8. Orthogonal bases

We have investigated the Heat Equation in one dimension with Neumann, Dirichlet, Robin, and periodic boundary conditions, as well as with a linear term added to the right-hand side. We have also looked at the Wave Equation with Dirichlet boundary conditions. In all of these cases, separation of variables always led to orthogonal eigenfunctions: this cannot be a mere coincidence! In fact, there must be some general structure in the BVP that is responsible for orthogonality. The goal of this section is to uncover that structure.

Let us use the familiar device of discretization. It will be easier to see what needs to be proved in the continuous case if we first investigate orthogonality in the discrete setting. Suppose we want to solve the Neumann problem for the Heat Equation on the interval $[0,\pi]$. Partition the interval $[0,\pi]$ into N equal subintervals of length π/N. If N is sufficiently large, the temperature on each subinterval will not vary appreciably. We can therefore introduce N "temperature probes" at the midpoints of subintervals

$$u_n(t) = u(x_n,t), \quad x_n = \frac{\pi}{2N} + \frac{\pi}{N}(n-1), \quad n = 1,\dots,N$$

For large N we expect the points $(x_n, u_n(t))$ to lie close to the graph of $u(x,t)$ and, as we show later, this is indeed the case.

The temperature probes $u_n(t)$ satisfy the following system of ODE [21]:

$$\begin{aligned}
\frac{du_1}{dt} &= \frac{N}{\pi}(u_2 - u_1),\\
\frac{du_n}{dt} &= \frac{N^2}{\pi^2}\left(u_{n-1} - 2\,u_n + u_{n+1}\right), \quad n = 2,\dots,N-1,\\
\frac{du_N}{dt} &= \frac{N}{\pi}(u_{N-1} - u_N).
\end{aligned}$$

Write the ODE system in matrix-vector form

$$\frac{d}{dt}\mathbf{u} = \mathbf{A}\,\mathbf{u}$$

[21] Think of π/N as Δx. Then for the interior nodes $n = 2,\dots,N-1$ the right-hand side

$$\frac{N^2}{\pi^2}\left(u_{n-1} - 2\,u_n + u_{n+1}\right) = \frac{u(x-\Delta x,t) - 2\,u(x,t) + u(x+\Delta x,t)}{(\Delta x)^2}$$

is the approximation of the second derivative $\frac{\partial^2 u}{\partial x^2}$ with finite differences. The first and the last nodes exchange energy only with one neighbor and have right-hand sides consistent with the Neumann conditions and let $\{\lambda_n, \mathbf{g_n}\}_{\mathbf{n=1}}^{\mathbf{N}}$ denote the eigenvalue decomposition of A. Then the general solution of the ODE system can be written in the form:

$$\mathbf{u} = \sum_{\mathbf{n=1}}^{\mathbf{N}} \mathbf{C_n}\, \mathbf{e}^{\lambda_\mathbf{n}\, \mathbf{t}}\, \mathbf{g_n}.$$

We expect the discretized solution to be close to the continuous solution

$$u(x,t) = \sum_{n=1}^{\infty} c_n\, e^{-n^2\, t}\, \cos(n\, x).$$

Hence λ_n must be close to $(-n^2)$ and $\mathbf{g_n}$ must be close to discretized cosines $\cos(n\,x)$ in the limit as $N \to \infty$. Hence our expectation is that the eigenvectors of A are orthogonal or very nearly orthogonal. Yet, what would force the orthogonality of eigenvectors of a matrix?

To answer this let us examine the structure of A. For instance, for $N = 5$ the matrix A has the form:

$$\frac{1}{(\Delta x)^2} \begin{pmatrix} -\Delta x & \Delta x & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & \Delta x & -\Delta x \end{pmatrix}, \quad \Delta x = \frac{\pi}{5}.$$

The most salient feature of A is its symmetry: $A^t = A$. This suggests the following theorem.

Theorem 1. *Let A be a real-valued symmetric matrix. The eigenvectors of A corresponding to different eigenvalues are orthogonal.*

In order to prove the theorem we first need to relate the symmetry under transposition with the dot product. This leads to the definition of the adjoint matrix.

