/// 1 /// ONE-DIMENSIONAL GRIDS

A finite difference grid for solving ordinary or partial differential equations consists of rectilinear or curvilinear grid lines that can be regarded as conveying links intersecting at nodes. This interpretation provides us with a point of departure for making an analogy between numerical grids, mathematical graphs, and physical or abstract networks. We begin in this chapter by developing finite difference equations for an elementary ordinary equation with the objective of identifying similarities between grids and graphs, and then we generalize the framework to higher dimensions.

1.1 POISSON EQUATION IN ONE DIMENSION

Consider the Poisson equation in one dimension for an unknown function of one variable, $f(x)$,

$$\frac{d^2f}{dx^2} + g(x) = 0, \tag{1.1.1}$$

to be solved in a finite domain, $[a, b]$, where $g(x)$ is a given source function. When $g(x) = 0$, the Poisson equation reduces to Laplace's equation. When $g(x) = \alpha f(x)$, the Poisson equation reduces to Helmholtz's equation, where α is a real or complex constant.

A numerical solution can be found on a uniform finite difference grid with K divisions defined by $K + 1$ nodes, as shown in Figure 1.1.1. Nodes numbered 0 and

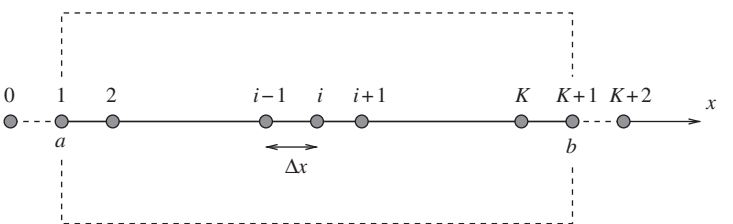

FIGURE 1.1.1 A finite difference with K uniform divisions along the x axis. Dirichlet or Neumann boundary conditions are specified at the two ends of the solution domain.

$K+2$ are phantom nodes, lying outside the solution domain, introduced to implement the Neumann boundary condition, when specified, as discussed later in this chapter.

Applying the Poisson equation at the ith node, approximating the second derivative with a central difference by setting

$$f''(x_i) \simeq \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2} + O(\Delta x^2) \tag{1.1.2}$$

with an error of order Δx^2, and rearranging, we obtain the difference equation

$$-f_{i-1} + 2f_i - f_{i+1} = \Delta x^2 g_i \tag{1.1.3}$$

to be applied at an appropriate number of nodes. To simplify the notation, we have denoted

$$f_i \equiv f(x_i), \quad g_i \equiv g(x_i). \tag{1.1.4}$$

The signs on the left- and right-hand sides of (1.1.3) were chosen intentionally to conform with standard notation in graph theory regarding the Laplacian, as discussed in Section 1.7.

Collecting all available difference equations and implementing the boundary conditions provides us with a system of linear algebraic equations for a suitable number of unknown nodal values contained in a solution vector, $\boldsymbol{\psi}$,

$$\mathbf{L} \cdot \boldsymbol{\psi} = \mathbf{b}, \tag{1.1.5}$$

where the centered dot denotes the matrix–vector product. The size and specific form of the coefficient matrix, $\mathbf{L}$, solution vector, $\boldsymbol{\psi}$, and vector on the right-hand side, $\mathbf{b}$, depend on the choice of boundary conditions. Several possibilities are discussed in this chapter.

Factorization

We will see that, for any type of boundary conditions—Neumann, Dirichlet, or periodic—the coefficient matrix of the linear system admits the factorization

$$\mathbf{L} = \mathbf{R} \cdot \mathbf{R}^T, \tag{1.1.6}$$

where $\mathbf{R}$ is a square or rectangular matrix, the superscript T denotes the matrix transpose, and the centered dot denotes the usual matrix product (e.g., [35]). This factorization can be regarded as the discrete counterpart of the definition of the second derivative as the sequential application of the first derivative,

$$\frac{d^2}{dx^2} = \frac{d}{dx}\frac{d}{dx}. \tag{1.1.7}$$

It is important to note that the commutative property $\mathbf{R} \cdot \mathbf{R}^T = \mathbf{R}^T \cdot \mathbf{R}$ is not always satisfied.

The counterpart of the factorization (1.1.6) in n dimensions is

$$\nabla^2 = \nabla \cdot \nabla, \tag{1.1.8}$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2} \tag{1.1.9}$$

is the scalar Laplacian operator,

$$\nabla = \left(\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} + \cdots + \frac{\partial}{\partial x_n} \right) \tag{1.1.10}$$

is the vectorial gradient operator, and the centered dot denotes the inner vector product. In two dimensions $n = 2$, and in three dimensions $n = 3$.

Exercise

1.1.1 *Helmholtz equation*

Write the counterpart of the difference equation (1.1.3) for the Helmholtz equation in one dimension,

$$\frac{d^2 f}{dx^2} + \alpha f = 0, \tag{1.1.11}$$

where α is a real or complex constant.

1.2 DIRICHLET BOUNDARY CONDITION AT BOTH ENDS

When the Dirichlet boundary condition is specified at both ends of the solution domain, the first and last values, f_1 and f_{K+1}, are known. Collecting the difference equations (1.1.3) for the interior nodes, $i = 2, \ldots, K$, we obtain a system of linear equations,

$$\mathbf{L}^{\mathrm{DD}} \cdot \boldsymbol{\psi}^{\mathrm{DD}} = \mathbf{b}^{\mathrm{DD}}, \tag{1.2.1}$$

where

$$\boldsymbol{\psi}^{\mathrm{DD}} \equiv \begin{bmatrix} f_2 \\ f_3, \\ \vdots \\ f_{K-1} \\ f_K \end{bmatrix}, \quad \mathbf{b}^{\mathrm{DD}} = \begin{bmatrix} \Delta x^2 g_2 + f_1 \\ \Delta x^2 g_3 \\ \vdots \\ \Delta x^2 g_{K-1} \\ \Delta x^2 g_K + f_{K+1} \end{bmatrix}, \tag{1.2.2}$$

are $(K-1)$-dimensional vectors and

$$\mathbf{L}^{\mathrm{DD}} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix} \tag{1.2.3}$$

is $(K-1) \times (K-1)$ symmetric tridiagonal Toeplitz matrix. By definition, a Toeplitz matrix consists of constant diagonal lines. The superscript DD emphasizes that the Dirichlet condition is specified at both ends.

