Discrete Models of Diffusion and Vibration

1. Heat Conduction in an Interval

Consider the diffusion of heat energy through a long thin rod G, which we shall identify with the interval (a, b) in the *real number* line $\mathbb{R}$. Assume this rod has uniform cross section S and it is insulated along its length.

Experiment 1. A *small* section of the rod experiences an increase in the temperature $u(t)$ during the time interval $[t_1, t_2]$ when a quantity of heat Q is supplied to it. We find that this quantity is proportional to the mass and the temperature increment, that is, for some constant c we have

$$Q = c\rho Sh(u(t_2) - u(t_1)) ,$$

where h is the length, so Sh is the volume of the section, and ρ is the volume-distributed *density*. The constant c is a material property called *specific heat*, and it provides a measure of the amount of heat energy required to raise the temperature of a unit mass of the material by a degree. The temperature is then a measure of heat energy. Taking the limit as $t_2 - t_1 \to 0$, we see the *rate* at which heat is supplied to this segment is $c\rho Sh\dot{u}(t)$. The superscript dot will be used to denote a time derivative.

We observe that heat (thermal energy) flows from the hotter portions to the cooler portions of the rod by a process called *conduction*. The rate of this transfer depends on the material of the rod.

Experiment 2. The ends $x = x_1$ and $x = x_2$ of a section of the homogeneous rod of length $h = x_2 - x_1$ and cross section S are maintained at temperatures u_1 and u_2, respectively. After a period of time (which depends on the material) the temperature distribution is observed to be linear: the temperature at the position x is given by

$$u(x) = (\frac{x_2 - x}{h})u_1 + (\frac{x - x_1}{h})u_2, \quad x_1 \le x \le x_2 .$$

The quantity of heat per unit time and unit area which flows to the right is called the *flux*, and it is observed to be given by

$$q = -k\frac{u_2 - u_1}{h} \tag{1}$$

for some constant k which is called *conductivity*. The conductivity is a property of the material that is a measure of the flow rate per unit area, *i.e.*, the *flux* q induced by a given temperature gradient, $\frac{\partial u}{\partial x}$. The equation (1) defining k is known as *Fourier's law*. The minus sign arises since the heat flow is directed toward the lower temperature.

1.1. The Initial-Value Problem. We shall use the two preceding experimental observations to formulate a discrete model of the flow of heat through the rod. Partition the rod $G = (a, b)$ into N sections of equal length h, so $Nh = b - a$. Here we are assuming that the mesh size h of the partition is so small that we can approximate the temperature distribution in each section by a constant. Thus, let $u_j(t)$ be the temperature in the j-th section $[x_{j-1}, x_j]$ at the time $t \geq 0$, where the endpoints are given by $x_j = a + jh$, $0 \leq j \leq N$. In particular, $x_0 = a$ and $x_N = b$. The heat flux past x_j is given by

$$q_j(t) = -k\frac{u_{j+1}(t) - u_j(t)}{h}, \quad 1 \leq j \leq N - 1\,. \tag{2a}$$

If we have a source of volume intensity $f_j(t)$ in the jth section, this contributes heat at the rate $Shf_j(t)$. The total flux into the jth section from left and right adjoining sections and the additional heat supply rate from internal sources is given by $q_{j-1}(t) - q_j(t) + Shf_j(t)$. Setting this equal to the rate at which heat is stored, we arrive at the *conservation of energy* in the jth section in the form

$$c\rho Sh\dot{u}_j(t) = S(q_{j-1}(t) - q_j(t) + hf_j(t))\,, \quad 1 \leq j \leq N\,. \tag{2b}$$

In order to complete this system, it remains to determine the flux terms q_0 and q_N at the ends. The resulting ordinary differential equations are to be supplemented with the *initial conditions*

$$c\rho u_j(0) = c\rho u_j, \quad 1 \leq j \leq N, \tag{2c}$$

where the initial temperatures u_j for $1 \leq j \leq N$ are also given. This is an *initial-value problem* for the N unknown functions $u_j(t)$, $1 \leq j \leq N$.

Note that we can eliminate the interior flux terms (2a) to obtain an equivalent form of (2b), the *system of ordinary differential equations*

$$c\rho\dot{u}_j(t) = \frac{k}{h^2}(u_{j+1}(t) + u_{j-1}(t) - 2u_j(t)) + f_j(t), \quad 2 \leq j \leq N - 1. \tag{3}$$

These will remain the same for any choice of q_0 and q_N. However the first and last of the energy equations (2b) will depend on these choices.

