8. The analogy between matrices and operators

In the typical problem of linear algebra, we solve

$$(1) \qquad \mathbf{L}\mathbf{u} = \mathbf{f}$$

for **u**, where **L** is an $n \times n$ matrix, and **u** and **f** are $(n \times 1)$ column vectors. This problem has a unique solution if det $\mathbf{L} \neq 0$. One method—usually not the best method—of solving (1) is to first find the inverse \mathbf{L}^{-1} of **L**, that is, to solve

(2)
$$\mathbf{L}(\mathbf{L}^{-1}) = \mathbf{I}$$

for \mathbf{L}^{-1} and then compute $\mathbf{u}=\mathbf{L}^{-1}\mathbf{f}$. A better method—though not always possible—is to transform the variables into a new system in which \mathbf{L} takes a simple form. The ultimate simplification is one in which the transformed \mathbf{L} is purely diagonal.

Our interest is differential equations. Hence we wish to solve

(3) $Lu(\mathbf{x}) = f(\mathbf{x})$ with the appropriate boundary conditions

where *L* is a linear partial differential operator, and $u(\mathbf{x})$ and $f(\mathbf{x})$ are functions. The linear algebra problem (1) and the system (3) are analogous. The analogy is between:

$$\{u_1, u_2, \dots, u_n\}$$
, the *n* components of **u**; and $\{u(\mathbf{x}), \text{ all } \mathbf{x}\}$, an infinite set $\{f_1, f_2, \dots, f_n\}$, and $\{f(\mathbf{x}), \text{ all } \mathbf{x}\}$
L, an $n \times n$ matrix; and L, an $\infty \times \infty$ operator.

In this section we explore the analogy between (1) and (3). The main benefit of this is a better understanding of the relationship between the various solution strategies for (3).

In the "transformation approach" to simplifying (1), one lets

(4)
$$\mathbf{u} = \mathbf{T}\hat{\mathbf{u}}$$
, i.e. $\hat{\mathbf{u}} = \mathbf{T}^{-1}\mathbf{u}$

where **T** is an $n \times n$ matrix and $\hat{\mathbf{u}}$ are the new variables. (We require det $\mathbf{T} \neq 0$ for an invertible transformation.) Then (1) takes the form $\mathbf{LT}\hat{\mathbf{u}} = \mathbf{T}\hat{\mathbf{f}}$, which implies

(5) $\hat{\mathbf{L}}\hat{\mathbf{u}} = \hat{\mathbf{f}}$ where $\hat{\mathbf{L}} = \mathbf{T}^{-1}\mathbf{L}\mathbf{T}$ is the transformation of \mathbf{L} .

The strategy is to find a T that makes \hat{L} simpler than L. Special properties of L may allow a spectacular simplification.

We rewrite (4) as

(6)
$$u_i = \sum_{j=1}^n T_{ij} \ \hat{u}_j$$
, which is analogous to

(7)
$$u(\mathbf{x}) = \iiint d\mathbf{x}' T(\mathbf{x}, \mathbf{x}') \hat{u}(\mathbf{x}').$$

The arrows point to the corresponding things. For example,

(8)
$$u(\mathbf{x}) = \iiint d\mathbf{k} \ e^{i\mathbf{k}\cdot\mathbf{x}} \ \hat{u}(\mathbf{k})$$

fits the form of (7) with $T(\mathbf{x}, \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}}$. The analog of $\hat{\mathbf{u}} = \mathbf{T}^{-1}\mathbf{u}$ is

(9)
$$\hat{u}(\mathbf{k}) = \iiint d\mathbf{x} \frac{1}{(2\pi)^3} e^{-i\mathbf{k}\cdot\mathbf{x}} u(\mathbf{x}).$$

Thus

(10)
$$T^{-1}(\mathbf{k},\mathbf{x}) = \frac{1}{(2\pi)^3} e^{-i\mathbf{k}\cdot\mathbf{x}}.$$

The (Fourier) transformation from $u(\mathbf{x})$ to $\hat{u}(\mathbf{k})$ is useful for all equations with constant coefficients in unbounded domains. For example, it transforms

 $\nabla^2 u = Q$ into $-\mathbf{k} \cdot \mathbf{k} \,\hat{u} = \hat{Q}$, a completely diagonal form.

