

Chapter 9

A General Framework for Linear Partial Differential Equations

Before pressing on to the higher dimensional versions of the heat, the wave, and the Laplace and Poisson equations, it will be worth pausing to establish a very general framework that exposes the common features of a large range of linear partial differential equations appearing in applications. While the development this chapter is in a more abstract vein than usual, all the results are immediately applicable to the boundary and initial value problems governed by partial differential equations, and aid our comprehension of the degree of generality of and the interconnections between the various solution techniques. A more applications oriented reader may wish to skip ahead to the following two chapters, referring back to the material here as necessary.

Most equilibrium equations are boundary value problems involving a linear partial differential operator that satisfies the two key conditions of being “self-adjoint” and either “positive definite” or, more generally, “positive semi-definite”. So, our first task is to formulate the definition of 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 definition relies on the specification of inner products on both the domain and target spaces of the operator, and, when 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 to formulate the Fredholm Alternative, which provides the key constraints required for the existence of solutions to linear systems.

A linear operator that equals its own adjoint is called self-adjoint. The simplest example of a self-adjoint linear operator 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 see how to construct self-adjoint positive (semi-)definite operators in a canonical manner. Almost all of the linear differential operators studied in this text — in particular 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 or is not unique. In their dynamical counterparts, positive definite operators provide stable vibrational systems, whereas the positive semi-definite cases lead to unstable systems.

In addition, the solutions to positive definite linear systems can be characterized by a minimization principle, given by a certain quadratic functional. In physical contexts, the functional represents the potential energy of the system, and the solution minimizes the energy among all possible functions satisfying the prescribed boundary conditions. Nature is always conservative, and inevitably seeks to minimize energy! The minimization principle also underlies the powerful finite element numerical method to be presented in Section 10.5.

For 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 equations. In the simple, one-dimensional cases discussed in Chapter 4, the eigenfunctions are trigonometric, leading to the classical Fourier expansions for the solutions. The effectuality of the Fourier method relies on the orthogonality of the eigenfunctions. We already hinted that this is not an accident. Rather, it follows from their status as the eigenfunctions of a self-adjoint boundary value problem. Not only are the eigenvectors/eigenfunctions of a self-adjoint linear operator automatically mutually orthogonal with respect to the underlying inner product, the eigenvalues are necessarily real and, in the case the operator is also positive definite, also positive. Orthogonality underlies the general Fourier expansion of a function in terms of the eigenfunctions. Its convergence 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 with a general framework for dynamics, that explains how to construct the general Fourier series solutions for diffusion equations, vibration equations and quantum mechanical Schrödinger equations in terms of the eigenfunctions of the underlying equilibrium operator. The following two chapters will specialize these very general constructions to the two- and three-dimensional heat, wave, and Schrödinger equations in simple geometries.

9.1. Adjoints.

Our starting point is a linear function

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

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 regime. 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 elasto-mechanics, 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 contains potential functions and V contains 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

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

and a double angle bracket

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

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

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

To understand the definition, let's first look at the finite-dimensional case.

Example 9.2. According to Theorem B.32, every linear function $L: \mathbb{R}^n \rightarrow \mathbb{R}^m$ is given by matrix multiplication, $L[\mathbf{u}] = A\mathbf{u}$, where A is an $m \times n$ matrix. The adjoint function $L^*: \mathbb{R}^m \rightarrow \mathbb{R}^n$ is also linear, and goes in the reverse direction, so it is represented by matrix multiplication, $L^*[\mathbf{v}] = A^*\mathbf{v}$, by an $n \times m$ matrix A^* .

Suppose first that we impose the ordinary Euclidean dot products

$$\langle \mathbf{u}; \tilde{\mathbf{u}} \rangle = \mathbf{u} \cdot \tilde{\mathbf{u}} = \mathbf{u}^T \tilde{\mathbf{u}}, \quad \mathbf{u}, \tilde{\mathbf{u}} \in \mathbb{R}^n, \quad \langle\langle \mathbf{v}; \tilde{\mathbf{v}} \rangle\rangle = \mathbf{v} \cdot \tilde{\mathbf{v}} = \mathbf{v}^T \tilde{\mathbf{v}}, \quad \mathbf{v}, \tilde{\mathbf{v}} \in \mathbb{R}^m,$$

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

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

Since these expressions must agree for all \mathbf{u}, \mathbf{v} , we conclude 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: $A^* = A^T$* . Thus, the very simplest example of the adjoint operation is provided by the matrix transpose.

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

$$\langle \mathbf{u}; \tilde{\mathbf{u}} \rangle = \mathbf{u}^T M \tilde{\mathbf{u}}, \quad \mathbf{u}, \tilde{\mathbf{u}} \in \mathbb{R}^n, \quad \langle\langle \mathbf{v}; \tilde{\mathbf{v}} \rangle\rangle = \mathbf{v}^T C \tilde{\mathbf{v}}, \quad \mathbf{v}, \tilde{\mathbf{v}} \in \mathbb{R}^m, \quad (9.4)$$

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

$$\begin{aligned} \langle\langle L[\mathbf{u}]; \mathbf{v} \rangle\rangle &= \langle\langle A\mathbf{u}; \mathbf{v} \rangle\rangle = (A\mathbf{u})^T C \mathbf{v} = \mathbf{u}^T A^T C \mathbf{v}, \\ \langle \mathbf{u}; L^*[\mathbf{v}] \rangle &= \langle \mathbf{u}; A^*\mathbf{v} \rangle = \mathbf{u}^T M A^* \mathbf{v}. \end{aligned} \quad (9.5)$$

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

$$A^* = M^{-1}A^T C. \quad (9.6)$$

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

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

Example 9.3. Consider the derivative $v = D[u] = du/dx$, which, in elasto-mechanics, [104], defines a linear operator $D:U \rightarrow V$ from the vector space U of possible displacements $u(x)$ to the vector space V of possible strains $v(x)$. We assume that the functions in question are defined on an interval $a \leq x \leq b$.

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

$$\langle u; \tilde{u} \rangle = \int_a^b u(x) \tilde{u}(x) dx, \quad \langle\langle v; \tilde{v} \rangle\rangle = \int_a^b v(x) \tilde{v}(x) dx, \quad (9.7)$$

on both vector spaces. According to the defining equation (9.2), the adjoint D^* of the derivative operator must satisfy the inner product identity

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

First, we compute the left hand side:

$$\langle\langle D[u]; v \rangle\rangle = \left\langle\left\langle \frac{du}{dx}; v \right\rangle\right\rangle = \int_a^b \frac{du}{dx} v dx. \quad (9.9)$$

On the other hand, the right hand side should equal

$$\langle u; D^*[v] \rangle = \int_a^b u D^*[v] dx. \quad (9.10)$$

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

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

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

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

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

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

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

$$D^* = -D. \tag{9.13}$$

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

$$u(b)v(b) - u(a)v(a) = 0, \tag{9.14}$$

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

$$u(a) = 0, \quad u(b) = 0, \tag{9.15}$$

on the displacement $u(x)$ will ensure that (9.14) holds, and therefore validate (9.13). In this case, the domain space of $D:U \rightarrow V$ 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 $D:U \rightarrow V$ is required to map a function $u(x)$ to an *allowable* function $v(x)$, the domain space 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).

- Dirichlet boundary conditions: $u(a) = u(b) = 0$.
- Mixed boundary conditions: $u(a) = u'(b) = 0$ or $u'(a) = u(b) = 0$.
- Neumann boundary conditions: $u'(a) = u'(b) = 0$.
- Periodic boundary conditions: $u(a) = u(b), \quad u'(a) = u'(b)$.

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

Remark: In the preceding discussion, we were purposefully vague about the required differentiability of the functions. In finite dimensions, every linear function $L: \mathbb{R}^n \rightarrow \mathbb{R}^m$ 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 $L = D: U \rightarrow V$ requires the function $u \in U$ to be differentiable — or at least piecewise. On the other hand, the target function $v = D[u] = u'$ is not as smooth, and so belongs to a different function space; for instance if $u \in C^1[a, b]$, then $v = u' \in C^0[a, b]$. On the other hand, the adjoint $D^* = -D$ is only defined on differentiable functions v , so if $v \in C^1[a, b]$, then $u = -v' \in C^0[a, b]$. 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 only constrained by the imposed boundary conditions. When we write $L: U \rightarrow V$, we allow the possibility that the linear operator L may only be defined on a “dense” subspace of the domain space U . For instance, we will write $D: U \rightarrow V$ with $U = V = C^0[a, b]$, even though $D[u] = u' \in V$ only if u belongs to the subspace $C^1[a, b] \subset U = C^0[a, b]$. Similarly, $D^*: V \rightarrow U$ is also only defined on the subspace $C^1[a, b] \subset V = C^0[a, b]$. The term *dense* refers to the fact that any continuous function in the full space $U = C^0[a, b]$ can be arbitrarily closely approximated in norm by a continuously differentiable function in the subspace $C^1[a, b]$. Or, to put it another way, given $u \in C^0[a, b]$, there exists a sequence of functions $u_1, u_2, u_3, \dots \in C^1[a, b]$ such that $\|u_k - u\| \rightarrow 0$ as $k \rightarrow \infty$. A similar density result can be proved for $U = L^2[a, b]$, [111].

Warning: In more advanced analysis, our notion of adjoint is usually called the *formal adjoint*. A true adjoint requires more subtle analytical hypotheses on the operator and its domain of definition, cf. [108].

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

$$\langle u; \tilde{u} \rangle = \int_a^b u(x) \tilde{u}(x) \rho(x) dx, \quad \langle\langle v; \tilde{v} \rangle\rangle = \int_a^b v(x) \tilde{v}(x) c(x) dx, \quad (9.16)$$

where $\rho(x) > 0$ and $c(x) > 0$ are strictly positive functions which, physically, represent the density and stiffness of a non-uniform bar. Now we need to compare

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

Integrating the first expression by parts, we find

$$\int_a^b \frac{du}{dx} c v dx = [c(b) u(b) v(b) - c(a) u(a) v(a)] - \int_a^b u \frac{d(cv)}{dx} dx = \int_a^b u \left(-\frac{1}{\rho} \frac{d(cv)}{dx} \right) \rho dx, \quad (9.17)$$

provided that we choose our boundary conditions so that

$$c(b) u(b) v(b) - c(a) u(a) v(a) = 0. \quad (9.18)$$

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

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

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 result 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 $L:U \rightarrow V$ and $M:V \rightarrow W$ are linear functions, with $L^*:V \rightarrow U$ and $M^*:W \rightarrow V$ their respective adjoints. Then the composite linear function $M \circ L:U \rightarrow W$ has adjoint $(M \circ L)^* = L^* \circ M^*:W \rightarrow U$.*

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

$$(D^2)^* = D^* \circ D^* = (-D) \circ (-D) = D^2, \quad (9.20)$$

and so 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 $D:U \rightarrow V$ could be $U = \{u(x) \mid u(a) = 0 = u(b)\}$ while its target space V is unconstrained; the second D could then map V to $W = \{w(x) \mid w(a) = 0 = w(b)\}$. Another option would be to impose Neumann conditions on the first D , with $U = \{u'(a) = u'(b) = 0\}$ and $V = \{v(a) = v(b) = 0\}$, while W remains unconstrained. Under either these or other compatible constraints, both adjoint identifications $D^* = -D$ are valid, thus justifying (9.20). Keep in mind that, as per the earlier remark, the differentiation operators are, in fact, only defined on the dense subspaces containing sufficiently smooth functions.

