in (6.83). The left-hand side is just $\langle\!\langle\,\nabla u\,,\mathbf{v}\,\rangle\!\rangle$. If the boundary line integral vanishes,

$$\oint_{\partial\Omega} u\,(\mathbf{v}\cdot\mathbf{n})\,ds = 0, \tag{9.25}$$

then the right-hand side of formula (9.24) reduces to

$$-\iint_\Omega u\,(\nabla\cdot\mathbf{v})\,dx\,dy = -\,\langle\, u\,,\nabla\cdot\mathbf{v}\,\rangle = \langle\, u\,,-\nabla\cdot\mathbf{v}\,\rangle.$$

Therefore, subject to the boundary constraint (9.25), we deduce the L^2 inner product identity

$$\langle\!\langle\, \nabla u\,,\mathbf{v}\,\rangle\!\rangle = \langle\, u\,,-\nabla\cdot\mathbf{v}\,\rangle, \tag{9.26}$$

which implies that the L^2 adjoint of the gradient operator is minus the *divergence operator*:

$$\nabla^* \mathbf{v} = -\nabla \cdot \mathbf{v}. \tag{9.27}$$

The vanishing of the boundary integral (9.25) will be ensured by the imposition of suitable homogeneous boundary conditions on the scalar field u and/or the vector field $\mathbf{v}$. Clearly the line integral will vanish if either $u = 0$ or $\mathbf{v} \cdot \mathbf{n} = 0$ at each point on the boundary. These possibilities lead immediately to the three principal types of (homogeneous) boundary conditions. The first are the *Dirichlet boundary conditions*, which require

$$u = 0 \qquad \text{on} \qquad \partial\Omega. \tag{9.28}$$

Alternatively, we can set

$$\mathbf{v} \cdot \mathbf{n} = 0 \qquad \text{on} \qquad \partial\Omega, \tag{9.29}$$

which requires that $\mathbf{v}$ be everywhere tangent to the boundary. Since ∇ must map the scalar field $u \in U$ to an admissible vector field $\mathbf{v} = \nabla u \in V$, the boundary condition (9.29) requires that u satisfy the homogeneous *Neumann boundary conditions*

$$\frac{\partial u}{\partial \mathbf{n}} = \nabla u \cdot \mathbf{n} = 0 \qquad \text{on} \qquad \partial\Omega. \tag{9.30}$$

One can evidently also mix the boundary conditions, imposing Dirichlet conditions on part of the boundary and Neumann conditions on the complementary part:

$$u = 0 \quad \text{on} \quad D \subset \partial\Omega, \qquad \mathbf{v} \cdot \mathbf{n} = \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on} \quad N = \partial\Omega \setminus D, \tag{9.31}$$

with neither D nor N empty.

More generally, when modeling deflections of nonuniform membranes, heat flow through heterogeneous media, and similar physical equilibria, we replace the L^2 inner product between scalar and vector fields (9.23) by suitably weighted versions[†]

$$\begin{aligned}
\langle u, \widetilde{u} \rangle &= \iint_\Omega u(x,y)\, \widetilde{u}(x,y)\, \rho(x,y)\, dx\, dy, \\
\langle\!\langle \mathbf{v}, \widetilde{\mathbf{v}} \rangle\!\rangle &= \iint_\Omega \left[v_1(x,y)\, \widetilde{v}_1(x,y)\, \kappa_1(x,y) + v_2(x,y)\, \widetilde{v}_2(x,y)\, \kappa_2(x,y) \right] dx\, dy,
\end{aligned} \tag{9.32}$$

in which $\rho(x,y), \kappa_1(x,y), \kappa_2(x,y) > 0$ are strictly positive functions for $(x,y) \in \Omega$. In applications, ρ represents a density, while κ_1, κ_2 represent stiffnesses or thermal conductivities. To compute the weighted adjoint of the gradient operator, we apply a similar integration by parts argument based on (6.83):

$$\begin{aligned}
\langle\!\langle \nabla u, \mathbf{v} \rangle\!\rangle &= \iint_\Omega \left(\kappa_1 v_1 \frac{\partial u}{\partial x} + \kappa_2 v_2 \frac{\partial u}{\partial y} \right) dx\, dy \tag{9.33} \\
&= \oint_{\partial\Omega} u \left(-\kappa_2 v_2\, dx + \kappa_1 v_1\, dy \right) - \iint_\Omega u \left(\frac{\partial(\kappa_1 v_1)}{\partial x} + \frac{\partial(\kappa_2 v_2)}{\partial y} \right) dx\, dy \\
&= \iint_\Omega u \left[-\frac{1}{\rho} \left(\frac{\partial(\kappa_1 v_1)}{\partial x} + \frac{\partial(\kappa_2 v_2)}{\partial y} \right) \right] \rho\, dx\, dy,
\end{aligned}$$

[†] Exercise 9.2.14 treats an even more general pair of inner products.

provided the boundary integral vanishes. Equating the left-hand side to

$$\langle\, u\,,\nabla^*\mathbf{v}\,\rangle = \iint_\Omega u\,(\nabla^*\mathbf{v})\,\rho\;dx\,dy,$$

we deduce that the adjoint of the gradient operator with respect to the weighted inner products (9.32) is minus the "weighted divergence operator":

$$\nabla^*\mathbf{v} = -\frac{1}{\rho}\left(\frac{\partial(\kappa_1 v_1)}{\partial x} + \frac{\partial(\kappa_2 v_2)}{\partial y}\right) = -\frac{\kappa_1}{\rho}\frac{\partial v_1}{\partial x} - \frac{\kappa_2}{\rho}\frac{\partial v_2}{\partial y} - \frac{1}{\rho}\frac{\partial\kappa_1}{\partial x}\,v_1 - \frac{1}{\rho}\frac{\partial\kappa_2}{\partial y}\,v_2. \quad (9.34)$$

The vanishing of the boundary integral,

$$0 = \oint_{\partial\Omega} u\bigl(-\kappa_2 v_2\,dx + \kappa_1 v_1\,dy\bigr) = \oint_{\partial\Omega} u\,\widetilde{\mathbf{v}}\cdot\mathbf{n}\,ds, \qquad\text{where}\qquad \widetilde{\mathbf{v}} = \begin{pmatrix}\kappa_1 v_1\\ \kappa_2 v_2\end{pmatrix},$$

is ensured if either $u = 0$ or $\widetilde{\mathbf{v}}\cdot\mathbf{n} = 0$ on $\partial\Omega$. The former is the usual homogeneous Dirichlet condition, but the latter is a "weighted" version of the homogeneous Neumann boundary condition, requiring that $\widetilde{\nabla}u \cdot \mathbf{n} = 0$ on the boundary, where $\widetilde{\nabla}u = \bigl(\kappa_1 u_x, \kappa_2 u_y\bigr)^T$ represents a "weighted normal flux vector".

Example 9.8. Let us compute the adjoint of the second-order Laplacian operator $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ with respect to the L^2 inner products on both its domain and target spaces. The computation is a simple consequence of the double integral identity (6.88), which we rewrite as

$$\langle\,\Delta u\,,v\,\rangle = \iint_\Omega v\,\Delta u\,dx\,dy = \oint_{\partial\Omega}\left(u\,\frac{\partial v}{\partial\mathbf{n}} - v\,\frac{\partial u}{\partial\mathbf{n}}\right)ds \;+\; \iint_\Omega u\,\Delta v\,dx\,dy = \langle\,u\,,\Delta v\,\rangle.$$

Thus, provided the boundary integral vanishes, we can conclude that the Laplacian equals its own adjoint: $\Delta^* = \Delta$. This is assured when $u\,\partial v/\partial\mathbf{n} = v\,\partial u/\partial\mathbf{n}$ at each point in $\partial\Omega$. For example, the adjoint computation is valid if either $u = v = 0$ or $\partial u/\partial\mathbf{n} = \partial v/\partial\mathbf{n} = 0$ at every point of the boundary of the domain. Keep in mind that if we require $v = 0$ on some or all of $\partial\Omega$, then this imposes the condition $\Delta u = 0$ there in order that Δ map u to an admissible v; similar considerations apply when $\partial v/\partial\mathbf{n} = 0$.

Exercises

9.1.1. Choose one from the following list of inner products on $\mathbb{R}^2$. Then find the adjoint of $A = \begin{pmatrix} 1 & 2 \\ -1 & 3 \end{pmatrix}$ when your inner product is used on both its domain and target space.

    (a) The Euclidean dot product; (b) the weighted inner product $\langle\,\mathbf{v}\,,\mathbf{w}\,\rangle = 2v_1 w_1 + 3v_2 w_2$;
    (c) the inner product $\langle\,\mathbf{v}\,,\mathbf{w}\,\rangle = \mathbf{v}^T C\,\mathbf{w}$ defined by the symmetric positive definite matrix
        $C = \begin{pmatrix} 2 & -1 \\ -1 & 4 \end{pmatrix}$.

9.1.2. From the list in Exercise 9.1.1, choose a different inner product on the domain and the target space, and then determine the adjoint of the matrix A.

9.1.3. Choose one from the following list of inner products on $\mathbb{R}^3$ for both the domain and target space, and find the adjoint of $A = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 2 \end{pmatrix}$. (a) The Euclidean dot product on $\mathbb{R}^3$; (b) the weighted inner product $\langle\, \mathbf{v}\,, \mathbf{w}\,\rangle = v_1\, w_1 + 2\, v_2\, w_2 + 3\, v_3\, w_3$; (c) the inner product $\langle\, \mathbf{v}\,, \mathbf{w}\,\rangle = \mathbf{v}^T C\, \mathbf{w}$ defined by the symmetric positive definite matrix $C = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}$.

9.1.4. From the list in Exercise 9.1.3, choose different inner products on the domain and target space, and then compute the adjoint of the matrix A.

9.1.5. Choose an inner product on $\mathbb{R}^2$ from the list in Exercise 9.1.1 and an inner product on $\mathbb{R}^3$ from the list in Exercise 9.1.3, and then compute the adjoint of $A = \begin{pmatrix} 1 & 3 \\ 0 & 2 \\ -1 & 1 \end{pmatrix}$.

$\diamondsuit$ 9.1.6. (a) Let C be an $m \times n$ matrix. Suppose $\mathbf{u}^T C\, \mathbf{v} = 0$ for all $\mathbf{u} \in \mathbb{R}^m$ and $\mathbf{v} \in \mathbb{R}^n$. Prove that $C = \mathrm{O}$ must be the zero matrix. (b) Let A, B be $m \times n$ matrices such that $\mathbf{u}^T A \mathbf{v} = \mathbf{u}^T B \mathbf{v}$ for all $\mathbf{u} \in \mathbb{R}^m$ and $\mathbf{v} \in \mathbb{R}^n$. Prove that $A = B$. (c) Find an $n \times n$ matrix $C \neq \mathrm{O}$ such that $\mathbf{u}^T C\, \mathbf{u} = 0$ for all $\mathbf{u} \in \mathbb{R}^n$.

9.1.7. Let $U = \mathrm{C}^0[0, 1]$. Find the adjoint I^* of the identity operator $\mathrm{I} : U \to U$ under the weighted inner products (9.16).

9.1.8. Compute the adjoint of the derivative operator $v = D[u] = u'$ under the weighted inner products $\langle\, u\,, \tilde{u}\,\rangle = \int_0^1 e^x\, u(x)\, \tilde{u}(x)\, dx$, $\langle\!\langle\, v\,, \tilde{v}\,\rangle\!\rangle = \int_0^1 (1 + x)\, v(x)\, \tilde{v}(x)\, dx$. Clearly state any boundary conditions that you are imposing.

9.1.9. Let $L[u] = x\, u'(x) + u(x)$ and $0 < a < x < b$. When subject to homogeneous Dirichlet boundary conditions $u(a) = u(b) = 0$, determine the adjoint $L^*[v]$ with respect to
      (a) the L^2 inner products (9.7); (b) the weighted inner products (9.16).

9.1.10. Consider the linear operator $L[u] = \begin{pmatrix} u' \\ u \end{pmatrix}$ that maps $u(x) \in \mathrm{C}^1$ to the vector-valued function whose components consist of the function and its first derivative. Imposing the boundary conditions $u(0) = u(1)$, compute the adjoint L^* with respect to the L^2 inner products on both the domain and target spaces.

9.1.11. *True or false*: The adjoint of the divergence operator $\nabla \cdot \mathbf{v}$ with respect to the L^2 inner products (9.22, 23) is minus the gradient operator: $(\nabla \cdot)^* u = -\nabla u$. If true, what boundary conditions do you need to assume? If false, what is the adjoint?

9.1.12. Find the adjoint of the two-dimensional curl operator $\nabla \times \mathbf{v}$, as defined in (6.73), with respect to the L^2 inner products (9.22, 23). Carefully state any required boundary conditions.

$\diamondsuit$ 9.1.13. Prove that (a) the adjoint of a linear operator is also a linear operator;
      (b) the adjoint is unique.

$\diamondsuit$ 9.1.14. Let $L, M : U \to V$ be linear operators on the same inner product spaces. Prove that
      (a) $(L + M)^* = L^* + M^*$, (b) $(c\,L)^* = c\,L^*$ for $c \in \mathbb{R}$.

$\diamondsuit$ 9.1.15. Prove Proposition 9.5.

$\diamondsuit$ 9.1.16. Prove Proposition 9.6.

9.1.17. *True or false*: If $L : U \to U$ is invertible, then $(L^{-1})^* = (L^*)^{-1}$.

The Fredholm Alternative

Given a linear operator $L: U \to V$ between inner product spaces U, V, a fundamental problem is to solve the associated inhomogeneous linear system

$$L[u] = f \tag{9.35}$$

for various forcing functions $f \in V$. In finite dimensions, this reduces to a linear algebraic system, $A\mathbf{u} = \mathbf{f}$, defined by a coefficient matrix A. For the linear ordinary and partial differential operators of interest to us, (9.35) represents a linear boundary value problem. In general, an inhomogeneous linear system will not be solvable unless its right-hand side satisfies certain constraints, ensuring that f belongs to the range of L. These conditions can be readily characterized using the adjoint operator via the so-called *Fredholm Alternative*, named after the early-twentieth-century Swedish mathematician Ivar Fredholm. Fredholm's primary interest was in solving linear integral equations, but his solvability criterion was then recognized to be a completely general property of linear systems, including linear algebraic systems, linear differential equations, linear boundary value problems, and so on.

Recall that the *kernel* of a linear operator L is the set of solutions to the homogeneous linear system $L[u] = 0$.

Definition 9.9. The *cokernel* of a linear operator $L: U \to V$ between inner product spaces is defined as the kernel of its adjoint:

$$\operatorname{coker} L = \ker L^* = \left\{ \, v \in V \mid L^*[v] = 0 \, \right\}. \tag{9.36}$$

We can now state and prove the *Fredholm Alternative*.

Theorem 9.10. *If the linear system $L[u] = f$ has a solution, then the right-hand side must be orthogonal to the cokernel of L, i.e.,*

$$\langle\!\langle \, v \, , f \, \rangle\!\rangle = 0 \qquad \text{for all} \qquad v \in \operatorname{coker} L. \tag{9.37}$$

Proof: If $L[u] = f$, then, given $v \in \operatorname{coker} L$, the adjoint equation (9.2) implies

$$\langle\!\langle \, v \, , f \, \rangle\!\rangle = \langle\!\langle \, v \, , L[u] \, \rangle\!\rangle = \langle \, L^*[v] \, , u \, \rangle = 0,$$

since $L^*[v] = 0$ by the definition of the cokernel.   *Q.E.D.*

Remark: In practice, one needs to check the orthogonality constraints (9.37) only when v runs through a basis of the cokernel. In particular, if the only solution to the homogeneous adjoint system $L^*[v] = 0$ is the trivial solution $v = 0$, then there are no constraints, and we expect that the inhomogeneous linear system (9.35) can be solved for any "reasonable" forcing function f. In finite dimensions, this is certainly the case, [**89**]. For boundary value problems defined by linear differential operators, one needs to determine what "reasonable" means, and then prove an appropriate existence theorem. Although valid for all of the boundary value problems presented here, when subject to continuous or even piecewise continuous forcing functions f, rigorous proofs of the existence of solutions for partial differential equations involve the advanced mathematical machinery of functional analysis — see, e.g., [**38, 44, 61, 99**] — and lie beyond the scope of this introductory text.

Example 9.11. Consider the linear algebraic system

$$u_1 - u_3 = f_1, \qquad u_2 - 2\,u_3 = f_2, \qquad u_1 - 2\,u_2 + 3\,u_3 = f_3. \tag{9.38}$$

Using Gaussian Elimination (or by inspection), one easily sees that (9.38) admits a solution if and only if the compatibility condition

$$-f_1 + 2\,f_2 + f_3 = 0 \tag{9.39}$$

holds. Moreover, when this occurs, a solution exists but is not unique. To connect this to the Fredholm Alternative, we write the system in matrix form $L[\mathbf{u}] = \mathbf{f}$, where $L[\mathbf{u}] = A\,\mathbf{u}$ represents multiplication by the coefficient matrix

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

Using the dot product on $\mathbb{R}^3$, the adjoint linear function $L^*[\mathbf{v}] = A^T \mathbf{v}$ is represented by the transposed matrix

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

Therefore, the cokernel is found by solving the homogeneous adjoint linear system $A^T \mathbf{y} = 0$, i.e.,

$$v_1 + v_3 = 0, \qquad v_2 - 2\,v_3 = 0, \qquad -v_1 - 2\,v_2 + 3\,v_3 = 0,$$

whose solutions consist of all scalar multiples of $\mathbf{v} = (-1, 2, 1)^T$. We recognize the compatibility condition (9.39) as requiring that the right-hand side be orthogonal (under the dot product) to the cokernel basis vector,

$$\mathbf{v} \cdot \mathbf{f} = -f_1 + 2\,f_2 + f_3 = 0,$$

in accordance with the Fredholm Alternative constraint (9.37).

Example 9.12. Let us solve the boundary value problem

$$u'' = f(x), \qquad u'(0) = 0, \qquad u'(\ell) = 0, \tag{9.40}$$

modeling the displacement, under an external force, of a uniform elastic bar of length ℓ both of whose ends are free. Solving the differential equation by direct integration, we find that

$$u(x) = a\,x + b + \int_0^x \left(\int_0^y f(z)\,dz \right) dy,$$

where the constants a, b are to be determined by the boundary conditions. Since

$$u'(x) = a + \int_0^x f(z)\,dz,$$

the boundary condition $u'(0) = 0$ implies that $a = 0$. The second boundary condition requires

$$u'(\ell) = \int_0^\ell f(x)\,dx = 0. \tag{9.41}$$

If this fails, then the boundary value problem has no solution. On the other hand, if the forcing function $f(x)$ satisfies the constraint (9.41), then the resulting solution of the boundary value problem has the form

$$u(x) = b + \int_0^x \left(\int_0^y f(z) \, dz \right) dy, \tag{9.42}$$

where the constant b is arbitrary. Thus, when it exists, the solution to the boundary value problem is not unique. The constant b solves the corresponding homogeneous problem, and represents a rigid translation of the entire bar by a distance b.

The solvability constraint (9.41) follows from the Fredholm Alternative. Indeed, according to Example 9.7, under the L^2 inner products and the given boundary conditions, $(D^2)^* = D^2$, and hence the adjoint system is the unforced homogeneous boundary value problem

$$v'' = 0, \qquad v'(0) = 0, \qquad v'(\ell) = 0,$$

with solution $v(x) = c$ for any constant c. Thus, the cokernel consists of all scalar multiples of the constant function $v_\star(x) \equiv 1$. The Fredholm Alternative requires that the forcing function in the original boundary value problem be orthogonal to the cokernel functions, and so

$$\langle 1, f \rangle = \int_0^\ell f(x) \, dx = 0,$$

which is precisely the condition (9.41) required for existence of a (nonunique) equilibrium solution.

Example 9.13. Consider the homogeneous Neumann boundary value problem for the Poisson equation on a bounded domain $\Omega \subset \mathbb{R}^2$, namely,

$$-\Delta u = f \quad \text{in} \quad \Omega, \qquad \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \partial \Omega. \tag{9.43}$$

According to Example 9.8, the Laplacian is self-adjoint under the L^2 inner product and the prescribed boundary conditions: $\Delta^* = \Delta$. Thus, the homogeneous adjoint system is merely

$$-\Delta v = 0 \quad \text{in} \quad \Omega, \qquad \frac{\partial v}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \partial \Omega.$$

Theorem 6.15 tells us that the only solutions to the adjoint problem are the constant functions, $v(x, y) \equiv c$. Thus, a basis for the cokernel consists of the function $v(x, y) \equiv 1$, and so the Fredholm Alternative requires that the forcing function in (9.43) satisfy

$$\langle 1, f \rangle = \iint_\Omega f(x, y) \, dx \, dy = 0, \tag{9.44}$$

reproducing our earlier constraint (6.90) for the homogeneous Neumann case.

Exercises

9.1.18. Use the Fredholm Alternative to determine whether the following linear systems are compatible. When compatible, write down the general solution.

(a) $\begin{array}{l} 2x - 4y = -2, \\ -x + 2y = 3, \end{array}$ (b) $\begin{array}{l} 6x - 3y + 9z = 6, \\ 2x - y + 3z = 2, \end{array}$ (c) $\begin{array}{l} 2x + 3y = -1, \\ 3x + 7y = 1, \\ x + 4y = 2, \\ -x + y = 3, \end{array}$

(d) $\begin{array}{l} 2x_1 - 3x_2 - x_3 = -1, \\ 3x_1 - x_2 = 1, \\ 4x_1 + x_2 + x_3 = 2, \end{array}$ (e) $\begin{array}{l} 2x_1 + 3x_2 - x_4 = -1, \\ 3x_1 + 2x_3 - x_4 = 0, \\ x_1 - x_2 + x_3 = 1. \end{array}$

9.1.19. Use the Fredholm Alternative to find the compatibility conditions for the following systems of linear equations.
(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) $x - 3y + 2z + w = a$, $4x - 2y + 2z + 3w = b$, $5x - 5y + 4z + 4w = c$, $2x + 4y - 2z + w = d$.