Next we ask: What is the analogue of matrix inversion? Clearly the analogue of

(11)
$$u_i = \sum_j L_{ij}^{-1} f_j$$

is

(12)
$$u(\mathbf{x}) = \iiint d\mathbf{x}' \ G(\mathbf{x}, \mathbf{x}') \ f(\mathbf{x}').$$

Thus the Green's function is analogous to the inverse matrix \mathbf{L}^{-1} . Applying the operator *L* to (12) we obtain

(13)
$$Lu(\mathbf{x}) = \iiint d\mathbf{x}' \ LG(\mathbf{x}, \mathbf{x}') \ f(\mathbf{x}')$$

which agrees with (3) provided that

(14)
$$LG(\mathbf{x},\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}').$$

(Note that L operates on x and not x'.) Thus (14) appears to be the analogue of

$$(15) \qquad \mathbf{L} \ \mathbf{L}^{-1} = \mathbf{I}.$$

This is not quite true! While we know that (15) has a unique solution for \mathbf{L}^{-1} provided that det $\mathbf{L} \neq 0$, (14) may be solved uniquely for *G* only if it is accompanied by the appropriate boundary conditions. In other words, the operator *L* is invertible only if it is defined in such a way as to incorporate the boundary conditions.

To clarify this we first note that the analogy between **L** and *L* can be turned into an equivalence if we agree to replace *L* by a finite-difference approximation. To keep things as simple as possible, suppose that $L = \partial^2 / \partial x^2$ so that our equation is the one-dimensional Poisson equation,

(16)
$$u_{xx} = f$$
.

The finite-difference version is

(17)
$$\frac{u_{i+1} + u_{i-1} - 2u_i}{\Delta^2} = f_i$$

where Δ is the spacing between gridpoints. If we let **u** be the column vector of gridded values, then, on the infinite domain, (16) takes the form

(18)
$$\begin{bmatrix} \ddots & & & \\ & \frac{1}{\Delta^2} & \frac{-2}{\Delta^2} & \frac{1}{\Delta^2} \\ & & & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ u_{i-1} \\ u_i \\ u_{i+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ f_{i-1} \\ f_i \\ f_{i+1} \\ \vdots \end{bmatrix}$$

We see that **L** is an $\infty \times \infty$ tridiagonal matrix. We also see that **L** must be singular, because we can add a constant to any solution of (18) and obtain another solution. (This corresponds to one null vector of **L**. What is the other null vector?)

If we make the domain finite and impose Dirichlet boundary conditions at the endpoints, then we obtain the *nonsingular* problem

(19)
$$\begin{bmatrix} 1 & & & & & \\ 1/\Delta^2 & -2/\Delta^2 & 1/\Delta^2 & & & \\ & & \ddots & \ddots & & \\ & & & 1/\Delta^2 & -2/\Delta^2 & 1/\Delta^2 \\ & & & & & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} 0 \\ f_2 \\ \vdots \\ f_{n-1} \\ 0 \end{bmatrix}$$

The matrix **L** in (19) is the analogue of *L* plus the boundary conditions u=0. Let $\mathbf{L}^{-1} = \mathbf{G}$ be the inverse of the matrix in (19). To find **G** we must solve

$$(20) \quad \mathbf{LG} = \mathbf{I}.$$

We may solve for G "one column at a time" by writing

(21)
$$\begin{bmatrix} 1 & & & & & \\ 1/\Delta^2 & -2/\Delta^2 & 1/\Delta^2 & & & \\ & \ddots & \ddots & & & \\ & & & 1/\Delta^2 & -2/\Delta^2 & 1/\Delta^2 \\ & & & & & 1 \end{bmatrix} \begin{bmatrix} G_{1j} \\ G_{2j} \\ \vdots \\ G_{n-1,j} \\ G_{nj} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

where the 1 on the right-hand side appears in the *j*-th row. We recognize (21) as the finitedifference analogue of