Higher Dimensional Operators

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

$$\nabla u = \text{grad } u = \begin{pmatrix} u_x \\ u_y \end{pmatrix}.$$

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 $(x, y) \in \Omega$. 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 before, the gradient operator $\nabla: U \rightarrow V$ is only well-defined on the dense subspace $C^1(\Omega) \subset U$ 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 $z(x, y) = \nabla^* \mathbf{v}$. The defining equation for the adjoint

$$\langle\langle \nabla u; \mathbf{v} \rangle\rangle = \langle u; \nabla^* \mathbf{v} \rangle \quad (9.21)$$

relies on the choice of inner products on the two vector spaces. Let's first look at the L^2 inner product between scalar fields:

$$\langle u; \tilde{u} \rangle = \iint_{\Omega} u(x, y) \tilde{u}(x, y) dx dy. \quad (9.22)$$

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

$$\langle\langle \mathbf{v}; \tilde{\mathbf{v}} \rangle\rangle = \iint_{\Omega} \mathbf{v}(x, y) \cdot \tilde{\mathbf{v}}(x, y) dx dy = \iint_{\Omega} [v_1(x, y) \tilde{v}_1(x, y) + v_2(x, y) \tilde{v}_2(x, y)] dx dy. \quad (9.23)$$

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

$$\begin{aligned} \langle\langle \nabla u; \mathbf{v} \rangle\rangle &= \iint_{\Omega} \nabla u \cdot \mathbf{v} dx dy = \iint_{\Omega} \left(\frac{\partial u}{\partial x} v_1 + \frac{\partial u}{\partial y} v_2 \right) dx dy, \\ \langle u; \nabla^* \mathbf{v} \rangle &= \iint_{\Omega} u \nabla^* \mathbf{v} dx dy. \end{aligned}$$

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 secret is the *integration by parts* formula for double integrals,

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

already noted in (5.86). The left hand side is just $\langle\langle \nabla u; \mathbf{v} \rangle\rangle$. If the boundary line integral vanishes,

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

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

$$\langle\langle \nabla u; \mathbf{v} \rangle\rangle = \langle u; -\nabla \cdot \mathbf{v} \rangle, \quad (9.26)$$

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

$$\nabla^* \mathbf{v} = -\nabla \cdot \mathbf{v}. \quad (9.27)$$

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 lead immediately to the three principle types of (homogeneous) boundary conditions. The first are the *Dirichlet boundary conditions*, which require

$$u = 0 \quad \text{on} \quad \partial\Omega. \quad (9.28)$$

Alternatively, we can require that

$$\mathbf{v} \cdot \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega \quad (9.29)$$

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

$$\frac{\partial u}{\partial \mathbf{n}} = \nabla u \cdot \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega. \quad (9.30)$$

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

$$u = 0 \quad \text{on} \quad D, \quad \mathbf{v} \cdot \mathbf{n} = \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on} \quad N, \quad \text{where} \quad \partial\Omega = D \cup N \quad (9.31)$$

is the disjoint union of the Dirichlet and Neumann parts.

More generally, when modeling deflections of heterogeneous 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 weighted versions[†]

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

in which $\rho(x, y), \kappa_1(x, y), \kappa_2(x, y) > 0$ are strictly positive functions when $(x, y) \in \Omega$. 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 the same

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

integration by parts argument based on (5.86):

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

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”:

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

The vanishing of the boundary integral,

$$0 = \oint_{\partial\Omega} u (-\kappa_2 v_2 dx + \kappa_1 v_1 dy) = \oint_{\partial\Omega} u \tilde{\mathbf{v}} ds, \quad \text{where} \quad \tilde{\mathbf{v}} = \begin{pmatrix} \kappa_1 v_1 \\ \kappa_2 v_2 \end{pmatrix}$$

is assured if either $u = 0$ or $\tilde{\mathbf{v}} \cdot \mathbf{n} = 0$ on $\partial\Omega$. The first condition is the usual homogeneous Dirichlet condition, but the second represents a “weighted” version of the homogeneous Neumann boundary condition, requiring that $\tilde{\nabla} u \cdot \mathbf{n} = 0$ on the boundary, where $\tilde{\nabla} u = (\kappa_1 u_x, \kappa_2 u_y)^T$ represents a “weighted normal flux vector”.

Example 9.8. Let us compute the adjoint of the Laplacian $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ with respect to the L^2 inner products on both its domain and target spaces. The computation is a simple consequence of an earlier double integral identity (5.91), 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.

The Fredholm Alternative

Given a linear operator $L: U \rightarrow V$ between inner product spaces, we are interested in solving the associated linear systems

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

for various inhomogeneities f . In finite dimensions, this reduces to a linear algebraic system, $A\mathbf{u} = \mathbf{f}$, defined by a matrix A . For the linear ordinary and partial differential operators of interest to us, (9.35) represents a linear boundary value problem. In general, a linear system will not be solvable unless its right hand side satisfies certain constraints. These constraints can be readily characterized using the adjoint operator via the so-called *Fredholm Alternative*, named after the Swedish mathematician Ivar Fredholm. Fredholm's primary interest was in solving linear integral equations, but his solvability criterion was soon recognized to be a 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 $L[u] = 0$. Elements of the kernel of its adjoint, that is the set of solutions to the *homogeneous adjoint system*

$$L^*[v] = 0, \tag{9.36}$$

provide the required solvability constraints to the original inhomogeneous system. Keep in mind that, just as the original system (9.35) will involve boundary conditions, so will the adjoint system (9.36); see below for explicit examples.

Definition 9.9. The *cokernel* of L is defined as the kernel of its adjoint:

$$\text{coker } L = \ker L^* = \{ v \in V \mid L^*[v] = 0 \}. \tag{9.37}$$

The statement and proof of the Fredholm Alternative follow:

Theorem 9.10. *If the linear system (9.35) has a solution, then the right hand side f must be orthogonal to the cokernel of L , i.e.,*

$$\langle\langle v; f \rangle\rangle = 0 \quad \text{for all } v \in \text{coker } L. \tag{9.38}$$

Proof: If $L[u] = f$, then, by (9.2),

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

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

Q.E.D.

Remark: In practice, one only needs to check the orthogonality constraints (9.38) when v runs through a basis of the cokernel. In particular, if the only solution to the homogeneous adjoint system (9.36) 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. 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 existence of solutions for partial differential equations require the advanced mathematical machinery of functional analysis — see, e.g., , [45, 52, 73] — and so lie beyond the scope of this text.

Example 9.11. Consider the linear algebraic system

$$u_1 - u_3 = f_1, \quad u_2 - 2u_3 = f_2, \quad u_1 - 2u_2 + 3u_3 = f_3.$$

Using Gaussian Elimination (or by inspection), one easily sees that the system admits a solution if and only if the inhomogeneities satisfy the constraint

$$-f_1 + 2f_2 + f_3 = 0. \quad (9.39)$$

To connect this to the Fredholm Alternative, we write the system in matrix form $A\mathbf{u} = \mathbf{f}$ with 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 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.,

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

Its 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 single cokernel basis vector:

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

which is in accordance with the Fredholm Alternative (9.38).

Example 9.12. Let us solve the boundary value problem

$$u'' = f(x), \quad u'(0) = 0, \quad u'(\ell) = 0, \quad (9.40)$$

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

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

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

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

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

$$u'(\ell) = \int_0^\ell f(x) dx = 0. \quad (9.41)$$

If this fails, then the boundary value problem has no solution. On the other hand, if the right hand side satisfies the constraint (9.41), then the resulting solution of the boundary value problem has the form

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

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 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

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

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

Example 9.13. Consider the homogeneous Neumann boundary value problem for the Poisson equation, namely,

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

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

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

Theorem 5.15 tells us that the only solutions to the adjoint problem are the constant functions, $u(x, y) \equiv c$. Thus, a basis for the cokernel consists of the function $u(x, y) \equiv 1$, and so Fredholm Alternative requires that the forcing function in (9.43) must satisfy

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

reproducing our earlier constraint (5.93) for the homogeneous Neumann case.

9.2. Self-Adjoint and Positive Definite Linear Functions.

In applied linear algebra, [104], there are two particularly important classes of matrices: those that are symmetric, i.e., equal their own transpose, and those that are positive definite, as in Definition B.12. The goal of this section is to generalize both concepts to more general linear functions, paying particular attention to the case of linear differential operators.

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 analog of a symmetric matrix is a linear operator that equals its own adjoint.

Definition 9.14. A linear function $K:U \rightarrow U$ is called *self-adjoint* if $K^* = K$.

Thus, by (9.2), K is self-adjoint if and only if

$$\langle K[u]; \tilde{u} \rangle = \langle u; K[\tilde{u}] \rangle \quad \text{for all } u, \tilde{u} \in U. \quad (9.45)$$

Example 9.15. In the finite-dimensional case, a linear function $K:\mathbb{R}^n \rightarrow \mathbb{R}^n$ is realized by matrix multiplication: $K[\mathbf{u}] = P\mathbf{u}$, where P 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 $K^*:\mathbb{R}^n \rightarrow \mathbb{R}^n$ is given by multiplication by the transposed matrix: $K^*[\mathbf{u}] = P^T\mathbf{u}$. Thus, the function is self-adjoint with respect to the dot product if and only if it is represented by a symmetric matrix: $P^T = P$. On the other hand, if we adopt a weighted inner product $\langle \mathbf{u}; \tilde{\mathbf{u}} \rangle = \mathbf{u}^T C \tilde{\mathbf{u}}$ provided by the symmetric, positive definite matrix $C > 0$, then, according to (9.6), the adjoint K^* has matrix representative $C^{-1}P^T C$, and hence K is self-adjoint under the weighted inner product if and only if the matrix P satisfies $P^T C = C P$.

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

$$\int_a^b K[u] v dx = \langle\langle K[u]; v \rangle\rangle = \langle u; K^*[v] \rangle = \int_a^b u K^*[v] dx. \quad (9.46)$$

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

$$\begin{aligned} \langle\langle K[u]; v \rangle\rangle &= \int_a^b \frac{d^2 u}{dx^2} v dx = \left[\frac{du}{dx} v \right] \Big|_{x=a}^b - \int_a^b \frac{du}{dx} \frac{dv}{dx} dx \\ &= \left[\frac{du}{dx} v - u \frac{dv}{dx} \right] \Big|_{x=a}^b + \int_a^b u \frac{d^2 v}{dx^2} dx. \end{aligned}$$

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

$$\left[\frac{du}{dx} v - u \frac{dv}{dx} \right] \Big|_{x=a}^b = [u'(b)v(b) - u(b)v'(b)] - [u'(a)v(a) - u(a)v'(a)] = 0. \quad (9.47)$$

We need to impose two boundary conditions at each endpoint. Some common possibilities are to require either:

$$u(a) = v(a) = 0, \quad u(a) = v'(a) = 0, \quad v(a) = v'(a) = 0, \quad \text{or} \quad u'(a) = v'(a) = 0,$$

at the left hand endpoint, along with a second pair

$$u(b) = v(b) = 0, \quad u(b) = v'(b) = 0, \quad v(b) = v'(b) = 0, \quad \text{or} \quad u'(b) = v'(b) = 0,$$

at the other end. You are allowed to mix or match the options in any combination.

Positive Definiteness

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

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

$$\langle u; K[u] \rangle > 0 \quad \text{for all} \quad u \neq 0. \quad (9.48)$$

The function K is *positive semi-definite*, written $K \geq 0$, if

$$\langle u; K[u] \rangle \geq 0 \quad \text{for all} \quad u. \quad (9.49)$$

Observe that, on the finite dimensional space $U = \mathbb{R}^n$ equipped with the dot product, the linear function $K[\mathbf{u}] = P\mathbf{u}$ is positive (semi-)definite if and only if $P > 0$ 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 P ; see Exercise ■.) In the infinite-dimensional situations involving differential operators, the domain of the operator may only be a dense subspace of the full inner product space U , and one imposes the positivity conditions (9.48) or (9.49) only on those functions u lying in the domain of K . This technicality has no serious effect on the subsequent development.