9.1.20. Suppose A is a symmetric matrix. Show that the linear system $A\mathbf{x} = \mathbf{b}$ has a solution if and only if $\mathbf{b}$ is orthogonal to $\ker A$.

9.1.21. Use the Fredholm Alternative to determine whether or not there exists a solution to the following boundary value problem: $x u'' + u' = 1 - \frac{2}{3}x$, $u'(1) = u'(2) = 0$. If so, write down all solutions.

9.1.22. Analyze the periodic boundary value problem
$$-u'' = f(x), \qquad u(0) = u(2\pi), \qquad u'(0) = u'(2\pi),$$
along the same lines as in Example 9.12. Characterize the forcing functions for which the problem has a solution. Explain why the constraints, if any, are in accordance with the Fredholm Alternative. Write down a forcing function $f(x)$ that satisfies all your constraints, and then find all corresponding solutions.

9.1.23. Answer Exercise 9.1.22 for the boundary value problems:
(a) $u'''' = f(x)$, $u''(0) = u'''(0) = 0$, $u''(1) = u'''(1) = 0$;
(b) $u'''' = f(x)$, $u''(0) = u'''(0) = 0$, $u(1) = u''(1) = 0$.

♡ 9.1.24. Let λ be a real parameter. (a) For which values of λ does the boundary value problem $u'' + \lambda u = h(x)$, $u(0) = 0$, $u(1) = 0$, have a unique solution? (b) Construct the Green's function for all such λ. (c) In the nonunique cases, use the Fredholm Alternative to find conditions on the forcing function $h(x)$ that are required for the existence of a solution.

9.1.25. Let $\Omega \subset \mathbb{R}^2$ be a bounded, connected domain. Using the L^2 inner products (9.22, 23) on scalar and vector fields, write out the Fredholm Alternative constraints for the solvability of the boundary value problem $\nabla \cdot \mathbf{v} = f$ in Ω, subject to the homogeneous boundary conditions $\mathbf{v} \cdot \mathbf{n} = 0$ on $\partial\Omega$.

9.1.26. Let $\Omega \subset \mathbb{R}^2$ be a bounded simply connected domain. Using the L^2 inner products (9.22, 23) on scalar and vector fields on a domain $\Omega \subset \mathbb{R}^2$, write out the Fredholm Alternative constraints for the solvability of the boundary value problem $\nabla u = \mathbf{f}$ in Ω, subject to the homogeneous boundary conditions $u = 0$ on $\partial\Omega$.

9.2 Self–Adjoint and Positive Definite Linear Functions

In finite-dimensional linear algebra, there are two particularly important classes of matrices: symmetric, equal to their own transpose, and positive definite, as prescribed by Definition B.12. The goal of this section is to adapt both concepts to more general linear operators, paying particular attention to the case of linear differential operators. The resulting classes of self-adjoint and positive (semi-)definite differential operators are ubiquitous in applications of ordinary and partial differential equations.

Self–Adjointness

Throughout this section, U will be a fixed inner product space. We have already seen that the transpose of a matrix is a very special case of the adjoint operation. Thus, the natural analogue of a symmetric matrix is a linear operator that equals its own adjoint.

Definition 9.14. A linear operator $S: U \to U$ is called *self-adjoint* if $S^* = S$.

Thus, according to (9.2), S is self-adjoint if and only if

$$\langle\, S[u]\,,\widetilde{u}\,\rangle = \langle\, u\,,S[\widetilde{u}\,]\,\rangle \qquad \text{for all} \qquad u, \widetilde{u} \in U. \tag{9.45}$$

Example 9.15. In the finite-dimensional case, a linear function $S: \mathbb{R}^n \to \mathbb{R}^n$ is realized by matrix multiplication: $S[\mathbf{u}] = K\,\mathbf{u}$, where K is a square matrix of size $n \times n$. If we use the ordinary dot product on $\mathbb{R}^n$, then, according to Example 9.2, the adjoint function $S^*: \mathbb{R}^n \to \mathbb{R}^n$ is given by multiplication by the transposed matrix: $S^*[\mathbf{u}] = K^T\mathbf{u}$. Thus, a linear function is self-adjoint with respect to the dot product if and only if it is represented by a symmetric matrix: $K^T = K$.

On the other hand, if we adopt the weighted inner product $\langle\, \mathbf{u}\,,\widetilde{\mathbf{u}}\,\rangle = \mathbf{u}^T C\,\widetilde{\mathbf{u}}$ provided by the symmetric positive definite matrix $C > 0$, then, according to (9.6), the adjoint function S^* has matrix representative $C^{-1}K^T C$, and hence S is self-adjoint under the weighted inner product if and only if the matrix K satisfies $K = C^{-1}K^T C$.

Example 9.16. In Example 9.7, we argued that the second-order derivative operator $S = D^2$ is self-adjoint with respect to the L^2 inner product, when subject to suitable homogeneous boundary conditions. A direct verification of this result is instructive. According to the general adjoint equation (9.2), we need to equate

$$\int_a^b S[u]\,\widetilde{u}\,dx = \langle\, S[u]\,,\widetilde{u}\,\rangle = \langle\, u\,,S^*[\widetilde{u}\,]\,\rangle = \int_a^b u\,S^*[\widetilde{u}]\,dx. \tag{9.46}$$

As before, the computation relies on (in this case two) integration by parts:

$$\langle\, S[u]\,,\widetilde{u}\,\rangle = \int_a^b \frac{d^2u}{dx^2}\,\widetilde{u}\,dx = \frac{du}{dx}\,\widetilde{u}\,\bigg|_{x=a}^b - \int_a^b \frac{du}{dx}\,\frac{d\widetilde{u}}{dx}\,dx$$

$$= \left[\frac{du}{dx}\,\widetilde{u} - u\,\frac{d\widetilde{u}}{dx}\right]\bigg|_{x=a}^b + \int_a^b u\,\frac{d^2\widetilde{u}}{dx^2}\,dx.$$

Comparing with (9.46), we conclude that $S^* = D^2 = S$, *provided* the boundary terms vanish:

$$\left[\frac{du}{dx}\,\widetilde{u} - u\,\frac{d\widetilde{u}}{dx}\right]\bigg|_{x=a}^b = \big[\,u'(b)\,\widetilde{u}(b) - u(b)\,\widetilde{u}'(b)\,\big] - \big[\,u'(a)\,\widetilde{u}(a) - u(a)\,\widetilde{u}'(a)\,\big] = 0. \tag{9.47}$$

This requires that we impose suitable boundary conditions at the endpoints, which will serve to characterize the underlying vector space U on which $S = D^2$ acts. One possibility is to set $U = \{\,u(a) = u(b) = 0\,\}$, thereby imposing homogeneous Dirichlet boundary conditions. Since $\widetilde{u} \in U$ also, $\widetilde{u}(a) = \widetilde{u}(b) = 0$, and hence (9.47) holds, proving self-adjointness. Alternatively, one can impose homogeneous Neumann, mixed, or periodic boundary conditions to specify the space U and similarly establish self-adjointness of $S = D^2$.

Positive Definiteness

Let us turn to the characterization of positive definite, and, slightly less stringently, positive semi-definite linear operators. These serve to extend the notions of positive definite and semi-definite matrices to linear differential operators defining boundary value problems.

Definition 9.17. A linear operator $S: U \to U$ on an inner product space is called *positive definite*, written $S > 0$, if

$$\langle\, u\,, S[u]\,\rangle > 0 \qquad \text{for all} \qquad u \neq 0. \tag{9.48}$$

The operator S is *positive semi-definite*, written $S \geq 0$, if

$$\langle\, u\,, S[u]\,\rangle \geq 0 \qquad \text{for all} \qquad u. \tag{9.49}$$

Observe that, on the finite-dimensional space $U = \mathbb{R}^n$ equipped with the dot product, the linear function $S[\mathbf{u}] = K\,\mathbf{u}$ is positive (semi-)definite if and only if K is a positive (semi-)definite matrix, as per Definition B.12. (However, changing the inner product on $\mathbb{R}^n$ will result in an alternative notion of positive definiteness for the matrix K; see Exercise 9.2.5.) In the infinite-dimensional situations involving differential operators, the domain of the operator may be only a dense subspace of the full inner product space U, and one imposes the positivity condition (9.48) or (9.49) only on those functions u lying in the domain of S. Fortunately, this technicality has no serious effect on the subsequent development.

Example 9.18. Consider the operator $S = -\,D^2$ acting on the space U consisting of all C^2 functions defined on a bounded interval $[a, b]$ and subject to homogeneous Dirichlet boundary conditions $u(a) = u(b) = 0$. To establish positive definiteness, we evaluate

$$\langle\, S[u]\,, u\,\rangle = \int_a^b \left(-\,\frac{d^2 u}{dx^2}\, u \right) dx = -\,\frac{du}{dx}\, u \,\bigg|_{x=a}^{b} + \int_a^b \left(\frac{du}{dx} \right)^2 dx = \int_a^b \left(\frac{du}{dx} \right)^2 dx,$$

where we integrated by parts and then used the boundary conditions to eliminate the boundary terms. The final expression is clearly ≥ 0, and hence S is at least positive semi-definite. Moreover, since $u'(x)$ is continuous, the only way the final integral could vanish is if $u'(x) \equiv 0$, which means $u(x) \equiv c$ is constant. However, the only constant function satisfying the homogeneous Dirichlet boundary conditions is $u(x) \equiv 0$. Thus, $\langle\, S[u]\,, u\,\rangle > 0$ for all $0 \neq u \in U$, which implies $S > 0$. A similar argument implies positive definiteness when the functions are subject to the mixed boundary conditions $u(a) = u'(b) = 0$. On the other hand, any constant function satisfies the Neumann boundary conditions $u'(a) = u'(b) = 0$, and hence in this case $S \geq 0$ is only positive semi-definite.

Proposition 9.19. *If $S > 0$, then $\ker S = \{0\}$. As a consequence, a positive definite linear system $S[u] = f$ with f in the range of S, so $f \in \operatorname{rng} S$, must have a unique solution.*

Proof: If $S[u] = 0$, then $\langle\, u\,, S[u]\,\rangle = 0$, which, according to (9.48), is possible only if $u = 0$. The second statement follows directly from Theorem 1.6.   *Q.E.D.*

Thus, in the finite-dimensional case, positive definiteness implies that the coefficient matrix of $S[\mathbf{u}] = K\,\mathbf{u}$ is nonsingular, and hence existence of a solution is automatic. In the infinite-dimensional cases of boundary value problems, existence of solutions usually requires some further analysis, [**63**].

The most common means of producing self-adjoint, positive (semi-)definite linear operators is provided by the following general construction. From here on, in order to distinguish the possibly different norms resulting from the inner products on the domain and target spaces of a linear operator $L : U \to V$, we employ, respectively, the following double and triple bar notation:

$$\| u \| = \langle u, u \rangle, \qquad u \in U, \qquad \| | v | \| = \langle\!\langle v, v \rangle\!\rangle, \qquad v \in V. \qquad (9.50)$$

Theorem 9.20. *Let $L : U \to V$ be a linear map between inner product spaces with adjoint $L^* : V \to U$. Then the composite map*

$$S = L^* \circ L : U \longrightarrow U$$

is always self-adjoint, $S = S^*$, and positive semi-definite, $S \geq 0$, with $\ker S = \ker L$. Moreover, $S > 0$ is positive definite if and only if $\ker L = \{0\}$.

Proof: First, by Propositions 9.5 and 9.6,

$$S^* = (L^* \circ L)^* = L^* \circ (L^*)^* = L^* \circ L = S,$$

proving self-adjointness. Furthermore,

$$\langle u, S[u] \rangle = \langle u, L^*[L[u]] \rangle = \langle\!\langle L[u], L[u] \rangle\!\rangle = \| | L[u] | \|^2 \geq 0 \qquad (9.51)$$

for all u, proving positive semi-definiteness. Moreover, the result is > 0 as long as $L[u] \neq 0$. Thus, if $\ker L = \{ u \mid L[u] = 0 \} = \{0\}$, then $\langle u, S[u] \rangle > 0$ for all $u \neq 0$, and hence S is positive definite. Finally, the same computation proves that $\ker S = \ker L$. Indeed, if $L[u] = 0$, then $S[u] = L^*[L[u]] = L^*[0] = 0$. On the other hand, if $S[u] = 0$, then $0 = \langle u, S[u] \rangle = \| | L[u] | \|^2$, and hence $L[u] = 0$.   *Q.E.D.*

We are particularly interested in linear systems that are based on the construction of Theorem 9.20, namely

$$S[u] = L^*[L[u]] = f. \qquad (9.52)$$

We will refer to the system (9.52) as *positive definite* or *positive semi-definite* according to the status of its defining operator S. Thus, the system is positive definite if and only if $\ker S = \ker L = \{0\}$, i.e., the only solution to the homogeneous system $S[z] = 0$ is the trivial solution $z = 0$. In this case, the solution to (9.52) (provided it exists) is unique. On the other hand, if there are nonzero solutions to $S[z] = 0$, then (9.52) is only positive semi-definite, and does not admit a unique solution. Moreover, unless the Fredholm Alternative constraints (9.37) hold, then there are no solutions. By Theorem 9.20, we can identify

$$\operatorname{coker} S = \ker S^* = \ker S = \ker L, \qquad (9.53)$$

which thus implies the following:

Theorem 9.21. *Let $S = L^* \circ L$. If the linear system $S[u] = f$ has a solution, then $\langle z, f \rangle = 0$ for all $z \in \ker L$. Moreover, if $S[u] = f$ and $S[\widetilde{u}] = f$ are two solutions to the same linear system, then $\widetilde{u} = u + z$, where $z \in \ker L$ is any solution to $L[z] = 0$.*

Example 9.22. In the finite-dimensional case, any linear function $L : \mathbb{R}^n \to \mathbb{R}^m$ is represented by matrix multiplication: $L[\mathbf{u}] = A \mathbf{u}$. For the dot product on both the domain and target spaces, $L^*[\mathbf{v}] = A^T \mathbf{v}$, and so the self-adjoint combination $S = L^* \circ L : \mathbb{R}^n \to \mathbb{R}^n$ is represented by the $n \times n$ symmetric matrix $K = A^T A$. According to Theorem 9.20, the

matrix K is always positive semi-definite, and is positive definite if and only if the only solution to the homogeneous linear system $A\mathbf{z} = \mathbf{0}$ is the trivial solution $\mathbf{z} = \mathbf{0}$. In the positive semi-definite case, the Fredholm Alternative of Theorem 9.21 states that the linear system $K\mathbf{u} = \mathbf{f}$ has a solution if and only if $\mathbf{z} \cdot \mathbf{f} = 0$ for all $\mathbf{z} \in \ker A$. (As noted before, existence of solutions in the finite-dimensional case is not an issue.) Moreover, if $\mathbf{u}$ is any solution, so is $\widetilde{\mathbf{u}} = \mathbf{u} + \mathbf{z}$ for any $\mathbf{z} \in \ker A$.

More generally, if we adopt the weighted inner products (9.4) on the domain and target spaces represented by the respective positive definite matrices $M > 0$ and $C > 0$, then the adjoint map L^* has matrix representative $M^{-1} A^T C$, and hence $S = L^* \circ L$ is given by multiplication by the (not necessarily symmetric) $n \times n$ matrix $K = M^{-1} A^T C A$. Again, $K \geq 0$ in all cases, and $K > 0$ if and only if $\ker A = \{\mathbf{0}\}$. Now, the Fredholm Alternative states that the linear system $K\mathbf{u} = M^{-1} A^T C A\mathbf{u} = \mathbf{f}$ has a solution if and only if $\langle\, \mathbf{z}\,,\mathbf{f}\,\rangle = \mathbf{z}^T M \mathbf{f} = 0$ for all $\mathbf{z} \in \ker A$. See [**89**, **112**] for applications of this construction in mechanics, electrical networks, and the stability of structures.

Example 9.23. Consider next the differentiation operator $D[u] = u'$. According to Example 9.3, if we impose suitable homogeneous boundary conditions on the space of allowable functions — Dirichlet, Neumann, mixed, or periodic — and use the L^2 inner products on both domain and target space, then $D^*[v] = -v'$. Therefore, the self-adjoint operator of Theorem 9.20 is given by $S = D^* \circ D = -D^2$.

According to Theorem 9.20, the resulting boundary value problem

$$S[u] = -u'' = f$$

is always positive semi-definite, and is positive definite if and only if $\ker D = \{0\}$, i.e., the only function that satisfies $D[u] = u' = 0$ along with the boundary conditions is the zero function. Consider first the Dirichlet boundary conditions $u(a) = u(b) = 0$. On a connected interval, $u' = 0$ if and only if $u = c$ is a constant function. However, the boundary conditions require that $c = 0$, and hence only the zero function appears in the kernel. We conclude that the Dirichlet boundary value problem is positive definite, and its solution unique. A similar argument applies to the mixed boundary conditions, e.g., $u(a) = u'(b) = 0$, since the condition at $x = a$ is enough to ensure that the constant function must be zero. On the other hand, *any* constant function satisfies the Neumann boundary conditions $u'(a) = u'(b) = 0$, and hence in this case, $\ker D$ consists of all constant functions. Therefore, the Neumann boundary value problem is only positive semi-definite. And, as we saw, the solution, when it exists, is not unique, since we can add any constant function to a solution and obtain another solution. A similar argument proves that the periodic boundary value problem, with $u(a) = u(b)$, $u'(a) = u'(b)$, is also positive semi-definite, with the same kinds of existence and uniqueness properties.

More generally, if we use weighted inner products (9.16) on the domain and target spaces, then, again subject to suitable boundary conditions, the adjoint is given by (9.19), and so the self-adjoint boundary value problem $S[u] = D^* \circ D[u] = f$ is based on the more general differential equation

$$S[u] = -\frac{1}{\rho(x)} \left(\frac{d}{dx}\, \kappa(x)\, \frac{du}{dx} \right) = f(x). \tag{9.54}$$

Such boundary value problems model the deformations of a nonuniform elastic bar with density $\rho(x)$ and stiffness $\kappa(x)$, when subject to the external forcing function $f(x)$. Again, the positive definiteness of the problem depends on whether $\ker D = \{0\}$, and so the exact

same classification holds as in the unweighted case: the Dirichlet and mixed boundary value problems are positive definite and have a unique solution, whereas the Neumann and periodic boundary value problems are only positive semi-definite, and the existence of a solution requires the Fredholm conditions to be satisfied.

Self-adjointness underlies the symmetry of the associated Green's function. As a function of x, the Green's function $G_\xi(x) = G(x; \xi)$ satisfies the boundary value problem with delta function forcing concentrated at position $x = \xi$:

$$S[G_\xi] = \delta_\xi, \quad \text{or, explicitly,} \quad -\frac{1}{\rho(x)} \frac{\partial}{\partial x} \left(\kappa(x) \frac{\partial G}{\partial x} \right) = \delta(x - \xi), \tag{9.55}$$

along with the required homogeneous boundary conditions. Suppose first that we are using the L^2 inner product on the interval $[a, b]$, so that $\rho(x) \equiv 1$. Using the definition of the delta function $\delta_\xi(x) = \delta(x - \xi)$ and the self-adjointness of S, we have, for any $a < x, \xi < b$,

$$\begin{aligned}
G(x; \xi) = G_\xi(x) &= \int_a^b G_\xi(y)\, \delta_x(y)\, dy = \langle\, G_\xi, \delta_x\,\rangle = \langle\, G_\xi, S[G_x]\,\rangle \\
&= \langle\, S[G_\xi], G_x\,\rangle = \langle\, \delta_\xi, G_x\,\rangle = \int_a^b \delta_\xi(y)\, G_x(y)\, dy = G_x(\xi) = G(\xi; x).
\end{aligned} \tag{9.56}$$

This establishes[†] the symmetry equation

$$G(x; \xi) = G(\xi; x) \tag{9.57}$$

for the Green's function of a self-adjoint boundary value problem under the L^2 inner product. This can be regarded as the differential operator version of the fact that the inverse of a symmetric matrix is also symmetric.

On the other hand, if we adopt a weighted inner product

$$\langle\, u, \widetilde{u}\,\rangle = \int_a^b u(y)\, \widetilde{u}(y)\, \rho(y)\, dy,$$

then the preceding argument must be slightly modified:

$$\begin{aligned}
\rho(x)\, G(x; \xi) = \rho(x)\, G_\xi(x) &= \int_a^b \rho(y)\, G_\xi(y)\, \delta_x(y)\, dy = \langle\, G_\xi, \delta_x\,\rangle = \langle\, G_\xi, S[G_x]\,\rangle \\
&= \langle\, S[G_\xi], G_x\,\rangle = \langle\, \delta_\xi, G_x\,\rangle = \int_a^b \delta_\xi(y)\, G_x(y)\, \rho(y)\, dy = \rho(\xi)\, G_x(\xi) = \rho(\xi)\, G(\xi; x),
\end{aligned}$$

and so the Green's function associated with a weighted self-adjoint boundary value problem satisfies a "weighted symmetry condition"

$$\rho(x)\, G(x; \xi) = \rho(\xi)\, G(\xi; x). \tag{9.58}$$

Remark: Equation (9.58) implies that the *modified Green's function*

$$\widehat{G}(x; \xi) = \frac{G(x; \xi)}{\rho(\xi)} \quad \text{is genuinely symmetric:} \quad \widehat{G}(x; \xi) = \widehat{G}(\xi; x). \tag{9.59}$$

[†] Symmetry at the endpoints is a consequence of continuity.