(22)
$$LG(x,x') = \delta(x-x')$$

and the boundary conditions

(23)
$$G(0, x') = G((n-1)\Delta, x') = 0$$

This proves that the inversion operation includes the imposition of the same boundary conditions on G that were applied to u. Of course solving (21) by (say) Gaussian elimination requires n times as much work as solving (19) directly for **u**. Thus Green's functions are impractical unless the symmetry of the problem makes them easy to find.

Everything we have said so far applies to general L and L. Now we consider the special case of symmetric L. If L is symmetric, then we know from section 5 that its eigenvalues are real, and the corresponding eigenvectors are (or can be made) orthogonal. This means that the eigenvectors span the whole *n*-dimensional space. Thus any column vector, including u and f, can be represented as a weighted sum of the eigenvectors. *The eigenvectors form a complete set*. Furthermore, if L is symmetric then so is L^{-1} . Finally, if L is symmetric, then

$$(24) \qquad \sum_{j} L_{ij} u_j = f_i$$

may be written

(25)
$$\frac{\partial}{\partial u_k} \left(\sum_i \sum_j \frac{1}{2} u_i L_{ij} u_j - \sum_i f_i u_i \right) = 0 \quad \text{for } k=1 \text{ to } n.$$

In other words, the problem **Lu=f** is equivalent to the *variational principle*

(26)
$$\delta\left(\frac{1}{2}\mathbf{u}^T\mathbf{L}\mathbf{u}-\mathbf{u}^T\mathbf{f}\right)=0$$

where δ stands for arbitrary independent variations in the components of the column vector **u**. These facts provide the motivation to seek the analogous properties for operators that are the analogues of symmetric matrices. Such operators are called *self-adjoint*. But how exactly do we define self-adjointness?

One approach is this: If the matrix corresponding to the finite-difference form of the differential equation is symmetric, then the operator is said to be self-adjoint. For

example, we note that the matrix in (19) is *not* symmetric (but only because of its first and last rows). Thus the problem

(27)
$$u_{xx} = f, \quad 0 < x < 1$$
$$u(0) = u(1) = 0$$

is not self-adjoint in the sense defined above. Suppose however that we change the boundary conditions to $u_x(0) = u_x(1) = 0$. Then the matrix in (19) becomes

(28)
$$\begin{bmatrix} -1/\Delta^{2} & 1/\Delta^{2} & & & \\ 1/\Delta^{2} & -2/\Delta^{2} & 1/\Delta^{2} & & \\ & \ddots & \ddots & & \\ & & 1/\Delta^{2} & -2/\Delta^{2} & 1/\Delta^{2} \\ & & & 1/\Delta^{2} & -1/\Delta^{2} \end{bmatrix} \begin{bmatrix} u_{1} \\ u_{2} \\ \vdots \\ u_{n-1} \\ u_{n} \end{bmatrix} = \begin{bmatrix} 0 \\ f_{2} \\ \vdots \\ f_{n-1} \\ 0 \end{bmatrix}$$

which *is* symmetric. Thus the problem

(29)
$$u_{xx} = f, \quad 0 < x < 1$$
$$u_{x}(0) = u_{x}(1) = 0$$

is self-adjoint. But wait! If we simply use the fact that $u_1 = u_n = 0$ to rewrite (19) as an $(n-2) \times (n-2)$ matrix equation,

$$(30) \begin{bmatrix} -1/\Delta^{2} & 1/\Delta^{2} \\ 1/\Delta^{2} & -2/\Delta^{2} & 1/\Delta^{2} \\ & \ddots & \ddots \\ & & 1/\Delta^{2} & -2/\Delta^{2} & 1/\Delta^{2} \\ & & & 1/\Delta^{2} & -1/\Delta^{2} \end{bmatrix} \begin{bmatrix} u_{2} \\ u_{3} \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{bmatrix} = \begin{bmatrix} f_{2} \\ f_{3} \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{bmatrix}$$

then the lower-dimensional matrix is symmetric. So is the problem (27) self-adjoint or not? The answer clearly depends on the size of the function space. If the function space includes only those u(x) that vanish at the endpoints, then the problem is self-adjoint.