Proposition 9.18. *If $K > 0$, then $\ker K = \{0\}$. As a consequence, a positive definite linear system $K[u] = f$ with $f \in \text{rng } K$ must have a unique solution.*

Proof: If $K[u] = 0$, then $\langle u; K[u] \rangle = 0$, which, according to (9.48), is only possible 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 is non-singular, $\det P \neq 0$, 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.

The most common means of producing self-adjoint, positive (semi-)definite linear operators is provided by the following result.

Theorem 9.19. *Let $L: U \rightarrow V$ be a linear map between inner product spaces with adjoint $L^*: V \rightarrow U$. Then the composite map*

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

is self-adjoint and positive semi-definite, with $\ker K = \ker L$. Moreover, K is positive definite if and only if $\ker L = \{0\}$.

Proof: First, by Propositions 9.5 and 9.6,

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

proving self-adjointness. Furthermore,

$$\langle u; K[u] \rangle = \langle u; L^*[L[u]] \rangle = \langle L[u]; L[u] \rangle = \|L[u]\|^2 \geq 0 \quad (9.50)$$

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 $\langle u; K[u] \rangle > 0$ for all $u \neq 0$, and hence K is positive definite. Finally, the same computation proves that $\ker K = \ker L$. Indeed, if $L[u] = 0$, then $K[u] = L^*[L[u]] = L^*[0] = 0$. On the other hand, if $K[u] = 0$, then $0 = \langle u; K[u] \rangle = \|L[u]\|^2$, and hence $L[u] = 0$. *Q.E.D.*

We are particularly interested in linear systems that are based on the construction of Theorem 9.19, namely

$$K[u] = L^*[L[u]] = f. \quad (9.51)$$

We will refer to the system (9.51) as *positive definite* or *positive semi-definite* according to the status of its defining operator K . Thus, the system is positive definite if and only if $\ker K = \ker L = \{0\}$, i.e., the only solution to the homogeneous system $K[z] = 0$ is the trivial solution $z = 0$. In this case the solution to (9.51) (provided it exists) is unique. On the other hand, if there are non-zero solutions to $K[z] = 0$, then (9.51) is only positive semi-definite, and does not admit a unique solution. Moreover, unless the Fredholm Alternative constraints (9.38) hold, then there are no solutions. By self-adjointness and Theorem 9.19, we can identify

$$\operatorname{coker} K = \ker K^* = \ker K = \ker L, \quad (9.52)$$

which thus implies the following:

Theorem 9.20. *Let $K = L^* \circ L$. If the linear system $K[u] = f$ has a solution, then $\langle z; f \rangle = 0$ for all $z \in \ker L$. Moreover, if $K[u] = f$ and $K[\tilde{u}] = f$ are two solutions to the same linear system, then $\tilde{u} = u + z$, where z is any solution to $L[z] = 0$.*

The Fredholm Alternative provides *necessary conditions* for the solvability of the system, but, in infinite-dimensional problems, the actual existence must still be proved by some additional analysis. Again, for the positive semi-definite boundary value problems treated in this text, this can be established, and hence the Fredholm conditions are both necessary and sufficient for the existence of a (perhaps non-unique) solution.

Example 9.21. In the finite-dimensional case, any linear $L: \mathbb{R}^n \rightarrow \mathbb{R}^m$ 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 hence the self-adjoint combination $K = L^* \circ L: \mathbb{R}^n \rightarrow \mathbb{R}^n$ is represented by the $n \times n$ symmetric matrix $P = A^T A$. According to Theorem 9.19, the matrix P 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 9.20 states that the linear system $P\mathbf{u} = \mathbf{f}$ 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 $\tilde{\mathbf{u}} = \mathbf{u} + \mathbf{z}$ 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 $K = L^* \circ L$ is given by multiplication by the (not necessarily symmetric) $n \times n$ matrix $P = M^{-1}A^T C A$. Again, $P \geq 0$ in all cases, and is positive definite if and only if $\ker A = \{\mathbf{0}\}$. Now, the Fredholm Alternative states that the linear system $P\mathbf{u} = M^{-1}A^T C A\mathbf{u} = \mathbf{f}$ 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 [104] for many applications of this construction in mechanics, electrical networks, and the stability of structures.

Example 9.22. Consider next the differentiation operator $D[u] = u'$. According to Example 9.3, if we impose suitable homogeneous boundary conditions on the space of functions — Dirichlet, Neumann, mixed, 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 9.19 is given by $K = D^* \circ D = -D^2$.

According to Theorem 9.19, the resulting boundary value problem

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

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 an 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 $u(a) = u(b)$, $u'(a) = u'(b)$, is also positive semi-definite.

More generally, if we use weighted inner products (9.16), then, again subject to suitable boundary conditions, the adjoint is given by (9.19), and so the self-adjoint boundary value

problem $K[u] = D^* \circ D[u] = f$ is based on the more general differential equation

$$K[u] = -\frac{1}{\rho(x)} \left(\frac{d}{dx} c(x) \frac{du}{dx} \right) = f(x). \quad (9.53)$$

Such boundary value problems model the deformations of a non-uniform elastic bar with density $\rho(x)$, stiffness $c(x)$, 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 also underlies the observed symmetry of the Green's function of a positive definite boundary value problem $K[u] = f$. (Indeed, this is the differential operator version of the statement that the inverse of a symmetric matrix is also symmetric.) We begin by assuming that K is a self-adjoint ordinary differential operator under the L^2 inner product on the interval $[a, b]$. As a function of x , the Green's function $G_\xi(x) = G(x; \xi)$ satisfies

$$K[G_\xi] = \delta_\xi, \quad \text{or, explicitly,} \quad -\frac{1}{\rho(x)} \left(\frac{\partial}{\partial x} c(x) \frac{\partial}{\partial x} \right) G(x; \xi) = \delta(x - \xi), \quad (9.54)$$

along with the required homogeneous boundary conditions. Thus, by the definition of the delta function $\delta_\xi(x) = \delta(x - \xi)$ and the self-adjointness identity (9.45),

$$\begin{aligned} G(x; \xi) = G_\xi(x) &= \int_a^b G_\xi(y) \delta_x(y) dy = \langle G_\xi; \delta_x \rangle = \langle G_\xi; K[G_x] \rangle \\ &= \langle K[G_\xi]; G_x \rangle = \langle \delta_\xi; G_x \rangle = \int_a^b \delta_\xi(y) G_x(y) dy = G_x(\xi) = G(\xi; x), \end{aligned} \quad (9.55)$$

for any $a < x, \xi < b$, which establishes[†] the symmetry equation

$$G(x; \xi) = G(\xi; x) \quad (9.56)$$

for such a Green's function. On the other hand, if we adopt a weighted inner product

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

then the preceding argument must be slightly modified:

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

[†] Symmetry at the endpoints follows from continuity.

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

$$\rho(x) G(x; \xi) = \rho(\xi) G(\xi; x). \quad (9.57)$$

Remark: Equation (9.57) implies that the *modified Green's function*

$$\widehat{G}(x; \xi) = \frac{G(x; \xi)}{\rho(\xi)} \quad \text{is genuinely symmetric:} \quad \widehat{G}(x; \xi) = \widehat{G}(\xi; x). \quad (9.58)$$

The modified function also has the effect of recasting the superposition formula for the solution to the boundary value problem $K[u] = f$ as a suitably weighted inner product:

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

Two-Dimensional Boundary Value Problems

Let us next apply the self-adjoint formalism to study boundary value problems on a two-dimensional domain $\Omega \subset \mathbb{R}^2$, which we assume to be both bounded and connected. (Similar considerations apply to three- and even higher dimensional problems.) 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 use 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 9.19 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

$$-\Delta u = -\nabla \cdot (\nabla u) = \nabla^* \circ \nabla u = f, \quad (9.59)$$

subject to the chosen boundary conditions.

According to Theorem 9.19, $-\Delta = \nabla^* \circ \nabla$ 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 5.16 tells us that the only functions which could show up in $\ker \nabla$, and thus prevent positive definiteness, are the constants. The boundary conditions will tell us whether or not 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 that means that its solution is uniquely defined. On the other hand, any constant function satisfies the homogeneous Neumann boundary conditions $\partial u / \partial \mathbf{n} = 0$, 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, according to (9.34), the corresponding self-adjoint equation boundary value problem takes the more general form

$$\nabla^* \circ \nabla u = -\frac{1}{\rho(x, y)} \frac{\partial}{\partial x} \left(\kappa_1(x, y) \frac{\partial u}{\partial x} \right) - \frac{1}{\rho(x, y)} \frac{\partial}{\partial x} \left(\kappa_2(x, y) \frac{\partial u}{\partial y} \right) = f(x, y), \quad (9.60)$$

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 (9.60) arises in various physical contexts. For example, consider a steady-state fluid flow described by a vector field \mathbf{v} moving in a domain $\Omega \subset \mathbb{R}^2$. The flow is called *irrotational* if it has zero curl, $\nabla \times \mathbf{v} = \mathbf{0}$, and hence, assuming Ω is simply connected, is a gradient $\mathbf{v} = \nabla u$. The function $u(x, y)$ 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

$$-\nabla \cdot (\kappa \nabla u) = f, \quad \text{or} \quad -\frac{\partial}{\partial x} \left(\kappa(x, y) \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left(\kappa(x, y) \frac{\partial u}{\partial y} \right) = f(x, y), \quad (9.61)$$

which is (9.60) with $\kappa \rightarrow 1$ and $\kappa_1, \kappa_2 \rightarrow \kappa$. The most common case of a homogeneous (constant density) fluid thus reduces to the Poisson equation (4.73), with f replaced by f/κ .

Symmetry of the Green's function for the Poisson equation and the more general boundary value problem (9.60) follows by an adaptation of the one-dimensional argument presented above. Details are left as an exercise for the reader.

9.3. Minimization Principles.

One of the most important features of positive definite linear problems is that their solution can be characterized by a minimization principle. In many physical contexts, both linear and nonlinear, the 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 halted its motion, the ball will be left sitting in equilibrium at the bottom of the bowl — the position that minimizes the potential gravitational energy.

When the equilibrium equations form a linear system, the energy depends quadratically on the solution. Let us thus begin by stating and proving the basic minimization theorem for quadratic function(al)s.

Theorem 9.23. *Let $K: U \rightarrow U$ be a self-adjoint and positive definite linear operator on an inner product space U . Assume that the linear system*

$$K[u] = f \quad (9.62)$$

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

$$Q[u] = \frac{1}{2} \langle u; K[u] \rangle - \langle f; u \rangle, \quad (9.63)$$

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

This characterization of the solutions to positive definite linear systems as the minimizers of an associated quadratic functional is of fundamental importance for the analysis of solutions to (positive definite) boundary value problems defined by both ordinary and partial differential equations, including proofs of existence of solutions, as well as forming the basis of one of the most powerful numerical solution techniques — the finite element method — to be studied in Chapter 10. Explicit examples will appear after the proof.

