3. Linearity

The Heat Equation (2.5) is an example of a *linear* PDE. Many other PDE of Mathematical Physics also happen to be linear. Therefore understanding linearity is key to the success of our entire enterprize.

Linearity is a universal concept. It pervades Calculus and ODE, so you have already encountered it multiple times. Still we should talk about linearity because it is often misunderstood in low-level courses. In this section you will see that linearity in the context of PDE is actually no different from the linearity you remember from your ODE course.

3.1. **Linear ODE.** Consider the following familiar second order ODE:

$$\frac{d^2y}{dt^2} + y = 0. \tag{3.1}$$

Recall that Equation (3.1) is classified as *linear homogeneous*[4] (with constant coefficients).

Now, here is why we are having this discussion. A common misconception is that terms like 'linear homogeneous' just serve to describe how an ODE (or some other object) *looks*: 'linear' means that the unknown function and its derivatives are present as "first powers"; 'homogeneous' means that the right-hand side is zero. Yet, think about it: it does not help to know how some equation *looks*, does it? For instance, it does not help to know that the right-hand side of an equation is zero. In fact, any equation can be rewritten so that all of its nonzero terms are collected on the left. Yet, not every equation is homogeneous.

Classification of Equation (3.1) as linear homogeneous has nothing to do with the way it looks but rather has to do with the *algebraic structure* of its solution set. Let us call that set V, which will stand for *vector space*. If y_1 and y_2 are arbitrary elements of V then, by definition:

$$\begin{aligned} \frac{d^2y_1}{dt^2} + y_1 &= 0 \\ \frac{d^2y_2}{dt^2} + y_2 &= 0 \end{aligned}$$

If we add these equations and use *linearity of differentiation*, we can write:

$$\frac{d^2(y_1+y_2)}{dt^2} + (y_1+y_2) = 0.$$

[4]Notice the difference in spelling between *homogeneous* and *homogenous*. The former is an adjective used to describe an ODE; the latter is a term commonly used in general chemistry to describe mixtures of gases and liquids.

In words, the sum of any two solutions of (3.1) is another solution of (3.1). More generally, for any numbers c_1 and c_2 the *linear combination* $(c_1\, y_1 + c_2\, y_2)$ is readily seen to be another solution of Equation (3.1). Thus V contains all linear combinations of its elements and for that reason is said to be a *vector space*.

For now, we will adopt an informal[5] definition of a vector space which is given below.

Definition 1 (Vector Space)**.** A vector space is a collection of objects, called vectors, which can be added and scaled. A vector space must be closed under vector operations: that is, it must contain all possible linear combinations of its vectors.

The connection between classification of ODE as linear homogeneous and Definition 1 is the following:

> *An ODE is said to be linear homogeneous if its set of solutions forms a vector space.*

From the point of view of Linear Algebra, solving Equation (3.1), or any linear homogeneous equation for that matter, amounts to describing the vector space of its solutions. Which leads to the question:

> *How does one describe a vector space?*

As one learns in Linear Algebra, all vector spaces are described using *bases*. Again, we will give an informal definition.

Definition 2 (Basis)**.** A basis of a vector space V is a minimal collection of vectors $\{e_1, e_2, \ldots, e_n\}$ that suffices to express any vector $v \in V$ as a linear combination: $v = c_1\, e_1 + c_2\, e_2 + \ldots + c_n\, e_n$.

The keyword 'minimal' is very important: it means that we whittled down the collection $\{e_1, e_2, \ldots, e_n\}$ to the bare minimum necessary for describing *all* elements of V. Alternatively, we could say that basis elements must be *linearly independent* while *spanning* the entire vector space. Since linear independence and span will prominently feature in later discussion, we continue with the parade of informal definitions.

Definition 3 (Independence)**.** The vectors $\{e_1, e_2, \ldots, e_n\}$ are said to be linearly independent if $c_1\, e_1 + c_2\, e_2 + \ldots + c_n\, e_n = 0$ implies that all coefficients c_1, c_2, …, c_n are zero.

[5]The rigorous definition includes nine axioms of the defining vector space operations—vector addition and scalar multiplication: e.g., vector addition should be associative, commutative, and so on. You can find these axioms in any standard linear algebra book.

Definition 4 (Span)**.** The span of vectors $\{e_1, e_2, \ldots, e_n\}$ is the set of all possible linear combinations:

$$\text{span}\{e_1, e_2, \ldots, e_n\} = \{c_1\, e_1 + c_2\, e_2 + \ldots + c_n\, e_n\}.$$

Using Definitions 3 and 4, we can define a basis of V as a *maximal* collection of *linearly independent* vectors whose span is V.