The modified Green's function also has the advantage of recasting the superposition formula for the solution to the boundary value problem $S[u] = f$ as the appropriate weighted inner product:

$$u(x) = \int_a^b G(x;\xi)\, f(\xi)\, d\xi = \int_a^b \widehat{G}(x;\xi)\, f(\xi)\, \rho(\xi)\, d\xi = \langle\, \widehat{G}_x\,, f\,\rangle, \quad \text{where} \quad \widehat{G}_x(\xi) = \widehat{G}(x;\xi).$$

Two–Dimensional Boundary Value Problems

Let us next apply the self-adjoint formalism to study boundary value problems on a bounded, connected, two-dimensional domain $\Omega \subset \mathbb{R}^2$. We take $L = \nabla$ to be the gradient operator, mapping a scalar field u to a vector field $\mathbf{v} = \nabla u$. We impose a suitable set of homogeneous boundary conditions, i.e., Dirichlet, Neumann, or mixed. According to the calculation in Section 9.1, if we adopt the basic L^2 inner products (9.22, 23) between scalar and vector fields, then the adjoint of the gradient is the negative of the divergence: $\nabla^* \mathbf{v} = -\nabla \cdot \mathbf{v}$. Therefore, the self-adjoint combination of Theorem 9.20 yields

$$\nabla^* \circ \nabla[u] = -\nabla \cdot (\nabla u) = -\Delta u,$$

where Δ is the Laplacian operator. In this manner, we are able to write the two-dimensional Poisson equation in self-adjoint form

$$-\Delta u = -\nabla \cdot (\nabla u) = \nabla^* \circ \nabla u = f, \tag{9.60}$$

as always subject to the selected boundary conditions.

According to Theorem 9.20, $-\Delta = \nabla^* \circ \nabla$ is positive definite if and only if the kernel of the gradient operator — restricted to the appropriate space of scalar fields — is trivial: $\ker \nabla = \{0\}$. Since we are assuming that the domain Ω is connected, Lemma 6.16 tells us that the only functions that could show up in $\ker \nabla$, and thus prevent positive definiteness, are the constants. The boundary conditions will tell us whether this occurs. The only constant function that satisfies either homogeneous Dirichlet or homogeneous mixed boundary conditions is the zero function, and thus, just as in the one-dimensional case, the boundary value problem for the Poisson equation subject to Dirichlet or mixed boundary conditions is positive definite. In particular, this means that its solution is uniquely defined. On the other hand, any constant function satisfies the homogeneous Neumann boundary condition $\partial u / \partial \mathbf{n} = 0$, and hence such boundary value problems are only positive semi-definite. Existence of a solution relies on the Fredholm Alternative, as we discussed in Example 9.13; moreover, when it exists, the solution is no longer unique, because one can add in any constant without affecting either the equation or the boundary conditions.

More generally, if we impose weighted inner products (9.32) on our spaces of scalar and vector fields, then, recalling (9.34), the corresponding self-adjoint boundary value problem takes the more general form

$$\nabla^* \circ \nabla u = -\frac{1}{\rho(x,y)}\frac{\partial}{\partial x}\left(\kappa_1(x,y)\frac{\partial u}{\partial x}\right) - \frac{1}{\rho(x,y)}\frac{\partial}{\partial y}\left(\kappa_2(x,y)\frac{\partial u}{\partial y}\right) = f(x,y), \tag{9.61}$$

along with the chosen boundary conditions on $\partial\Omega$. Again, the Dirichlet and mixed boundary value problems are positive definite, with unique solutions, while the (suitably weighted) Neumann problem is only positive semi-definite.

The partial differential equation (9.61) arises in various physical contexts. For example, consider a steady-state fluid flow moving in a domain $\Omega \subset \mathbb{R}^2$ described by a vector field $\mathbf{v}$. The flow is called *irrotational* if it has zero curl, $\nabla \times \mathbf{v} = \mathbf{0}$, and hence, assuming that Ω is simply connected, is a gradient $\mathbf{v} = \nabla u$, where $u(x, y)$ is known as the fluid *velocity potential*. The constitutive assumptions connect the fluid velocity with its rate of flow $\mathbf{w} = \kappa \mathbf{v}$, where $\kappa(x, y) > 0$ is the scalar density of the fluid. Conservation of mass provides the final equation, namely $\nabla \cdot \mathbf{w} + f = 0$, where $f(x, y)$ represents fluid sources ($f > 0$) or sinks ($f < 0$). Therefore, the basic equilibrium equations take the form

$$-\nabla \cdot (\kappa \nabla u) = f, \qquad \text{or} \qquad -\frac{\partial}{\partial x}\left(\kappa(x, y)\frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(\kappa(x, y)\frac{\partial u}{\partial y}\right) = f(x, y), \quad (9.62)$$

which is (9.61) with $\rho \to 1$ and $\kappa_1, \kappa_2 \to \kappa$. The case of a homogeneous (constant density) fluid thus reduces to the Poisson equation (4.84), with f replaced by f/κ.

Symmetry of the Green's function for the Poisson equation and the more general boundary value problems (9.61, 62) follows by an evident adaptation of the one-dimensional argument presented above. Details are left as Exercise 9.2.17.

Exercises

9.2.1. Which of the following matrices define self-adjoint linear functions $S \colon \mathbb{R}^2 \to \mathbb{R}^2$ relative to the dot product? (a) $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, (b) $\begin{pmatrix} 0 & 3 \\ 2 & 2 \end{pmatrix}$, (c) $\begin{pmatrix} 1 & 0 \\ 2 & -5 \end{pmatrix}$, (d) $\begin{pmatrix} 3 & 2 \\ 2 & 1 \end{pmatrix}$.

9.2.2. Answer Exercise 9.2.1 for the inner products
$$(i)\ \langle \mathbf{u}, \tilde{\mathbf{u}} \rangle = 2u_1\tilde{u}_1 + 3u_2\tilde{u}_2; \quad (ii)\ \langle \mathbf{u}, \tilde{\mathbf{u}} \rangle = \mathbf{u}^T C \tilde{\mathbf{u}}, \text{ where } C = \begin{pmatrix} 2 & -1 \\ -1 & 3 \end{pmatrix}.$$

9.2.3. *True or false*: Given an inner product $\langle \mathbf{u}, \mathbf{v} \rangle$ on $\mathbb{R}^n$:
   (a) The inverse of a nonsingular self-adjoint $n \times n$ matrix is self-adjoint.
   (b) The inverse of a nonsingular positive definite $n \times n$ matrix is positive definite.

9.2.4. Prove that $K > 0$ is a positive definite $n \times n$ matrix if and only if $J = K^T + K$ is a symmetric positive definite matrix.

$\diamond$ 9.2.5. (a) Prove that the $n \times n$ matrix K defines a self-adjoint linear function on $\mathbb{R}^n$ with respect to the inner product $\langle \mathbf{u}, \tilde{\mathbf{u}} \rangle = \mathbf{u}^T C \tilde{\mathbf{u}}$ for C a symmetric positive definite matrix if and only if the matrix $J = CK$ is symmetric, and hence defines a self-adjoint linear function with respect to the dot product. (b) Prove that $K > 0$ under the given inner product if and only if $J > 0$ under the dot product.

9.2.6. Let $D[u] = u'$ be the derivative operator acting on the vector space of C^2 scalar functions $u(x)$ defined for $0 \le x \le 1$ and satisfying the boundary conditions $u(0) = 0$, $u(1) = 0$.
   (a) Given the weighted inner product $\langle u, \tilde{u} \rangle = \int_0^1 u(x)\tilde{u}(x)e^x\,dx$ on both its domain and target spaces, determine the corresponding adjoint operator D^*.
   (b) Let $S = D^* \circ D$. Write down and solve the boundary value problem $S[u] = 2e^x$.

9.2.7. Let $c(x) \in \mathrm{C}^0[a, b]$ be a continuous function. Prove that the linear multiplication operator $S[u] = c(x)u(x)$ is self-adjoint with respect to the L^2 inner product. What sort of boundary conditions need to be imposed?

9.2.8. *True or false*: The Neumann boundary value problem $-u'' + u = x$, $u'(0) = u'(\pi) = 0$, admits a unique solution.

9.2.9. Prove that the complex differential operator $L[u] = \mathrm{i}\,\dfrac{du}{dx}$ is self-adjoint with respect to the L^2 Hermitian inner product $\langle\, u\,,v\,\rangle \;=\; \displaystyle\int_{-\pi}^{\pi} u(x)\,\overline{v(x)}\,dx$ on the space of continuously differentiable complex-valued 2π–periodic functions: $u(x + 2\pi) = u(x)$.

9.2.10. Let $L \;=\; D^2$. Using the L^2 inner products on both the domain and target spaces, write down a set of homogeneous boundary conditions that makes $L^* \;=\; D^2$. Then set $S = L^* \circ L = D^4$. Do your boundary conditions lead to a boundary value problem $S[u] = f$ that is (i) positive definite; (ii) positive semi-definite; or (iii) neither?

9.2.11. Let β be a real constant. *True or false*: The second derivative operator $S[u] = u''$ is self-adjoint with respect to the L^2 inner product on the space of functions
$$U = \big\{\, u(x) \in \mathrm{C}^2[0,1] \;\big|\; u(0) = 0,\ u'(1) + \beta\,u(1) = 0 \,\big\}$$
subject to Dirichlet boundary conditions at the left-hand endpoint and Robin boundary conditions at the right-hand endpoint.

♡ 9.2.12. Let β be a real constant. Consider the differential operator $S[u] = -\,u''$ acting on the space of functions
$$U = \big\{\, u(x) \in \mathrm{C}^2[0,1] \;\big|\; u(0) = 0,\ u'(1) + \beta\,u(1) = 0 \,\big\}$$
subject to Dirichlet boundary conditions at the left-hand endpoint and Robin boundary conditions at the right-hand endpoint. Prove that $S > 0$ is positive definite with respect to the L^2 inner product if and only if $\beta > -1$. *Hint*: Use the analysis following (4.48).

♡ 9.2.13. The equilibrium equations for a toroidal membrane (an inner tube) lead to the Poisson equation $-\,u_{xx} - u_{yy} = f(x,y)$ on a rectangle $0 < x < a$, $0 < y < b$, subject to periodic boundary conditions
$$u(x,0) = u(x,b), \qquad u_y(x,0) = u_y(x,b), \qquad u(0,y) = u(a,y), \qquad u_x(0,y) = u_x(a,y).$$
(a) Prove that the toroidal boundary value problem is self-adjoint. (b) Is it positive definite, positive semi-definite, or neither? (c) Are there any conditions that must be imposed on the forcing function $f(x,y)$ in order that a solution exist?

◇ 9.2.14. Find the adjoint of the gradient operator ∇ with respect to the L^2 inner product (9.22) between scalar fields, and the following weighted inner product between (column) vector fields $\mathbf{v} = (\,v_1(x,y), v_2(x,y)\,)^T$, $\tilde{\mathbf{v}} = (\,\tilde{v}_1(x,y), \tilde{v}_2(x,y)\,)^T$:
$$\langle\!\langle\, \mathbf{v}\,,\tilde{\mathbf{v}}\,\rangle\!\rangle = \iint_\Omega \mathbf{v}(x,y)^T C(x,y)\,\tilde{\mathbf{v}}(x,y)\,dx\,dy,$$
where the 2×2 matrix $C(x,y) = \begin{pmatrix} \alpha(x,y) & \beta(x,y) \\ \beta(x,y) & \gamma(x,y) \end{pmatrix} > 0$ is symmetric, positive definite at all points $(x,y) \in \Omega$. What sort of boundary conditions do you need to impose? Write out the corresponding boundary value problem for the equilibrium equation $\nabla^* \circ \nabla u = f$.

9.2.15. Let $\Omega \subset \mathbb{R}^2$ be a bounded domain. Construct a set of homogeneous boundary conditions on $\partial\Omega$ that make the *biharmonic equation* $\Delta^2 u = f$: (a) self-adjoint, (b) positive definite, (c) positive semi-definite, but not positive definite.

9.2.16. Write down the boundary value problem $\widehat{S}_\xi[\widehat{G}_\xi] = \delta_\xi$ satisfied by the modified Green's function $\widehat{G}_\xi(x) = \widehat{G}(x;\xi)$ given in (9.59). Is the underlying linear operator $\widehat{S}_\xi$, which may depend on ξ, self-adjoint with respect to a suitable inner product?

◇ 9.2.17. Prove symmetry of the Green's function, $G(\boldsymbol{\xi};\mathbf{x}) = G(\mathbf{x};\boldsymbol{\xi})$, for the Poisson equation on a bounded domain $\Omega \subset \mathbb{R}^2$ subject to homogeneous Dirichlet boundary conditions. *Hint*: Look at how we established (9.56).

9.2.18. Generalize Exercise 9.2.17 to the partial differential equation (9.61).

9.3 Minimization Principles

One of the most important features of positive definite linear problems is that their solution can be characterized by a quadratic minimization priniciple. In many physical contexts, equilibrium configuration(s) serve to minimize the potential energy of the system. Think of a small ball rolling around in a bowl. After frictional effects have stopped its motion, the ball will be left sitting in equilibrium at the bottom of the bowl — the position that minimizes the gravitational potential energy. Minimization principles are employed in functional analytic proofs of existence of solutions, as well as providing a foundation for the powerful finite element numerical method to be studied in Chapter 10.

The basic theorem on quadratic minimization principles is as follows.

Theorem 9.24. *Let* $S: U \to U$ *be a self-adjoint and positive definite linear operator on an inner product space* U. *Suppose that the linear system*

$$S[u] = f \tag{9.63}$$

admits a (necessarily unique) solution $u_\star$. *Then* $u_\star$ *minimizes the value of the associated quadratic function(al)*

$$Q[u] = \tfrac{1}{2} \langle u, S[u] \rangle - \langle f, u \rangle, \tag{9.64}$$

meaning that $Q[u_\star] < Q[u]$ *for all admissible* $u \neq u_\star$ *in* U.

Proof: We are given that $S[u_\star] = f$, and so, for any $u \in U$,

$$Q[u] = \tfrac{1}{2} \langle u, S[u] \rangle - \langle u, S[u_\star] \rangle = \tfrac{1}{2} \langle u - u_\star, S[u - u_\star] \rangle - \tfrac{1}{2} \langle u_\star, S[u_\star] \rangle, \tag{9.65}$$

where we used linearity, along with our assumption that S is self-adjoint, to identify the terms $\langle u, S[u_\star] \rangle = \langle u_\star, S[u] \rangle$. Since $S > 0$, the first term on the right-hand side of (9.65) is always ≥ 0; moreover it equals 0 if and only if $u = u_\star$. On the other hand, the second term does not depend on u at all. Thus, to minimize $Q[u]$, we must make the first term as small as possible, which is accomplished by setting $u = u_\star$.   *Q.E.D.*

Example 9.25. Consider the the problem of minimizing a *quadratic function*

$$Q(u_1, \ldots, u_n) = \frac{1}{2} \sum_{i,j=1}^{n} k_{ij} u_i u_j - \sum_{i=1}^{n} f_i u_i + c, \tag{9.66}$$

depending on n variables $\mathbf{u} = (u_1, u_2, \ldots, u_n)^T \in \mathbb{R}^n$, with fixed real coefficients k_{ij}, f_i, and c. Since $u_i u_j = u_j u_i$, we can assume, without loss of generality, that the coefficients of the quadratic terms are symmetric: $k_{ij} = k_{ji}$. We rewrite (9.66) in matrix notation as

$$Q(\mathbf{u}) = \tfrac{1}{2} \mathbf{u} \cdot K \mathbf{u} - \mathbf{f} \cdot \mathbf{u} + c, \tag{9.67}$$

which, apart from the inessential constant term, agrees with (9.64) once we set $S[\mathbf{u}] = K \mathbf{u}$ and use the dot product $\langle \mathbf{u}, \tilde{\mathbf{u}} \rangle = \mathbf{u} \cdot \tilde{\mathbf{u}}$ as the inner product on $\mathbb{R}^n$. Thus, according to Theorem 9.24, if K is a symmetric positive definite matrix, then the quadratic function (9.67) has a unique minimizer $\mathbf{u}^\star = (u_1^\star, \ldots, u_n^\star)^T$, which is the solution to the linear system $K \mathbf{u}^\star = \mathbf{f}$.

If the positive definite linear operator in Theorem 9.24 comes from the self-adjoint construction of Theorem 9.20, so $S = L^* \circ L$, then, by (9.51), the quadratic term can be re-expressed as $\langle u, S[u] \rangle = \|\!| L[u] |\!\|^2$, using our notational convention (9.50) for the norm on the target space V of L. We can thus rephrase the minimization principle as follows.

Theorem 9.26. *Suppose* $L: U \to V$ *is a linear operator between inner product spaces with adjoint* $L^*: V \to U$. *Assume that* $\ker L = \{\mathbf{0}\}$, *and let* $S = L^* \circ L: U \to U$ *be the associated positive definite linear operator. If* $f \in \operatorname{rng} S$, *then the quadratic function*

$$Q[u] = \tfrac{1}{2} \, \| \, \| \, L[u] \, \| \, \|^2 - \langle \, f \,, u \, \rangle \tag{9.68}$$

has a unique minimizer $u_\star$, *which is the solution to the linear system* $S[u] = f$.

Warning: In (9.68), the first term $\| \, \| \, L[u] \, \| \, \|^2$ is computed using the norm based on the inner product on V, while the second term $\langle \, f \,, u \, \rangle$ employs the inner product on U.

One of the most important applications of minimization is the method of least squares, which is extensively applied in data analysis and approximation theory. We refer the interested reader to [**89**] for developments in this direction. Here we will concentrate on applications to differential equations.

Example 9.27. Consider the boundary value problem

$$-u'' = f(x), \qquad u(a) = 0, \qquad u(b) = 0. \tag{9.69}$$

The underlying differential operator $S = D^* \circ D = -D^2$, when acting on the space of functions satisfying the homogeneous Dirichlet boundary conditions, is self-adjoint and, in fact, positive definite, since $\ker D = \{0\}$. Explicitly, positive definiteness requires

$$\langle \, S[u] \,, u \, \rangle = \int_a^b \left[-u''(x) \, u(x) \right] dx = \int_a^b u'(x)^2 \, dx > 0 \tag{9.70}$$

for all nonzero $u(x) \not\equiv 0$ with $u(a) = u(b) = 0$. Notice how we used an integration by parts, invoking the boundary conditions to eliminate the boundary contributions, to expose the positivity of the integral. The associated quadratic functional is, using (9.68),

$$Q[u] = \tfrac{1}{2} \| \, \| \, u' \, \| \, \|^2 - \langle \, f \,, u \, \rangle = \int_a^b \left[\tfrac{1}{2} u'(x)^2 - f(x) \, u(x) \right] dx.$$

Its minimum value, taken over all C^2 functions that satisfy the homogeneous Dirichlet boundary conditions, occurs precisely when $u = u_\star$ is the solution to the boundary value problem.

Sturm–Liouville Boundary Value Problems

The most important class of boundary value problems governed by second-order ordinary differential equations was first systematically investigated by the nineteenth-century French mathematicians Jacques Sturm and Joseph Liouville. A *Sturm–Liouville boundary value problem* is based on a second-order ordinary differential equation of the form

$$S[u] = -\frac{d}{dx} \left(p(x) \, \frac{du}{dx} \right) + q(x) \, u = -p(x) \, \frac{d^2 u}{dx^2} - p'(x) \, \frac{du}{dx} + q(x) \, u = f(x), \tag{9.71}$$

on a bounded interval $a \le x \le b$, supplemented by Dirichlet, Neumann, mixed, or periodic boundary conditions. To avoid singular points of the differential equation (although we will later discover that most cases of interest have one or more singular points), we assume here that $p(x) > 0$ and, to ensure positive definiteness, $q(x) > 0$ for all $a \le x \le b$.

Sturm–Liouville equations and boundary value problems appear in a remarkably broad range of applications, and particularly in the analysis of partial differential equations by the method of separation of variables. Moreover, most of the important special functions, including Airy functions, Bessel functions, Legendre functions, hypergeometric functions, and so on, naturally appear as solutions to particular Sturm–Liouville equations, [**85**, **86**]. In the final two chapters, the analysis of basic linear partial differential equations in curvilinear coordinates, in both two and three dimensions, will require us to solve several particular examples, including the Bessel, Legendre, and Laguerre equations. For now, though, we concentrate on understanding how Sturm–Liouville boundary value problems fit into our self-adjoint and positive definite framework.

Our starting point is the linear operator

$$L[u] = \begin{pmatrix} u' \\ u \end{pmatrix} \tag{9.72}$$

that maps a scalar function $u(x) \in U$ to a vector-valued function $\mathbf{v}(x) = (v_1(x), v_2(x))^T \in V$, whose components are $v_1 = u'$, $v_2 = u$. To compute the adjoint of $L: U \to V$, we use the standard L^2 inner product (9.7) on U, but adopt the following weighted inner product on V:

$$\langle\!\langle \mathbf{v}, \widetilde{\mathbf{v}} \rangle\!\rangle = \int_a^b \left[p(x)\, v_1(x)\, \widetilde{v}_1(x) + q(x)\, v_2(x)\, \widetilde{v}_2(x) \right] dx, \quad \mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad \widetilde{\mathbf{v}} = \begin{pmatrix} \widetilde{v}_1 \\ \widetilde{v}_2 \end{pmatrix}. \tag{9.73}$$

The positivity assumptions on the weight functions p, q ensure that the latter is a bona fide inner product. As usual, the adjoint computation relies on integration by parts. Here, we only need to manipulate the first summand:

$$\langle\!\langle L[u], \mathbf{v} \rangle\!\rangle = \int_a^b (p\, u'\, v_1 + q\, u\, v_2)\, dx$$

$$= p(b)\, u(b)\, v_1(b) - p(a)\, u(a)\, v_1(a) + \int_a^b u \left[-(p v_1)' + q v_2 \right] dx.$$

The boundary terms will disappear, provided that, at each endpoint, either u or v_1 vanishes. Since for the linear operator $\mathbf{v} = L[u]$ given by (9.72), we can identify $v_1 = u'$, we conclude that any of our usual boundary conditions — Dirichlet, mixed, or Neumann — remain valid here. Under any of these conditions,

$$\langle\!\langle L[u], \mathbf{v} \rangle\!\rangle = \int_a^b u \left[-(p v_1)' + q v_2 \right] dx = \langle u, L^*[\mathbf{v}] \rangle,$$

and so the adjoint operator is given by

$$L^*[\mathbf{v}] = -\frac{d(p v_1)}{dx} + q v_2 = -p v_1' - p' v_1 + q v_2.$$

The canonical self-adjoint combination

$$S[u] = L^* \circ L[u] = L^* \begin{pmatrix} u' \\ u \end{pmatrix} = -\frac{d}{dx}\left(p\, \frac{du}{dx} \right) + q u \tag{9.74}$$

then reproduces the Sturm–Liouville differential operator (9.71). Moreover, since $\ker L = \{0\}$ is trivial (why?), the boundary value problem is positive definite for *all boundary conditions*, not only Dirichlet and mixed, but also Neumann!