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

$$Q[u] = \frac{1}{2} \langle u; K[u] \rangle - \langle u; K[u_\star] \rangle = \frac{1}{2} \langle u - u_\star; K[u - u_\star] \rangle - \frac{1}{2} \langle u_\star; K[u_\star] \rangle, \quad (9.64)$$

where we used linearity, along with our assumption that K is self-adjoint to identify the terms $\langle u; K[u_\star] \rangle = \langle u_\star; K[u] \rangle$. Since $K > 0$, the first term on the right hand side of (9.64) is always ≥ 0 ; moreover it equals 0 if and only if $u = u_\star$. On the other hand, the second term does not depend upon 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 9.24. Consider the the problem of minimizing a *quadratic function*

$$Q(u_1, \dots, u_n) = \frac{1}{2} \sum_{i,j=1}^n p_{ij} u_i u_j - \sum_{i=1}^n f_i u_i + c, \quad (9.65)$$

depending on n variables $\mathbf{u} = (u_1, u_2, \dots, u_n)^T \in \mathbb{R}^n$, with fixed real coefficients p_{ij}, b_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: $p_{ij} = p_{ji}$. We rewrite (9.65) in matrix notation as

$$Q(\mathbf{u}) = \frac{1}{2} \mathbf{u} \cdot P \mathbf{u} - \mathbf{f} \cdot \mathbf{u} + c, \quad (9.66)$$

which, apart from the inessential constant term, agrees with (9.63) once we set $K[\mathbf{u}] = P \mathbf{u}$ and use the dot product $\langle \mathbf{v}; \mathbf{w} \rangle = \mathbf{v} \cdot \mathbf{w}$ as the inner product on \mathbb{R}^n . Thus, according to Theorem 9.23, if $P > 0$ is a symmetric, positive definite matrix, then the quadratic function (9.66) has a unique minimizer $\mathbf{u}^\star = (u_1^\star, \dots, u_n^\star)^T$, which is the solution to the linear system $P \mathbf{u}^\star = \mathbf{f}$.

If the positive definite linear operator in Theorem 9.23 comes from the self-adjoint construction of Theorem 9.19, so $K = L^\star \circ L$, then, by (9.50), the quadratic term can be re-expressed as $\langle u; K[u] \rangle = \|L[u]\|^2$. We can thus rephrase the minimization principle as follows:

Theorem 9.25. *Suppose $L: U \rightarrow V$ is a linear function between inner product spaces with $\ker L = \{\mathbf{0}\}$, and adjoint $L^\star: V \rightarrow U$. Let $K = L^\star \circ L: U \rightarrow U$ be the associated positive definite linear function. Assuming $f \in \text{rng } K$, then the quadratic function*

$$Q[u] = \frac{1}{2} \|L[u]\|^2 - \langle f; u \rangle \quad (9.67)$$

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

Warning: In (9.67), 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 this result is the method of least squares, extensively applied in data analysis and approximation theory. We refer the interested reader to [104] for developments in this direction. Here we will concentrate on applications to differential equations.

Example 9.26. Consider the boundary value problem

$$-u'' = f(x), \quad u(0) = 0, \quad u(\ell) = 0. \quad (9.68)$$

The underlying differential operator $K = D^* \circ D = -D^2$, when acting on the functions satisfying the boundary conditions, is self-adjoint and positive definite. Explicitly, positive definiteness requires

$$\langle K[u]; u \rangle = \int_a^b [-u''(x)u(x)] dx = \int_a^b [u'(x)]^2 dx = \|L[u]\|^2 > 0 \quad (9.69)$$

for all nonzero $u(x) \not\equiv 0$ with $u(0) = u(\ell) = 0$. 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 (9.67),

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

Its minimum value, taken over all possible functions that satisfy the homogeneous Dirichlet boundary conditions, occurs precisely when $u = u_*$ is the solution to the boundary value problem.

Sturm–Liouville Boundary Value Problems

The most important general class of boundary value problems governed by second order ordinary differential equations were 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

$$K[u] = -\frac{d}{dx} \left(p(x) \frac{du}{dx} \right) + q(x)u = -p(x) \frac{d^2u}{dx^2} - p'(x) \frac{du}{dx} + q(x)u = f(x), \quad (9.70)$$

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 that $p(x) > 0$ for all $a \leq x \leq b$. To ensure positive definiteness, we will also assume that $q(x) > 0$. Actually, it is not difficult to relax these conditions to allow p and q vanish at isolated points.

Sturm–Liouville boundary value problems appear in a broad range of applications, particularly in the analysis of partial differential equations by the method of separation of variables. Moreover, most of the important special functions, including Bessel functions,

Legendre functions, hypergeometric functions, and so on, naturally appear as solutions to particular Sturm–Liouville equations, [3, 102]. A partial list of applications includes

- heat conduction in non-uniform bars;
- vibrations of non-uniform bars and strings;
- vibrations of circular membranes (drums) and cylinders — Bessel’s equation;
- oscillations of a sphere — Legendre’s equation;
- thermodynamics of cylindrical and spherical bodies;
- quantum mechanics — the one-dimensional Schrödinger equation; and
- scattering theory — Hill’s equation.

To place a Sturm–Liouville boundary value problem in our self-adjoint framework, we proceed as follows. Consider the linear operator

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

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 $L:U \rightarrow V$, we use the standard L^2 inner product (9.7) on U , but adopt the following weighted inner product

$$\langle\langle \mathbf{v}; \mathbf{w} \rangle\rangle = \int_a^b [p(x)v_1(x)w_1(x) + q(x)v_2(x)w_2(x)] dx, \quad \mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad \mathbf{w} = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}, \quad (9.71)$$

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

$$\begin{aligned} \langle\langle L[u]; \mathbf{v} \rangle\rangle &= \int_a^b (p u' v_1 + q u v_2) dx \\ &= p(b)u(b)v_1(b) - p(a)u(a)v_1(a) + \int_a^b u [-(pv_1)' + qv_2] dx. \end{aligned}$$

The boundary terms will disappear provided, at each endpoint, either u or v_1 vanishes. Since we can identify $v_1 = u'$, we conclude that any of our usual boundary conditions — Dirichlet, mixed, or Neumann — remain valid here. Under these conditions,

$$\langle\langle L[u]; \mathbf{v} \rangle\rangle = \int_a^b u [-(pv_1)' + qv_2] dx = \langle u; L^*[\mathbf{v}] \rangle,$$

and so the adjoint operator is given by

$$L^*[\mathbf{v}] = -\frac{d(pv_1)}{dx} + qv_2 = -pv_1' - p'v_1 + qv_2.$$

The canonical self-adjoint combination

$$K[u] = L^* \circ L[u] = L^* \begin{pmatrix} u' \\ u \end{pmatrix} = -\frac{d}{dx} \left(p \frac{du}{dx} \right) + qu \quad (9.72)$$

then reproduces the Sturm–Liouville differential operator (9.70). 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 Existence Theorem can be found in [78].

Theorem 9.27. *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 (9.70) admits a unique solution.*

As we know, the solutions to positive definite boundary value problems can be characterized by a minimization principle. Indeed, Theorem 9.25 implies that the solution to the Sturm–Liouville boundary value problem (9.70) can be characterized as the unique minimizer of the quadratic functional

$$Q[u] = \frac{1}{2} \|L[u]\|^2 - \langle f; u \rangle = \int_a^b \left[\frac{1}{2} p(x) u'(x)^2 + \frac{1}{2} q(x) u(x)^2 - f(x) u(x) \right] dx \quad (9.73)$$

among all C^1 functions satisfying the prescribed homogeneous boundary conditions.

Example 9.28. For example, consider the constant coefficient Sturm–Liouville problem

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

studied earlier in Example 5.10. Its solution yields the minimum possible value for the quadratic functional

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

among all functions satisfying the given boundary conditions.

More generally, suppose we adopt a weighted inner product

$$\langle u; \tilde{u} \rangle = \int_a^b u(x) \tilde{u}(x) \rho(x) dx \quad (9.74)$$

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,

$$L^*[\mathbf{v}] = \frac{1}{\rho} \left(-\frac{d(pv_1)}{dx} + qv_2 \right) = -\frac{p}{\rho} v_1' - \frac{p'}{\rho} v_1 + \frac{q}{\rho} v_2,$$

and so the weighted Sturm–Liouville differential operator is

$$K[u] = L^* \circ L[u] = \frac{1}{\rho} \left[-\frac{d}{dx} \left(p \frac{du}{dx} \right) + qu \right]. \quad (9.75)$$

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

$$K[u] = \frac{1}{\rho(x)} \left[-\frac{d}{dx} \left(p(x) \frac{du}{dx} \right) + q(x) u \right] = -\frac{p(x)}{\rho(x)} \frac{d^2 u}{dx^2} - \frac{p'(x)}{\rho(x)} \frac{du}{dx} + \frac{q(x)}{\rho(x)} u = f(x), \quad (9.76)$$

which is, in fact, the same as (9.70) after we replace f by ρf . On the other hand, the weighted generalization will become important when we discuss eigenvalue problems.

Example 9.29. Let $m > 0$ be a fixed parameter. Consider the differential equation

$$K[u] = -u'' - \frac{1}{x} u' + \frac{m^2}{x^2} u = f(x), \quad (9.77)$$

where K is known as the *Bessel differential operator of order m* . To place it in weighted Sturm–Liouville form (9.76), we must find $p(x)$, $q(x)$ and $\rho(x)$ that satisfy

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

Clearly, we can set

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

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

$$\langle u; \tilde{u} \rangle = \int_a^b u(x) \tilde{u}(x) x \, dx. \quad (9.78)$$

The Dirichlet Principle

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

$$-\Delta u = \nabla^* \circ \nabla u = f.$$

In the positive definite cases when the partial differential equation is supplemented by either homogeneous Dirichlet or homogeneous mixed boundary conditions, the solution can be characterized by the justly famous *Dirichlet Minimization Principle*.

Theorem 9.30. *The function $u(x, y)$ that minimizes the Dirichlet integral*

$$Q[u] = \frac{1}{2} \|\nabla u\|^2 - \langle f; u \rangle = \iint_{\Omega} \left(\frac{1}{2} u_x^2 + \frac{1}{2} u_y^2 - f u \right) dx \, dy, \quad (9.79)$$

among all C^1 functions that satisfy the prescribed homogeneous Dirichlet or mixed boundary conditions, is the solution to the corresponding boundary value problem for the Poisson equation $-\Delta u = f$.

Remark: The fact that a minimizer to the Dirichlet integral (9.79) satisfies the Poisson equation is an immediate consequence of our general Minimization Theorem 9.25. However, proving the *existence* of a minimizing function is a non-trivial issue. Indeed, this was not immediately recognized: Dirichlet originally thought existence to be self-evident, but it then took about 50 years until Hilbert supplied the first rigorous proof. (Indeed, this was one of his primary motivations for introducing Hilbert space.)

The Dirichlet principle (9.79) 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 inhomogeneous Dirichlet boundary conditions. However, if we have a mixed boundary value problem with inhomogeneous Neumann conditions on part of the boundary, then we must include an additional boundary term in the minimizing functional. The general result can be stated as follows:

Theorem 9.31. *The solution $u(x, y)$ to the boundary value problem*

$$-\Delta u = f \quad \text{in } \Omega, \quad u = h \quad \text{on } D, \quad \frac{\partial u}{\partial \mathbf{n}} = k \quad \text{on } N,$$

with $\partial\Omega = D \cup N$, $D \cap N = \emptyset$ and $D \neq \emptyset$, is characterized as the unique function that minimizes the modified Dirichlet integral

$$\widehat{Q}[u] = \iint_{\Omega} \left(\frac{1}{2} \|\nabla u\|^2 - f u \right) dx dy - \int_N u k ds \quad (9.80)$$

among all C^1 functions that satisfy the prescribed boundary conditions.