This agrees with something we discovered in Section 7. If (27) is self-adjoint it should have a variational principle. The variational principle is in fact

(31)
$$\delta \int_{0}^{1} dx \left(\frac{1}{2}u_{x}^{2} + fu\right) = 0$$

But the variational principle (31) only works if we constrain $u = \delta u = 0$ at the endpoints. If, on the other hand, we place no restrictions on u and δu at the endpoints, then the variational principle gives us the problem (29) with its boundary conditions of $u_x = 0$. The matrix in (28) corresponding to this problem is symmetric. Thus the problem (29) is self-adjoint on the *unrestricted* function space.

If self-adjointness really matters, then it is disturbing that it should depend on the manner in which we choose to incorporate the boundary conditions. It seems better to redefine self-adjointness as a property of the operator alone, and to leave the boundary conditions as a separate issue. Moreover, it seems a bad idea to define properties of the operator based on the form of the corresponding finite-difference equations. Not only are these non-unique, but we note that multiplying any row of (19) or (28) by a constant, or interchanging any 2 rows, would destroy the symmetry property without changing the problem at all. Finally, writing out the finite-differences in more than 1 space dimension becomes very tedious. Considering all this, we are on very thin ice!

We therefore proceed by manipulations that do not refer to matrices or finitedifferences at all, but simply use the matrix theory as a guide. That is, we pursue the analogy withou attempting to show an equivalence.

Definition. The operator L is self-adjoint if

(32)
$$\int dx \ v Lu = \int dx \ u Lv + \text{boundary terms}$$

for any 2 functions u(x) and v(x).

This is clearly the analogue of the statement $\mathbf{u}^T \mathbf{L} \mathbf{v} = \mathbf{v}^T \mathbf{L} \mathbf{u}$ for any 2 column vectors \mathbf{u} and \mathbf{v} , which in turn implies that $\mathbf{L} = \mathbf{L}^T$. However the definition (32) does not require us to determine the "components" of *L* by forming finite differences. By this definition $L = \partial^2 / \partial x^2$ is self-adjoint. More generally, $\nabla^2 = \partial^2 / \partial x^2 + \partial^2 / \partial y^2$ is self-adjoint within any closed domain. To prove this we note that

(33)
$$u\nabla^2 v = \nabla \cdot (u\nabla v) - \nabla u \cdot \nabla v$$
$$v\nabla^2 u = \nabla \cdot (v\nabla u) - \nabla u \cdot \nabla v$$

Subtracting and integrating we obtain

(34)
$$\iint dx \, dy \left\{ u \nabla^2 v - v \nabla^2 u \right\} = \iint dx \, dy \, \nabla \cdot \left(u \nabla v - v \nabla u \right).$$

By the divergence theorem this becomes

(35)
$$\iint dx \, dy \left\{ u \nabla^2 v - v \nabla^2 u \right\} = \oint ds \left(u \frac{\partial v}{\partial n} - v \frac{\partial u}{\partial n} \right),$$

which fits the form of (32).

Consider the problem

$$(36) \quad \nabla^2 u = f(x, y)$$

in an arbitrary domain with mixed boundary condition

(37)
$$\alpha u + \beta \frac{\partial u}{\partial n} = 0$$

where α and β are prescribed functions. (This includes Neumann and Dirichlet boundary conditions as the special cases $\alpha=0$ and $\beta=0$.)