1.2. The Boundary conditions. We consider a number of typical possibilities for determining the endpoint conditions. The first four of these will be illustrated with a condition at the right end, $x_N = b$. Note that in each of these cases another such condition will also be prescribed at the left end, $x_0 = a$. In the last example, the two conditions each involve data at both endpoints.

1. The value of the temperature could be specified at the end point. To obtain this situation, we append an additional section which is always at a known temperature, $u_b(t)$. Thus, we have

$$u_{N+1}(t) = u_b(t), \quad t > 0\,. \tag{4}$$

This is the *Dirichlet* boundary condition, or boundary condition of *first type* which describes *perfect contact* with the boundary value. It arises when the value of the end point temperature is known, usually from a direct measurement. Special cases can also correspond to fixing the boundary temperature at a prescribed value, for example, $u_b(t) = 0$

if the end is submerged in ice-water. Note that the Dirichlet condition (4) is equivalent to supplementing the flux equations (2a) with

$$q_N(t) = -k\frac{u_b(t) - u_N(t)}{h}$$

2. The heat flux into the rod could be specified at the end point:

$$-q_N(t)S = f_b(t), \quad t > 0\,.$$

This is the *Neumann* boundary condition, or boundary condition of *second type.* It depends on a given *source* of heat, $f_b(t)$ at the end. The homogeneous conditon with $f_b(t) = 0$ corresponds to an *insulated* end point.

3. The end of the rod is exposed to a known outside temperature $u_b(t)$, and the flux is determined by an exchange of heat through the end at a rate proportional to the difference between inside and outside temperatures:

$$-q_N(t)S + k_b(u_N(t) - u_b(t))S = f_b(t), \quad t > 0\,.$$

This is the *Robin* boundary condition, or boundary condition of *third type* which describes *partially insulated* end points. Here both $u_b(\cdot)$ and $f_b(\cdot)$ are prescribed. The first is the outside temperature and the second is a heat source concentrated on the end point. This model for heat loss determined by the difference $u_N(t) - u_b(t)$ is called *Newton's law* for cooling. It is merely a discrete form of the Fourier law and defines the *effective conductivity* k_b. For very large values $k_b \to \infty$, we obtain formally the Dirichlet boundary condition, while for very small values $k_b \to 0$ we get the Neumann condition. Thus the effective conductivity k_b is a new quantity which interpolates between the first two types.

4. Another type of boundary condition arises if there is a *concentrated capacity* at the end point, for instance, if the end of the rod is submerged in an insulated container of well-stirred fluid, or if the end is attached to a region of very highly conductive material. Then we introduce a *new unknown* $u_{N+1}(t)$ for the temperature of the water, or the temperature of the material, respectively, and we have the *dynamic* boundary condition

$$c_0\dot{u}_{N+1}(t)S + k_b(u_{N+1}(t) - u_N(t))S = f_b(t), \quad t > 0\,,$$

together with the flux condition

$$q_N(t) = -k_b(u_{N+1}(t) - u_N(t)) \quad t > 0\,.$$

This is the boundary condition of *fourth type* and defines the *effective specific heat* c_0. This boundary condition must be supplemented with an additional initial condition,

$$c_0 u_{N+1}(0) = c_0 u_{N+1}\,.$$

Note that each of the first three examples led to a system of ordinary differential equations of size $N \times N$, whereas this fourth example is of size $(N + 1) \times (N + 1)$. That is, an extra differential equation was necessarly introduced to account for the additional energy storeage at the end point, and its form is independent of the mesh size h.

Each of the preceding examples was a *local* boundary condition, *i.e.*, it involves only information at the one end. For each of these, another boundary condition needs to be prescribed for the other end.

5. Here is an example of a *nonlocal boundary condition.* If the rod is bent around and the ends are joined to form a large ring, we identify the end points $x_0 = a$ and $x_N = b$, and the N-th section is now situated to the left of the 1-st section. Thus at the endpoints we match the temperature and the flux:

$$u_0(t) = u_N(t), \quad t > 0\,,$$
$$q_0 = q_N = -k\frac{u_1(t) - u_N(t)}{h}\,.$$

These are *periodic* boundary conditions. Again, since the first is only naming another variable, we have a total of two boundary constraints to supplement the initial value problem.