In particular, the inhomogeneous Dirichlet problem has $D = \partial\Omega$ and so $N = \emptyset$, in which case the extra boundary integral does not appear.

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

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

Theorem 9.30 implies that \tilde{u} minimizes the Dirichlet functional

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

among all functions satisfying the homogeneous boundary conditions. We compute

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

where

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

does not depend on u . We then apply formula (5.86) to evaluate

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

Thus,

$$\tilde{Q}[\tilde{u}] = Q[u] - \int_N u k ds + C_1, \quad \text{where the final term } C_1 = C_0 + \int_D h \frac{\partial v}{\partial \mathbf{n}} ds$$

is fixed by the boundary conditions and the choice of v , and does not change when the function u is varied. Thus, minimizing $\tilde{Q}[\tilde{u}]$ over all \tilde{u} subject to the homogeneous boundary conditions is equivalent to minimizing $\hat{Q}[u]$ over all $u = \tilde{u} + v$ subject to the given inhomogeneous boundary conditions. *Q.E.D.*

9.4. 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 defining 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, based on the so-called Rayleigh quotient, to characterize the eigenvalues of a positive definite boundary value problem.

We begin with the *eigenvalue problem*

$$K[v] = \lambda v \tag{9.81}$$

for a linear operator $K: U \rightarrow U$ on[†] a vector space U . Clearly $v = 0$ solves the eigenvalue equation no matter what λ is. If the homogeneous linear system (9.81) admits a *non-zero* solution $0 \neq v \in U$, then λ is called an *eigenvalue* of the operator K and v a corresponding *eigenvector* or *eigenfunction*, depending on the context. If λ is an eigenvalue, then the corresponding *eigenspace* is the subspace

$$V_\lambda = \ker(K - \lambda I) = \{ v \mid K[v] = \lambda v \} \subset U, \tag{9.82}$$

consisting of all the eigenvectors/eigenfunctions along with 0. To avoid technical difficulties, we will assume that all the eigenspaces are finite-dimensional, and we call $1 \leq$

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

$\dim V_\lambda < \infty$ the *geometric multiplicity* of the eigenvalue λ . (We will later prove their finite dimensionality for regular boundary value problems on bounded intervals.)

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

Theorem 9.32. *If $K = K^*$ 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.*

Proof: To prove the first part of the theorem, suppose λ is a complex eigenvalue, so that $K[v] = \lambda v$ for some complex eigenvector/eigenfunction $v \neq 0$. Then, using the sesquilinearity (B.17) of the underlying Hermitian inner product and self-adjointness (9.45) of K , we find

$$\lambda \|v\|^2 = \langle \lambda v; v \rangle = \langle K[v]; v \rangle = \langle v; K[v] \rangle = \langle v; \lambda v \rangle = \bar{\lambda} \|v\|^2.$$

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

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

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

where the final equality relied 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 9.33. *If $K > 0$ is a self-adjoint, positive definite linear operator, then all its eigenvalues are strictly positive: $\lambda > 0$. If $K \geq 0$ is self-adjoint and positive semi-definite, then its eigenvalues are non-negative: $\lambda \geq 0$.*

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

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

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.*

Example 9.34. In finite dimensions, if we equip $U = \mathbb{R}^n$ with the dot product, then a self-adjoint linear transformation is given by multiplication by an $n \times n$ symmetric matrix: $K[u] = P\mathbf{u}$, where $P^T = P$. Theorem 9.32 implies the well-known result that a symmetric matrix has only real eigenvalues, [104]. 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, [104]. In other words, there exists an orthogonal basis $\mathbf{v}_1, \dots, \mathbf{v}_n$ of \mathbb{R}^n consisting of eigenvectors of P , so $P\mathbf{v}_j = \lambda_j \mathbf{v}_j$ for $j = 1, \dots, n$. If the eigenvalues $\lambda_1, \dots, \lambda_n$

are all simple, so $\lambda_i \neq \lambda_j$ for $i \neq j$, then the basis eigenvectors are automatically orthogonal. When P has a repeated eigenvalue, then one needs to select an orthogonal basis of the associated eigenspace $V_\lambda = \ker(P - \lambda I)$, e.g., by using the Gram–Schmidt process, [104]. Completeness implies that the number of linearly independent eigenvectors associated with an eigenvalue, i.e., the dimension of V_λ or geometric multiplicity, is the same as the eigenvalue’s algebraic multiplicity.

If, furthermore, the matrix $P > 0$ is symmetric and positive definite, then Theorem 9.33 implies that all the 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, [104].

Example 9.35. Consider the Dirichlet eigenvalue problem

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

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

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

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

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

on the 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,

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

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

Example 9.36. Similarly, the periodic boundary value problem

$$-v'' = \lambda v, \quad v(-\pi) = v(\pi), \quad v'(-\pi) = v'(\pi), \quad (9.83)$$

has eigenvalues $\lambda_0 = 0$, with eigenfunction $v_0(x) \equiv 1$, and $\lambda_n = n^2$ for $n = 1, 2, 3, \dots$, each possessing two independent eigenfunctions: $v_n(x) = \cos nx$ and $\tilde{v}_n(x) = \sin nx$. In this case, a zero eigenvalue appears because $K = D^* \circ D = -D^2$ is only positive semi-definite on the space of periodic functions. Theorem 9.32 implies the all-important orthogonality, under the L^2 inner product on $[-\pi, \pi]$, of the Fourier eigenfunctions corresponding to *different* eigenvalues: $\langle v_m; v_n \rangle = \langle v_m; \tilde{v}_n \rangle = \langle \tilde{v}_m; \tilde{v}_n \rangle = 0$ for $m \neq n$. However, since they have the same eigenvalue, the orthogonality of $v_n(x) = \cos nx$ and $\tilde{v}_n(x) = \sin nx$ must be checked by hand.

Example 9.37. On the other hand, the self-adjoint boundary value problem

$$-\frac{d^2u}{dx^2} = \lambda u, \quad \lim_{x \rightarrow \infty} u(x) = 0, \quad \lim_{x \rightarrow -\infty} u(x) = 0, \quad (9.84)$$

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. Exponential solutions that decay at one end become infinitely large at the other end. 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 $|x| \rightarrow \infty$, and so do not qualify as bona fide eigenfunctions. Rather, since they are bounded on the entire line, they represent the “continuous spectrum” of the underlying self-adjoint differential operator.

Example 9.38. The eigenvalue problem for the Bessel differential operator of order m (9.77) is governed by the following differential equation:

$$K[u] = -u'' - \frac{1}{x}u' + \frac{m^2}{x^2}u = \lambda u, \quad (9.85)$$

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 $0 \leq a < b$. Its eigenfunctions are not elementary, but, as we will learn in Chapter 11, can be expressed in terms of Bessel functions. Nevertheless, Theorem 9.33 guarantees the orthogonality of any two eigenfunctions v, \tilde{v} associated with distinct eigenvalues $\lambda \neq \tilde{\lambda}$ under the weighted inner product (9.78):

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

Example 9.39. According to equation (9.59), 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 non-zero solutions to the following boundary value problem

$$-\Delta v = \lambda v \quad \text{in } \Omega, \quad u = 0 \quad \text{in } \partial\Omega. \quad (9.86)$$

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* and, as we will see, plays a central role in the solution of the two-dimensional heat, wave, and Schrödinger equations.

Only in a few select cases, e.g., rectangles and circular disks, can the eigenfunctions and eigenvalues be determined exactly; see Chapter 11 for details. Nevertheless, thanks to Theorem 9.32, we know that the eigenvalues are all non-negative, $\lambda \geq 0$, with $\lambda_0 = 0$ being

an eigenvalue only in positive semi-definite cases, e.g., Neumann boundary conditions. Theorem 9.33 ensures the orthogonality of any two eigenfunctions v, \tilde{v} associated with distinct eigenvalues $\lambda \neq \tilde{\lambda}$, so that

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

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 the eigenvalues by a minimization principle, named after the prolific nineteenth century English applied mathematician Lord Rayleigh (John Strutt).

Definition 9.40. Let $K: U \rightarrow U$ be a self-adjoint linear function on an inner product space. The *Rayleigh quotient* of K is defined as

$$R[v] = \frac{\langle v; K[v] \rangle}{\|v\|^2}, \quad \text{for } 0 \neq v \in U. \quad (9.87)$$

We are, in fact, primarily interested in the Rayleigh quotient of positive (semi-)definite operators. In particular, if $K = L^* \circ L$, then, using (9.50), we can rewrite the Rayleigh quotient in the alternative form

$$R[v] = \frac{\|L[v]\|^2}{\|v\|^2}. \quad (9.88)$$

We will minimize the Rayleigh quotient over all non-zero elements $0 \neq v \in U$. The minimum value turns out to be the smallest eigenvalue of K .

Theorem 9.41. Let K be a self-adjoint linear operator. Then the minimum value of its Rayleigh quotient,

$$\lambda_{\star} = \min \{ R[v] \mid v \neq 0 \}, \quad (9.89)$$

is its smallest eigenvalue. Moreover, any $0 \neq v_{\star} \in U$ that achieves this minimum value, so $R[v_{\star}] = \lambda_{\star}$, is an associated eigenvector/eigenfunction: $K[v_{\star}] = \lambda_{\star} v_{\star}$.

Proof: Suppose that v_{\star} is a minimizing function, and

$$\lambda_{\star} = R[v_{\star}] = \frac{\langle v_{\star}; K[v_{\star}] \rangle}{\|v_{\star}\|^2} \quad (9.90)$$

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

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

[†] $g(t)$ may not be defined for all t , but it is defined for t sufficiently small, which suffices for the purposes of the proof.

where we used the self adjointness of K to identify the terms

$$\langle u; K[v_\star] \rangle = \langle K[u]; v_\star \rangle = \langle v_\star; K[u] \rangle.$$

Since

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

it will attain its minimum value at $t = 0$. Elementary calculus tell us that

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

Therefore, in view of (9.90), we must have

$$\langle u; K[v_\star] - \lambda_\star v_\star \rangle = 0. \quad (9.91)$$

The only way the inner product in (9.91) can vanish for all possible[‡] $u \in U$ is if

$$K[v_\star] = \lambda_\star v_\star, \quad (9.92)$$

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

On the other hand, if v is any eigenfunction, so $K[v] = \lambda v$, then the value of the Rayleigh quotient

$$R[v] = \frac{\langle v; K[v] \rangle}{\|v\|^2} = \frac{\langle v; \lambda v \rangle}{\|v\|^2} = \lambda \quad (9.93)$$

is its eigenvalue. Since λ_\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, one can, with some more analytical work, prove the existence of a minimizing eigenfunction, and hence a smallest positive eigenvalue.

We label the eigenvalues λ_n in increasing order, so that, assuming positive definiteness, $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$, 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 n^{th} eigenfunction v_n must be orthogonal to all its predecessors v_1, \dots, v_{n-1} , it makes sense to try minimizing the Rayleigh quotient over those elements that are orthogonal to the preceding $n - 1$ eigenfunctions.

Theorem 9.42. *Let v_1, \dots, v_{n-1} be eigenfunctions corresponding to the first $n - 1$ eigenvalues $\lambda_1, \dots, \lambda_{n-1}$ of the positive definite, self-adjoint linear operator K . Let*

$$V_{n-1} = \{ u \mid \langle u; v_1 \rangle = \dots = \langle u; v_{n-1} \rangle = 0 \} \quad (9.94)$$

[‡] Or, at least, all u in a dense subspace.