Decomposition

We can decompose

$$\mathbf{L}^{\mathrm{DD}} = 2\,\mathbf{I} - \boldsymbol{\Omega}^{\mathrm{DD}}, \tag{1.2.4}$$

where $\mathbf{I}$ is the $(K-1) \times (K-1)$ identity matrix and

$$\boldsymbol{\Omega}^{\mathrm{DD}} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \tag{1.2.5}$$

is a $(K-1) \times (K-1)$ symmetric bidiagonal Toeplitz matrix with zeros along the diagonal.

Eigenvalues and Eigenvectors

The eigenvalues of the matrices $\boldsymbol{\Omega}^{\mathrm{DD}}$ and $\mathbf{L}^{\mathrm{DD}}$ are

$$\lambda_m^{\Omega} = 2\,\cos\alpha_m \tag{1.2.6}$$

and

$$\lambda_m^{\mathrm{L}} = 2 - 2\,\cos\alpha_m = 4\,\sin^2\left(\tfrac{1}{2}\alpha_m\right), \tag{1.2.7}$$

where

$$\alpha_m = \frac{m}{K}\,\pi \tag{1.2.8}$$

for $m = 1, \ldots, K-1$.

The corresponding shared eigenvectors, $\mathbf{u}^{(m)}$, normalized so that their length is equal to unity, $\mathbf{u}^{(m)} \cdot \mathbf{u}^{(m)} = 1$, are

$$u_j^{(m)} = \left(\frac{2}{K}\right)^{1/2} \sin(j\alpha_m) \tag{1.2.9}$$

for $m, j = 1, \ldots, K-1$. It is interesting that all eigenvectors are pure harmonic waves, with higher-order eigenvalues corresponding to shorter wavelengths.

Factorization

We can factorize

$$\mathbf{L}^{\mathrm{DD}} = \mathbf{R}^{\mathrm{DD}} \cdot \mathbf{R}^{\mathrm{DD}^T}, \tag{1.2.10}$$

where

$$\mathbf{R}^{\mathrm{DD}} = \left[\begin{array}{ccccccc|c} -1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 & 0 & \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 1 \end{array}\right] \tag{1.2.11}$$

is a rectangular $(K-1) \times K$ matrix implementing forward difference approximations to the first derivative. The transpose of $\mathbf{R}^{\mathrm{DD}}$,

$$\mathbf{R}^{\mathrm{DD}^T} = \left[\begin{array}{ccccccc} -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -1 \\ \hline 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{array}\right], \tag{1.2.12}$$

is a rectangular $K \times (K-1)$ matrix implementing backward difference approximations to the first derivative.

Exercises

1.2.1 *Sinusoidal Source*

Solve the linear system (1.2.1) for $a = 0$ and $g(x) = \gamma \sin^2(2\pi x/b)$, where γ is a constant. The boundary conditions specify that $f(0) = 0$ and $f(b) = f_b$, where f_b is a

given constant. Carry out computations for $K = 2, 4, 8, 16$, and 32, and discuss the accuracy of the numerical results with reference to the exact solution.

1.2.2 *Factorization*

Confirm the factorization (1.2.10).

1.3 NEUMANN–DIRICHLET BOUNDARY CONDITIONS

Now assume that the Neumann boundary condition is prescribed at the right end of the solution domain, $x = a$, specifying that

$$f'(x_1) = -q_1, \tag{1.3.1}$$

where q_1 is a given constant, while the Dirichlet boundary condition is prescribed at the left end of the solution domain, $x = b$. specifying the value of f_{K+1}. Following standard practice, we introduce a phantom node labeled zero, as shown in Figure 1.1.1, approximate the first derivative with second-order accuracy using a central difference as

$$f'(x_1) \simeq \frac{f_2 - f_0}{2\Delta x} + O(\Delta x^2), \tag{1.3.2}$$

and write

$$f_0 = f_2 + 2\Delta x\, q_1. \tag{1.3.3}$$

The difference equations for $i = 1, \ldots, K$ provide us with a system of linear equations,

$$\mathbf{L}^{\mathrm{ND}} \cdot \boldsymbol{\psi}^{\mathrm{ND}} = \mathbf{b}^{\mathrm{ND}}, \tag{1.3.4}$$

where

$$\boldsymbol{\psi}^{\mathrm{ND}} \equiv \begin{bmatrix} f_1 \\ f_2, \\ \vdots \\ f_{K-1} \\ f_K \end{bmatrix}, \quad \mathbf{b}^{\mathrm{ND}} = \begin{bmatrix} \frac{1}{2}\Delta x^2 g_1 + \Delta x\, q_1 \\ \Delta x^2 g_2 \\ \vdots \\ \Delta x^2 g_{K-1} \\ \Delta x^2 g_K + f_{K+1} \end{bmatrix}, \tag{1.3.5}$$

are K-dimensional vectors and

$$\mathbf{L}^{\mathrm{ND}} = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix} \tag{1.3.6}$$

is a $K \times K$ symmetric, tridiagonal, nearly Toeplitz matrix. If the first diagonal element were equal to 2, this matrix would have been a perfect Toeplitz matrix.