EXERCISE 1. *The rod above is submerged in a perfectly insulated container of well-stirred water. It is partially insulated along its length, so there is some limited heat exchange with the surrounding water along the length, $a < x < b$. The rod is in perfect contact with the water at the end points. Find an initial value problem for the discrete model of this situation. (Hint: The temperature of the water is unknown.)*

1.3. Examples: Dirichlet Boundary Conditions. We compute solutions of some particular cases in order to see if our models are giving solutions which correspond to our intuition.

Example $N = 1$. Set $\alpha = \frac{k}{h^2 c\rho}$. The system is given by

$$\dot{u}_1(t) + 2\alpha u_1(t) = F_1(t)$$
$$u_1(0) = u_1$$

where $F_1(t) \equiv \alpha(u_0(t) + u_2(t)) + \frac{1}{c\rho} f_1(t)$. The solution is given explicitly by

$$u_1(t) = e^{-2\alpha t} u_1 + \int_0^t e^{-2\alpha(t-s)} F_1(s)\, ds\,.$$

Suppose that $f_1(t) = 0$ and consider the following cases.

$u_0(t) = u_2(t) = 0$, thus, $F_1(t) = 0$. Then we get $u_1(t) = e^{-2\alpha t} u_1$, so the solution dissipates to zero. The heat has been drained out of the end points.

$u_0(t) = u_0$, $u_2(t) = u_2$. Then we get

$$u_1(t) = e^{-2\alpha t} u_1 + \frac{u_0 + u_2}{2}(1 - e^{-2\alpha t})\,,$$

so the solution approaches the mean value of the endpoint temperatures. Heat has been lost or gained from the end points.

Example $N = 2$. The system of equations describing the discrete Dirichlet problem is given by

$$\dot{u}_1(t) + 2\alpha u_1(t) - \alpha u_2(t) = \frac{1}{c\rho} f_1(t) + \alpha u_0(t) \equiv F_1(t), \quad u_1(0) = u_1$$
$$\dot{u}_2(t) - \alpha u_1(t) + 2\alpha u_2(t) = \frac{1}{c\rho} f_2(t) + \alpha u_3(t) \equiv F_2(t), \quad u_2(0) = u_2\,.$$

Assume that $F_j(t) = 0$ and look for solutions in the form

$$u_1(t) = a_1 e^{-\lambda t},\ u_2(t) = a_2 e^{-\lambda t}.$$

This leads to the linear algebra problem

$$-\lambda a_1 + \alpha(2a_1 - a_2) = 0,$$
$$-\lambda a_2 + \alpha(-a_1 + 2a_2) = 0.$$

The eigenvalues are given by $\lambda = \alpha,\ 3\alpha$ with corresponding eigenvalues

$$\boldsymbol{\xi_1} \equiv \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \boldsymbol{\xi_2} \equiv \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

A family of solutions of the homogeneous system is given by

$$\begin{bmatrix} u_1(t) \\ u_2(t) \end{bmatrix} = c_1 e^{-\alpha t} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + c_2 e^{-3\alpha t} \begin{bmatrix} 1 \\ -1 \end{bmatrix},$$

that is,

$$\mathbf{u}(t) = c_1 e^{-\alpha t} \boldsymbol{\xi_1} + c_2 e^{-3\alpha t} \boldsymbol{\xi_2}.$$

A solution satisfying the given initial conditions $u_1,\ u_2$ can be obtained by choosing constants with

$$c_1 \begin{bmatrix} 1 \\ 1 \end{bmatrix} + c_2 \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}.$$

This system is solvable because the pair $\boldsymbol{\xi_1},\ \boldsymbol{\xi_2}$ is a *basis* for the plane, $\mathbb{R}^2$. This can be done to match any initial conditions. Note that the second term in the solution decays at a rate three times as fast as the first. This corresponds to the additional loss of heat between the two components in the second term, whereas the only loss of heat in the first term is to the end points.