Now we state and check properties of (36-37) which are expected from the analogy with the matrix problem:

• Since ∇^2 is self-adjoint, we expect its eigenfunctions to be orthogonal. To see that they are, let u_1 and u_2 be any 2 eigenfunctions. Then

•

(38)
$$\nabla^2 u_1 = \lambda_1 u_1$$
 with boundary conditions
$$\alpha u_1 + \beta \frac{\partial u_1}{\partial n} = 0$$
$$\alpha u_2 + \beta \frac{\partial u_2}{\partial n} = 0$$

where λ_1 and λ_2 are the eigenvalues. Multiplying (38a) by u_2 , (38b) by u_1 , subtracting, integrating and using the property (35) we obtain

(39)
$$\oint ds \left(u_2 \frac{\partial u_1}{\partial n} - u_1 \frac{\partial u_2}{\partial n} \right) = \left(\lambda_1 - \lambda_2 \right) \iint u_1 u_2 \, dx \, dy.$$

the left-hand side vanishes because of the boundary conditions (37). Thus if $\lambda_1 \neq \lambda_2$, the eigenfunctions are indeed orthogonal. (Note how this proof mirrors the corresponding proof for matrices in Section 5.)

• Since ∇^2 is self-adjoint [analogous statement: L is symmetric], we expect its Green's function to be symmetric in its arguments [analogous statement: \mathbf{L}^{-1} is symmetric]. The Green's function corresponding to (36-37) obeys

(40)
$$\nabla^2 G(\mathbf{x}, \mathbf{x}_0) = \delta(\mathbf{x} - \mathbf{x}_0)$$
 and the boundary conditions $\alpha G + \beta \frac{\partial G}{\partial n} = 0$.

From (40) it follows that

(41)
$$u(\mathbf{x}) = \iint d\mathbf{x}_0 \ G(\mathbf{x}, \mathbf{x}_0) f(\mathbf{x}_0).$$

To show that G is symmetric we multiply (40) by $u(\mathbf{x})$, and (36) by $G(\mathbf{x}, \mathbf{x}_0)$, and proceed as toward (39) to obtain

(42)
$$\oint ds \left(u \frac{\partial G}{\partial n} - G \frac{\partial u}{\partial n} \right) = \iint d\mathbf{x} \left\{ u(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}_0) - G(\mathbf{x}, \mathbf{x}_0) f(\mathbf{x}) \right\}$$

The left-hand side vanishes because of the boundary conditions on G and u. Thus

(43)
$$u(\mathbf{x}_0) = \iint d\mathbf{x} G(\mathbf{x}, \mathbf{x}_0) f(\mathbf{x}).$$

By interchanging \mathbf{x}_0 and \mathbf{x} in (43) and comparing the result with (41), we see that

(44)
$$G(\mathbf{x}, \mathbf{x}_0) = G(\mathbf{x}_0, \mathbf{x})$$

as expected.

• Since ∇^2 is self-adjoint, we expect the problem (36-37) to correspond to a variational principle. From Section 7 we know that it does.

• Finally since ∇^2 is self-adjoint, we expect that its eigenfunctions form a complete set of functions. (This is analogous to the statement that the eigenvectors of symmetric L span the whole *n*-dimensional space.) Unfortunately, completeness is a property that does not *automatically* accompany self-adjointness; it depends on the particular case. However, we can prove that the eigenfunctions of ∇^2 are complete using tools that arise from the self-adjointness.

Sketch of the proof.

For simplicity we assume Dirichlet boundary conditions, but the proof can be extended to Neumann or mixed boundary conditions. By definition the eigenfunctions obey

(45)
$$\nabla^2 u + \lambda u = 0$$
 with boundary condition $u=0$.

For example, if the domain is $0 < x, y < \pi$, then the eigenfunctions are $\theta_{nm}(x, y) = \sin nx \sin my$ with eigenvalues $\lambda_{nm} = n^2 + m^2$.

In general, the normalized eigenfunction u_1 with the smallest eigenvalue λ_1 is the function that minimizes

$$(46) \qquad \iint \nabla u \cdot \nabla u$$

subject to the constraints

(47) $\iint u^2 = 1$ and u=0 at the boundary.