Decomposition

We can decompose

$$\mathbf{L}^{\mathrm{ND}} = 2\,\mathbf{I} - \boldsymbol{\Omega}^{\mathrm{ND}}, \tag{1.3.7}$$

where $\mathbf{I}$ is the $K \times K$ identity matrix and

$$\boldsymbol{\Omega}^{\mathrm{ND}} = \begin{bmatrix} 1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \tag{1.3.8}$$

is a $K \times K$ square, symmetric, tridiagonal, nearly Toeplitz matrix. If the first diagonal element were equal to 0, this would have been a perfect Toeplitz matrix.

Eigenvalues and Eigenvectors

The eigenvalues of $\boldsymbol{\Omega}^{\mathrm{ND}}$ and $\mathbf{L}^{\mathrm{ND}}$ are

$$\lambda_m^{\Omega} = 2\cos\alpha_m \tag{1.3.9}$$

and

$$\lambda_m^{L} = 2 - 2\,\cos\alpha_m = 4\sin^2\left(\tfrac{1}{2}\,\alpha_m\right), \tag{1.3.10}$$

where

$$\alpha_m = \frac{m - 1/2}{K + 1/2}\,\pi \tag{1.3.11}$$

for $m = 1, \ldots, K$.

The corresponding shared eigenvectors, $\mathbf{u}^{(m)}$, normalized so that their length is equal to unity, $\mathbf{u}^{(m)} \cdot \mathbf{u}^{(m)} = 1$, are

$$u_j^{(m)} = \left(\frac{4}{2K+1}\right)^{1/2} \cos\left[\left(j - \tfrac{1}{2}\right)\,\alpha_m\right] \tag{1.3.12}$$

for $m, j = 1, \ldots, K$. All eigenvectors are pure harmonic waves.

Factorization

We can factorize

$$\mathbf{L}^{\mathrm{ND}} = \mathbf{R}^{\mathrm{ND}} \cdot \mathbf{R}^{\mathrm{ND}^T}, \tag{1.3.13}$$

where

$$\mathbf{R}^{\mathrm{ND}} = \begin{bmatrix} -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -1 \end{bmatrix} \tag{1.3.14}$$

is a $K \times K$ square lower bidiagonal $K \times K$ Toeplitz matrix implementing backward difference approximations to the first derivative. Its transpose,

$$\mathbf{R}^{\mathrm{ND}^T} = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -1 \end{bmatrix}, \tag{1.3.15}$$

is a $K \times K$ square upper bidiagonal $K \times K$ Toeplitz matrix implementing forward difference approximations to the first derivative.

Exercise

1.3.1 *Factorization*

Confirm by direct multiplication the factorization (1.3.13).

1.4 DIRICHLET–NEUMANN BOUNDARY CONDITIONS

In the third case study, we assume that a Dirichlet boundary condition specifying the value of f_1 is prescribed at the left end of the solution domain, and a Neumann boundary condition specifying that

$$f'(x_{K+1}) = q_{K+1} \tag{1.4.1}$$

is prescribed at the right end of the solution domain, where q_{K+1} is a given constant. We proceed by introducing a phantom node numbered $K + 2$, as shown in Figure 1.1.1, approximate the first derivative with second-order accuracy as

$$f'(x_{K+1}) \simeq \frac{f_{K+2} - f_K}{2\Delta x} + O(\Delta x^2), \tag{1.4.2}$$

and obtain

$$f_{K+2} = f_K + 2\Delta x\, q_{K+1}. \tag{1.4.3}$$

The difference equations for $i = 2, K+1$ provide us with a linear system,

$$\mathbf{L}^{\mathrm{DN}} \cdot \boldsymbol{\psi}^{\mathrm{DN}} = \mathbf{b}^{\mathrm{DN}}, \tag{1.4.4}$$

where

$$\boldsymbol{\psi}^{\mathrm{DN}} \equiv \begin{bmatrix} f_2 \\ f_3, \\ \vdots \\ f_K \\ f_{K+1} \end{bmatrix}, \quad \mathbf{b}^{\mathrm{DN}} = \begin{bmatrix} \Delta x^2 g_2 + f_1 \\ \Delta x^2 g_3 \\ \vdots \\ \Delta x^2 g_K \\ \frac{1}{2}\Delta x^2 g_{K+1} + \Delta x\, q_{K+1} \end{bmatrix} \tag{1.4.5}$$

are K-dimensional vectors and

$$\mathbf{L}^{\mathrm{DN}} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix} \tag{1.4.6}$$

is a $K \times K$ symmetric, tridiagonal, nearly Toeplitz matrix.

Decomposition

We can decompose

$$\mathbf{L}^{\mathrm{DN}} = 2\,\mathbf{I} - \boldsymbol{\Omega}^{\mathrm{DN}}, \tag{1.4.7}$$

where $\mathbf{I}$ is the $N \times N$ identity matrix and

$$\boldsymbol{\Omega}^{\mathrm{DN}} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 1 \end{bmatrix} \tag{1.4.8}$$

is a $K \times K$ symmetric, tridiagonal, nearly Toeplitz matrix.

Eigenvalues and Eigenvectors

The eigenvalues of $\mathbf{\Omega}^{\mathrm{DN}}$ and $\mathbf{L}^{\mathrm{DN}}$ are

$$\lambda_m^{\Omega} = 2\cos\alpha_m \tag{1.4.9}$$

and

$$\lambda_m^{L} = 2 - 2\cos\alpha_m = 4\sin^2\left(\tfrac{1}{2}\alpha_m\right), \tag{1.4.10}$$

where

$$\alpha_m = \frac{m-\frac{1}{2}}{K+\frac{1}{2}}\,\pi \tag{1.4.11}$$

for $m = 1, \ldots, K$.