A proof of the following general existence theorem can be found in [**63**].

Theorem 9.28. *Let $p(x) > 0$ and $q(x) > 0$ for $a \leq x \leq b$. Then, for any choice of boundary conditions (including Neumann), the Sturm–Liouville boundary value problem (9.71) admits a unique solution.*

Theorem 9.26 tells us that the solution to the Sturm–Liouville boundary value problem (9.71) can be characterized as the unique minimizer of the quadratic functional

$$Q[u] = \tfrac{1}{2} ||| L[u] |||^2 - \langle f, u \rangle = \int_a^b \left[\tfrac{1}{2} p(x) u'(x)^2 + \tfrac{1}{2} q(x) u(x)^2 - f(x) u(x) \right] dx \quad (9.75)$$

among all C^2 functions satisfying the prescribed homogeneous boundary conditions.

Example 9.29. Let $\omega > 0$. Consider the constant-coefficient Sturm–Liouville problem

$$-u'' + \omega^2 u = f(x), \qquad u(0) = u(1) = 0,$$

which we studied earlier in Example 6.10. Theorem 9.28 guarantees the existence of a unique solution. The solution achieves the minimum possible value for the quadratic functional

$$Q[u] = \int_0^1 \left[\tfrac{1}{2} u'^2 + \tfrac{1}{2} \omega^2 u^2 - f u \right] dx$$

among all C^2 functions satisfying the given boundary conditions.

More generally, suppose we adopt a weighted inner product

$$\langle u, \widetilde{u} \rangle = \int_a^b u(x)\, \widetilde{u}(x)\, \rho(x)\, dx \tag{9.76}$$

on the domain space U, where $\rho(x) > 0$ on $[a, b]$. The same integration by parts computation proves that, when subject to the homogeneous boundary conditions,

$$L^*[\mathbf{v}] = \frac{1}{\rho} \left(-\frac{d(p v_1)}{dx} + q v_2 \right) = -\frac{p}{\rho} v_1' - \frac{p'}{\rho} v_1 + \frac{q}{\rho} v_2,$$

and so the weighted Sturm–Liouville differential operator is

$$S[u] = L^* \circ L[u] = \frac{1}{\rho} \left[-\frac{d}{dx} \left(p\, \frac{du}{dx} \right) + q u \right]. \tag{9.77}$$

The corresponding weighted Sturm–Liouville equation $S[u] = f$ has the form

$$S[u] = \frac{1}{\rho(x)} \left[-\frac{d}{dx} \left(p(x)\, \frac{du}{dx} \right) + q(x)\, u \right] = -\frac{p(x)}{\rho(x)} \frac{d^2 u}{dx^2} - \frac{p'(x)}{\rho(x)} \frac{du}{dx} + \frac{q(x)}{\rho(x)}\, u = f(x), \tag{9.78}$$

which is, in fact, identical to the ordinary Sturm–Liouville equation (9.71) after we replace f by ρf. Be that as it may, the weighted generalization will become important when we study the associated eigenvalue problems.

Example 9.30. Let $m > 0$ be a fixed positive number. Consider the differential equation

$$B[u] = -u'' - \frac{1}{x} u' + \frac{m^2}{x^2} u = f(x), \tag{9.79}$$

where B is known as the *Bessel differential operator* of *order m*. To place it in weighted Sturm–Liouville form (9.78), we must find $p(x), q(x)$, and $\rho(x)$ that satisfy

$$\frac{p(x)}{\rho(x)} = 1, \qquad \frac{p'(x)}{\rho(x)} = \frac{1}{x}, \qquad \frac{q(x)}{\rho(x)} = \frac{m^2}{x^2}.$$

Dividing the second equation by the first, we see that $p'(x)/p(x) = 1/x$, and hence we can set

$$p(x) = x, \qquad q(x) = \frac{m^2}{x}, \qquad \rho(x) = x.$$

Thus, when subject to homogeneous Dirichlet, mixed, or even Neumann boundary conditions on an interval $0 < a \le x \le b$, the Bessel operator B is positive definite and self-adjoint with respect to the weighted inner product

$$\langle u, \widetilde{u} \rangle = \int_a^b u(x)\,\widetilde{u}(x)\, x\, dx. \tag{9.80}$$

Exercises

9.3.1. Consider the boundary value problem $-u'' = x$, $u(0) = u(1) = 0$. (i) Find the solution. (ii) Write down a minimization principle that characterizes the solution. (iii) What is the value of the minimized quadratic functional on the solution? (iv) Write down at least two other functions that satisfy the boundary conditions and check that they produce larger values for the energy.

9.3.2. Answer Exercise 9.3.1 for the boundary value problems
(a) $\dfrac{d}{dx}\left(\dfrac{1}{1+x^2}\dfrac{du}{dx}\right) = x^2$, $u(-1) = u(1) = 0$; (b) $-(e^x u')' = e^{-x}$, $u(0) = u'(1) = 0$;
(c) $x^2 u'' + 2x u' = 3x^2$, $u'(1) = u(2) = 0$; (d) $x u'' + 3 u' = 1$, $u(-2) = u(-1) = 0$.

9.3.3. Let $Q[u] = \displaystyle\int_0^1 \left[\tfrac{1}{2}(u')^2 - 5u\right] dx$. (a) Find the function $u_\star(x)$ that minimizes $Q[u]$ among all C^2 functions that satisfy $u(0) = u(1) = 0$.
(b) Test your answer by computing $Q[u_\star]$ and then comparing with the value of $Q[u]$ when $u(x) = $ (i) $x - x^2$, (ii) $\tfrac{3}{2}x - \tfrac{3}{2}x^3$, ($iii$) $\tfrac{2}{3}\sin \pi x$, (iv) $x^2 - x^4$.

9.3.4. For each of the following functionals and associated boundary conditions: (i) write down a boundary value problem satisfied by the minimizing function, and (ii) find the minimizing function $u_\star(x)$:
(a) $\displaystyle\int_0^1 \left[\tfrac{1}{2}(u')^2 - 3u\right] dx$, $u(0) = u(1) = 0$,

(b) $\displaystyle\int_0^1 \left[\tfrac{1}{2}(x+1)(u')^2 - 5u\right] dx$, $u(0) = u(1) = 0$,

(c) $\displaystyle\int_1^3 \left[x(u')^2 + 2u\right] dx$, $u(1) = u(3) = 0$,

(d) $\displaystyle\int_0^1 \left[\tfrac{1}{2}e^x (u')^2 - (1+e^x)u\right] dx$, $u(0) = u(1) = 0$,

(e) $\displaystyle\int_{-1}^1 \frac{(x^2+1)(u')^2 + x u}{(x^2+1)^2}\, dx$, $u(-1) = u(1) = 0$.

9.3.5. Which of the following quadratic functionals possess a unique minimizer among all C^2 functions satisfying the indicated boundary conditions? Find the minimizer if it exists.

(a) $\int_1^2 \left[\frac{1}{2} x\,(u')^2 + 2\,(x-1)\,u \right] dx$, $u(1) = u(2) = 0$;

(b) $\int_{-\pi}^{\pi} \left[\frac{1}{2} x\,(u')^2 - u\cos x \right] dx$, $u(-\pi) = u(\pi) = 0$;

(c) $\int_{-1}^1 \left[(u')^2 \cos x - u\sin x \right] dx$, $u(-1) = u'(1) = 0$;

(d) $\int_{-2}^2 \left[(1 - x^2)\,(u')^2 - u \right] dx$, $u(-2) = u(2) = 0$;

(e) $\int_0^1 \left[(x+1)\,(u')^2 - u \right] dx$, $u'(0) = u'(1) = 0$.

9.3.6. Let $D[u] = u'$ be the derivative operator acting on the vector space of C^2 scalar functions $u(x)$ defined for $0 \le x \le 1$ and satisfying the boundary conditions $u(0) = 0$, $u'(1) = 0$.

(a) Given the weighted inner product $\langle u, \tilde{u} \rangle = \int_0^1 u(x)\,\tilde{u}(x)\,e^x\,dx$ on both its domain and target spaces, determine the corresponding adjoint operator D^*.

(b) Let $S = D^* \circ D$. Write down and solve the boundary value problem $S[u] = 3e^x$.

(c) Write down a minimization principle that characterizes the solution you found in part (b), or explain why none exists.

9.3.7. Solve the Sturm–Liouville boundary value problem $-4u'' + 9u = 1$, $u(0) = 0$, $u(2) = 0$. Is your solution unique?

9.3.8. Answer Exercise 9.3.7 for the Neumann boundary conditions $u'(0) = 0$, $u'(2) = 0$.

9.3.9. (i) Write the following differential equations in Sturm–Liouville form. (ii) If possible, write down a minimization principle that characterizes the solutions to the Dirichlet boundary value problem on the interval $[1, 2]$. (a) $-e^x u'' - e^x u' = e^{2x}$, (b) $-x u'' - u' + 2u = 1$, (c) $-u'' - 2u' + u = e^x$, (d) $-x^2 u'' + 2xu' + 3u = 1$, (e) $xu'' + (1 - x)u' + u = 0$.

9.3.10. *True or false*: The Sturm–Liouville operator (9.71) is self-adjoint and positive definite when subject to periodic boundary conditions $u(a) = u(b)$, $u'(a) = u'(b)$.

9.3.11. Does the quadratic functional $Q[u] = \int_0^1 \left[\frac{1}{2}(u')^2 - \left(x - \frac{1}{2}\right)u \right] dx$ have a minimum value when $u(x)$ is subject to the homogeneous Neumann boundary value conditions $u'(0) = u'(1) = 0$? If so, determine the minimum value and find all minimizing functions.

♡ 9.3.12. (a) Determine the adjoint of the differential operator $L[u] = u' + 2xu$ with respect to the L^2 inner products on $[0,1]$ when subject to the fixed boundary conditions $u(0) = u(1) = 0$. (b) Is the self-adjoint operator $S = L^* \circ L$ positive definite? Explain your answer. (c) Write out the boundary value problem represented by $S[u] = f$. (d) Find the solution to the boundary value problem when $f(x) = e^{x^2}$. *Hint*: To integrate the differential equation, work with the factored form of the differential operator. (e) Discuss what happens if you instead impose the Neumann boundary conditions $u'(0) = u'(1) = 0$.

9.3.13. Discuss the self-adjointness and positive definiteness of boundary value problems associated with the Bessel operator (9.79) of order $m = 0$.

9.3.14. Let $u_\star(x)$ be the solution to the self-adjoint positive definite boundary value problem $S[u_\star] = f$. Prove that if $f(x) \not\equiv 0$, then the minimum of the associated quadratic functional is strictly negative: $Q[u_\star] < 0$.

9.3.15. Find a function $u(x)$ such that $\int_0^1 u''(x)\,u(x)\,dx > 0$. How do you reconcile this with the claimed positivity in (9.70)?

9.3.16. Does the inequality (9.70) hold when $u(x) \not\equiv 0$ is subject to the Neumann boundary conditions $u'(a) = u'(b) = 0$?

9.3.17. *True or false*: When subject to homogeneous Dirichlet boundary conditions on an interval $[a, b]$, every nonsingular second-order linear ordinary differential equation $a(x)\,u'' + b(x)\,u' + c(x)\,u = f(x)$ is (a) self-adjoint, (b) positive definite, (c) positive semi-definite, with respect to some weighted inner product (9.76).

The Dirichlet Principle

Let us now apply these ideas to boundary value problems governed by the Poisson equation

$$-\Delta u = \nabla^* \circ \nabla u = f. \tag{9.81}$$

In the positive definite cases in which the partial differential equation is supplemented by either homogeneous Dirichlet or homogeneous mixed boundary conditions, our general Minimization Theorem 9.24 implies that the solution can be characterized by the justly famous *Dirichlet Principle*.

Theorem 9.31. *The function $u(x, y)$ that minimizes the* Dirichlet integral

$$Q[u] = \tfrac{1}{2} \,\|\!| \nabla u \|\!|^2 - \langle\, f\,, u\,\rangle = \iint_\Omega \left(\, \tfrac{1}{2}\, u_x^2 + \tfrac{1}{2}\, u_y^2 - f\, u\,\right) dx\, dy \tag{9.82}$$

among all C^2 functions that satisfy the prescribed homogeneous Dirichlet or mixed boundary conditions is the solution to the corresponding boundary value problem for the Poisson equation $-\Delta u = f$.

The fact that a minimizer to the Dirichlet integral (9.82) satisfies the Poisson equation is an immediate consequence of our general Minimization Theorem 9.26. On the other hand, proving the *existence* of a C^2 minimizing function is a nontrivial issue. Indeed, the need for a rigorous existence proof was not immediately recognized: arguing from the finite-dimensional situation, Dirichlet deemed existence to be self-evident, but it was not until 50 years later that Hilbert supplied the first rigorous proof — which was one of his primary motivations for introducing the mathematical machinery of Hilbert space.

The Dirichlet principle (9.82) was derived under the assumption that the boundary conditions are homogeneous — either pure Dirichlet or mixed. As it turns out, the minimization principle, as stated, also applies to the inhomogeneous Dirichlet boundary value problem. However, the minimizing functional that characterizes the solution to a mixed boundary value problem with inhomogeneous Neumann conditions on part of the boundary acquires an additional boundary term.

Theorem 9.32. *The solution $u(x, y)$ to the boundary value problem*

$$-\Delta u = f \quad in \quad \Omega, \qquad u = h \quad on \quad D \subset \partial\Omega, \qquad \frac{\partial u}{\partial \mathbf{n}} = k \quad on \quad N = \partial\Omega \setminus D, \tag{9.83}$$

with $D \neq \varnothing$, is characterized as the unique function that minimizes the modified Dirichlet integral

$$\widehat{Q}[u] = \iint_\Omega \left(\, \tfrac{1}{2}\, u_x^2 + \tfrac{1}{2}\, u_y^2 - f\, u\,\right) dx\, dy \,-\, \int_N k\, u\, ds \tag{9.84}$$

among all C^2 functions that satisfy the prescribed boundary conditions.

In particular, the inhomogeneous Dirichlet problem has $N = \varnothing$, in which case the extra boundary integral does not appear.

Proof: Write $u(x,y) = \widetilde{u}(x,y) + v(x,y)$, where v is any function that satisfies the given boundary conditions: $v = h$ on D, while $\partial v / \partial \mathbf{n} = k$ on N. (We specifically do not require that v satisfy the Poisson equation.) Their difference $\widetilde{u} = u - v$ satisfies the corresponding homogeneous boundary conditions, along with the modified Poisson equation

$$-\Delta \widetilde{u} = \widetilde{f} \equiv f + \Delta v \quad \text{in} \quad \Omega, \qquad \widetilde{u} = 0 \quad \text{on} \quad D, \qquad \frac{\partial \widetilde{u}}{\partial \mathbf{n}} = 0 \quad \text{on} \quad N.$$

Theorem 9.31 implies that $\widetilde{u}$ minimizes the Dirichlet functional

$$\widetilde{Q}[\widetilde{u}] = \tfrac{1}{2} \, \| \nabla \widetilde{u} \|^2 - \langle\!\langle \widetilde{f}, \widetilde{u} \rangle\!\rangle = \iint_\Omega \left(\tfrac{1}{2} \widetilde{u}_x^2 + \tfrac{1}{2} \widetilde{u}_y^2 - \widetilde{f} \, \widetilde{u} \right) dx\, dy$$

among all functions satisfying the homogeneous boundary conditions. We compute

$$\begin{aligned}
\widetilde{Q}[\widetilde{u}] = \widetilde{Q}[u - v] &= \tfrac{1}{2} \, \| \nabla (u - v) \|^2 - \langle f + \Delta v, u - v \rangle \\
&= \tfrac{1}{2} \, \| \nabla u \|^2 - \langle \nabla u, \nabla v \rangle + \tfrac{1}{2} \, \| \nabla v \|^2 - \langle f, u \rangle - \langle \Delta v, u \rangle + \langle f + \Delta v, v \rangle \\
&= Q[u] - \iint_\Omega (\nabla u \cdot \nabla v + u\,\Delta v)\, dx\, dy + C_0,
\end{aligned}$$

where

$$C_0 = \tfrac{1}{2} \, \| \nabla v \|^2 + \langle f + \Delta v, v \rangle$$

does not depend on u. We then apply formula (6.83) to evaluate the middle terms:

$$\iint_\Omega (\nabla u \cdot \nabla v + u\,\Delta v)\, dx\, dy = \oint_{\partial \Omega} u \, \frac{\partial v}{\partial \mathbf{n}} \, ds = \int_D h \, \frac{\partial v}{\partial \mathbf{n}} \, ds + \int_N u\, k \, ds.$$

Thus,

$$\widetilde{Q}[\widetilde{u}] = Q[u] - \int_N k\, u \, ds + C_1 = \widehat{Q}[u] + C_1,$$

where the final term $C_1 = C_0 + \int_D h \, \dfrac{\partial v}{\partial \mathbf{n}} \, ds$ is fixed by the boundary conditions and the choice of v, and so its value does not change when the function u is varied. We conclude that $\widetilde{u}$ minimizes $\widetilde{Q}[\widetilde{u}]$ if and only if $u = \widetilde{u} + v$ minimizes $\widehat{Q}[u]$.   *Q.E.D.*

Exercises

$\heartsuit$ 9.3.18. (a) Show that the function $u(x,y) = \tfrac{1}{2}\left(-xy + xy^2 + x^2 y - x^2 y^2\right)$ solves the homogeneous Dirichlet boundary value problem for the Poisson equation $-\Delta u = x^2 + y^2 - x - y$ on the unit square $S = \{0 \le x \le 1,\ 0 \le y \le 1\}$. (b) Write down the Dirichlet integral (9.82) for this boundary value problem. What is its value for your solution? (c) Write down three other functions that satisfy the homogeneous Dirichlet boundary conditions on S, and check that all three have larger Dirichlet integrals.

9.3.19. (a) Suppose $u(x,y)$ solves the boundary value problem $-\Delta u = f$ in Ω and $u = 0$ on $\partial \Omega$, with $f(x,y) \not\equiv 0$. Prove that its Dirichlet integral (9.82) is strictly negative: $Q[u] < 0$. (b) Does this result hold for the inhomogeneous boundary value problem $u = h$ on $\partial \Omega$?

♡ 9.3.20. Consider the boundary value problem $-\Delta u = 1$, $x^2 + y^2 < 1$, $u = 0$, $x^2 + y^2 = 1$.
(a) Find all solutions. (b) Formulate the Dirichlet minimization principle for this problem. Carefully indicate the function space over which you are minimizing. Make sure your solution belongs to the function space. (c) Which of the following functions belong to your function space? (i) $1 - x^2 - y^2$, (ii) $1 - \frac{1}{2}x^2 - \frac{1}{2}y^2$, (iii) $x - x^3 - xy^2$, (iv) $x^4 - x^2 y^2 + y^4$, (v) $\frac{1}{2}e^{-x^2 - y^2} - \frac{1}{2}e^{-1}$. (d) For each function in part (c) that does belong to your function space, verify that its Dirichlet integral is larger than your solution's value.

9.3.21. Suppose $\lambda > 0$. Under what conditions does the inhomogeneous Neumann problem $-\Delta u + \lambda u = f$ in Ω, $\partial u / \partial \mathbf{n} = k$ on $\partial \Omega$, for the Helmholtz equation have a solution? Is the solution unique? *Hint*: Is the boundary value problem positive definite?

◇ 9.3.22. Suppose $\kappa(x) > 0$ for all $a \le x \le b$.

(a) Prove that the solution $u_\star(x)$ to the inhomogeneous Dirichlet boundary value problem

$$-\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right) = f(x), \qquad u(a) = \alpha, \qquad u(b) = \beta,$$

minimizes the functional $Q[u] = \int_a^b \left[\frac{1}{2}\kappa(x)\, u'(x)^2 - f(x)\, u(x)\right] dx$.

Hint: Mimic the proof of Theorem 9.32.

(b) Construct a minimization principle for the mixed boundary value problem

$$-\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right) = f(x), \qquad u(a) = \alpha, \qquad u'(b) = \beta.$$

9.3.23. Use the result of Exercise 9.3.22 to find the C^2 function $u_\star(x)$ that minimizes the integral $Q[u] = \int_1^2 \left[\frac{x}{2}\left(\frac{du}{dx}\right)^2 + x^2 u\right] dx$ when subject to the boundary conditions $u(1) = 0$, $u(2) = 1$.

9.3.24. Find the function $u(x)$ that minimizes the integral $Q[u] = \int_1^2 [x(u')^2 + x^2 u]\, dx$ subject to the boundary conditions $u(1) = 1$, $u'(2) = 0$. *Hint*: Use Exercise 9.3.22(b).

9.3.25. Prove that the functional $Q[u] = \int_0^1 (u')^2\, dx$, when subject to the mixed boundary conditions $u(0) = 0$, $u'(1) = 1$, has no minimizer.