Definition 5. Let A be any matrix. The adjoint matrix A^* is defined by the property:

$$\mathbf{v} \cdot (\mathbf{A}\,\mathbf{u}) = (\mathbf{A}^*\mathbf{v}) \cdot \mathbf{u},$$

which must hold for any two vectors $\mathbf{u}$ and $\mathbf{v}$ (of appropriate lengths).

As an exercise, you are asked to show that for real-valued matrices $A^* = A^t$. In particular, a symmetric matrix is its own adjoint, that is symmetric matrices are self-adjoint. We can now prove the theorem.

Proof of Theorem 1. Let $\mathbf{v_1}$ and $\mathbf{v_2}$ be two eigenvectors of A corresponding to distinct eigenvalues λ_1 and λ_2. Consider

$$\mathbf{v_1} \cdot (\mathbf{A}\,\mathbf{v_2})$$

On one hand, since $\mathbf{v_2}$ is an eigenvector with eigenvalue λ_2, we can write

$$\mathbf{v_1} \cdot (\mathbf{A}\,\mathbf{v_2}) = \mathbf{v_1} \cdot (\boldsymbol{\lambda_2}\,\mathbf{v_2}) = \boldsymbol{\lambda_2}\,\mathbf{v_1} \cdot \mathbf{v_2}.$$

On the other hand, since A is self-adjoint and v_1 is an eigenvector with eigenvalue λ_1,

$$\mathbf{v_1} \cdot (\mathbf{A}\,\mathbf{v_2}) = (\mathbf{A}\,\mathbf{v_1}) \cdot \mathbf{v_2} = \boldsymbol{\lambda_1}\,\mathbf{v_1} \cdot \mathbf{v_2}.$$

We conclude that

$$\lambda_1\,\mathbf{v_1} \cdot \mathbf{v_2} = \boldsymbol{\lambda_2}\,\mathbf{v_1} \cdot \mathbf{v_2},$$

which is possible only if

$$\mathbf{v_1} \cdot \mathbf{v_2} = \mathbf{0},$$

since $\lambda_1 \neq \lambda_2$ and eigenvectors cannot be zero. □

As follows from Theorem 1 the eigenvectors $\mathbf{g_n}$ corresponding to discretized eigenfunctions

$$g_n(x) = \cos(n\,x)$$

in the Neumann problem for the Heat Equation are orthogonal for all N due to the symmetry of the matrix A. We can now attempt to prove orthogonality in the continuous case. It must clearly have to do with the symmetry of the operator $\frac{d^2}{dx^2}$, or, to be more precise, with its *self-adjointness*. To make things interesting, let us prove the orthogonality of eigenfunctions in the Robin problem where eigenvalues cannot be obtained in close form.

Theorem 2 (Orthogonality)**.** *Consider the Heat Equation IBVP with Robin's boundary conditions:*

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} \quad \textit{(Heat Equation in 1 dimension)} \\
u(x,0) &= u_0(x) \quad \textit{(Initial condition)} \\
\alpha\, u(x,t) + \beta \left.\frac{\partial u}{\partial x}\right|_{x=0,L} &= 0 \quad \textit{(Robin boundary conditions)}
\end{aligned}$$

Let $g_n(x)$ denote the solution of the associated ordinary BVP that arises during separation of variables:

$$\frac{d^2 g_n}{dx^2} + \lambda_n^2\, g_n = 0, \quad \alpha\, g_n(x) + \beta \left.\frac{dg_n}{dx}(x)\right|_{x=0,L} = 0. \tag{8.1}$$