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 V_{n-1} is the n^{th} eigenvalue of K , i.e.,

$$\lambda_n = \min \{ R[v] \mid 0 \neq v \in V_{n-1} \}, \quad (9.95)$$

and any minimizer is an associated eigenfunction v_n .

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

$$\langle K[u]; v_j \rangle = \langle u; K[v_j] \rangle = \lambda_j \langle u; v_j \rangle = 0 \quad \text{for } j = 1, \dots, n-1.$$

Thus, (9.91) applies for arbitrary $u \in V_{n-1}$, which, by setting $u = K[v_*] - \lambda_* v_*$, immediately implies the eigenvalue equation (9.92). Thus, $0 \neq v_* \in V_{n-1}$ must be an eigenfunction that is orthogonal to the first $n-1$ eigenfunctions. Since the eigenfunctions of K are automatically orthogonal, this means that $\lambda_* = \lambda_n$ must be the next lowest eigenvalue and $v_* = v_n$ one of its associated eigenfunctions. *Q.E.D.*

Example 9.43. Return to the Dirichlet eigenvalue problem on the interval $[0, \ell]$ for the L^2 self-adjoint differential operator $-D^2 = D^* \circ D$ discussed in Example 9.35. Its Rayleigh quotient can be written as

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

where the second expression, based on the alternative form (9.88), can be deduced from the first via an integration by parts. According to Theorem 9.41 the minimum value of $R[v]$ over all non-zero functions $v(x) \not\equiv 0$, satisfying the boundary conditions $v(0) = v(\ell) = 0$ is the lowest eigenvalue, namely

$$\lambda_1 = \frac{\pi^2}{\ell^2} = \min \{ R[v] \mid v(0) = v(\ell) = 0, v(x) \not\equiv 0 \},$$

which is achieved if and only if $v(x)$ is a non-zero constant multiple of $\sin \frac{\pi x}{\ell}$, the corresponding eigenfunction. The reader is invited to numerically test this result by evaluating $R[v]$ on various functions $v(x)$ satisfying the boundary conditions and seeing that the 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:

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

and similarly for the higher eigenvalues.

Example 9.44. Consider the Helmholtz eigenvalue problem (9.86) on a bounded domain $\Omega \subset \mathbb{R}^2$, subject to Dirichlet boundary conditions. The associated Rayleigh quotient (9.88) can be written in the form

$$R[v] = \frac{\|\nabla v\|^2}{\|v\|^2} = \frac{\iint_{\Omega} \left[\left(\frac{\partial v}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 \right] dx dy}{\iint_{\Omega} v(x, y)^2 dx dy}. \quad (9.96)$$

Its minimum value among all nonzero functions $v(x, y) \not\equiv 0$ subject to the boundary conditions $v = 0$ on $\partial\Omega$ is the smallest eigenvalue $0 < \lambda_1$, and the minimizing function is any non-zero constant multiple of the associated eigenfunction $v_1(x, y)$. To obtain a higher eigenvalue λ_n , one minimizes $R[v]$ where $v(x, y) \not\equiv 0$ again satisfies the boundary conditions, and in addition is orthogonal to the preceding $n - 1$ eigenfunctions:

$$0 = \langle v; v_k \rangle = \iint_{\Omega} v(x, y) v_k(x, y) dx dy, \quad \text{for } k = 1, \dots, n - 1.$$

It can be proved, [35], that, as long as the domain is bounded, there is a solution to each of these minimization problems, and hence the Helmholtz equation admits an infinite number of eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$.

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. To fix notation, we will proceed as if we are 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 $K[v] = \lambda v$, where K is a self-adjoint operator relative to a weighted L^2 inner product

$$\langle v; \tilde{v} \rangle = \int_a^b v(x) \tilde{v}(x) \rho(x) dx, \quad (9.97)$$

with $\rho(x) > 0$ for $a \leq x \leq b$.

Let $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$ be the eigenvalues, and v_1, v_2, v_3, \dots , the corresponding eigenfunctions. Theorem 9.32 assures us that those corresponding to different eigenvalues are mutually orthogonal:

$$\langle v_j; v_k \rangle = 0, \quad j \neq k. \quad (9.98)$$

Orthogonality is not automatic if v_j and v_k belong to the same eigenvalue, but can be ensured by selecting an orthogonal basis of each eigenspace V_{λ} , if necessary by applying of the Gram–Schmidt process, [104].

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, as in (3.114), in the eigenfunctions:

$$f \sim \sum_k c_k v_k, \quad \text{where the coefficient } c_k = \frac{\langle f; v_k \rangle}{\|v_k\|^2} \quad (9.99)$$

is found by formally taking the inner product of both sides of (9.99) with the eigenfunction v_k and invoking their mutual orthogonality. (Note that our earlier formula (3.114) assumed orthonormality; here, it will be convenient to not necessarily impose the condition $\|v_k\| = 1$.) For example, in the case covered by Example 9.35, the result is the usual Fourier sine series for the function f ; for Example 9.36, we have the full periodic Fourier series. In a similar fashion, Example 9.39 leads to series in the eigenfunctions of the Laplacian on any bounded domain; 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 (9.99) requires completeness of the eigenfunctions. (Pointwise and uniform convergence are then implied by more restrictive hypotheses on the function and the domain, e.g., $f \in C^1$.) In the finite-dimensional context, when $K: \mathbb{R}^n \rightarrow \mathbb{R}^n$ is given by matrix multiplication $K[\mathbf{u}] = P\mathbf{u}$, there are only finitely many eigenvectors, and so the summation (9.99) has only finitely many terms; here, there is no issue with convergence, and completeness is always assured. For boundary value problems in infinite-dimensional function space, the completeness of the resulting eigensolutions is a more delicate issue. For example, the eigenvalue problem for $K = -D^2$ 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, considered in Example 9.37 has *no* eigenfunctions, and so completeness is out of the question. As we will see, the eigenfunctions for regular boundary value problems on bounded domains are automatically complete, whereas singular problems and problems on unbounded domains require a much more delicate analysis.

Whether or not the eigenfunctions are complete, we always have *Bessel's inequality*[†] (3.118):

$$\sum_k c_k^2 \|v_k\|^2 \leq \|f\|^2. \quad (9.100)$$

Theorem 3.38 says that the eigenfunctions are complete if and only if Bessel's inequality is an equality — the Plancherel formula for the eigenfunction expansion.

Green's Functions and Eigenfunctions

We now weave several strands together. Remarkably, the key to completeness of eigenfunctions for boundary value problems lies in the eigenfunction expansion of the Green's function! Assume that K is both self-adjoint and positive definite. Thus, by Theorem 9.33, all its eigenvalues are positive. We index the eigenvalues in increasing order:

$$0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots \quad (9.101)$$

where, as before, the eigenvalues are repeated according to their multiplicities.

[†] Formula (3.118) 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.

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

$$K[G_\xi(x)] = \delta_\xi(x), \quad (9.102)$$

with a delta function impulse on the right hand side. For each fixed ξ , let us write down the eigenfunction series (9.99) for the Green's function:

$$G(x; \xi) = \sum_{k=1}^{\infty} c_k(\xi) v_k(x), \quad \text{where the coefficient} \quad c_k(\xi) = \frac{\langle G_\xi; v_k \rangle}{\|v_k\|^2} \quad (9.103)$$

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

$$\begin{aligned} \lambda_k c_k(\xi) \|v_k\|^2 &= \langle G_\xi; \lambda_k v_k \rangle = \langle G_\xi; K[v_k] \rangle \\ &= \langle K[G_\xi]; v_k \rangle = \langle \delta_\xi; v_k \rangle = \int_a^b \delta(x - \xi) v_k(x) \rho(x) dx = v_k(\xi) \rho(\xi), \end{aligned}$$

where $\rho(x)$ is the weight function of our inner product (9.97), and we used the self-adjointness of K in the middle of the computation. Solving for

$$c_k(\xi) = \frac{v_k(\xi) \rho(\xi)}{\lambda_k \|v_k\|^2}, \quad (9.104)$$

and then substituting back into (9.103), we deduce the explicit eigenfunction series

$$G(x; \xi) \sim \sum_{k=1}^{\infty} \frac{v_k(x) v_k(\xi) \rho(\xi)}{\lambda_k \|v_k\|^2} \quad (9.105)$$

for the Green's function. Observe that this expression is in accordance with the weighted symmetry equation (9.57).

Example 9.45. According to Example 5.9, the Green's function for the L^2 self-adjoint boundary value problem

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

is

$$G(x; \xi) = \begin{cases} x(1 - \xi), & x \leq \xi, \\ \xi(1 - x), & x \geq \xi. \end{cases} \quad (9.106)$$

On the other hand, the eigenfunctions for

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

[‡] As usual, we are assuming the existence; Proposition 9.18 guarantees uniqueness.

are

$$v_k(x) = \sin k\pi x, \quad \text{with corresponding eigenvalues } \lambda_k = k^2\pi^2, \quad \text{for } k = 1, 2, 3, \dots \quad (9.107)$$

Since

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

formula (9.105) implies the eigenfunction expansion

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

This result can be checked by a direct computation of the Fourier sine series of (9.106).

Now, in general, let us apply Bessel's inequality (9.100) to the eigenfunction series for the Green's function; using (9.104), the result is

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

which is valid for any finite n . (And hence also true in the limit as $n \rightarrow \infty$.) We divide by $\rho(\xi) > 0$, and then integrate both sides of the resulting inequality from a to b . On the right hand side, the integrated summands are

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

As a result, we deduce the interesting inequality

$$\sum_{k=1}^n \frac{1}{\lambda_k^2} \leq \int_a^b \int_a^b G(x; \xi)^2 \frac{\rho(x)}{\rho(\xi)} \, dx \, d\xi. \quad (9.108)$$

To make the right hand side look less strange, we can replace $G(x; \xi)$ by the modified Green's function $\tilde{G}(x; \xi) = G(x; \xi)/\rho(\xi)$, cf. (9.58), whence

$$\int_a^b \int_a^b G(x; \xi)^2 \frac{\rho(x)}{\rho(\xi)} \, dx \, d\xi = \int_a^b \int_a^b \hat{G}(x; \xi)^2 \rho(x) \rho(\xi) \, dx \, d\xi \equiv \|\|\hat{G}\|\|^2, \quad (9.109)$$

which we can interpret as a "double weighted L^2 norm" of the modified Green's function $\hat{G}(x; \xi)$. Since the summands in (9.108) are all positive, we can let $n \rightarrow \infty$, and conclude that

$$\sum_{k=1}^{\infty} \frac{1}{\lambda_k^2} \leq \|\|\hat{G}\|\|^2. \quad (9.110)$$

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: $\lambda_k^{-2} \rightarrow 0$ as $k \rightarrow \infty$. We have thus proved the first statement of the following important result.

Theorem 9.46. If $\|\widehat{G}\|^2 < \infty$, then the eigenvalues of the positive definite, self-adjoint operator K are unbounded: $0 < \lambda_k \rightarrow \infty$ as $k \rightarrow \infty$. Moreover, the associated orthogonal eigenfunctions v_1, v_2, v_3, \dots , are complete.

Proof: Our remaining task is to prove that the eigenfunction series (9.99) of a function f converges in norm. For $n = 1, 2, 3, \dots$, 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

$$\|g_{n-1}\| \rightarrow 0 \quad \text{as} \quad n \rightarrow \infty. \quad (9.111)$$

We can assume that each $g_{n-1} \neq 0$, as otherwise the eigenfunction series terminates, with $0 = g_{n-1} = g_n = g_{n+1} = \dots$ (why?), and so (9.111) holds trivially.