♡ 9.3.26. Let $p_1(x, y), p_2(x, y), q(x, y) > 0$ be strictly positive functions on a closed, bounded, connected domain $\overline{\Omega} \subset \mathbb{R}^2$. Consider the boundary value problem for the second-order partial differential equation

$$-\frac{\partial}{\partial x}\left(p_1(x,y)\frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(p_2(x,y)\frac{\partial u}{\partial y}\right) + q(x,y)\, u = f(x,y), \qquad (x,y) \in \Omega, \qquad (9.85)$$

subject to homogeneous Dirichlet boundary conditions $u = 0$ on $\partial \Omega$.
(a) *True or false*: Equation (9.85) is an elliptic partial differential equation. (b) Write the boundary value problem in self-adjoint form $L^* \circ L[u] = f$. *Hint*: Regard (9.85) as a "two-dimensional Sturm–Liouville equation". (c) Prove that this boundary value problem is positive definite, and then find a minimization principle that characterizes the solution. (d) Find suitable homogeneous Neumann–type boundary conditions involving the values of the derivatives of u on $\partial \Omega$ that make the resulting boundary value problem for (9.85) self-adjoint. Is your boundary value problem positive definite? Why or why not?

9.4 Eigenvalues and Eigenfunctions

We have already come to appreciate the value of eigenfunctions for constructing separable solutions to dynamical partial differential equations such as the one-dimensional heat and wave equations. In both cases, the eigenfunctions are trigonometric, and are used to write the solution to the initial value problem in the form of a Fourier series. The most important feature is that the Fourier eigenfunctions are orthogonal with respect to the underlying L^2 inner product. As we remarked earlier, orthogonality is not an accident. Rather, it is a direct consequence of the self-adjointness of the linear differential operator prescribing the eigenvalue equation. The goal of this section is, in preparation for extending the eigenfunction method to higher-dimensional and more general dynamical problems, to establish the orthogonality property of eigenfunctions in general, discuss how positive (semi-)definiteness affects the eigenvalues, and present the basic theory of eigenfunction series expansions, thereby significantly generalizing basic Fourier series. As an application, we deduce a general formula for the Green's function of a positive definite boundary value problem as an infinite series in the eigenfunctions, and use this to formulate a condition that guarantees completeness of the eigenfunctions. Along the way, we also need to introduce an important minimization principle, the Rayleigh quotient, that characterizes the eigenvalues of a positive definite linear system.

We begin with the *eigenvalue problem*

$$S[v] = \lambda\, v \tag{9.86}$$

for a linear operator $S\colon U \to U$ on† a real or complex vector space U. Clearly, $v = 0$ solves the eigenvalue equation no matter what the scalar λ is. If the homogeneous linear system (9.86) admits a *nonzero* solution $0 \neq v \in U$, then $\lambda \in \mathbb{C}$ is called an *eigenvalue* of the operator S and v a corresponding *eigenvector* or *eigenfunction*, depending on the context. If λ is an eigenvalue, then the corresponding *eigenspace* is the subspace

$$V_\lambda = \ker(S - \lambda\, \mathrm{I}) = \{\, v \mid\ S[v] = \lambda\, v\,\} \subset U, \tag{9.87}$$

consisting of all the eigenvectors/eigenfunctions along with the zero element. To avoid technical difficulties, we will work under the assumption that all the eigenspaces are finite-dimensional, and we call $1 \le \dim V_\lambda < \infty$ the *geometric multiplicity* of the eigenvalue λ. Finite-dimensionality is almost always valid, and indeed, will be later established for regular boundary value problems on bounded domains.

Self–Adjoint Operators

In the applications considered here, the vector space U comes equipped with an inner product, and S is a self-adjoint linear operator. In such instances, one can readily establish the basic orthogonality property of the eigenvectors/eigenfunctions.

Theorem 9.33. *If $S = S^*$ is a self-adjoint linear operator on an inner product space U, then all its eigenvalues are real. Moreover, the eigenvectors/eigenfunctions associated with* different *eigenvalues are automatically orthogonal.*

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† As discussed earlier, in the infinite-dimensional case, the differential operator S might be only defined on a dense subspace of U consisting of sufficiently smooth functions.

Proof: To prove the first part of the theorem, suppose λ is a complex eigenvalue, so that $S[v] = \lambda v$ for some complex eigenvector/eigenfunction $v \neq 0$. Then, using the sesquilinearity (B.19) of the underlying Hermitian inner product[‡] and self-adjointness (9.45) of S, we find

$$\lambda \, \| \, v \, \|^2 = \langle \, \lambda \, v \, , v \, \rangle = \langle \, S[v] \, , v \, \rangle = \langle \, v \, , S[v] \, \rangle = \langle \, v \, , \lambda \, v \, \rangle = \overline{\lambda} \, \| \, v \, \|^2.$$

Since $v \neq 0$, this immediately implies that $\lambda = \overline{\lambda}$, its complex conjugate, and hence λ must necessarily be real.

To prove orthogonality, suppose $S[u] = \lambda \, u$ and $S[v] = \mu \, v$. Again by self-adjointness,

$$\lambda \, \langle \, u \, , v \, \rangle = \langle \, \lambda \, u \, , v \, \rangle = \langle \, S[u] \, , v \, \rangle = \langle \, u \, , S[v] \, \rangle = \langle \, u \, , \mu \, v \, \rangle = \mu \, \langle \, u \, , v \, \rangle,$$

where the final equality relies on the fact that the eigenvalue μ is real. Therefore, the assumption that $\lambda \neq \mu$ immediately implies orthogonality: $\langle \, u \, , v \, \rangle = 0$.   *Q.E.D.*

Thus, the eigenvalues of self-adjoint linear operators are necessarily real. If, in addition, the operator is positive definite, then its eigenvalues must, in fact, be positive.

Theorem 9.34. *If $S > 0$ is a self-adjoint positive definite linear operator, then all its eigenvalues are strictly positive: $\lambda > 0$. If $S \geq 0$ is self-adjoint and positive semi-definite, then its eigenvalues are nonnegative: $\lambda \geq 0$.*

Proof: Self-adjointness assures us that all of the eigenvalues are real. Suppose $S[u] = \lambda \, u$ with $u \neq 0$ a real eigenfunction. Then

$$\lambda \, \| \, u \, \|^2 = \lambda \, \langle \, u \, , u \, \rangle = \langle \, \lambda \, u \, , u \, \rangle = \langle \, S[u] \, , u \, \rangle > 0,$$

by positive definiteness. Since $\| \, u \, \|^2 > 0$, this immediately implies that $\lambda > 0$. The same argument implies that $\lambda \geq 0$ in the positive semi-definite case.   *Q.E.D.*

All the linear operators to be considered in this text are real, and, at the very least, self-adjoint, and often either positive definite or semi-definite. Thus, we will restrict our attention from here on (at least until we reach the Schrödinger equation in the final subsection) to real operators defined on real vector spaces, knowing a priori that we are not overlooking any eigenvalues or eigenfunctions by this restriction.

Example 9.35. In finite dimensions, if we equip $U = \mathbb{R}^n$ with the dot product, then any self-adjoint linear function is given by multiplication by an $n \times n$ symmetric matrix: $S[u] = K \mathbf{u}$, where $K^T = K$. Theorem 9.33 implies the well-known result that a symmetric matrix has only real eigenvalues. Moreover, the eigenvectors associated with different eigenvalues are mutually orthogonal.

In fact, it can be proved that, in general, the eigenvectors of a symmetric matrix are complete, [**89**]. In other words, there exists an orthogonal basis $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of $\mathbb{R}^n$ consisting of eigenvectors of K, so $K \mathbf{v}_j = \lambda_j \mathbf{v}_j$ for $j = 1, \ldots, n$. If the eigenvalues $\lambda_1, \ldots, \lambda_n$ are all simple, so $\lambda_i \neq \lambda_j$ for $i \neq j$, then the basis eigenvectors are automatically orthogonal. When K has repeated eigenvalues, this requires selecting an orthogonal basis of each of the associated eigenspaces $V_\lambda = \ker(K - \lambda \, \mathrm{I})$, e.g., using the Gram–Schmidt process.

[‡]   We are temporarily working in the vector space of complex-valued functions. Once we establish reality of the eigenvalues and eigenfunctions, we can shift our focus back to the real function space.

Completeness implies that the number of linearly independent eigenvectors associated with an eigenvalue, i.e., its geometric multiplicity, is the same as the eigenvalue's algebraic multiplicity. If, furthermore, the matrix $K > 0$ is symmetric and positive definite, then Theorem 9.34 implies that all its eigenvalues are positive: $\lambda_j > 0$. In this case, thanks to completeness, the converse is also valid: a symmetric matrix is positive definite if and only if it has all positive eigenvalues. These results can all be immediately generalized to self-adjoint matrices under general inner products on $\mathbb{R}^n$.

Example 9.36. Consider the Dirichlet eigenvalue problem

$$ -\frac{d^2 v}{dx^2} = \lambda\, v, \qquad v(0) = 0, \qquad v(\ell) = 0, $$

for the differential operator $S = -D^2$ on an interval of length $\ell > 0$. As we know — see, for instance, Section 4.1 — the eigenvalues and eigenfunctions are

$$ \lambda_n = \left(\frac{n\pi}{\ell}\right)^2, \qquad v_n(x) = \sin\frac{n\pi x}{\ell}, \qquad n = 1, 2, 3, \ldots. $$

We now understand this example in our general framework. The fact that the eigenvalues are real and positive follows from the fact that the boundary value problem is defined by the self-adjoint positive definite operator

$$ S[u] = D^* \circ D[u] = -D^2[u] = -u'', $$

acting on the vector space $U = \{\, u(0) = u(\ell) = 0\,\}$, equipped with the L^2 inner product:

$$ \langle\, u\,, v\,\rangle = \int_0^\ell u(x)\, v(x)\, dx. $$

The orthogonality of the Fourier sine functions,

$$ \langle\, v_m\,, v_n\,\rangle = \int_0^\ell \sin\frac{m\pi x}{\ell}\,\sin\frac{n\pi x}{\ell}\, dx = 0 \qquad \text{for} \qquad m \neq n, $$

is also an automatic consequence of their status as eigenfunctions of this self-adjoint boundary value problem.

Example 9.37. Similarly, the periodic boundary value problem

$$ -v'' = \lambda\, v, \qquad v(-\pi) = v(\pi), \qquad v'(-\pi) = v'(\pi), \tag{9.88} $$

has eigenvalues $\lambda_0 = 0$, with eigenfunction $v_0(x) \equiv 1$, and $\lambda_n = n^2$, for $n = 1, 2, 3, \ldots$, each possessing two independent eigenfunctions: $v_n(x) = \cos nx$ and $\widetilde{v}_n(x) = \sin nx$. In this case, a zero eigenvalue appears because $S = D^* \circ D = -D^2$ is only positive semi-definite on the space of periodic functions. Theorem 9.33 implies the all-important orthogonality of the Fourier eigenfunctions corresponding to *different* eigenvalues: $\langle\, v_m\,, v_n\,\rangle = \langle\, v_m\,, \widetilde{v}_n\,\rangle = \langle\, \widetilde{v}_m\,, \widetilde{v}_n\,\rangle = 0$ for $m \neq n$, under the L^2 inner product on $[-\pi, \pi]$. However, since they have the same eigenvalue, the orthogonality of $v_n(x) = \cos nx$ and $\widetilde{v}_n(x) = \sin nx$, while true, is not ensured and must be checked by hand.

Example 9.38. On the other hand, the self-adjoint boundary value problem

$$ -\frac{d^2 u}{dx^2} = \lambda\, u, \qquad \lim_{x\to\infty} u(x) = 0, \qquad \lim_{x\to-\infty} u(x) = 0, \tag{9.89} $$

on the real line has no eigenvalues: no matter what the value of λ, the only solution decaying to 0 at both $\pm\infty$ is the zero solution. Indeed, exponential solutions that decay at one end become infinitely large at the other. The trigonometric functions $u(x) = \cos\omega\,x$ and $\sin\omega\,x$ satisfy the differential equation when $\lambda = \omega^2 > 0$, but do not go to zero as $|x| \to \infty$, and so do not qualify as bona fide eigenfunctions. Rather, because they are bounded on the entire line, they represent the "continuous spectrum" of the underlying self-adjoint differential operator, [**95**]. In this particular context, the continuous spectrum leads directly to the Fourier transform.

Example 9.39. The eigenvalue problem for the Bessel differential operator of order m, given in (9.79), is governed by the following differential equation:

$$S[u] = -u'' - \frac{1}{x}\,u' + \frac{m^2}{x^2}\,u = \lambda\,u, \tag{9.90}$$

or, equivalently,

$$x^2\,\frac{d^2u}{dx^2} + x\,\frac{du}{dx} + (\lambda\,x^2 - m^2)\,u = 0,$$

supplemented by appropriate homogeneous boundary conditions at the endpoints of the interval $0 \le a < b$. Its eigenfunctions are not elementary, but, as we will learn in Chapter 11, can be expressed in terms of Bessel functions. Nevertheless, no matter what their eventual formula, Theorem 9.33 guarantees the orthogonality of any two eigenfunctions $v, \widetilde{v}$ associated with distinct eigenvalues $\lambda \ne \widetilde{\lambda}$ under the weighted inner product (9.80):

$$\langle\, v\,,\widetilde{v}\,\rangle = \int_a^b v(x)\,\widetilde{v}(x)\,x\,dx = 0.$$

Example 9.40. According to equation (9.60), on a bounded domain $\Omega \subset \mathbb{R}^2$, the (negative) Laplacian $-\Delta$ forms a self-adjoint positive (semi-)definite operator under the L^2 inner product (9.22) when subject to one of the usual sets of homogeneous boundary conditions. Let us, for specificity, concentrate on the Dirichlet case. The *eigenfunctions* of the Laplacian are the nonzero solutions to the following boundary value problem:

$$-\Delta v = \lambda\,v \qquad \text{in} \quad \Omega, \qquad u = 0 \qquad \text{on} \quad \partial\Omega. \tag{9.91}$$

The underlying partial differential equation, namely

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \lambda\,v = 0,$$

is known as the *Helmholtz equation*, named after the influential and wide-ranging German applied mathematician Hermann von Helmholtz. As we will see, the Helmholtz equation plays a central role in the solution of the two-dimensional heat, wave, and Schrödinger equations.

Only in a few special cases, e.g., rectangles and circular disks, can the eigenfunctions and eigenvalues be determined exactly; see Chapter 11 for details. Nevertheless, Theorem 9.34 guarantees that, for all domains, the eigenvalues are always nonnegative, $\lambda \ge 0$, with $\lambda_0 = 0$ being an eigenvalue only in positive semi-definite cases, e.g., Neumann boundary conditions. Moreover, Theorem 9.33 ensures the orthogonality of any two eigenfunctions,

$$\langle\, v\,,\widetilde{v}\,\rangle = \iint_\Omega v(x,y)\,\widetilde{v}(x,y)\,dx\,dy = 0,$$

that are associated with distinct eigenvalues $\lambda \ne \widetilde{\lambda}$.

The Rayleigh Quotient

We have already learned how to characterize the solutions of positive definite boundary value problems by a minimization principle. One can also characterize their eigenvalues by a minimization principle, named after the prolific nineteenth-century English applied mathematician Lord Rayleigh (John Strutt).

Definition 9.41. Let $S : U \to U$ be a self-adjoint linear operator on an inner product space. The *Rayleigh quotient* of S is defined as

$$R[u] = \frac{\langle u, S[u] \rangle}{\| u \|^2} \qquad \text{for} \qquad 0 \neq u \in U. \tag{9.92}$$

We are, in fact, primarily interested in the Rayleigh quotient of positive definite operators, for which $R[u] > 0$ for all $u \neq 0$. If $S = L^* \circ L$, then, using (9.51), we can rewrite the Rayleigh quotient in the alternative form

$$R[u] = \frac{\| | L[u] | \|^2}{\| u \|^2}, \tag{9.93}$$

keeping in mind our notational convention (9.50) for the respective norms on U and V.

Theorem 9.42. *Let S be a self-adjoint linear operator. Then the minimum value of its Rayleigh quotient,*

$$\lambda_\star = \min \{ R[u] \mid u \neq 0 \}, \tag{9.94}$$

is the smallest eigenvalue of the operator S. Moreover, any $0 \neq v_\star \in U$ that achieves this minimum value, $R[v_\star] = \lambda_\star$, is an associated eigenvector/eigenfunction: $S[v_\star] = \lambda_\star v_\star$.

Proof: Suppose that $v_\star \in U$ is a minimizing element, and

$$\lambda_\star = R[v_\star] = \frac{\langle v_\star, S[v_\star] \rangle}{\| v_\star \|^2} \tag{9.95}$$

the minimum value. Given any $u \in U$, define the scalar function[†]

$$
\begin{aligned}
g(t) = R[v_\star + t\,u] &= \frac{\langle v_\star + t\,u, S[v_\star + t\,u] \rangle}{\| v_\star + t\,u \|^2} \\
&= \frac{\langle v_\star, S[v_\star] \rangle + 2t \langle u, S[v_\star] \rangle + t^2 \langle u, S[u] \rangle}{\| v_\star \|^2 + 2t \langle u, v_\star \rangle + t^2 \| u \|^2},
\end{aligned}
$$

where we used the self-adjointness of S and the fact that we are working in a real inner product space to identify the terms

$$\langle u, S[v_\star] \rangle = \langle S[u], v_\star \rangle = \langle v_\star, S[u] \rangle.$$

Since

$$g(0) = R[v_\star] \leq R[v_\star + t\,u] = g(t),$$

the function $g(t)$ will attain its minimum value at $t = 0$. Elementary calculus tells us that

$$0 = g'(0) = 2 \, \frac{\langle u, S[v_\star] \rangle \| v_\star \|^2 - \langle v_\star, S[v_\star] \rangle \langle u, v_\star \rangle}{\| v_\star \|^4}.$$

[†] $g(t)$ is not defined if $v_\star + t\,u = 0$, but this does not affect the argument.

Therefore, using (9.95) to replace $\langle v_\star , S[v_\star] \rangle$ by $\lambda_\star \| v_\star \|^2$, we must have

$$\langle u , S[v_\star] \rangle - \lambda_\star \langle u , v_\star \rangle = \langle u , S[v_\star] - \lambda_\star v_\star \rangle = 0. \tag{9.96}$$

The only way the inner product in (9.96) can vanish for all possible $u \in U$ is if

$$S[v_\star] = \lambda_\star v_\star, \tag{9.97}$$

which means that $0 \neq v_\star$ is an eigenfunction and $\lambda_\star$ its associated eigenvalue.

On the other hand, if v is any eigenfunction, so $S[v] = \lambda v$, where, by self-adjointness, the eigenvalue λ is necessarily real, then the value of its Rayleigh quotient is

$$R[v] = \frac{\langle v , S[v] \rangle}{\| v \|^2} = \frac{\langle v , \lambda v \rangle}{\| v \|^2} = \lambda. \tag{9.98}$$

Since $\lambda_\star$ was, by definition, the smallest possible value of the Rayleigh quotient, it thus must necessarily be the smallest eigenvalue.   Q.E.D.

Remark: The existence of a minimizing function is not addressed in this result, and, indeed, there may be no minimum eigenvalue; the infimum of the set of eigenvalues could be $-\infty$ or, even if finite, not an eigenvalue. However, for the positive definite boundary value problems considered here, the eigenvalues are all strictly positive, and one can, with some additional analysis, [**44**], prove the existence of a minimizing eigenfunction, and hence a smallest positive eigenvalue.

We label the eigenvalues in increasing order, so that, assuming positive definiteness, $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots$, with λ_1 the minimum eigenvalue and hence the minimum value of the Rayleigh quotient. To characterize the other eigenvalues, we need to restrict the class of functions over which one minimizes. Indeed, since the nth eigenfunction v_n must be orthogonal to all its predecessors $v_1, \ldots, v_{n-1}$, it makes sense to try minimizing the Rayleigh quotient over such elements.

Theorem 9.43. *Let $v_1, \ldots, v_{n-1}$ be eigenfunctions corresponding to the first $n-1$ eigenvalues $0 < \lambda_1 \leq \cdots \leq \lambda_{n-1}$ of the positive definite self-adjoint linear operator S. Let*

$$U_{n-1} = \left\{ u \mid \langle u , v_1 \rangle = \cdots = \langle u , v_{n-1} \rangle = 0 \right\} \subset U \tag{9.99}$$

be the set of functions that are orthogonal to the indicated eigenfunctions. Then the minimum value of the Rayleigh quotient function restricted to the subspace U_{n-1} is the nth eigenvalue of S, that is,

$$\lambda_n = \min \left\{ R[u] \mid 0 \neq u \in U_{n-1} \right\}, \tag{9.100}$$

and any minimizer is an associated eigenfunction v_n.

Proof: We follow the preceding proof, but now restrict $v_\star$ and u to belong to the subspace U_{n-1}. Observe that $S[u] \in U_{n-1}$ whenever $u \in U_{n-1}$, because, by self-adjointness,

$$\langle S[u] , v_j \rangle = \langle u , S[v_j] \rangle = \lambda_j \langle u , v_j \rangle = 0 \qquad \text{for} \qquad j = 1, \ldots, n-1.$$

Thus, if $0 \neq v_\star \in U_{n-1}$ minimizes the Rayleigh quotient, then (9.96) holds for arbitrary $u \in U_{n-1}$. In particular, choosing $u = S[v_\star] - \lambda_\star v_\star$, we conclude that $v_\star$ satisfies the eigenvalue equation (9.97), and hence must be an eigenfunction that is orthogonal to the first $n-1$ eigenfunctions. This means that $\lambda_\star = \lambda_n$ must be the next-lowest eigenvalue and $v_\star = v_n$ one of its associated eigenfunctions.   Q.E.D.