The corresponding shared eigenvectors, $\mathbf{u}^{(m)}$, normalized so that their length is equal to unity, $\mathbf{u}^{(m)} \cdot \mathbf{u}^{(m)} = 1$, are

$$u_j^{(m)} = \left(\frac{4}{2K+1}\right)^{1/2} \cos\left[\left(K - j + \tfrac{1}{2}\right)\alpha_m\right] \tag{1.4.12}$$

for $m, j = 1, \ldots, K$. All eigenvectors are pure harmonic waves.

Factorization

We can factorize

$$\mathbf{L}^{\mathrm{DN}} = \mathbf{R}^{\mathrm{DN}} \cdot \mathbf{R}^{\mathrm{DN}^T} = \mathbf{R}^{\mathrm{ND}^T} \cdot \mathbf{R}^{\mathrm{ND}}, \tag{1.4.13}$$

where $\mathbf{R}^{\mathrm{DN}} = \mathbf{R}^{\mathrm{ND}^T}$ and the matrix $\mathbf{R}^{\mathrm{ND}}$ is given in (1.3.15).

Exercise

1.4.1 *Eigenvalues and eigenvectors*

Confirm by direct substitution the eigenvalues and eigenvectors given in (1.4.10) and (1.4.12).

1.5 NEUMANN BOUNDARY CONDITIONS

In the fourth and most important case, the Neumann boundary condition is prescribed at both ends of the solution domain,

$$f'(x_1) = -q_1, \quad f'(x_{K+1}) = q_{K+1}. \tag{1.5.1}$$

where q_1 and q_{K+1} are two given constants. Working in the familiar way, we collect the difference equations for $i = 1, \ldots, K+1$ into a linear system,

$$\mathbf{L}^{\mathrm{NN}} \cdot \boldsymbol{\psi}^{\mathrm{NN}} = \mathbf{b}^{\mathrm{NN}}, \tag{1.5.2}$$

where

$$\boldsymbol{\psi}^{\mathrm{NN}} \equiv \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_K \\ f_{K+1} \end{bmatrix}, \quad \mathbf{b}^{\mathrm{NN}} = \begin{bmatrix} \frac{1}{2}\Delta x^2 g_1 + \Delta x\, q_1 \\ \Delta x^2 g_2 \\ \vdots \\ \Delta x^2 g_K \\ \frac{1}{2}\Delta x^2 g_{K+1} + \Delta x\, q_{K+1} \end{bmatrix} \tag{1.5.3}$$

are $(K+1)$-dimensional vectors and

$$\mathbf{L}^{\mathrm{NN}} = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix} \tag{1.5.4}$$

is a $(K+1) \times (K+1)$ symmetric tridiagonal matrix. If the first and last diagonal elements were equal to 2, this would have been a perfect Toeplitz matrix.

Decomposition

We can decompose

$$\mathbf{L} = 2\,\mathbf{I} - \boldsymbol{\Omega}^{\mathrm{NN}}, \tag{1.5.5}$$

where $\mathbf{I}$ is the $(K+1) \times (K+1)$ identity matrix and

$$\boldsymbol{\Omega}^{\mathrm{NN}} = \begin{bmatrix} 1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 1 \end{bmatrix} \tag{1.5.6}$$

is a nearly upper and lower bidiagonal matrix. Note the presence of two nonzero top and bottom diagonal elements.

Eigenvalues and Eigenvectors

The eigenvalues of $\mathbf{\Omega}^{\mathrm{NN}}$ and $\mathbf{L}^{\mathrm{NN}}$ are

$$\lambda_m^{\Omega} = 2\,\cos\alpha_m \tag{1.5.7}$$

and

$$\lambda_m^{L} = 2 - 2\,\cos\alpha_m = 4\,\sin^2\left(\tfrac{1}{2}\alpha_m\right), \tag{1.5.8}$$

where

$$\alpha_m = \frac{m-1}{K+1}\,\pi \tag{1.5.9}$$

for $m = 1, \ldots, K+1$.

The corresponding shared eigenvectors, $\mathbf{u}^{(m)}$, normalized so that their length is equal to unity, $\mathbf{u}^{(m)} \cdot \mathbf{u}^{(m)} = 1$, are

$$u_j^{(m)} = A_m \left(\frac{2}{K+1}\right)^{1/2} \cos\left[\left(j - \tfrac{1}{2}\right)\alpha_m\right] \tag{1.5.10}$$

for $m, j = 1, \ldots, K+1$, where $A_m = 1$, except that $A_1 = 1/\sqrt{2}$. The presence of a zero eigenvalue of the Laplacian, $\lambda_1^L = 0$, corresponding to a constant eigenvector, confirms that the Laplacian matrix is singular. The rest of the eigenvectors are pure harmonic waves.

Cursory inspection reveals the interesting identity

$$\mathbf{f} \cdot \mathbf{L}^{\mathrm{NN}} \cdot \mathbf{f} = \sum_{i=1}^{K} (f_i - f_{i+1})^2 \geq 0 \tag{1.5.11}$$

for any arbitrary nodal field, $\mathbf{f}$, which demonstrates that the matrix $\mathbf{L}^{\mathrm{NN}}$ is positive semidefinite. If $\mathbf{u}$ is an eigenvector of $\mathbf{L}^{\mathrm{NN}}$ with corresponding eigenvector λ, then

$$\mathbf{u} \cdot \mathbf{L}^{\mathrm{NN}} \cdot \mathbf{u} = \lambda\,\mathbf{u} \cdot \mathbf{u} \geq 0. \tag{1.5.12}$$

This inequality confirms that the eigenvalues of $\mathbf{L}^{\mathrm{NN}}$ are zero or positive.