We call the function g_n an eigenfunction corresponding to the eigenvalue λ_n *and tacitly assume that the eigenvalues λ_n form a discrete sequence. Let g_n and g_m be two eigenfunctions corresponding to two* *distinct eigenvalues. Then g_n and g_m are orthogonal with respect to the usual dot product on* $[0, L]$*:*

$$g_n(x) \cdot g_m(x) = \int_0^L g_n(x)\, g_m(x)\, dx = 0.$$

Proof. Notice that the theorem asserts orthogonality of Fourier modes without reference to any trigonometry: the eigenfunctions g_n do not need to be known explicitly. This suggests that we should work with the BVP (8.1) rather than its trigonometric solution. In the light of Equation (8.1), what we do know about g_n and g_m can be restated as follows:

$$\begin{aligned} \frac{d^2 g_n}{dx^2} &= -\lambda_n^2\, g_n \\ \frac{d^2 g_m}{dx^2} &= -\lambda_m^2\, g_m \end{aligned}$$

Further, we know that both g_n and g_m satisfy symmetric Robin boundary conditions. If we multiply the first ODE (for g_n) by g_m and the second by g_m and subtract one from another, the results will be

$$g_n \frac{d^2 g_m}{dx^2} - g_m \frac{d^2 g_n}{dx^2} = (\lambda_n^2 - \lambda_m^2)\, g_n\, g_m.$$

Now integrate both sides from 0 to L to get

$$\int_0^L \left[g_n(x) \frac{d^2 g_m}{dx^2}(x) - g_m(x) \frac{d^2 g_n}{dx^2}(x) \right] dx = (\lambda_n^2 - \lambda_m^2)$$
$$\times \int_0^L g_n(x)\, g_m(x)\, dx = (\lambda_n^2 - \lambda_m^2)\, g_n \cdot g_m.$$

Notice that we have essentially obtained an expression for the dot product of $g_n \cdot g_m$ which we can now manipulate as follows:

$$\begin{aligned} &\int_0^L \left[g_n(x) \frac{d^2 g_m}{dx^2}(x) - g_m(x) \frac{d^2 g_n}{dx^2}(x) \right] dx \\ &= \int_0^L \frac{d}{dx} \left[g_n(x) \frac{d g_m}{dx}(x) - g_m(x) \frac{d g_n}{dx}(x) \right] dx \\ &= g_n(x) \frac{d g_m}{dx}(x) - g_m(x) \frac{d g_n}{dx}(x) \Bigg|_{x=0}^{x=L} \\ &= \left| \begin{array}{cc} g_n(x) & g_m(x) \\ \frac{dg_n}{dx}(x) & \frac{dg_m}{dx}(x) \end{array} \right| \Bigg|_{x=0}^{x=L} \end{aligned}$$

We now argue that the determinant vanishes at both endpoints due to Robin's boundary conditions: indeed, at the endpoints of $[0, L]$ we can substitute derivatives with scaled functions

$$\frac{dg_{n,m}}{dx} = -\frac{\alpha}{\beta}\, g_{n,m}(x)\bigg|_{x=0,L}$$

and then the determinant vanishes (if $\beta = 0$, we have the already investigated Dirichlet case.) We have thus shown that

$$(\lambda_n^2 - \lambda_m^2)\, g_n \cdot g_m = 0, \quad n \neq m.$$

Since $\lambda_n \neq \lambda_m$ we must have

$$g_n \cdot g_m = 0,$$

which shows that the eigenfunctions corresponding to distinct eigenvalues are orthogonal. $\square$

Exercises

(1) Present an argument showing that for real square matrices $A^* = A^t$. Explain how adjoint needs to be defined for complex matrices.

(2) Let

$$f(x) = \begin{cases} +1, & 0 \leq x \leq \pi \\ -1, & -\pi < x < 0. \end{cases}$$

Think of $f(x)$ as a function on a unit circle. Find the coefficients in the complex Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n\, e^{i\,n\,x}.$$

Note: Exercise care with the complex dot product.

(3) Solve the Heat Equation with Robin's boundary conditions:

$$u(x,t) + 2\,\frac{\partial u}{\partial x}\bigg|_{x=0,L} = 0.$$

Use software to confirm the orthogonality of the first three Fourier modes numerically.

(4) Let

$$V = \{f \in C^1([0,1]) \mid f(0) = f(1) = 0\}$$

and let $L = \frac{d}{dx}$. That is, V is the space of continuously differentiable functions on $[0,1]$ which vanish at the endpoints; L is the derivative operator. Find the adjoint L^*.