Example 9.44. Return to the Dirichlet eigenvalue problem on the interval $[0, \ell]$ for the self-adjoint (under the L^2 inner product) differential operator $-D^2 = D^* \circ D$ discussed in Example 9.36. Its Rayleigh quotient can be written as

$$R[u] = \frac{\langle u, -u'' \rangle}{\| u \|^2} = -\frac{\displaystyle\int_0^\ell u(x)\, u''(x)\, dx}{\displaystyle\int_0^\ell u(x)^2\, dx} = \frac{\displaystyle\int_0^\ell u'(x)^2\, dx}{\displaystyle\int_0^\ell u(x)^2\, dx} = \frac{\|\|\, u' \,\|\|^2}{\| u \|^2},$$

where the second expression, based on the alternative form (9.93), can be readily deduced from the first via an integration by parts. (Here, both domain and target space of $L = D$ use the same L^2 norm.) According to Theorem 9.42, the minimum value of $R[u]$ over all nonzero functions $u(x) \not\equiv 0$ satisfying the boundary conditions $u(0) = u(\ell) = 0$ is the lowest eigenvalue, namely

$$\lambda_1 = \frac{\pi^2}{\ell^2} = \min \left\{ R[u] \,\Big|\, u(0) = u(\ell) = 0,\ u(x) \not\equiv 0 \right\},$$

which is achieved if and only if $u(x)$ is a nonzero constant multiple of $\sin(\pi x/\ell)$, the corresponding eigenfunction. The reader is invited to numerically test this result by fixing a value of ℓ, and then evaluating $R[u]$ on various functions $u(x)$ satisfying the boundary conditions to check that the numerical value is always larger than π^2/ℓ^2, the smallest eigenvalue. The second eigenvalue can be found by minimizing over all nonzero functions that are orthogonal to the first eigenfunction:

$$\lambda_2 = \frac{4\pi^2}{\ell^2} = \min \left\{ R[u] \,\Big|\, u(0) = u(\ell) = 0,\ \int_0^\ell u(x) \sin \frac{\pi}{\ell} x\, dx = 0,\ u(x) \not\equiv 0 \right\},$$

and similarly for the higher eigenvalues.

Example 9.45. Consider the Helmholtz eigenvalue problem (9.91) on a bounded domain $\Omega \subset \mathbb{R}^2$, subject to Dirichlet boundary conditions. The associated Rayleigh quotient (9.93) can be written in the form

$$R[u] = \frac{\|\|\, \nabla u \,\|\|^2}{\| u \|^2} = \frac{\displaystyle\iint_\Omega \left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 \right] dx\, dy}{\displaystyle\iint_\Omega u(x,y)^2\, dx\, dy}. \tag{9.101}$$

Its minimum value among all nonzero functions $u(x,y) \not\equiv 0$ subject to the boundary conditions $u = 0$ on $\partial\Omega$ is the smallest eigenvalue λ_1, and the minimizing function is any nonzero constant multiple of the associated eigenfunction $v_1(x,y)$. To obtain a higher eigenvalue λ_n, one minimizes $R[u]$, where $u(x,y) \not\equiv 0$ again satisfies the boundary conditions and, in addition, is orthogonal to the preceding $n-1$ eigenfunctions:

$$0 = \langle u, v_k \rangle = \iint_\Omega u(x,y)\, v_k(x,y)\, dx\, dy, \qquad \text{for} \qquad k = 1, \ldots, n-1.$$

It can be proved, [**34**, **44**], that, as long as the domain is bounded with, as always, a reasonably nice boundary, there is a solution to each of these minimization problems, and hence the Helmholtz equation admits an infinite sequence of positive eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots$, with $\lambda_n \to \infty$ becoming arbitrarily large as $n \to \infty$; see also Theorem 9.47 below.

Eigenfunction Series

For our applications to dynamical partial differential equations, we will be particularly interested in expanding more general functions in terms of the orthogonal eigenfunctions, the simplest case being the classical Fourier series. To fix notation, we will proceed as if we were treating a one-dimensional boundary value problem, although the formulas are equally valid for higher-dimensional problems, e.g., those governed by the Helmholtz equation. Thus, we consider an eigenvalue problem of the form $S[v] = \lambda v$, where S is a positive definite or semi-definite operator that is self-adjoint relative to a weighted L^2 inner product

$$\langle\, v\,, \widetilde{v}\,\rangle = \int_a^b v(x)\, \widetilde{v}(x)\, \rho(x)\, dx, \tag{9.102}$$

with $\rho(x) > 0$ on the bounded interval $a \leq x \leq b$.

Let $0 \leq \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots$ be the eigenvalues, and $v_1, v_2, v_3, \ldots$, the corresponding eigenfunctions. Theorem 9.33 assures us that those corresponding to different eigenvalues are mutually orthogonal:

$$\langle\, v_j\,, v_k\,\rangle = 0, \qquad j \neq k. \tag{9.103}$$

Orthogonality is not automatic if v_j and v_k belong to the same eigenvalue, but it can be ensured by selecting an orthogonal basis of each eigenspace V_λ, if necessary by applying the Gram–Schmidt orthogonalization process, [**89**].

Let $f \in U$ be an arbitrary function in our inner product space. The *eigenfunction series* of f is, by definition, its generalized Fourier series:

$$f \;\sim\; \sum_k c_k\, v_k, \qquad \text{where the coefficient} \qquad c_k = \frac{\langle\, f\,, v_k\,\rangle}{\|\, v_k\,\|^2} \tag{9.104}$$

is found by formally taking the inner product of both sides of (9.104) with the eigenfunction v_k and invoking their mutual orthogonality. (Note that our earlier eigenfunction series formula (3.108) assumed orthonormality; here, it will be convenient to not necessarily impose the condition $\|\, v_k\,\| = 1$.) For example, in the case covered by Example 9.36, (9.104) becomes the usual Fourier sine series for the function f, whereas for Example 9.37, it represents its full periodic Fourier series. In a similar fashion, Example 9.40 leads to series in the eigenfunctions of the Laplacian operator on a bounded domain subject to appropriate homogeneous boundary conditions; explicit examples of the latter can be found in Chapters 11 and 12.

As we learned in Section 3.5, convergence (in norm) of the series (9.104) requires completeness of the eigenfunctions. (Pointwise and uniform convergence are then implied by more restrictive hypotheses on the function and the domain, e.g., $f \in \mathrm{C}^1$.) In the finite-dimensional context, when $S \colon \mathbb{R}^n \to \mathbb{R}^n$ is given by matrix multiplication, $S[\mathbf{u}] = K\,\mathbf{u}$, there are only finitely many eigenvectors, and so the summation (9.104) has only finitely many terms. There are, hence, no convergence considerations, and completeness is automatic. For boundary value problems in infinite-dimensional function space, the completeness of the resulting eigensolutions is a more delicate issue. In Example 9.36, the eigenvalue problem for $S = -\,D^2$ subject to homogeneous Dirichlet boundary conditions on a bounded interval leads to the Fourier sine eigenfunctions, which we know to be complete. On the other hand, the corresponding eigenvalue problem on the real line, treated in Example 9.38, has *no* eigenfunctions, and so completeness is out of the question. As we will

see, the eigenfunctions associated with regular boundary value problems on bounded domains are automatically complete, whereas singular problems and problems on unbounded domains require additional analysis.

Whether or not the eigenfunctions are complete, we always have *Bessel's inequality*[†] (3.117):

$$\sum_k c_k^2 \, \| \, v_k \, \|^2 \;\leq\; \| \, f \, \|^2. \tag{9.105}$$

Theorem 3.43 says that the eigenfunctions are complete if and only if Bessel's inequality is an equality, which is then the Plancherel formula for the eigenfunction expansion.

Green's Functions and Completeness

We now combine two of our principal themes. Remarkably, the key to the completeness of eigenfunctions for boundary value problems lies in the eigenfunction expansion of the Green's function! Assume that S is both self-adjoint and positive definite. Thus, by Theorem 9.34, all its eigenvalues are positive. We index them in increasing order:

$$0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \;\cdots\;, \tag{9.106}$$

where each eigenvalue is repeated according to its multiplicity.

By positive definiteness, the boundary value problem $S[u] = f$ has a unique solution.[‡] Therefore, it admits a Green's function $G_\xi(x) = G(x; \xi)$, which satisfies the boundary value problem

$$S[G_\xi] = \delta_\xi, \tag{9.107}$$

with a delta function impulse on the right-hand side. For each fixed ξ, let us write down the eigenfunction series (9.104) for the Green's function:

$$G(x;\xi) = \sum_{k=1}^{\infty} c_k(\xi) \, v_k(x), \qquad \text{where the coefficient} \qquad c_k(\xi) = \frac{\langle \, G_\xi \, , v_k \, \rangle}{\| \, v_k \, \|^2} \tag{9.108}$$

depends on the impulse point ξ. Since $S[v_k] = \lambda_k v_k$, the coefficients can be explicitly evaluated by means of the following calculation:

$$\lambda_k \, c_k(\xi) \, \| \, v_k \, \|^2 = \langle \, G_\xi \, , \lambda_k v_k \, \rangle = \langle \, G_\xi \, , S[v_k] \, \rangle$$

$$= \langle \, S[G_\xi] \, , v_k \, \rangle = \langle \, \delta_\xi \, , v_k \, \rangle = \int_a^b \delta(x - \xi) \, v_k(x) \, \rho(x) \, dx = v_k(\xi) \, \rho(\xi),$$

where $\rho(x)$ is the weight function of our inner product (9.102), and we invoked the self-adjointness of S. Solving for

$$c_k(\xi) = \frac{v_k(\xi) \, \rho(\xi)}{\lambda_k \| \, v_k \, \|^2} \tag{9.109}$$

[†] Formula (3.117) assumed orthonormality of the functions; here we are stating the analogous result for orthogonal elements. Moreover, here, the eigenfunctions and hence the coefficients c_k are all real, so we don't need absolute value signs.

[‡] As usual, we are assuming existence of the solution; Proposition 9.19 guarantees uniqueness.

and then substituting back into (9.108), we deduce the explicit eigenfunction series

$$G(x;\xi) \;\sim\; \sum_{k=1}^{\infty} \frac{v_k(x)\,v_k(\xi)\,\rho(\xi)}{\lambda_k\,\|\,v_k\,\|^2} \tag{9.110}$$

for the Green's function. Observe that this expression is compatible with the weighted symmetry equation (9.58).

Example 9.46.   According to Example 6.9, the Green's function for the L^2 self-adjoint boundary value problem

$$-u'' = f(x), \qquad u(0) = 0 = u(1),$$

is

$$G(x;\xi) = \begin{cases} x(1-\xi), & x \le \xi, \\ \xi(1-x), & x \ge \xi. \end{cases} \tag{9.111}$$

On the other hand, the eigenfunctions for

$$-v'' = \lambda\,v, \qquad v(0) = 0 = v(1),$$

are $v_k(x) = \sin k\pi x$, with corresponding eigenvalues $\lambda_k = k^2\pi^2$, for $k = 1, 2, 3, \ldots$. Since

$$\|\,v_k\,\|^2 = \int_0^1 \sin^2 k\pi x\,dx = \tfrac{1}{2}\,,$$

formula (9.110) implies the eigenfunction expansion

$$G(x;\xi) = \sum_{k=1}^{\infty} \frac{2\sin k\pi x\,\sin k\pi\xi}{k^2\pi^2}\,. \tag{9.112}$$

This result can be checked by a direct computation of the Fourier sine series of (9.111).

Let us now apply Bessel's inequality (9.105) to the eigenfunction series (9.108) for the Green's function; using (9.109), the result is

$$\sum_{k=1}^{n} c_k(\xi)^2\,\|\,v_k\,\|^2 \;=\; \sum_{k=1}^{n} \frac{v_k(\xi)^2\,\rho(\xi)^2}{\lambda_k^2\,\|\,v_k\,\|^2} \le \|\,G_\xi\,\|^2 = \int_a^b G(x;\xi)^2\,\rho(x)\,dx. \tag{9.113}$$

We divide by $\rho(\xi) > 0$, and then integrate both sides of the resulting inequality from a to b. On the left-hand side, the integrated summands are

$$\int_a^b \frac{v_k(\xi)^2\,\rho(\xi)}{\lambda_k^2\,\|\,v_k\,\|^2}\,d\xi = \frac{1}{\lambda_k^2\,\|\,v_k\,\|^2}\,\int_a^b v_k(\xi)^2\,\rho(\xi)\,d\xi = \frac{1}{\lambda_k^2}\,.$$

Substituting back into (9.113) establishes the interesting inequality

$$\sum_{k=1}^{n} \frac{1}{\lambda_k^2} \;\le\; \int_a^b \int_a^b G(x;\xi)^2\,\frac{\rho(x)}{\rho(\xi)}\,dx\,d\xi. \tag{9.114}$$

To make the right-hand side look less strange, we can replace $G(x;\xi)$ by the symmetric

modified Green's function $\widehat{G}(x;\xi) = G(x;\xi)/\rho(\xi) = \widehat{G}(\xi;x)$, cf. (9.59), whence

$$\int_a^b \int_a^b G(x;\xi)^2 \, \frac{\rho(x)}{\rho(\xi)} \, dx \, d\xi = \int_a^b \int_a^b \widehat{G}(x;\xi)^2 \rho(x)\,\rho(\xi)\,dx\,d\xi \equiv \| \widehat{G} \|^2, \qquad (9.115)$$

which we can interpret as a "double weighted L^2 norm" of the modified Green's function $\widehat{G}(x;\xi)$. Since the summands in (9.114) are all positive, we can let $n \to \infty$, and conclude that

$$\sum_{k=1}^{\infty} \frac{1}{\lambda_k^2} \le \| \widehat{G} \|^2. \qquad (9.116)$$

Thus, assuming that the right-hand side of this inequality is finite, the summation on the left converges. This implies that its summands must go to zero: $\lambda_k^{-2} \to 0$ as $k \to \infty$. We have thus proved the first statement of the following important result.

Theorem 9.47. *If $\| \widehat{G} \|^2 < \infty$, then the eigenvalues of the positive definite self-adjoint operator S are unbounded: $0 < \lambda_k \to \infty$ as $k \to \infty$. Moreover, the associated orthogonal eigenfunctions $v_1, v_2, v_3, \ldots$, are complete.*

Proof: Our remaining task is to prove completeness — that is, that the eigenfunction series (9.104) of any function $f \in U$ converges in norm. For $n = 2, 3, 4, \ldots$, consider the function

$$g_{n-1} = f - \sum_{k=1}^{n-1} c_k v_k,$$

i.e., the difference between the function f and the $(n-1)^{\text{st}}$ partial sum of its eigenfunction series. Completeness requires that

$$\| g_{n-1} \| \longrightarrow 0 \qquad \text{as} \qquad n \to \infty. \qquad (9.117)$$

We can assume that $g_{n-1} \ne 0$, since otherwise, the eigenfunction series terminates, with $0 = g_{n-1} = g_n = g_{n+1} = \cdots$ (why?), and so (9.117) holds trivially.

First, note that, for any $j = 1, \ldots, n-1$,

$$\langle\, g_{n-1}\,, v_j \,\rangle = \langle\, f\,, v_j \,\rangle - \sum_{k=1}^{n-1} c_k \langle\, v_k\,, v_j \,\rangle = \langle\, f\,, v_j \,\rangle - c_j \| v_j \|^2 = 0,$$

by the orthogonality of the eigenfunctions combined with the formula (9.104) for the coefficient c_j. Thus, $g_{n-1} \in V_{n-1}$, the subspace (9.99) of functions orthogonal to the first $n-1$ eigenfunctions used in the Rayleigh Minimization Theorem 9.43. Since, according to (9.100), λ_n is the *minimum* value of the Rayleigh quotient among all nonzero elements of V_{n-1}, we must have

$$\lambda_n \le R[g_{n-1}] = \frac{\langle\, g_{n-1}\,, S[g_{n-1}] \,\rangle}{\| g_{n-1} \|^2},$$

and hence

$$\lambda_n \| g_{n-1} \|^2 \leq \langle\, g_{n-1}\,, S[g_{n-1}]\,\rangle$$

$$= \left\langle\, f - \sum_{k=1}^{n-1} c_k v_k\,, \ S\left[\, f - \sum_{k=1}^{n-1} c_k v_k\,\right]\,\right\rangle$$

$$= \left\langle\, f - \sum_{k=1}^{n-1} c_k v_k\,, \ S[f] - \sum_{k=1}^{n-1} c_k S[v_k]\,\right\rangle$$

$$= \left\langle\, f - \sum_{k=1}^{n-1} c_k v_k\,, \ S[f] - \sum_{k=1}^{n-1} c_k \lambda_k v_k\,\right\rangle$$

$$= \langle\, f\,, S[f]\,\rangle - \sum_{k=1}^{n-1} \lambda_k c_k \langle\, f\,, v_k\,\rangle - \sum_{k=1}^{n-1} c_k \langle\, v_k\,, S[f]\,\rangle + \sum_{k=1}^{n-1} \lambda_k c_k^2 \| v_k \|^2$$

$$= \langle\, f\,, S[f]\,\rangle - \sum_{k=1}^{n-1} \lambda_k \frac{\langle\, f\,, v_k\,\rangle^2}{\| v_k \|^2}\,.$$

In the final equality, we used the self-adjointness of S to identify

$$\langle\, v_k\,, S[f]\,\rangle = \langle\, S[v_k]\,, f\,\rangle = \lambda_k \langle\, v_k\,, f\,\rangle = \lambda_k \langle\, f\,, v_k\,\rangle,$$

coupled with the formula in (9.104) for the coefficients c_k. Since the summands in the final expression are all positive, we conclude that

$$\| g_{n-1} \|^2 \ \leq \ \frac{\langle\, f\,, S[f]\,\rangle}{\lambda_n}\,.$$

Since we already know that $\lambda_n \to \infty$, the right-hand side of the final inequality goes to 0 as $n \to \infty$. This implies (9.117) and hence establishes completeness.   *Q.E.D.*

One important corollary of this theorem is that, since each eigenvalue is repeated according to its geometric multiplicity, the multiplicity cannot be infinite (why?), and hence each eigenspace of such an S is necessarily finite-dimensional.

Example 9.48. For the eigenvalue problem considered in Example 9.46, since $\rho(x) \equiv 1$, the double norm of the (modified) Green's function $G(x;\xi) = \widehat{G}(x;\xi)$ is

$$\| G \|^2 = \int_0^1 \int_0^1 G(x;\xi)^2\, dx\, d\xi = 2 \int_0^1 \int_0^\xi x^2 (1-\xi)^2\, dx\, d\xi = \frac{1}{90} < \infty.$$

Thus, Theorem 9.47 re-establishes the completeness of the sine eigenfunctions, meaning that the eigenfunction series, which is just the ordinary Fourier sine series on $[0,1]$, converges in norm.

Indeed, for any regular Sturm–Liouville boundary value problem on a bounded interval, the (modified) Green's function is automatically continuous, and hence its double weighted norm is finite. Thus, Theorem 9.47 implies the completeness of the Sturm–Liouville eigenfunctions. In Chapters 11 and 12, we will extend this result to some important singular boundary value problems.

Example 9.49. The completeness result of Theorem 9.47 doesn't directly apply to the periodic boundary value problem of Example 9.37, because it is not positive definite, and hence there is no Green's function. However, we can convert it into a positive definite problem by a simple trick. As you are asked to prove in Exercise 9.4.4, if $S \geq 0$ is any positive semi-definite operator and $\mu > 0$ any positive constant, then $\widehat{S} = S + \mu\,\mathrm{I}$ is positive definite, where $\mathrm{I}[u] = u$ is the identity operator. Thus, we replace the original periodic boundary value problem (9.88) by the following modification:

$$-v'' + \mu\,v = \lambda\,v, \qquad v(-\pi) = v(\pi), \qquad v'(-\pi) = v'(\pi). \qquad (9.118)$$

This does not alter the eigenfunctions, while adding μ to each of the eigenvalues, and hence the modified problem has eigenvalues $\lambda_0 = \mu$, with eigenfunction $v_0(x) \equiv 1$, and $\lambda_n = n^2 + \mu$, with two independent eigenfunctions: $v_n(x) = \cos nx$ and $\widetilde{v}_n(x) = \sin nx$.

The Green's function for the periodic boundary value problem

$$-v'' + \mu\,v = \delta(x - \xi), \qquad v(-\pi) = v(\pi), \qquad v'(-\pi) = v'(\pi),$$

where $\mu > 0$ is a fixed constant, is derived along the same lines as in Example 6.10. Setting $\mu = \omega^2$, the result is

$$G(x; \xi) = \frac{\cosh \omega\,(\pi - |x - \xi|)}{2\,\omega \sinh \pi \omega}. \qquad (9.119)$$

Its double L^2 norm is clearly finite, and, although unnecessary, can even be computed:

$$\|\,G\,\|^2 = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} G(x; \xi)^2\, dx\, d\xi = \frac{\pi\,(2\,\pi\omega + \sinh 2\,\pi\omega)}{4\omega^3 \sinh^2 \pi\omega} < \infty.$$

As a result, Theorem 9.47 reconfirms the completeness of the trigonometric eigenfunctions.

Example 9.50. According to (6.120), the Green's function $G(\mathbf{x}; \boldsymbol{\xi})$ for the Dirichlet boundary value problem for the Poisson equation on a domain $\Omega \subset \mathbb{R}^2$ is the sum of a logarithmic potential (6.106) and a harmonic function. Thus $G(\mathbf{x}; \boldsymbol{\xi})^2$ is a sum of three terms: the first two, involving $(\log r)^2$ and $\log r$ with $r = \|\,\mathbf{x} - \boldsymbol{\xi}\,\|$, have mild singularities when $\mathbf{x} = \boldsymbol{\xi}$, while the last term is smooth (indeed analytic) everywhere. Using this information, it is not hard to prove that its double L^2 norm

$$\|\,G\,\|^2 = \iint_{\Omega} \left[\iint_{\Omega} G(x, y; \xi, \eta)^2\, dx\, dy \right] d\xi\, d\eta < \infty$$

is finite. Indeed, the only problematic point is the logarithmic singularity at $\mathbf{x} = \boldsymbol{\xi}$, but a polar coordinate computation, similar to that used in the proof of Theorem 6.17, shows that such logarithmic singularities still have finite integrals. Therefore, Theorem 9.47 implies that the Helmholtz eigenvalues $\lambda_n \to \infty$, and the corresponding Helmholtz eigenfunctions $v_n(x, y)$ form a complete orthogonal system.