It is worth remarking that the eigenvalues of the Laplacian matrix are approximations of those of the Laplace equation, ℓ, in the interval $[a, b]$, satisfying the equation

$$\frac{d^2u}{dx^2} + \frac{\ell}{\Delta x^2}\,u = 0 \tag{1.5.13}$$

with homogeneous Neumann boundary conditions at both ends, $u'(a) = 0$ and $u'(b) = 0$, where $u(x)$ is an eigenfunction, $L = K\Delta x$, and $L = b - a$. We find that

$$\ell_m = \left(\frac{m-1}{K}\right)^2 \pi^2, \quad u_m(x) = \cos\left(\frac{m-1}{K}\,\frac{\pi x}{\Delta x}\right), \tag{1.5.14}$$

for $m \geq 1$. The eigenvalues of the Laplacian matrix, λ_m^L, agree with the eigenvalues ℓ_m for small m and large K.

Factorization

We can factorize

$$\mathbf{L}^{\mathrm{NN}} = \mathbf{R}^{\mathrm{NN}} \cdot \mathbf{R}^{\mathrm{NN}^T}, \tag{1.5.15}$$

where

$$\mathbf{R}^{\mathrm{NN}} = \begin{bmatrix} -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -1 \\ \hline 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{bmatrix} \tag{1.5.16}$$

is a $(K+1)\times K$ rectangular matrix implementing backward difference approximations to the first derivative. Its transpose,

$$\mathbf{R}^{\mathrm{NN}^T} = \left[\begin{array}{ccccccc|c} -1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 1 \end{array}\right], \tag{1.5.17}$$

is a $K \times (K+1)$ matrix implementing forward difference approximations to the first derivative.

Exercise

1.5.1 *Eigenvalues of the Laplacian*

(*a*) Derive the eigenvalues and eigenvectors shown in (1.5.14). (*b*) Prepare and discuss a plot of the eigenvalues given in (1.5.14) and those of the Laplacian matrix for $K = 2, 4, 8, 16$, and 32.

1.6 PERIODIC BOUNDARY CONDITIONS

When the solution of the differential equation (1.1.1) is required to be periodic, we specify that $f_1 = f_{K+1}$ and compile the difference equations for $i = 1, \ldots, K$ to obtain a linear system,

$$\mathbf{L}^{\mathrm{P}} \cdot \boldsymbol{\psi}^{\mathrm{P}} = \mathbf{b}^{\mathrm{P}}, \tag{1.6.1}$$

where

$$\boldsymbol{\psi}^{\mathrm{P}} \equiv \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{K-1} \\ f_K \end{bmatrix}, \quad \mathbf{b}^{\mathrm{P}} = \Delta x^2 \begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_{K-1} \\ g_K \end{bmatrix}, \tag{1.6.2}$$

are K-dimensional vectors and

$$\mathbf{L}^{\mathrm{P}} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & -1 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ -1 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}, \tag{1.6.3}$$

is a $K \times K$ symmetric and nearly tridiagonal matrix. Note the presence of a northeastern and a southwestern element, both equal to –1, implementing the periodicity condition.

Decomposition

We can decompose

$$\mathbf{L}^{\mathrm{P}} = 2\,\mathbf{I} - \boldsymbol{\Omega}^{\mathrm{P}}, \tag{1.6.4}$$

where $\mathbf{I}$ is the $K \times K$ identity matrix and

$$\boldsymbol{\Omega}^{\mathrm{P}} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \tag{1.6.5}$$

is a $K \times K$ symmetric, nearly bidiagonal Toeplitz matrix. Note the presence of two unit corner elements, equal to 1, implementing the periodicity condition.

Eigenvalues and Eigenvectors

The eigenvalues of $\mathbf{\Omega}^{\mathrm{P}}$ and $\mathbf{L}^{\mathrm{P}}$ are

$$\lambda_m^{\Omega} = 2\cos\alpha_m \tag{1.6.6}$$

and

$$\lambda_m^{L} = 2 - 2\cos\alpha_m = 4\,\sin^2\left(\tfrac{1}{2}\,\alpha_m\right) \tag{1.6.7}$$

for $m = 1, \ldots, K$, where

$$\alpha_m = \frac{m-1}{K}\,2\pi\,. \tag{1.6.8}$$

The corresponding shared eigenvectors, $\mathbf{u}^{(m)}$, normalized so that their norm is equal to unity, $\mathbf{u}^{(m)} \cdot \mathbf{u}^{(m)^*} = 1$, are

$$u_j^{(m)} = \frac{1}{\sqrt{K}}\exp\left(-\mathrm{i}\,j\,\alpha_m\right) \tag{1.6.9}$$

for $m, j = 1, \ldots, K$, where i is the imaginary unit and an asterisk denotes the complex conjugate. The presence of a zero eigenvalue of the Laplacian, $\lambda_1^L = 0$, corresponding to a constant eigenvector, confirms that the matrix $\mathbf{L}^{\mathrm{P}}$ is singular. The rest of the eigenvectors are pure harmonic waves.

Complex eigenvectors appear because two eigenvalues, λ_{m_1} and λ_{m_2}, are identical when

$$m_1 + m_2 = K + 2. \tag{1.6.10}$$

The real part of the complex exponential in (1.6.9) can be retained for one eigenvalue, yielding a cosine, and the imaginary part can be retained for the other eigenvalue, yielding a sine.