Let's review this procedure. Define the matrix and the (column) vector

$$\mathbf{A} = \alpha \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, \qquad \mathbf{u}(t) = \begin{bmatrix} u_1(t) \\ u_2(t) \end{bmatrix}.$$

Then the system can be written in matrix form

$$\dot{\mathbf{u}}(t) + \mathbf{A}\mathbf{u}(t) = \mathbf{F}(t). \tag{5}$$

To look for a solution $\mathbf{u}(t) = \boldsymbol{\xi} e^{-\lambda t}$ of the homogeneous equation with $\mathbf{F}(t) = \mathbf{0}$, substitute this into the differential equation to get the *eigenvalue problem*

$$\mathbf{A}\boldsymbol{\xi} = \lambda \boldsymbol{\xi}. \tag{6}$$

If $\boldsymbol{\xi_1},\ \lambda_1$ and $\boldsymbol{\xi_2},\ \lambda_2$ are solutions, we obtain the corresponding solutions of the ordinary differential equation (5) in the form

$$\mathbf{u}(t) = c_1 e^{-\lambda_1 t} \boldsymbol{\xi_1} + c_2 e^{-\lambda_2 t} \boldsymbol{\xi_2}. \tag{7}$$

If the pair $\boldsymbol{\xi_1},\ \boldsymbol{\xi_2}$ is a basis, we can choose the constants to satisfy any initial condition

$$\mathbf{u}(0) = c_1 \boldsymbol{\xi_1} + c_2 \boldsymbol{\xi_2} + = \mathbf{u}_0.$$

It follows that every solution of the system can be obtained this way, so we can say the representation (7) gives the *general solution* of the homogeneous equation.

It is clear how we would like to extend this procedure to larger N's. For the case of Dirichlet boundary conditions, the matrix form of the problem is given by (5) where the unknown, matrix, and data are given by

$$\mathbf{u}(t) = \begin{bmatrix} u_1(t) \\ u_2(t) \\ u_3(t) \\ \dots \\ u_{N-1}(t) \\ u_N(t) \end{bmatrix}, \quad \mathbf{A} = \alpha \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & -1 & 2 & -1 \\ 0 & \dots & \dots & 0 & -1 & 2 \end{pmatrix},$$

$$\mathbf{F}(t) = \begin{bmatrix} \frac{1}{c\rho} f_1(t) + \alpha u_a(t) \\ \frac{1}{c\rho} f_2(t) \\ \frac{1}{c\rho} f_3(t) \\ \dots \\ \frac{1}{c\rho} f_{N-1}(t) \\ \frac{1}{c\rho} f_N(t) + \alpha u_b(t) \end{bmatrix}.$$

Example $N = 3$. For our final example of the discrete Dirichlet problem, consider the case with $N = 3$ sections. The matrix is given by

$$\mathbf{A} = \alpha \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix},$$

and the matrix of the eigenvalue problem has the form

$$\mathbf{A} - \lambda \mathbf{I} = \begin{pmatrix} 2\alpha - \lambda & -\alpha & 0 \\ -\alpha & 2\alpha - \lambda & -\alpha \\ 0 & -\alpha & 2\alpha - \lambda \end{pmatrix},$$

so the characteristic equation is

$$det(\mathbf{A} - \lambda \mathbf{I}) = (2\alpha - \lambda)((2\alpha - \lambda)^2 - 2\alpha^2) = 0 .$$

The characteristic values are

$$\lambda_1 = (2 - \sqrt{2})\alpha, \ \lambda_2 = 2\alpha, \ \lambda_3 = (2 + \sqrt{2})\alpha ,$$

and the corresponding vectors are

$$\boldsymbol{\xi_1} = \begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}, \ \boldsymbol{\xi_2} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}, \ \boldsymbol{\xi_3} = \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix}.$$

Thus, the solution of the system (5) with $\mathbf{F}(t) = \mathbf{0}$ is given by

$$\mathbf{u}(t) = c_1 e^{-\lambda_1 t} \boldsymbol{\xi_1} + c_2 e^{-\lambda_2 t} \boldsymbol{\xi_2} + c_3 e^{-\lambda_3 t} \boldsymbol{\xi_3} ,$$

where the constants are chosen to satisfy the initial condition

$$c_1 \boldsymbol{\xi_1} + c_2 \boldsymbol{\xi_2} + c_3 \boldsymbol{\xi_3} = \mathbf{u}_0 .$$

Note that the characteristic values are arranged in increasing magnitude and the corresponding eigenvectors have more and more dissipation of heat between adjacent components. This can be quantified by the number of sign changes between adjacent components of the successive eigenvalues.