Remark: In problems involving unbounded domains, such as the Schrödinger equation for the hydrogen atom to be discussed in Section 12.7, the eigenfunctions are typically not complete, and one needs to introduce additional solutions corresponding to what is known as the *continuous spectrum* of the operator. Functions are now represented by combinations of discrete Fourier-like sums over the eigenfunctions (the bound states in the quantum-mechanical system) plus a Fourier integral-like term involving the continuous spectrum (the scattering states), [**66**, **72**]. A full discussion of completeness and convergence in such cases must be deferred to an advanced course in analysis, [**95**].

Exercises

9.4.1. Find the eigenvalues and an orthonormal eigenvector basis for the following symmetric matrices:

(a) $\begin{pmatrix} 2 & 6 \\ 6 & -7 \end{pmatrix}$, (b) $\begin{pmatrix} 5 & -2 \\ -2 & 5 \end{pmatrix}$, (c) $\begin{pmatrix} 2 & -1 \\ -1 & 5 \end{pmatrix}$, (d) $\begin{pmatrix} 1 & 0 & 4 \\ 0 & 1 & 3 \\ 4 & 3 & 1 \end{pmatrix}$, (e) $\begin{pmatrix} 6 & -4 & 1 \\ -4 & 6 & -1 \\ 1 & -1 & 11 \end{pmatrix}$.

9.4.2. Determine whether the following symmetric matrices are positive definite by computing their eigenvalues.

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

9.4.3. Suppose $S[\mathbf{u}] = K\,\mathbf{u}$, where $K = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. (a) Show that $S \colon \mathbb{R}^2 \to \mathbb{R}^2$ is positive semi-definite under the dot product. (b) Find the eigenvalues of S. (c) Explain why your result in part (b) does not contradict Theorem 9.34.

◇ 9.4.4. Suppose that $S \colon U \to U$ is a positive semi-definite linear operator. Let $I \colon U \to U$ be the identity operator, so $I[u] = u$. (a) Prove that, for any positive scalar $\mu > 0$, the operator $S_\mu = S + \mu\,I$ is positive definite. (b) Show that S and S_μ have the same eigenfunctions. Do they have the same eigenvalues? If not, how are their eigenvalues related?

9.4.5. Find the minimum value of $R[v] = \dfrac{\displaystyle\int_0^1 v'^2\,dx}{\displaystyle\int_0^1 v^2\,dx}$ on the space of C^2 functions $v(x)$ defined

on $0 \le x \le 1$ that are subject to one of the following pairs of boundary conditions:

(a) $v(0) = v(1) = 0$, (b) $v(0) = v'(1) = 0$, (c) $v'(0) = v'(1) = 0$.

9.4.6. Find the minimum value of $R[v] = \dfrac{\displaystyle\int_1^e x^2 v'^2\,dx}{\displaystyle\int_1^e v^2\,dx}$ on the space of C^2 functions defined on

$[1, e]$ subject to the boundary conditions $v(1) = v(e) = 0$.

9.4.7. Show that the Rayleigh quotient $R[v]$ has the same value for all nonzero scalar multiples of an element $0 \ne v \in U$, i.e., $R[cv] = R[v]$ for all $c \ne 0$.

9.4.8. Prove that the minimum value of the Rayleigh quotient of a positive semi-definite, but not positive definite, operator is 0.

♡ 9.4.9. (a) Find the eigenfunctions and eigenvalues for the boundary value problem
$$-x^2 u'' - x\,u' = \lambda\,u, \qquad u(1) = u(e) = 0.$$
(b) Under which inner product are the eigenfunctions orthogonal? Justify your answer by direct computation.
(c) Write down the eigenfunction expansion of a function $f(x)$ defined for $1 \le x \le e$.
(d) Find the Green's function for
$$-x^2 u'' - x\,u' = f(x), \qquad u(1) = u(e) = 0,$$
both in closed form and as a series in the eigenfunctions you found in part (a).
(e) Is your Green's function symmetric? Discuss.
(f) Prove the completeness of the eigenfunctions.

9.4.10. Discuss completeness of the eigenfunctions of the boundary value problem
$$-x^2 u'' - 2x\,u' = \lambda\,u, \qquad |u(0)| < \infty, \qquad u(1) = 0.$$

9.4.11. Consider the eigenvalue problem $-u'' = \lambda u$, $u(0) = 0$, $u'(1) = 0$. (a) Is the problem self-adjoint? positive definite? Which inner product are you referring to? (b) Find all eigenvalues and eigenfunctions. (c) Write down the explicit formula for the eigenfunction expansion of a function $f(x)$ defined on $[0, 1]$. (d) Find the Green's function and use it to prove completeness of the eigenfunctions.

♡ 9.4.12. (a) Find the eigenfunctions and eigenvalues for the *Chebyshev boundary value problem*
$$(x^2 - 1)u'' + x u' = \lambda u, \qquad u(-1) = u(1) = 0.$$
Hint: Let $x = \cos\theta$. (b) Under what inner product are the eigenfunctions orthogonal? Justify your answer by direct computation. (c) Find the Green's function for
$$(x^2 - 1)u'' + x u' = f(x), \qquad u(-1) = u(1) = 0,$$
both in closed form and as a series in the eigenfunctions you found in part (a).
(d) Discuss completeness of the eigenfunctions.

9.4.13. Consider the differential operator $S[u] = -u'' + u$ on the space of C^2 functions $u(x)$ defined for all x and subject to the boundary conditions $\lim\limits_{x \to \infty} u(x) = \lim\limits_{x \to -\infty} u(x) = 0$.
(a) Find the Green's function $G(x; \xi)$. (b) Compute its double L^2 norm: $\| G \|^2$. What does this indicate about the completeness of the eigenfunctions of S? (c) Justify your conclusion in part (b) by determining the eigenfunctions.

9.4.14. Find all (real and complex) eigenvalues of the first-derivative operator $D = d/dx$ on the interval $[0, 1]$ subject to the single periodic boundary condition $v(0) = v(1)$. Are the corresponding eigenfunctions orthogonal? For which inner product?

♡ 9.4.15. Consider the Dirichlet boundary value problem
$$-\Delta u = h(x, y), \quad u(x, 0) = 0, \quad u(x, 1) = 0, \quad u(0, y) = 0, \quad u(1, y) = 0, \quad 0 < x, y < 1,$$
for the Poisson equation on the unit square. (a) Find the eigenfunction series expansion for the Green's function of this problem. (b) Does your series coincide with that derived in Exercise 6.3.22? Explain any discrepancies. (c) For the impulse points $(\xi, \eta) = (.5, .5)$ and $(.7, .8)$, graph the result of summing the first 9, 25, and 100 terms in your series, and discuss what you observe in light of what you expect the Green's function to look like.

9.4.16. Find the eigenfunction series expansion for the Green's function of the following mixed boundary value problems:
(a) $-\Delta u = h(x, y), \quad u(x, 0) = 0, \quad u(x, 1) = 0, \quad u_x(0, y) = 0, \quad u_x(1, y) = 0, \quad 0 < x, y < 1$;
(b) $-\Delta u = h(x, y), \quad u(x, 0) = 0, \quad u_y(x, 1) = 0, \quad u(0, y) = 0, \quad u_x(1, y) = 0, \quad 0 < x, y < 1$.

9.4.17. Find the eigenfunction series expansion for the Green's function of the following Helmholtz boundary value problem:
$$-\Delta u + u = h(x, y), \qquad u(x, 0) = u(x, \pi) = u(0, y) = u(\pi, y) = 0, \qquad 0 < x, y < \pi.$$

◇ 9.4.18. If the eigenvalues of a self-adjoint linear operator satisfy $\lambda_n \to \infty$ as $n \to \infty$, explain why each eigenspace is necessarily finite-dimensional.

9.4.19. *True or false*: If $S: \mathbb{R}^n \to \mathbb{R}^n$ is any linear function, then one can find an inner product on $\mathbb{R}^n$ that makes S self-adjoint.

9.5 A General Framework for Dynamics

In this final section, we show how to use general eigenfunction expansions to analyze three important classes of linear dynamical systems: parabolic diffusion equations such as the heat equation, hyperbolic vibration equations such as the wave equation, and the Schrödinger equation, a complex evolution equation that governs the dynamical processes

of quantum mechanics. In all three cases we can, assuming completeness, write the general solution to the initial-boundary value problem as a convergent eigenfunction series with time-dependent coefficients, and thereby establish several general properties governing their dynamics.

Evolution Equations

In all cases, our starting point is the basic *equilibrium equation*, which is a linear system of the form

$$S[u] = f, \tag{9.120}$$

where f represents an external forcing. The linear operator S is assumed to be of the usual self-adjoint form

$$S = L^* \circ L, \tag{9.121}$$

which is either positive definite, when $\ker L = \{0\}$, or positive semi-definite, the latter case being characterized by the existence of null eigenfunctions $0 \neq v \in \ker L = \ker S$. In finite dimensions, (9.120) represents a linear algebraic system consisting of n equations in n unknowns with positive (semi-)definite coefficient matrix. In infinite-dimensional function space, it represents a self-adjoint positive (semi-)definite boundary value problem for the unknown function u.

With the equilibrium operator in hand, there are two principal classical dynamical systems of importance as physical models. The first are the (unforced) *diffusion processes* modeled by an evolution equation of the form

$$\frac{\partial u}{\partial t} = -S[u] = -L^* \circ L[u]. \tag{9.122}$$

In the discrete case, this represents a first-order system of ordinary differential equations, known as a linear *gradient flow*. In the continuous case, S is a linear differential operator equipped with homogeneous boundary conditions, and (9.122) represents a linear partial differential equation for the time-varying function $u = u(t, x)$, the heat equation being the prototypical example. (As in the preceding section, the notation employed below indicates that we are working in a single space dimension, but the methods and results apply equally well to higher-dimensional problems.) The addition of external forcing to the diffusion process is treated in Exercise 9.5.6.

The basic separation of variables solution technique was already outlined in Section 3.1. To recap, the separable solutions are of exponential form

$$u(t, x) = e^{-\lambda t}\, v(x), \tag{9.123}$$

where $v \in U$ is a fixed function. Since the operator S is linear and does not involve t differentiation, we find

$$\frac{\partial u}{\partial t} = -\lambda\, e^{-\lambda t}\, v, \qquad \text{while} \qquad S[u] = e^{-\lambda t}\, S[v].$$

Substituting back into (9.122) and canceling the common exponential factors, we are led to the eigenvalue problem

$$S[v] = \lambda\, v. \tag{9.124}$$

Thus, (9.123) defines a solution if and only if v is an eigenfunction for the linear operator S, with λ the corresponding eigenvalue.

We let $v_k(x)$, $k = 1, 2, \ldots$, be the orthogonal eigenfunctions and $0 \leq \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots \to \infty$ the corresponding eigenvalues. Assuming completeness, the solution to the initial value problem

$$u(0, x) = f(x) \tag{9.125}$$

can be expanded in terms of the eigensolutions:

$$u(t, x) = \sum_{k=1}^{\infty} e^{-\lambda_k t} c_k v_k(x), \qquad \text{where} \qquad c_k = \frac{\langle f, v_k \rangle}{\| v_k \|^2} \tag{9.126}$$

are the eigenfunction coefficients of the initial data. In particular, the *fundamental solution* of the diffusion equation is defined as the solution $u = F(t, x; \xi)$ to the initial value problem

$$u(0, x) = \delta_\xi(x) \tag{9.127}$$

induced by an initial delta impulse at the point ξ. Its eigenfunction coefficients are

$$c_k = \frac{\langle \delta_\xi, v_k \rangle}{\| v_k \|^2} = \frac{1}{\| v_k \|^2} \int_a^b \delta(x - \xi) v_k(x) \rho(x) \, dx = \frac{v_k(\xi) \rho(\xi)}{\| v_k \|^2} .$$

Thus,

$$F(t, x; \xi) = \sum_{k=1}^{\infty} e^{-\lambda_k t} \frac{v_k(x) v_k(\xi) \rho(\xi)}{\| v_k \|^2}, \tag{9.128}$$

where the denominator denotes the appropriately weighted L^2 norm of the eigenfunction:

$$\| v_k \|^2 = \int_a^b v_k(x)^2 \rho(x) \, dx.$$

As with the one-dimensional heat equation, if the equilibrium operator is positive definite, $S > 0$, then all the eigenvalues are strictly positive, and hence, generically, solutions decay to 0 at the exponential rate prescribed by the smallest eigenvalue, which can be characterized as the minimum value of the Rayleigh quotient. On the other hand, if S is only positive semi-definite, then the solution will tend to a null eigenmode, that is, an element of $\ker S = \ker L$, as its asymptotic equilibrium state. If $\dim \ker S = p$, the first p eigenvalues are all $0 = \lambda_1 = \cdots = \lambda_p < \lambda_{p+1}$, and the solution

$$u(t, x) \longrightarrow \sum_{k=1}^{p} c_k v_k(x) \qquad \text{as} \qquad t \longrightarrow \infty$$

will tend to its eventual equilibrium configuration at an exponential rate determined by the smallest positive eigenvalue $\lambda_{p+1} > 0$. In almost all applications, $p = 1$ and there is a single, constant null eigenfunction. The Neumann and periodic boundary value problems for the heat equation are prototypical examples.

Exercises

9.5.1. Find the eigenfunction series of the fundamental solution for the heat equation
$u_t = \gamma\, u_{xx}$ on the interval $0 \le x \le 1$ subject to homogeneous Dirichlet boundary conditions.

9.5.2. Solve Exercise 9.5.1 for (a) the mixed boundary conditions $u(t,0) = u_x(t,1) = 0$;
(b) homogeneous Neumann boundary conditions.

9.5.3. Let $D[u] = u'$ be the derivative operator acting on the vector space of C^1 scalar functions $u(x)$ defined for $0 \le x \le 1$ and satisfying the boundary conditions $u(0) = u'(1) = 0$.
(a) Given the L^2 inner product on its domain space and the weighted inner product
$\langle\, v\,, \tilde{v}\,\rangle = \int_0^1 v(x)\,\tilde{v}(x)\,x\,dx$ on its target space, determine the adjoint operator D^*.
(b) Let $S = D^* \circ D$. Write out the diffusion equation $u_t = -\,S[u]$ explicitly, as a partial differential equation plus boundary conditions.
(c) Given the initial condition $u(0,x) = x - x^2$, what is the asymptotic equilibrium
$u_\star(x) = \lim\limits_{t\,\to\,\infty} u(t,x)$ of the resulting solution to the diffusion equation?

9.5.4. Write down an eigenfunction series for the solution $u(t,x)$ to the initial value problem
$u(0,x) = f(x)$ for the fourth-order evolution equation $u_t = -\,u_{xxxx}$ subject to the boundary
conditions $u(t,0) = u_{xx}(t,0) = u(t,1) = u_{xx}(t,1) = 0$. Does your solution tend to an
equilibrium state? If so, at what rate?

9.5.5. Answer Exercise 9.5.4 for the boundary conditions
$$u_x(t,0) = u_{xxx}(t,0) = u_x(t,1) = u_{xxx}(t,1) = 0.$$

$\diamond$ 9.5.6. Explain how to solve the forced diffusion equation $u_t = -\,S[u] + f$, subject to homogeneous boundary conditions, when $f(x)$ does not depend on time t. Does the solution tend to equilibrium as $t \to \infty$? If so, what is the rate of decay, and what is the equilibrium?

9.5.7. Show that if $u(t,x)$ solves the diffusion equation (9.122), then $\|\, u(t,\,\cdot\,)\,\| \ge \|\, u(s,\,\cdot\,)\,\|$
whenever $t \le s$.

$\diamond$ 9.5.8. Let $S > 0$ be a positive definite operator. Suppose $F(t,x;\xi)$ is the fundamental
solution for the diffusion equation (9.122). Prove that $G(x;\xi) = \int_0^\infty F(t,x;\xi)\,dt$ is
the Green's function for the corresponding equilibrium equation $S[u] = f$.

Vibration Equations

The second important class of dynamical systems comprises the second-order (in time)
vibration equations
$$\frac{\partial^2 u}{\partial t^2} = -\,S[u], \tag{9.129}$$
which we initially analyze in the absence of external forcing. Vibrational systems arise as
a consequence of Newton's equations of motion in the absence of frictional forces. Their
continuum versions model the propagation of waves in solids and fluids, electromagnetic
waves, plasma waves, and many other related physical systems.

For a general vibration equation, the separable solutions are of trigonometric form
$$u(t,x) = \cos(\omega\, t)\, v(x) \qquad \text{or} \qquad \sin(\omega\, t)\, v(x). \tag{9.130}$$

Substituting either ansatz back into (9.129) results in the same eigenvalue problem (9.124) for $v(x)$ with eigenvalue $\lambda = \omega^2$ equal to the square of the vibrational frequency. We conclude that the *normal modes* or *eigensolutions* take the form

$$u_k(t, x) = \cos(\omega_k t)\, v_k(x), \qquad \widetilde{u}_k(t, x) = \sin(\omega_k t)\, v_k(x),$$

provided $\lambda_k = \omega_k^2 > 0$ is a nonzero eigenvalue and v_k an associated eigenfunction. Thus, the natural vibrational frequencies of the system are the square roots of the nonzero eigenvalues, a fact that we already observed in the context of the one-dimensional wave equation.

In the positive definite case, the eigenvalues are all strictly positive, and so the general solution is built up as a linear combination of vibrational eigenmodes:

$$
\begin{aligned}
u(t, x) &= \sum_{k=1}^{\infty} \left[c_k u_k(t, x) + d_k \widetilde{u}_k(t, x) \right] \\
&= \sum_{k=1}^{\infty} \left[c_k \cos(\omega_k t) + d_k \sin(\omega_k t) \right] v_k(x) = \sum_{k=1}^{\infty} r_k \cos(\omega_k t + \delta_k)\, v_k,
\end{aligned}
\tag{9.131}
$$

where

$$r_k = \sqrt{c_k^2 + d_k^2}, \qquad \delta_k = \tan^{-1} \frac{d_k}{c_k}. \tag{9.132}$$

The initial conditions

$$g(x) = u(0, x) = \sum_{k=1}^{\infty} c_k v_k(x), \qquad h(x) = u_t(0, x) = \sum_{k=1}^{\infty} d_k \omega_k v_k(x), \tag{9.133}$$

are used to specify the coefficients:

$$c_k = \frac{\langle\, g\,,v_k\,\rangle}{\|\, v_k\,\|^2}, \qquad d_k = \frac{\langle\, h\,,v_k\,\rangle}{\omega_k \|\, v_k\,\|^2}. \tag{9.134}$$

In the unstable, positive semi-definite cases, any null eigenfunction $v_0 \in \ker S = \ker L$ contributes two aperiodic eigensolutions:

$$u_0(t, x) = v_0(x), \qquad \widetilde{u}_0(t, x) = t\, v_0(x),$$

as can be readily checked. The first is constant in time, while the second is an unstable, linearly growing mode, which is excited if and only if the initial velocity is *not* orthogonal to the null eigenfunction: $\langle\, h\,, v_0\,\rangle \neq 0$.

If, as occurred in the one-dimensional wave equation, the natural frequencies happen to be integer multiples of a common frequency, $\omega_k = n_k \omega_\star$ for $n_k \in \mathbb{N}$, then the solution (9.131) is a periodic function of t with period $p_\star = 2\pi/\omega_\star$. On the other hand, in most cases the frequencies are not rationally related, and the solution is only *quasiperiodic*. Although it is the sum of individually periodic modes, it is not periodic, and never exactly reproduces its initial behavior; see the illustrative Example 2.20 for additional details.

Forcing and Resonance

Periodically forcing an undamped mechanical structure, modeled by a vibrational system of ordinary differential equations, at a frequency that is distinct from its natural vibrational frequencies, leads, in general, to a quasiperiodic response. The solution is a sum of the

unforced vibrational modes superimposed with an additional component that vibrates at the forcing frequency. However, if forced at one of its natural frequencies, the system may experience a catastrophic resonance. See [**89**; §9.6] for details.

The same type of quasiperiodic/resonant response is also observed in the partial differential equations governing the vibrations of continuous media. Consider the forced vibrational equation

$$\frac{\partial^2 u}{\partial t^2} = - S[u] + F(t, x), \tag{9.135}$$

subject to specified homogeneous boundary conditions. The external forcing function $F(t, x)$ may depend on both time t and position x. We will be particularly interested in a periodically varying external force of the form

$$F(t, x) = \cos(\omega t) \, h(x), \tag{9.136}$$

where ω is the forcing frequency, while the forcing profile $h(x)$ is unvarying.

As always, the solution to an inhomogeneous linear equation can be written as a combination,

$$u(t, x) = u_\star(t, x) + z(t, x), \tag{9.137}$$

of a particular solution $u_\star(t, x)$ to the inhomogeneous forced equation combined with the general solution $z(t, x)$ to the homogeneous equation, namely

$$\frac{\partial^2 z}{\partial t^2} = - S[z]. \tag{9.138}$$

The boundary and initial conditions will serve to uniquely prescribe the solution $u(t, x)$, but there is some flexibility in its two constituents (9.137). For instance, we may ask that the particular solution $u_\star$ satisfy the homogeneous boundary conditions along with zero (homogeneous) initial conditions and thus represent the pure response of the system to the forcing. The homogeneous solution $z(t, x)$ will then reflect the effect of the initial and boundary conditions unadulterated by the external forcing. The final solution is the combined sum of the two individual responses.