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

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

by the orthogonality of the eigenfunctions combined with the formula (9.99) for the coefficient c_j . Thus, $g_{n-1} \in V_{n-1}$, the subspace (9.94) of functions orthogonal to the first $n-1$ eigenfunctions used in the Rayleigh Minimization Theorem 9.42. Since, according to (9.95), λ_n is the *minimum* value of the Rayleigh quotient among all nonzero elements of V_{n-1} , we must have

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

and hence

$$\begin{aligned} \lambda_n \|g_{n-1}\|^2 &\leq \langle g_{n-1}; K[g_{n-1}] \rangle \\ &= \left\langle f - \sum_{k=1}^{n-1} c_k v_k; K \left[f - \sum_{k=1}^{n-1} c_k v_k \right] \right\rangle \\ &= \left\langle f - \sum_{k=1}^{n-1} c_k v_k; K[f] - \sum_{k=1}^{n-1} c_k K[v_k] \right\rangle \\ &= \left\langle f - \sum_{k=1}^{n-1} c_k v_k; K[f] - \sum_{k=1}^{n-1} c_k \lambda_k v_k \right\rangle \\ &= \langle f; K[f] \rangle - \sum_{k=1}^{n-1} \lambda_k c_k \langle f; v_k \rangle - \sum_{k=1}^{n-1} c_k \langle v_k; K[f] \rangle + \sum_{k=1}^{n-1} \lambda_k c_k^2 \|v_k\|^2 \\ &= \langle f; K[f] \rangle - \sum_{k=1}^{n-1} \lambda_k \frac{\langle f; v_k \rangle^2}{\|v_k\|^2}. \end{aligned}$$

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

$$\langle v_k; K[f] \rangle = \langle K[v_k]; f \rangle = \lambda_k \langle f; v_k \rangle,$$

along with the formula in (9.99) for the coefficients c_k . Since the summands are all positive, we conclude that

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

Since we already know that $\lambda_n \rightarrow \infty$, the right hand side of the final inequality goes to 0 as $n \rightarrow \infty$. This implies (9.111) 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 K is necessarily finite-dimensional.

Example 9.47. For the eigenvalue problem considered in Example 9.45, 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 9.46 re-establishes the completeness of the sine eigenfunctions (9.107), 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 9.46 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 9.48. The completeness result of Theorem 9.46 doesn't directly apply to the periodic boundary value problem of Example 9.36 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 ■, if $K \geq 0$ is any positive semi-definite operator and $\mu > 0$ any positive constant, then $\widehat{K} = K + \mu I$, where $I[u] = u$ is the identity operator, is positive definite. Thus, we replace the original periodic boundary value problem (9.83) by the following modification

$$-v'' + \mu v = \lambda v, \quad v(-\pi) = v(\pi), \quad v'(-\pi) = v'(\pi). \quad (9.112)$$

This does not alter the eigenfunctions, but adds μ to 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 $\tilde{v}_n(x) = \sin nx$.

The Green's function for the periodic boundary value problem

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

is derived along the same lines as in Example 5.10. Setting $\mu = \omega^2$, the result is

$$G(x; \xi) = \frac{\cosh \omega (\pi - |x - \xi|)}{2 \omega \sinh \pi \omega}. \quad (9.113)$$

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

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

As a result, Theorem 9.46 reconfirms the completeness of the trigonometric eigenfunctions.

Example 9.49. According to (5.123), 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 (5.107) 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

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

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 Lemma 5.17 shows that such logarithmic singularities still have finite integrals. Therefore, Theorem 9.46 implies that the Helmholtz eigenvalues $\lambda_k \rightarrow \infty$, and the corresponding Helmholtz eigenfunctions $v_k(x, y)$ form a complete 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 not complete, and one needs to introduce additional solutions corresponding to the *continuous spectrum* of the operator. Functions are now represented by combinations of discrete Fourier-like sums over the eigenfunctions (the bound states in quantum mechanics) plus a Fourier integral-like term involving the continuous spectrum (the scattering states). A full discussion of completeness and convergence in such cases must be relegated to an advanced course in analysis, [35, 108].

9.5. A General Framework for Dynamics.

In this section, we show how to apply the results on eigenfunction expansions to three important classes of linear dynamical systems: parabolic evolution equations such as the heat equation, hyperbolic vibration equations such as the wave equation, and the Schrödinger equation, which is the fundamental equation of quantum mechanics. In all three cases we can, assuming completeness, write the general solution to the initial-boundary value problem in an eigenfunction series with time-dependent coefficients.

Evolution Equations

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

$$K[u] = f, \quad (9.114)$$

where f represents an external forcing function. The linear operator

$$K = L^* \circ L \quad (9.115)$$

is self-adjoint, and either positive definite, when $\ker L = \{0\}$, or, more generally, positive semi-definite. In finite dimensions, (9.114) represents a linear system consisting of n equations in n unknowns with positive (semi-)definite coefficient matrix. In function space, it becomes a self-adjoint boundary value problem for the unknown function u .

With the equilibrium operator K in hand, there are two principle types of classical dynamical systems of importance as physical models. The first are the (unforced) *diffusion processes* modeled by a dynamical system of the form

$$\frac{\partial u}{\partial t} = -K[u]. \quad (9.116)$$

In the discrete case, this represents a first order system of ordinary differential equations. In the continuous case, K is a differential operator equipped with boundary conditions, and (9.116) represents a partial differential equation for the time-varying function $u = u(t, x)$.

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

$$u(t, x) = e^{-\lambda t} v(x), \quad (9.117)$$

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

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

Substituting back into (9.116) and canceling the common exponential factors, we are led to the eigenvalue problem

$$K[v] = \lambda v. \quad (9.118)$$

Thus, (9.117) defines a solution if and only if v is an eigenfunction for the linear operator K , with λ the corresponding eigenvalue.

Assuming completeness, we let $v_k(x)$, $k = 1, 2, \dots$, be the eigenfunctions and $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots \rightarrow \infty$ the corresponding eigenvalues. The solution to the initial value problem

$$u(0, x) = f(x) \quad (9.119)$$

can be expanded in terms of the eigensolutions:

$$u(t, x) = \sum_{k=1}^{\infty} e^{-\lambda_k t} c_k v_k(x), \quad \text{where} \quad c_k = \frac{\langle f; v_k \rangle}{\|v_k\|^2} \quad (9.120)$$

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

$$u(0, x) = \delta_\xi(x) \quad (9.121)$$

induced by a unit impulse at the point ξ . Its eigenfunction coefficients are

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

and hence

$$F(t, x; \xi) = \sum_{k=1}^{\infty} e^{-\lambda_k t} \frac{v_k(x) v_k(\xi) \rho(\xi)}{\|v_k\|^2}, \quad (9.122)$$

where the denominator denotes the weighted L^2 norm of the eigenfunction.

As with the one-dimensional heat equation, if the equilibrium operator $K > 0$ is positive definite, then the solutions decay to 0 at an exponential rate given by the smallest eigenvalue (and hence also the minimum value of the Rayleigh quotient). On the other hand, if $K \geq 0$, then the solution will tend to a null eigenmode (or, equivalently, element of $\ker K$) as its asymptotic equilibrium state. Thus, if K has a p -dimensional kernel, the first p eigenvalues are all $0 = \lambda_1 = \dots = \lambda_p < \lambda_{p+1}$, and

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

will tend to its eventual equilibrium configuration at an exponential rate given by the smallest positive eigenvalue λ_{p+1} . In almost all applications, though, $p = 1$ and there is a single, constant null eigenfunction.

Vibration Equations

The second important class of dynamical systems consists of second order (in time) vibration equations

$$\frac{\partial^2 u}{\partial t^2} = -K[u]. \quad (9.123)$$

Newton's equations of motion in the absence of non-conservative frictional forces, the propagation of waves in fluids and solids, as well as electromagnetic waves, and many other related physical problems all lead to such vibrational systems. For a general vibration equation, the separable solutions are of trigonometric form

$$u(t, x) = \cos(\omega t) v(x) \quad \text{or} \quad \sin(\omega t) v(x). \quad (9.124)$$

Substituting this ansatz back into the vibration equation (9.123) results in the same eigenvalue problem (9.118) with eigenvalue $\lambda = \omega^2$ equal to the square of the vibrational frequency. We conclude that the *normal modes* or *eigensolutions* take the form

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

provided $\lambda_k = \omega_k^2 > 0$ is a non-zero eigenvalue and v_k an associated eigenfunction.

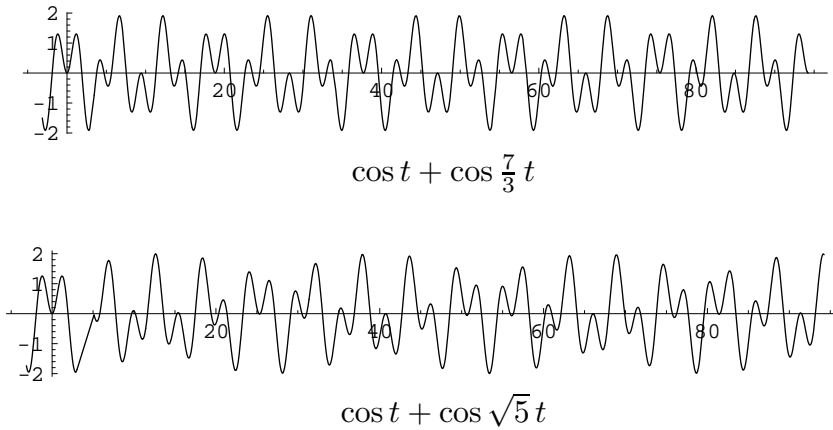


Figure 9.1. Periodic and Quasi-Periodic Functions.

In the positive definite case, there are no zero eigenvalues, and so the general solution is built up as a combination of the eigenmodes:

$$\begin{aligned}
 u(t, x) &= \sum_{k=1}^{\infty} [c_k u_k(t, x) + d_k \tilde{u}_k(t, x)] \\
 &= \sum_{k=1}^{\infty} [c_k \cos(\omega_k t) + d_k \sin(\omega_k t)] v_k(x) = \sum_{k=1}^{\infty} r_k \cos(\omega_k t + \delta_k) v_k,
 \end{aligned} \tag{9.125}$$

where $r_k = \sqrt{c_k^2 + d_k^2}$, $\delta_k = \tan^{-1}(d_k/c_k)$. The initial conditions

$$g(x) = u(0, x) = \sum_{k=1}^{\infty} c_k v_k(x), \quad h(x) = u_t(0, x) = \sum_{k=1}^{\infty} d_k \omega_k v_k(x), \tag{9.126}$$

are used to specify the coefficients:

$$c_k = \frac{\langle f; v_k \rangle}{\|v_k\|^2}, \quad d_k = \frac{\langle f; v_k \rangle}{\omega_k \|v_k\|^2}. \tag{9.127}$$

In the unstable, positive semi-definite cases, any null eigenfunction $v_0 \in \ker K = \ker L$ contributes two non-periodic eigensolutions

$$u_0(t, x) = v_0(x), \quad \tilde{u}_0(t, x) = t v_0(x).$$

The first is constant in time, while the second contributes an unstably growing mode \tilde{u}_0 , 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 eigen-frequencies happen to be integer multiples of a common frequency: $\omega_k = n_k \omega_*$ for $n_k \in \mathbb{N}$, then the solution (9.125) is a periodic function of t with period $p_* = 2\pi/\omega_*$. On the other hand, in most cases the frequencies are not rationally related, and the solution is only *quasi-periodic*, since, although it is the sum of individually periodic modes, it never exactly repeats itself over time.