1.4. Examples: Other Boundary Conditions. For all the other boundary conditons, the matrix is changed, but the change occurs *only* in the first or last row, depending on whether the condition was changed at $x = a$ or at $x = b$. For example, with the Dirichlet condition at the left and the Neumann condition at the right end, this leads to the system of ordinary differential equations (5) as before, but the matrix is given by

$$\mathbf{A} = \alpha \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & -1 & 2 & -1 \\ 0 & \dots & \dots & 0 & -1 & 1 \end{pmatrix}.$$

Example $N = 3$. For the case of Neumann conditions at *both* ends, the matrix is given by

$$\mathbf{A} = \alpha \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix},$$

and the matrix of the eigenvalue problem has the form

$$\mathbf{A} - \lambda\mathbf{I} = \begin{pmatrix} \alpha - \lambda & -\alpha & 0 \\ -\alpha & 2\alpha - \lambda & -\alpha \\ 0 & -\alpha & \alpha - \lambda \end{pmatrix},$$

so the characteristic equation is

$$det(\mathbf{A} - \lambda\mathbf{I}) = (\alpha - \lambda)(3\alpha - \lambda)\lambda = 0\,.$$

The characteristic values are

$$\lambda_1 = 0,\ \lambda_2 = \alpha,\ \lambda_3 = 3\alpha\,,$$

and the corresponding vectors are

$$\boldsymbol{\xi_1} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix},\ \boldsymbol{\xi_2} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix},\ \boldsymbol{\xi_3} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}.$$

Thus, the solution of the system (5) with $\mathbf{F}(t) = \mathbf{0}$ is given by

$$\mathbf{u}(t) = c_1\boldsymbol{\xi_1} + c_2 e^{-\alpha t}\boldsymbol{\xi_2} + c_3 e^{-3\alpha t}\boldsymbol{\xi_3}\,,$$

where the constants are chosen to satisfy the initial condition

$$c_1\boldsymbol{\xi_1} + c_2\boldsymbol{\xi_2} + c_3\boldsymbol{\xi_3} = \mathbf{u}_0\,.$$

The characteristic value $\lambda = 0$ indicates the matrix is *singular*, and the 'constant' vector $\boldsymbol{\xi_1}$ corresponds to the *stationary* solution of the heat conduction problem with insulated ends. Again note that the characteristic values are arranged in increasing magnitude and the corresponding eigenvectors have more and more dissipation of heat between adjacent components. This can be quantified by the number of sign changes between adjacent components of the successive eigenvalues.

Example $N = 3$. For the case of *periodic boundary conditions*, there is an essential choice to make concerning the number of points to take in the model. If we eliminate $u_{N+1}(t)$ in order to get an $N \times N$ problem, the first row is $\frac{3}{2}\ -1\ 0\ \ldots\ 0\ -\frac{1}{2}$. However, if instead we write the problem as an $(N+1) \times (N+1)$ problem, the matrix takes the more amenable form

$$\mathbf{A} = \alpha \begin{pmatrix} 2 & -1 & 0 & 0 & \ldots & 0 & -1 \\ -1 & 2 & -1 & 0 & \ldots & 0 & 0 \\ 0 & -1 & 2 & -1 & \ldots & 0 & 0 \\ \multicolumn{7}{c}{\dotfill} \\ 0 & 0 & \ldots & 0 & -1 & 2 & -1 \\ -1 & 0 & \ldots & 0 & 0 & -1 & 2 \end{pmatrix}.$$

The periodic structure of this matrix is clear.

Exercise 2. *Write out the matrix* $\mathbf{A}$ *and forcing term* $\mathbf{F}(t)$ *that arise in the system* (5) *for each of the boundary conditions of Section 1.2 at both ends.*

Exercise 3. *Write out the matrix* $\mathbf{A}$ *and forcing term* $\mathbf{F}(t)$ *corresponding to the boundary conditions of Exercise 1.*

Exercise 4. *Find the general solution of the homogeneous system* (5) *for* $N = 2$ *and with Dirichlet condition at* $x = a$ *and Neumann condition at* $x = b$.

Exercise 5. *Find the general solution of the homogeneous system* (5) *for* $N = 2$ *and with Neumann conditions at both* $x = a$ *and* $x = b$.