In the case of periodic forcing (9.136), we look for a particular solution

$$u_\star(t, x) = \cos(\omega t) \, v_\star(x) \tag{9.139}$$

that vibrates at the forcing frequency. Substituting the ansatz (9.139) into the equation (9.135) and canceling the common cosine factors, we discover that $v_\star(x)$ must satisfy the boundary value problem prescribed by a forced differential equation

$$S[v_\star] - \omega^2 \, v_\star = h(x), \tag{9.140}$$

supplemented by the relevant homogeneous boundary conditions: Dirichlet, Neumann, mixed, or periodic.

At this juncture, there are two possibilities. If the unforced homogeneous boundary value problem

$$S[v] - \omega^2 \, v = 0 \tag{9.141}$$

has only the trivial solution $v \equiv 0$, then, according to the Fredholm Alternative Theorem 9.10, a solution to the forced boundary value problem will exist[†] for any form of the

---

[†]   Existence is immediate in finite-dimensional systems. For boundary value problems, this relies on an analytic existence theorem, e.g., Theorem 9.28.

forcing function $h(x)$. In other words, if ω^2 is *not* an eigenvalue, then the particular solution (9.139) will vibrate with the forcing frequency, and the general solution will be a periodic or quasiperiodic combination (9.137) of the natural vibrational modes along with the vibrational response to the periodic forcing.

On the other hand, if $\omega^2 = \lambda_k$ is an eigenvalue, and so $\omega = \omega_k$ coincides with one of the natural vibrational frequencies of the homogeneous problem, then (9.141) admits nontrivial solutions, namely the eigenfunction[†] $v_k(x)$. In such cases, the Fredholm Alternative tells us that the boundary value problem (9.140) admits a solution if and only if the forcing function is orthogonal to the eigenfunction:

$$\langle\, h\,, v_k\,\rangle = 0. \tag{9.142}$$

If this holds, then the resulting particular solution (9.139) still vibrates with the forcing frequency, and resonance doesn't occur.

If we force in a resonant manner — meaning that the Fredholm condition (9.142) does *not* hold — then the solution will be a resonantly growing vibration of the form

$$u_\star(t, x) = a\,t \sin(\omega_k\,t)\,v_k(x) + \cos(\omega_k\,t)\,v_\star(x), \tag{9.143}$$

in which a is a constant to be specified as follows. By direct calculation,

$$\frac{\partial^2 u_\star}{\partial t^2} + S[u_\star] = a\,t \sin(\omega_k\,t)\,\big(\,S[v_k] - \omega_k^2\,v_k(x)\,\big)$$
$$+ \cos(\omega_k\,t)\,\big(\,S[v_\star] - \omega_k^2\,v_\star(x) + 2\,a\,\omega_k\,v_k(x)\,\big).$$

The first term vanishes, since $v_k(x)$ is an eigenfunction with eigenvalue $\lambda_k = \omega_k^2$. Therefore, (9.143) satisfies the forced boundary value problem if and only if $v_\star(x)$ satisfies the forced boundary value problem

$$S[v_\star] - \omega_k^2\,v_\star(x) = h(x) - 2\,a\,\omega_k\,v_k(x). \tag{9.144}$$

Again, the Fredholm Alternative implies that (9.144) admits a solution $v_\star(x)$ if and only if

$$0 = \langle\, h - 2\,a\,\omega_k v_k\,, v_k\,\rangle = \langle\, h\,, v_k\,\rangle - 2\,a\,\|\,v_k\,\|^2, \quad \text{and hence} \quad a = \frac{\langle\, h\,, v_k\,\rangle}{2\,\|\,v_k\,\|^2}, \tag{9.145}$$

which serves to fix the value of the constant in the resonant solution ansatz (9.143). In a real-world situation, such large resonant (or even near resonant) vibrations will, if unchecked, eventually either leads to a catastrophic breakdown of the system or to a transition into the nonlinear regime.

Example 9.51. As a specific example, consider the initial-boundary value problem modeling the forced vibrations of a uniform string of unit length that is fixed at both ends:

$$u_{tt} = c^2\,u_{xx} + \cos(\omega\,t)\,h(x),$$
$$u(t, 0) = 0 = u(t, 1), \quad u(0, x) = f(x), \quad u_t(0, x) = g(x). \tag{9.146}$$

[†] For simplicity, we assume that the eigenvalue λ_k is simple, and so there is a unique, up to constant multiple, eigenfunction v_k. Modifications for multiple eigenvalues proceed analogously.

The particular solution $u_\star(t, x)$ will have the nonresonant form (9.139), provided there exists a solution $v_\star(x)$ to the boundary value problem

$$S[v_\star] - \omega^2 v_\star = -c^2 v_\star'' - \omega^2 v_\star = h(x), \qquad\qquad v_\star(0) = 0 = v_\star(1). \qquad\qquad (9.147)$$

The natural frequencies and associated eigenfunctions of the unforced Dirichlet boundary value problem are

$$\omega_k = kc\pi, \qquad\qquad v_k(x) = \sin k\pi x, \qquad\qquad k = 1, 2, 3, \ldots .$$

Thus, the boundary value problem (9.147) will admit a solution, and hence the forcing is not resonant, if either $\omega \neq \omega_k$ is not a natural frequency or $\omega = \omega_k$ for some k but the forcing profile is orthogonal to the associated eigenfunction:

$$0 = \langle\, h\,, v_k\,\rangle = \int_0^1 h(x)\sin k\pi x\, dx. \qquad\qquad (9.148)$$

Otherwise, the system will undergo a resonant response.

For example, under periodic forcing of frequency ω with trigonometric sine profile $h(x) \equiv \sin k\pi x$, for k a positive integer, the particular solution to (9.147) is

$$v_\star(x) = \frac{\sin k\pi x}{\omega^2 - k^2\pi^2 c^2}, \qquad \text{so that} \qquad u_\star(t, x) = \frac{\cos\omega t\,\sin k\pi x}{\omega^2 - k^2\pi^2 c^2}, \qquad\qquad (9.149)$$

which is valid provided $\omega \neq \omega_k = k\pi c$. Observe that we may allow the forcing frequency to coincide with any of the other natural frequencies, $\omega = \omega_n$ for $n \neq k$, because the sine profiles are mutually orthogonal, and so the nonresonance condition (9.148) holds. On the other hand, if $\omega = \omega_k = k\pi c$, then the particular solution

$$u_\star(t, x) = \frac{t\,\sin k\pi ct\,\sin k\pi x}{2k\pi c} \qquad\qquad (9.150)$$

is resonant and grows linearly in time.

To obtain the full solution to the initial-boundary value problem, we write $u = u_\star + z$, where $z(t, x)$ must satisfy

$$z_{tt} - c^2 z_{xx} = 0, \qquad\qquad z(t, 0) = 0 = z(t, 1),$$

along with the modified initial conditions

$$z(0, x) = f(x) - \frac{\sin k\pi x}{\omega^2 - k^2\pi^2 c^2}, \qquad\qquad \frac{\partial z}{\partial t}(0, x) = g(x),$$

stemming from the fact that the particular solution (9.149) has a nontrivial initial displacement. (In the resonant case (9.150), there is no extra term in the initial data.) Note that the closer ω is to the resonant frequency, the larger the modification of the initial data, and hence the larger the response of the system to the periodic forcing. As before, the solution $z(t, x)$ to the homogeneous equation can be written as a Fourier sine series (4.68). The final formulas are left for the reader to write out in detail; see Exercise 9.5.14.

Exercises

9.5.9. Which of the following forcing functions $F(t, x)$ excites resonance in the wave equation $u_{tt} = u_{xx} + F(t, x)$ when subject to homogeneous Dirichlet boundary conditions on the interval $0 \leq x \leq 1$?   (a) $\sin 3t$, (b) $\sin 3\pi t$, (c) $\sin \frac{3}{2}\pi t$, (d) $\sin \pi t \, \sin \pi x$,
$\qquad\qquad\qquad$ (e) $\sin \pi t \, \sin 2\pi x$, (f) $\sin 2\pi t \, \cos \pi x$, (g) $x(1 - x)\sin 2\pi t$.

9.5.10. Answer Exercise 9.5.9 when the solution is subject to the mixed boundary conditions $u(t, 0) = u_x(t, 1) = 0$.

♡ 9.5.11. Let $\omega > 0$. Find the solution to the initial-boundary value problem
$$u_{tt} = u_{xx} + \cos \omega t, \quad u(t, 0) = 0 = u(t, 1), \quad u(0, x) = 0 = u_t(0, x).$$

9.5.12. Answer Exercise 9.5.11 for homogeneous Neumann boundary conditions.

9.5.13. A piano wire of length 1 m and wave speed $c = 2$ m/sec can support a maximal deflection of 5 cm before breaking. Suppose the wire starts at rest, with both ends fixed, and then is subject to a uniform periodic force $F(t, x) = \frac{1}{10}\cos \omega t \, \sin \pi x$. What range of frequencies will cause the wire to break?

◇ 9.5.14. Write out the eigenfunction series solution to the initial-boundary value problem in Example 9.51 with $h(x) \equiv \sin k\pi x$.

9.5.15. How should the solution formulas (9.131, 134) be modified when there are unstable modes? Write down explicit conditions on the initial data that prevent an instability from being excited.

◇ 9.5.16. Explain how to convert the homogeneous wave equation with inhomogeneous Dirichlet boundary conditions $u(t, 0) = \alpha(t)$, $u(t, \ell) = \beta(t)$, into a homogeneous boundary value problem for the forced wave equation. *Hint*: Mimic (4.46).

♡ 9.5.17. Two children hold a jump rope taut, while one of them periodically shakes their end of the rope. Use the inhomogeneous boundary value problem
$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \quad u(t, 0) = 0, \quad u(t, 1) = \sin \omega t,$$
to model the motion of the rope, adopting units in which the wave speed $c = 1$.
(a) What are the resonant frequencies of this system?
(b) Apply the method of Exercise 9.5.16 to find a particular solution to the boundary value problem when ω is a nonresonant frequency.
(c) Suppose the rope starts at rest. Find a series solution to the corresponding initial-boundary value problem when ω is a nonresonant frequency.
(d) Answer parts (b,c) when ω is a resonant frequency. *Hint*: Use the ansatz (9.143).

9.5.18. Explain how to solve the periodically forced *telegrapher's equation*
$$u_{tt} + a\,u_t = c^2\,u_{xx} + h(x)\cos \omega t$$
on the interval $0 \leq x \leq 1$ when subject to homogeneous Dirichlet boundary conditions. At which frequencies does the forcing function excite a resonant response?
Hint: First solve Exercise 4.2.9.

9.5.19. The fourth-order evolution equation $u_{tt} = -c^2 u_{xxxx}$, subject to the boundary conditions $u(t, 0) = u_{xx}(t, 0) = u(t, 1) = u_{xx}(t, 1) = 0$, models the transverse vibrations of a simply supported uniform thin elastic beam, in which $c > 0$ represents the wave speed. Write down an eigenfunction series for the solution to the initial value problem $u(0, x) = f(x)$, $u_t(0, x) = 0$. Is the solution
$\qquad\qquad$ (i) periodic, (ii) quasiperiodic, (iii) chaotic, (iv) none of the above?

The Schrödinger Equation

The fundamental dynamical system that governs all quantum-mechanical systems is known as the *Schrödinger equation*, first written down by the great twentieth-century German physicist Erwin Schrödinger, one of the preeminent founders of modern quantum physics. His original series of papers in which, by fits and starts, he arrives at his fundamental equation, makes for fascinating reading, [**101**].

Unlike classical mechanics, quantum mechanics is a completely linear theory, governed by linear systems of partial differential equations. The abstract form of the linear *Schrödinger equation* is

$$\mathrm{i}\,\hbar\,\frac{\partial\psi}{\partial t} = S[\psi], \tag{9.151}$$

where S is a linear operator of the usual self-adjoint form (9.121). In this equation, $\mathrm{i} = \sqrt{-1}$, while $\hbar$ is Planck's constant (7.69). The operator S is known as the *Hamiltonian* for the quantum-mechanical system, and, typically, represents the quantum energy operator. For physical systems such as atoms and nuclei, the relevant Hamiltonian operator is constructed from the classical energy through the rather mysterious process of "quantization".

At each time t, the solution $\psi(t, x)$ to the Schrödinger equation represents the wave function of the quantum system, and so should be a complex-valued square-integrable function having unit L^2 norm: $\|\psi\| = 1$. (The reader may wish to revisit Sections 3.5 and 7.1 for a discussion of the basics of quantum mechanics and Hilbert space.) We interpret the wave function as a probability density on the possible quantum states, and so the Schrödinger equation governs the dynamical evolution of quantum probabilities. The interested reader should consult a basic text on quantum mechanics, e.g., [**66, 72, 115**], for full details on both the physics and underlying mathematics.

Proposition 9.52. *If $\psi(t, x)$ is a solution to the Schrödinger equation, its Hermitian* L^2 *norm* $\|\psi(t, \cdot)\|$ *is fixed for all time.*

Proof: Since the solution is complex-valued, we use the sesquilinearity of the underlying Hermitian inner product, as in (B.19), to compute

$$\frac{d}{dt}\,\|\psi(t, \cdot)\|^2 = \left\langle\,\frac{\partial\psi}{\partial t}\,,\,\psi\,\right\rangle + \left\langle\,\psi\,,\,\frac{\partial\psi}{\partial t}\,\right\rangle = \left\langle\,-\frac{\mathrm{i}}{\hbar}\,S[\psi]\,,\,\psi\,\right\rangle + \left\langle\,\psi\,,\,-\frac{\mathrm{i}}{\hbar}\,S[\psi]\,\right\rangle$$

$$= -\frac{\mathrm{i}}{\hbar}\,\langle\,S[\psi]\,,\psi\,\rangle + \frac{\mathrm{i}}{\hbar}\,\langle\,\psi\,,S[\psi]\,\rangle = 0,$$

which vanishes because S is self-adjoint. This implies that $\|\psi(t, \cdot)\|^2$ is constant. *Q.E.D.*

As a result, if the initial data $\psi(t_0, x) = \psi_0(x)$ is a quantum-mechanical wave function, meaning that $\|\psi_0\| = 1$, then, at each time t, the solution $\psi(t, x)$ to the Schrödinger equation also has norm 1, and hence remains a wave function throughout the evolutionary process.

Apart from the extra factor of $\mathrm{i}\,\hbar$, the Schrödinger equation looks like a diffusion equation (9.122). This inspires us to seek separable solutions with an exponential ansatz:

$$\psi(t, x) = e^{\alpha\,t}\,v(x).$$

Substituting this expression into the Schrödinger equation (9.151) and canceling the common exponential factors reduces us to the usual eigenvalue problem

$$S[v] = \lambda v, \qquad \text{with eigenvalue} \qquad \lambda = i\hbar\alpha.$$

By self-adjointness, the eigenvalues are necessarily real. Let v_k denote the normalized eigenfunction, so $\| v_k \| = 1$, associated with the kth eigenvalue λ_k. The corresponding eigensolution of the Schrödinger equation is the complex-valued function

$$\psi_k(t, x) = e^{-i\lambda_k t/\hbar}\, v_k(x).$$

Observe that, in contrast to the exponentially decaying solutions to the diffusion equation, the eigensolutions to the Schrödinger equation are periodic, with vibrational frequencies $\omega_k = -\lambda_k/\hbar$ proportional to the eigenvalues. (Along with constant solutions corresponding to the null eigenmodes, if any.) The general solution is a (quasi)periodic series in the fundamental eigensolutions,

$$\psi(t, x) = \sum_k c_k \psi_k(t, x) = \sum_k c_k e^{-i\lambda_k t/\hbar}\, v_k(x), \qquad (9.152)$$

whose coefficients are prescribed by the initial conditions. The periodicity of the summands has the additional implication that, again unlike the diffusion equation, the Schrödinger equation can be run backwards in time, i.e., it remains well-posed in the past. Consequently, we can determine both the past and future behavior of a quantum system from its present configuration.

The eigenvalues represent the energy levels of the system described by the Schrödinger equation and can be experimentally detected by exciting the system. For instance, when an excited electron orbiting a nucleus jumps back to a lower energy level, it emits a photon whose observed electromagnetic spectral line corresponds to the difference between the energies of the two quantum levels. This motivates the use of the term *spectrum* to describe the eigenvalues of a linear Hamiltonian operator.

Example 9.53. The simplest version of the Schrödinger equation is based on the derivative operator $L = D$, leading to the self-adjoint combination $S = L^* \circ L = -D^2$ when subject to appropriate boundary conditions. In this case, the Schrödinger equation (9.151) reduces to the second-order partial differential equation

$$i\hbar\, \frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2}. \qquad (9.153)$$

If we impose the Dirichlet boundary conditions $\psi(t, 0) = \psi(t, \ell) = 0$, then the Schrödinger equation (9.153) governs the dynamics of a quantum particle that is confined to the interval $0 < x < \ell$; the boundary conditions imply that there is zero probability of the particle escaping from the interval.

According to Section 4.1, the eigenfunctions of the Dirichlet eigenvalue problem

$$v'' + \lambda v = 0, \qquad v(0) = v(\ell) = 0,$$

are

$$v_k(x) = \sqrt{\frac{2}{\ell}}\, \sin\frac{k\pi}{\ell}x, \quad \text{with eigenvalue} \quad \lambda_k = \frac{k^2\pi^2}{\ell^2}, \quad \text{for} \quad k = 1, 2, \ldots,$$

where the initial factor ensures that v_k has unit L^2 norm, and hence is a bona fide wave function. The corresponding oscillatory eigenmodes are

$$\psi_k(t, x) = \sqrt{\frac{2}{\ell}} \, \exp\left(-i \, \frac{k^2 \pi^2}{\hbar \, \ell^2} \, t \right) \sin \frac{k \pi}{\ell} \, x. \qquad (9.154)$$

Since the temporal frequencies $\omega_k = -k^2 \pi^2 / (\hbar \, \ell^2)$ depend nonlinearly on the wave number $k \pi / \ell$, the Schrödinger equation, is, in fact, *dispersive*, sharing many similarities with the third-order linear equation (8.90); see, for instance, Exercises 9.5.25, 27.

Exercises

9.5.20. (a) Solve the following initial boundary value problem:

$$i \, \hbar \, \psi_t = -\psi_{xx}, \qquad \psi(t, 0) = \psi(t, 1) = 0, \qquad \psi(0, x) = 1.$$

   (b) Using your solution formula, verify that $\| \psi(t, \cdot) \| = 1$ for all t.

9.5.21. Answer Exercise 9.5.20 for the initial condition $\psi(0, x) = \sqrt{30} \, x(1 - x)$.

9.5.22. Answer Exercise 9.5.20 when the solution is subject to Neumann boundary conditions $\psi_x(t, 0) = \psi_x(t, 1) = 0$.

9.5.23. Write down the eigenseries solution for the Schrödinger equation on a bounded interval $[0, \ell]$ when subject to homogeneous Neumann boundary conditions.

9.5.24. Given the solution formula (9.152), and assuming completeness of the eigenfunctions, prove that $\| \psi(t, \cdot) \|^2 = \sum_k | c_k |^2$ for all t.

$\Diamond$ 9.5.25. Write down the dispersion relation, phase velocity, and group velocity for the one-dimensional Schrödinger equation (9.153).

9.5.26. Show that the real and imaginary parts of the solution $\psi(t, x) = u(t, x) + i \, v(t, x)$ to the one-dimensional Schrödinger equation (9.153) are solutions to the beam equation of Exercise 9.5.19. What is the wave speed?

$\Diamond$ 9.5.27. *The Talbot effect for the linear Schrödinger equation*: Let $u(t, x)$ solve the periodic initial-boundary value problem

$$i \, u_t = u_{xx}, \quad u(t, -\pi) = u(t, \pi), \quad u_x(t, -\pi) = u_x(t, \pi),$$

with initial data $u(0, x) = \sigma(x)$ given by the unit step function. Prove that when $t = \pi p / q$, where p, q are integers, the solution $u(t, x)$ is constant on each interval $\hbar \pi j / q < x < \hbar \pi (j + 1) / q$ for integers $j \in \mathbb{Z}$. *Hint*: Use Exercise 6.1.29(d).

9.5.28. The wave function $\psi(t, x)$ of a one-dimensional free quantum particle of mass m satisfies the Schrödinger equation $i \psi_t = - \hbar \psi_{xx} / (2m)$ on the real line $-\infty < x < \infty$. Assuming that ψ and its x derivatives decay reasonably rapidly to zero as $| x | \to \infty$, prove that the particle's expected position $\langle x \rangle = \int_{-\infty}^{\infty} x \, | \psi(t, x) |^2 \, dx$ moves on a straight line.

Hint: Prove that $\dfrac{d^2 \langle x \rangle}{dt^2} = 0$.

♡ 9.5.29. Consider the periodically forced Schrödinger equation $i\hbar\psi_t = -\psi_{xx} + e^{i\omega t}$ on the interval $0 \le x \le 1$, subject to homogeneous Dirichlet boundary conditions. (a) At which frequencies ω does the forcing function excite a resonant response? (b) Find the solution to the general initial value problem for a nonresonant forcing frequency. (c) Find the solution to the general initial value problem for a resonant forcing frequency. What are the conditions on $\hbar$ that ensure that the resulting solution remains a wave function?

♡ 9.5.30. The Schrödinger equation for the *harmonic oscillator* is $i\hbar\psi_t = \psi_{xx} - x^2\psi$. Write this equation in the self-adjoint form (9.151) under a suitable choice of boundary conditions. Write down the self-adjoint boundary value problem for the eigenfunctions.
Remark: The eigenfunctions are not elementary functions. After studying Section 11.3, you may wish to return here to investigate its solutions.