Cursory inspection reveals the interesting identity

$$\mathbf{f} \cdot \mathbf{L}^{\mathrm{P}} \cdot \mathbf{f} = \sum_{i=1}^{K} (f_i - f_{i+1})^2 \geq 0, \tag{1.6.11}$$

where $\mathbf{f}$ is an arbitrary nodal field satisfying the mandatory periodicity condition $f_{K+1} = f_1$, which demonstrates that the matrix $\mathbf{L}^{\mathrm{NN}}$ is positive semidefinite. Consequently, the eigenvalues of $\mathbf{L}^{\mathrm{P}}$ are zero or positive.

Factorization

We can factorize

$$\mathbf{L}^{\mathrm{P}} = \mathbf{R}^{\mathrm{P}^T} \cdot \mathbf{R}^{\mathrm{P}} = \mathbf{R}^{\mathrm{P}} \cdot \mathbf{R}^{\mathrm{P}^T}, \tag{1.6.12}$$

where

$$\mathbf{R}^{\mathrm{P}} = \begin{bmatrix} -1 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -1 \end{bmatrix} \tag{1.6.13}$$

is a $K \times K$ square nearly lower bidiagonal matrix implementing backward difference approximations. Its transpose,

$$\mathbf{R}^{\mathrm{P}^T} = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 0 & -1 \end{bmatrix}, \tag{1.6.14}$$

is a $K \times K$ square nearly upper bidiagonal matrix implementing forward difference approximations. Note the presence of one nonzero corner element implementing the periodicity condition.

Exercise

1.6.1 *Eigenvalues and eigenvectors*

Confirm by direct substitution the eigenvalues and eigenvectors given in (1.6.7) and (1.6.9).

1.7 ONE-DIMENSIONAL GRAPHS

The finite difference grid discussed previously in this chapter is now regarded as a graph consisting of N nodes, also called vertices, connected by $L = N - 1$ links (edges), as illustrated in Figure 1.7.1. In an alternative interpretation, the finite difference grid is a network consisting of conducting or conveying links. For example, the links can be regarded as segments of a fluid-carrying pipe.

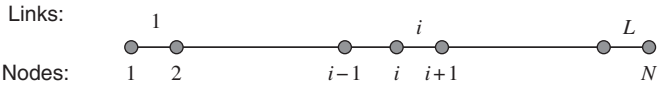

FIGURE 1.7.1 Illustration of a one-dimensional graph consisting of N nodes connected by $L = N - 1$ links.

1.7.1 Graph Laplacian

The $N \times N$ matrix $\mathbf{L} \equiv \mathbf{L}^{\mathrm{NN}}$, corresponding to two Neumann boundary conditions discussed in Section 1.5, is the Laplacian of the one-dimensional network, given by

$$\mathbf{L} = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}. \tag{1.7.1}$$

Note that the sum of the elements in each row or column is zero. Sometimes, the graph Laplacian is also called the combinatorial Laplacian.

The eigenvalues of $\mathbf{L}$ are given by

$$\lambda_m = 2 - 2\cos\alpha_n = 4\sin^2\left(\tfrac{1}{2}\alpha_n\right) \tag{1.7.2}$$

for $n = 1, \ldots, N$, where

$$\alpha_n = \frac{n-1}{N}\pi. \tag{1.7.3}$$

The corresponding eigenvectors, $\mathbf{u}^{(n)}$, normalized so that $\mathbf{u}^{(n)} \cdot \mathbf{u}^{(n)} = 1$, are given by

$$u_i^{(n)} = A_n \left(\frac{2}{N}\right)^{1/2} \cos\left[(2j-1)\alpha_n\right] \tag{1.7.4}$$

for $i, n = 1, \ldots, N$, where $A_n = 1$, except that $A_1 = 1/\sqrt{2}$. The presence of a zero eigenvalue, $\lambda_1 = 0$, corresponding to a uniform eigenvector with equal elements, confirms that the Laplacian matrix is singular. The rest of the eigenvectors are pure harmonic waves.

1.7.2 Adjacency Matrix

In graph theory, an $N \times N$ adjacency matrix is introduced, $\mathbf{A}$, defined such that $A_{ij} = 1$ if nodes i and j are connected by a grid line or link, and $A_{ij} = 0$ otherwise, with the convention that $A_{ii} = 0$. Thus, by convention, the diagonal line of the adjacency matrix is zero.

In the case of the one-dimensional grid presently considered, the adjacency matrix is

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}. \tag{1.7.5}$$

The eigenvalues of this matrix are

$$\mu_n = 2\,\cos\left(\frac{n}{N+1}\,\pi\right) \tag{1.7.6}$$

for $n = 1, \ldots, N$.

The eigenvalues of the adjacency matrix provide us with measure of the network properties, independent of node and link labeling. In particular, the number of paths that return to an arbitrary node after s steps have been made, summed over all starting nodes, is

$$n_s = \sum_{n=1}^{N} \mu_n^s, \tag{1.7.7}$$

where s is an integer. We observe that $n_0 = N$, in agreement with physical intuition. In our one-dimensional network, $n_s = 0$ if s is an odd integer and $n_s \neq 0$ if s is an even integer. Physically, an even number of steps are necessary for an equal number of forward and backward steps. For a one-dimensional network with $N = 13$ nodes, we find that

$$n_2 = 26, \quad n_4 = 74, \quad n_6 = 236, \quad n_8 = 794, \quad n_{10} = 2756. \tag{1.7.8}$$

Node Degrees

The degree of the ith node, denoted by d_i, is defined as the number of links attached to the node, which is equal to the sum of the elements in the corresponding row or

column of the adjacency matrix, **A**. In the case of the one-dimensional grid presently considered, we have

$$d_1 = 1, \quad d_i = 2, \quad d_N = 1, \tag{1.7.9}$$

for $i = 2, \ldots N - 1$.