That is, of all the functions satisfying (47), u_1 is the one that minimizes (46). Similarly, the eigenfunction u_2 with the next-smallest eigenvalue is the function that minimizes (46) subject to

(48)
$$\iint u^2 = 1$$
, $\iint uu_1 = 0$, and $u=0$ at the boundary.

Proceeding in the obvious way, the n-th eigenfunction minimizes (46) subject to

(49)
$$\iint u^2 = 1$$
, $\iint uu_1 = \cdots \iint uu_{n-1}$, and $u=0$ at the boundary.

Within the set of functions satisfying (49) u_n gives (46) its minimum value.

To see that this procedure is equivalent to (45), consider the "amplitudeinsensitive" functional

(50)
$$R[u] = \frac{\iint \nabla u \cdot \nabla u}{\iint u^2}$$

We shall show that solutions of (45) are stationary points of (50). Using $u=\delta u=0$ at the boundary,

(51)
$$\delta R = 2 \frac{\iint \nabla u \cdot \nabla \delta u}{\iint u^2} - \frac{\iint \nabla u \cdot \nabla u}{\left(\iint u^2\right)^2} 2 \iint u \, \delta u = 0$$

implies

(52)
$$\iint \left(-\nabla^2 u - \lambda u\right) \delta u = 0$$

where

(53)
$$\lambda = \frac{\iint \nabla u \cdot \nabla u}{\iint u^2}.$$

Thus the variational principle $\delta R=0$ yields (45); and, moreover, the value of R at the solution of (45) is the eigenvalue λ .

Returning to the subject of completeness, we let f(x,y) be an arbitrary function satisfying the boundary condition f=0. If the eigenfunctions are complete, then

(54)
$$f(x, y) = \sum_{i=1}^{\infty} c_i u_i(x, y)$$
 where $c_i = \iint f u_i$.

To test this we define the partial sum

(55)
$$f_n(x,y) = \sum_{i=1}^n c_i u_i(x,y)$$

and the remainder $r_n(x,y) = f - f_n$. Our task is to show that $r_n \to 0$ (in some sense) as $n \to \infty$. But r_n belongs to the class (49) except for the normalization requirement. Thus

(56)
$$R[r_n] \ge \lambda_{n+1} \quad \Leftrightarrow \quad \frac{\iint \nabla r_n \cdot \nabla r_n}{\iint r_n^2} \ge \lambda_{n+1}$$

The proof proceeds by showing that $\iint \nabla r_n \cdot \nabla r_n$ is bounded as $n \to \infty$. Then since $\lambda_{n+1} \to \infty$, we must have $\iint r_n^2 \to 0$, i.e.

(57)
$$\iint \left(f - \sum_{i=1}^{n} c_i u_i \right)^2 \to 0 \quad \text{as} \quad n \to \infty$$

(convergence in the mean square). To see that $\iint \nabla r_n \cdot \nabla r_n$ is bounded, we compute

$$\iint \nabla r_n \cdot \nabla r_n = \iint \left[\nabla f \cdot \nabla f - 2 \nabla f \cdot \nabla f_n + \nabla f_n \cdot \nabla f_n \right]$$
$$= \iint \left[\nabla f \cdot \nabla f + 2 f \nabla^2 f_n - f_n \nabla^2 f_n \right]$$
$$(58) = \iint \left[\nabla f \cdot \nabla f - 2 f \sum_{i=1}^n \lambda_i c_i u_i + \sum_{i=1}^n \sum_{i=1}^n c_i u_i \lambda_j c_j u_j \right]$$
$$= \iint \nabla f \cdot \nabla f - 2 \sum_{i=1}^n \lambda_i c_i^2 + \sum_{i=1}^n \lambda_i c_i^2$$
$$= \iint \nabla f \cdot \nabla f - \sum_{i=1}^n \lambda_i c_i^2 < \iint \nabla f \cdot \nabla f$$

Since only mean square convergence has been proved, we can even relax the condition that f=0 at the boundaries. That is, any f(x,y) can be represented as an infinite series of the eigenfunctions in a mean-square sense.

Reference. The book by Lanczos.