To appreciate the difference between periodic and quasi-periodic vibrations, consider the function

$$u(t) = \cos t + \cos \omega t,$$

which is a linear combination of two simple periodic vibrations, of frequencies 1 and ω . If $\omega = p/q$ is a rational number, then $u(t)$ is a periodic function of period $2\pi q$, so $u(t+2\pi q) = u(t)$. However, if ω is an irrational number, then $u(t)$ is not periodic, and will never precisely repeat itself. You are encouraged to inspect the graphs in Figure 9.1. The first is periodic — can you spot where it begins to repeat? — whereas the second is only quasi-periodic and never quite succeeds in reproducing its behavior. To the uninitiated, such quasi-periodic motions may appear to be rather chaotic, even though they are built from a few simple periodic constituents. However, quasi-periodic motion is *not* true chaos, which is an inherently nonlinear phenomenon, [92].

Forcing and Resonance

Periodically forcing an undamped mechanical structure (or a resistanceless electrical circuit) at a frequency that is distinct from its natural vibrational frequencies leads, in general, to a quasi-periodic response. The solution is a sum of the unforced vibrations superimposed with an additional vibrational mode at the forcing frequency. However, if forced at one of its natural frequencies, the system may go into a catastrophic resonance.

The same type of quasi-periodic/resonant response is also observed in the partial differential equations governing the vibrations of continuous media. To keep the analysis as simple as possible, we restrict our attention to the forced wave equation for a homogeneous string

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} + F(t, x), \quad (9.128)$$

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

$$F(t, x) = \cos(\omega t) h(x), \quad (9.129)$$

where the function $h(x)$ is fixed.

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

$$u(t, x) = u_\star(t, x) + z(t, x) \quad (9.130)$$

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

$$\frac{\partial^2 z}{\partial t^2} = c^2 \frac{\partial^2 z}{\partial x^2}. \quad (9.131)$$

The boundary and initial conditions will serve to uniquely prescribe the solution $u(t, x)$, but there is some flexibility in its two constituents (9.130). For instance, we may ask that the particular solution u_\star satisfy the homogeneous boundary conditions along with zero (homogeneous) initial conditions, and thus represents 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 will equal the sum of the two individual responses.

In the case of periodic forcing (9.129), we look for a particular solution

$$u_{\star}(t, x) = \cos(\omega t) v_{\star}(x) \quad (9.132)$$

that vibrates at the forcing frequency. Substituting the ansatz (9.132) into the equation (9.128), and canceling the common cosine factors, we discover that $v_{\star}(x)$ must satisfy the boundary value problem prescribed by a forced differential equation

$$-c^2 v_{\star}'' - \omega^2 v_{\star} = h(x), \quad (9.133)$$

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 has only the trivial solution $v \equiv 0$, then a solution to the forced boundary value problem exists for any form of the forcing function $h(x)$. Thus, if ω^2 is *not* an eigenvalue, then the particular solution (9.132) will vibrate with the forcing frequency, and the general solution will be a combination (9.130) of the free vibrations and the forced vibrations.

On the other hand, if ω^2 is an eigenvalue, and so ω is a natural frequency of vibration to the homogeneous problem, then the homogeneous boundary value problem admits a non-trivial solution, namely the corresponding eigenfunction $v(x)$. In such cases, either the forced boundary value problem (9.133) has no solution, or the solution is no longer unique, depending on the form of the forcing function.

The solution $v(x)$ is the corresponding eigenfunction appearing in the solution series (4.58). In this case, according to the Fredholm Alternative, Theorem 9.10, the boundary value problem (9.133) has a solution if and only if the forcing function $h(x)$ is orthogonal to the eigenfunction(s):

$$\langle h; v \rangle = 0. \quad (9.134)$$

If we force in a resonant manner — meaning that (9.134) is not satisfied — then the solution will be a resonantly growing vibration of the form

$$u_{\star}(t, x) = at \sin(\omega t) v(x) + \cos(\omega t) v_{\star}(x). \quad (9.135)$$

In a real-world situation, such large resonant (or near resonant) vibrations will, if unchecked, eventually lead to a catastrophic breakdown, e.g., the string snaps. Indeed, by direct calculation,

$$\begin{aligned} \frac{\partial^2 u_{\star}}{\partial t^2} - c^2 \frac{\partial^2 u_{\star}}{\partial x^2} &= -at \sin(\omega t) [c^2 v''(x) + \omega^2 v(x)] - \\ &\quad - \cos(\omega t) [c^2 v_{\star}''(x) + \omega^2 v_{\star}(x) - 2a\omega v(x)]. \end{aligned}$$

The first term vanishes since $v(x)$ is the eigenfunction. Therefore, (9.135) satisfies the forced the boundary value problem if and only if $v_{\star}(x)$ satisfies the ordinary differential equation

$$-c^2 v_{\star}''(x) - \omega^2 v_{\star}(x) = h(x) - 2a\omega v(x)$$

along with the relevant boundary conditions. Again, the Fredholm Alternative implies that the latter boundary value problem admits a solution $v_*(x)$ if and only if

$$0 = \langle h - 2a\omega v; v \rangle = \langle h; v \rangle - 2a \|v\|^2, \quad \text{and hence} \quad a = \frac{\langle h; v \rangle}{2 \|v\|^2} \quad (9.136)$$

fixes the value of the constant in the resonant solution ansatz (9.135).

Example 9.50. As a specific example, consider the initial-boundary value problem modeling the forced vibrations of a uniform string of unit length and fixed at both ends:

$$\begin{aligned} u_{tt} &= c^2 u_{xx} + \cos(\omega t) h(x), \\ u(t, 0) = 0 &= u(t, 1), \quad u(0, x) = f(x), \quad u_t(0, x) = g(x). \end{aligned} \quad (9.137)$$

The particular solution will have the nonresonant form (9.132) provided there exists a solution $v_*(x)$ to the boundary value problem

$$c^2 v_*'' + \omega^2 v_* = -h(x), \quad v_*(0) = 0 = v_*(1). \quad (9.138)$$

The natural frequencies and associated eigenfunctions are

$$\omega_n = n c \pi, \quad v_n(x) = \sin n \pi x, \quad n = 1, 2, 3, \dots$$

The boundary value problem (9.138) will have a solution, and hence the forcing is not resonant, provided either $\omega \neq \omega_n$ is not a natural frequency, or $\omega = \omega_n$, but

$$0 = \langle h; v_n \rangle = \int_0^1 h(x) \sin n \pi x \, dx \quad (9.139)$$

is orthogonal to the associated eigenfunction. Otherwise, the forcing profile will induce a resonant response.

For example, under periodic forcing of frequency ω with trigonometric profile $h(x) \equiv \sin k \pi x$, the particular solution to (9.138) is

$$v_*(x) = \frac{\sin k \pi x}{\omega^2 - k^2 \pi^2 c^2}, \quad \text{so that} \quad u_*(t, x) = \frac{\cos \omega t \sin k \pi x}{\omega^2 - k^2 \pi^2 c^2}, \quad (9.140)$$

which is a valid solution as long as $\omega \neq \omega_k = k \pi c$. Note that we may allow the forcing frequency $\omega = \omega_n$ to coincide with any other resonant forcing frequency, $n \neq k$, because the sine profiles are mutually orthogonal and so the nonresonance condition (9.139) holds. On the other hand, if $\omega = \omega_k = k \pi c$, then the particular solution

$$u_*(t, x) = \frac{t \sin k \pi c t \sin k \pi x}{2 k \pi c}, \quad (9.141)$$

is resonant, and grows linearly in time.

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

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

along with the modified initial conditions

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

stemming from the fact that the particular solution (9.140) has non-trivial initial data. (In the resonant case (9.141), 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 (4.58). The final formulae are left to the reader to write out.

The Schrödinger Equation

In quantum mechanics, the basic dynamical system is known as the *Schrödinger equation*, first written down by the German physicist Erwin Schrödinger, one of the founding fathers of the subject. His original series of papers in which, by fits and starts, he arrives at his fundamental equation, make for fascinating reading, [116].

The abstract form of the Schrödinger equation is

$$i \hbar \frac{\partial \psi}{\partial t} = K[\psi], \quad (9.142)$$

where K is a linear operator of the usual self-adjoint[†] form (9.115). In this equation, $i = \sqrt{-1}$, while \hbar is Planck's constant (7.64). At each time t , the solution $\psi(t, \mathbf{x})$ to the Schrödinger equation represents the wave function of the quantum system, and so should be a complex-valued square integrable function of constant L^2 norm: $\|\psi\| = 1$. (The reader may wish to refer back to 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 operator K 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”. The interested reader should consult a basic text on quantum mechanics, e.g., [83, 89], for full details on both the physics and underlying mathematics.

Proposition 9.51. *If $\psi(t, \mathbf{x})$ is a solution to the Schrödinger equation, its Hermitian L^2 norm $\|\psi(t, \cdot)\|$ is constant.*

Proof: Since the solution is complex-valued, we use the sesquilinearity of the under-

[†] Although, since K acts on a complex vector space, the adjoint really refers to the Hermitian adjoint, [104]. But the reader will not lose anything by viewing K as a real linear operator here.

lying Hermitian inner product, as in (B.17), to compute

$$\begin{aligned} \frac{d}{dt} \|\psi\|^2 &= \left\langle \frac{\partial\psi}{\partial t}; \psi \right\rangle + \left\langle \psi; \frac{\partial\psi}{\partial t} \right\rangle \\ &= \left\langle -\frac{i}{\hbar} K[\psi]; \psi \right\rangle + \left\langle \psi; -\frac{i}{\hbar} K[\psi] \right\rangle = -\frac{i}{\hbar} \langle K[\psi]; \psi \rangle + \frac{i}{\hbar} \langle \psi; K[\psi] \rangle = 0, \end{aligned}$$

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

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

Apart from the extra factor of $i\hbar$, the Schrödinger equation looks like a diffusion equation (9.116). (*Warning:* Despite this superficial similarity, their solutions have radically different behavior. Indeed, the Schrödinger equation behaves much more like a hyperbolic wave equation than a parabolic heat equation.) This inspires us to seek separable solutions with an exponential ansatz:

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

Substituting this expression into the Schrödinger equation (9.142) and canceling the common exponential factors reduces us to the usual eigenvalue problem

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

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

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

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

$$\psi(t, \mathbf{x}) = \sum_k c_k \psi_k(t, \mathbf{x}) = \sum_k c_k e^{-i\lambda_k t/\hbar} v_k(\mathbf{x}), \quad (9.143)$$

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. So, we can determine both the past and future behavior of a quantum system from its present configuration.

Example 9.52. In a single space dimension, the simplest version of the Schrödinger equation is based on the derivative operator $L = D_x$, for which, assuming appropriate boundary conditions, the self-adjoint combination $K = L^* \circ L = -D_x^2$. Thus, (9.142) reduces to the second order partial differential equation

$$i\hbar \frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2}. \quad (9.144)$$

When subject to the Dirichlet boundary conditions

$$\psi(t, 0) = \psi(t, \ell) = 0,$$

the Schrödinger equation 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

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

are

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

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

$$\psi_k(t, x) = \sqrt{\frac{2}{\ell}} \exp\left(-i \frac{k^2\pi^2}{\hbar\ell^2} t\right) \sin \frac{k\pi}{\ell} x. \quad (9.145)$$

The eigenvalues represent the energy levels of the particle, which can be deduced from the spectral lines that are emitted when the system is excited. For instance, when an electron jumps from one level to another, it emits a photon whose energy equals the difference between the energies of the two quantum levels. These emitted photons form the observed electromagnetic spectral lines, which explains the adoption of the physics term “spectrum” to describe the eigenvalues of the linear operator K .