Laplacian in Terms of the Adjacency Matrix

The graph Laplacian of the one-dimensional grid is given by

$$\mathbf{L} = \mathbf{D} - \mathbf{A}, \tag{1.7.10}$$

where **D** is a diagonal matrix whose ith diagonal element is equal to the corresponding node degree, d_i.

1.7.3 Connectivity Lists and Oriented Incidence Matrix

The number of links in the one-dimensional network is $L = N - 1$. It is useful to introduce two L-dimensional connectivity lists, **k** and **l**, defined such that the label of the first node of the mth link is k_m and the label of the second node of the mth link is l_m. In the case of the one-dimensional grid presently considered, we have

$$k_m = m, \quad l_m = m + 1 \tag{1.7.11}$$

for $m = 1, \ldots, L$. An $N \times L$ oriented incidence matrix can be introduced, **R**, defined such that $R_{i,m} = 0$, except that

$$R_{k_m,m} = -1, \quad R_{l_m,m} = 1. \tag{1.7.12}$$

If nodes and links are labeled sequentially, as shown in Figure 1.7.1, we obtain the rectangular $N \times (N - 1)$ matrix

$$\mathbf{R} = \left[\begin{array}{ccccccc} -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -1 \\ \hline 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{array}\right] \tag{1.7.13}$$

encountered previously in Section 1.5.

Laplacian in Terms of the Oriented Incidence Matrix

The graph Laplacian is given by

$$\mathbf{L} = \mathbf{R} \cdot \mathbf{R}^T. \tag{1.7.14}$$

In fact, this factorization is valid for arbitrary node and link labeling and for general higher-dimensional graphs.

Exercise

1.7.1 *Node and link labeling*

Derive the connectivity lists and the oriented incidence matrix for an arbitrary node and link labeling scheme of your choice.

1.8 PERIODIC ONE-DIMENSIONAL GRAPHS

Shown in Figure 1.8.1 is a closed or periodic one-dimensional graph consisting of N unique nodes connected by $L = N$ links. The $N \times N$ periodic graph Laplacian is

$$\mathbf{L} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & -1 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ -1 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}, \tag{1.8.1}$$

where the two nonzero northeastern and southwestern corner elements implement the periodicity condition, as discussed in Section 1.6.

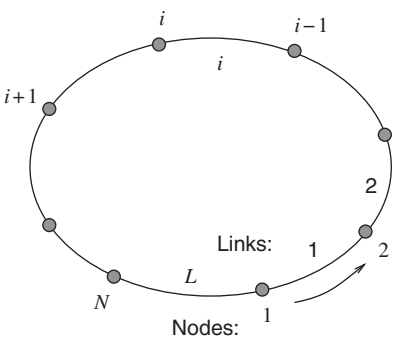

FIGURE 1.8.1 Illustration of a periodic one-dimensional graph consisting of N unique nodes connected by $L = N$ links. The first and last nodes numbered 1 and $N + 1$ coincide.

The periodic Laplacian is a circulant matrix. By definition, each row of an arbitrary circulant matrix derives from the previous row by shifting each element to the right by one place and then returning the last element to the first place, as discussed in Section A.4, Appendix A.

The eigenvalues of the periodic Laplacian are

$$\lambda_n = 2 - 2\,\cos\alpha_n = 4\,\sin^2\left(\tfrac{1}{2}\,\alpha_n\right) \tag{1.8.2}$$

for $n = 1, \ldots, N$, where

$$\alpha_n = \frac{n-1}{N}\,2\pi\,. \tag{1.8.3}$$

The corresponding eigenvectors, $\mathbf{u}^{(n)}$, normalized so that $\mathbf{u}^{(n)} \cdot \mathbf{u}^{(n)^*} = 1$, are

$$u_i^{(n)} = \frac{1}{\sqrt{N}}\,\exp(-\mathrm{i}\,i\alpha_n) \tag{1.8.4}$$

for $n, j = 1, \ldots, N$, where i is the imaginary unit and an asterisk denotes the complex conjugate. The presence of a zero eigenvalue, $\lambda_1 = 0$, corresponding to a uniform eigenvector, confirms that the periodic Laplacian is singular. The rest of the eigenvectors are pure harmonic waves.

A discrete Fourier orthogonality property states that

$$\sum_{j=1}^{N} \exp\left(\mathrm{i}\,jp\frac{2\pi}{N}\right) = \begin{cases} N & \text{if} \quad p = sN, \\ 0 & \text{otherwise}, \end{cases} \tag{1.8.5}$$

where p and s are zero or arbitrary integers. This property ensures that

$$\mathbf{u}^{(s)} \cdot \mathbf{u}^{(r)^*} = \delta_{sr}, \tag{1.8.6}$$

that is, the eigenvectors comprise an orthonormal set.

1.8.1 Periodic Adjacency Matrix

The $N \times N$ periodic adjacency matrix is a circulant matrix,

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}. \tag{1.8.7}$$

Two nonzero corner elements appear due to the periodicity condition. The degrees of all nodes are the same, $d_i = 2$ for $i = 1, \ldots, N$.

The eigenvalues of the periodic adjacency matrix are

$$\mu_n = 2\cos\left(\frac{n-1}{N}2\pi\right) \tag{1.8.8}$$

for $n = 1, \ldots, N$.

The number of steps defined in (1.7.7) are zero when s is zero or an odd integer and nonzero when s is an even integer. When $N = 13$, we find that

$$n_2 = 26, \quad n_4 = 78, \quad n_6 = 260, \quad n_8 = 910, \quad n_{10} = 3276. \tag{1.8.9}$$

1.8.2 Periodic Oriented Incidence Matrix

If we label nodes and links sequentially, as shown in Figure 1.8.1, we will obtain a square $N \times N$ oriented incidence matrix,

$$\mathbf{R} = \begin{bmatrix} -1 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -1 \end{bmatrix}. \tag{1.8.10}$$

The periodic Laplacian is given by

$$\mathbf{L} = \mathbf{D} - \mathbf{A} = \mathbf{R} \cdot \mathbf{R}^T, \tag{1.8.11}$$

where $\mathbf{D} = 2\,\mathbf{I}$ is a diagonal matrix hosting the degree of the N nodes.

1.8.3 Fourier Expansions

A real periodic nodal field, ψ, can be expanded in a Fourier series so that

$$\psi_i = \sum_{p=-M}^{M} c_p \exp\left[-\mathrm{i}\,pk(i-1)\right] \tag{1.8.12}$$

for $i = 1, \ldots, N$, where $k \equiv 2\pi/N$ is the wave number of the longest wave, i is the imaginary unit, and c_p are complex Fourier coefficients. To ensure that the expanded nodal field is real, we require that $c_{-p} = c_p^*$, where an asterisk denotes the complex conjugate. The truncation level, M, is discussed later in this section.

An equivalent representation in terms of sines and cosines, arising by resolving the Fourier coefficients and complex exponentials into their real and imaginary parts, is

$$\psi_i = \frac{1}{2}\, a_0 + \sum_{p=1}^{M} \Big(a_p \cos\big[(i-1)pk\,\big] + b_p \sin\big[(i-1)pk\,\big] \Big), \tag{1.8.13}$$

where

$$a_p = 2\,\Re(c_p), \qquad b_p = 2\,\Im(c_p) \tag{1.8.14}$$

for $p = 0, \ldots, M$, with the understanding that $b_0 = 0$, where $\Re$ and $\Im$ denote the real and imaginary parts. Accordingly,

$$c_p = \tfrac{1}{2}\,(a_p + \mathrm{i}\, b_p). \tag{1.8.15}$$

Using Fourier orthogonality properties (e.g., [35]), we find that

$$c_p = \frac{1}{N} \sum_{i=1}^{N} \omega^{(i-1)p}\, \psi_i \tag{1.8.16}$$

or

$$c_p = \frac{1}{N} \Big(\psi_1 + \psi_2\, \omega^p + \psi_3\, \omega^{2p} + \cdots + \psi_N\, \omega^{(N-1)p} \Big), \tag{1.8.17}$$

where

$$\omega = \exp(\mathrm{i}k). \tag{1.8.18}$$

These formulas indicate that

$$c_0 = a_0 = \frac{1}{N} \sum_{i=1}^{N} \psi_i, \tag{1.8.19}$$

that is, the Fourier constant a_0 is the mean of all nodal values.

When N is odd, we truncate the Fourier sum at $M = (N-1)/2$ and compute c_p for $p = 0, \ldots, M$. When N is even, we truncate the Fourier sum at $M = N/2$, compute c_p and b_p for $p = 0, \ldots, M-1$, using formula (1.8.17), and set

$$c_M = \frac{1}{N} \Big(\psi_1 - \psi_2 + \psi_3 - \cdots - \psi_N \Big). \tag{1.8.20}$$

The alternating signs arise because $\omega^{N/2} = \exp(\mathrm{i}\pi) = -1$.

1.8.4 Cosine Fourier Expansion

If a real periodic nodal field, ψ, is symmetric with respect to the midpoint of the network, that is,

$$\psi_i = \psi_{N+2-i}, \tag{1.8.21}$$

we may use the cosine Fourier expansion

$$\psi_i = \tfrac{1}{2}\, a_0 + \sum_{p=1}^{N-1} a_p \cos[(i-1)pk\,], \tag{1.8.22}$$

where a_p are cosine Fourier coefficients.

Using Fourier orthogonality properties, we find that

$$a_p = \frac{1}{N}\Big(\psi_1 + \psi_2\, \cos(kp) + \psi_3\, \cos(2kp) + \cdots + \psi_N\, \cos[(N-1)kp]\Big) \tag{1.8.23}$$

for $p = 1, \ldots, N-1$, and

$$a_0 = \frac{2}{N} \sum_{i=1}^{N} \psi_i \tag{1.8.24}$$

that is, the Fourier constant a_0 is twice the arithmetic mean of the nodal values.

The associated complex Fourier series is

$$\psi_i = \sum_{p=-(N-1)}^{N-1} c_p \exp\big[-\mathrm{i}\,(i-1)pk\,\big], \tag{1.8.25}$$

where $c_p = \frac{1}{2} a_p$.

1.8.5 Sine Fourier Expansion

If a real periodic nodal field, ψ, is antisymmetric with respect to the midpoint of the network, that is,

$$\psi_i = -\psi_{N+2-i}, \tag{1.8.26}$$

we may use the sine Fourier expansion

$$\psi_i = \sum_{p=1}^{N-1} b_p \sin[(i-1)\,pk\,], \tag{1.8.27}$$

where a_p are cosine Fourier coefficients.

Using Fourier orthogonality properties, we find that

$$b_p = \frac{1}{N}\Big(\psi_2 \ \sin(kp) + \psi_3 \ \sin(2kp) + \cdots + \psi_N \ \sin[(N-1)kp]\Big) \tag{1.8.28}$$

for $p = 1, \ldots, N-1$.

The associated complex Fourier series is

$$\psi_i = \sum_{p=-(N-1)}^{N-1} c_p \exp\big[-\mathrm{i}\,(i-1)\,pk\,\big], \tag{1.8.29}$$

where $c_p = \frac{1}{2}\mathrm{i}\,a_p$ for $p = 1, \ldots, N-1$ and $c_p = 0$.

Exercise

1.8.1 *Link labeling*

Confirm that the factorization $\mathbf{L} = \mathbf{R} \cdot \mathbf{R}^T$ is independent of link labeling.