When working with bases, keep in mind the following facts from Linear Algebra:

(1) Any nontrivial[6] vector space has *infinitely many* bases. In particular, the familiar $\mathbb{R}^3$ has infinitely many bases other than the standard $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$.
(2) All bases are equivalent in the sense that any basis completely describes the vector space. Therefore, at the abstract level, it does not matter which basis is chosen. In particular, every basis of V has the same number of elements. That number is called the *dimension* of V and is denoted $\dim(V)$.
(3) While all bases are abstractly equivalent, in practice some bases are more suitable for computations than others. Some of the most important theorems in Applied Linear Algebra can be regarded as consequences of choosing the right bases.

Returning to Equation (3.1), we have shown that its solutions form a vector space. We now require a basis for that space. As you will recall, in your ODE course that basis was constructed by "guessing" exponential solutions: $y = e^{\lambda t}$. Substituting the exponential "guess"[7] into (3.1) one obtains the so-called *Characteristic Equation*

$$\lambda^2 + 1 = 0,$$

which has two roots

$$\lambda_1 = i, \quad \lambda_2 = -i.$$

These roots, called *eigenvalues*, correspond to two linearly independent *eigenfunctions* (see Exercises at the end):

$$y_1 = e^{\lambda_1 t} = e^{i t}, \quad y_2 = e^{\lambda_2 t} = e^{-i t}.$$

[6]That is, not consisting just of the zero vector.

[7]The idea of looking for exponential solutions is often introduced in ODE courses in *ad hoc* manner, as a method that "works" for linear equations with constant coefficients. The method is actually based on the fact that the derivative of an exponential is a scalar multiple of itself:

$$\frac{d}{dt}(e^{\lambda t}) = \lambda\, e^{\lambda t}.$$

As a consequence, any operation constructed by means of repeated differentiation, addition, and scaling, maps exponentials into exponentials.

The eigenfunctions form a "correct" basis for describing the solution space of Equation (3.1). Put differently, the general solution of Equation (3.1) is given by

$$y = c_1\, y_1 + c_2\, y_2 = c_1\, e^{i\,t} + c_2\, e^{-i\,t}.$$

The exponentials form a correct basis rather than *the* correct basis because, as we have already remarked, bases are not unique and there are other possibilities. For instance, another equally correct basis can be constructed from trigonometric functions:

$$y = c_1\, \cos(t) + c_2\, \sin(t).$$

In case you have forgotten the connection between complex exponentials and trigonometry, review *Euler's formula*. You will need very soon.

3.2. **Linear PDE.** Let us now turn our attention to the Neumann problem for the Heat Equation where, for simplicity, we set the thermal conductivity constant to unity:

$$\begin{aligned} &\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < L, \quad t > 0, \\ &\frac{\partial u}{\partial x}(0,t) = 0, \quad \frac{\partial u}{\partial x}(L,t) = 0. \end{aligned} \tag{3.2}$$

For the time being we are not concerned with the initial temperature as it does not have any bearing on linearity.

Suppose u_1 and u_2 are two solutions of Equation (3.2). It is straightforward to show (exercise) that so is the linear combination $c_1\, u_1 + c_2\, u_2$. The difference from the analogous proof in Section 3.1 is that one must use partial differentiation and check that linear combinations satisfy Neumann boundary conditions. We conclude that the PDE (3.2) is *linear homogeneous* because its solutions form a *vector space*.

According to the logic of Section 3.1, we now need to find a basis. Furthermore, the theory of linear ODE suggests that we may want to consider exponential functions as candidates for basis elements. Let us give it a try. Substituting the exponential "guess"

$$u = e^{\lambda\, t + \mu\, x}$$

into the Heat Equation, leads to a Characteristic Equation of the form:

$$\lambda = \mu^2.$$

Using the Characteristic Equation, we can construct an immense[8] number of independent solutions of the Heat Equation of the form

$$u = e^{\mu^2 t + \mu x}, \tag{3.3}$$

where μ is any complex number. Yet not all exponential solutions (3.3) qualify: we are interested only in the ones that satisfy Neumann boundary conditions. And here we run into an unpleasant surprise. Applying the boundary condition at $x = 0$, we get:

$$\frac{\partial}{\partial x}\left(e^{\mu^2 t + \mu x}\right)_{x=0} = \mu\, e^{\mu^2 t} = 0.$$

This forces $\mu = 0$ with the implication that all basis solutions are constant which manifestly cannot be true.

It may be that the failure of the exponential guess for Equation (3.2) is the reason why introductory PDE books make no attempt at it. Instead, the reader is instructed to make a more general guess on the grounds that it "works". I assume that you are not the kind of student who needs to be constantly told what to "guess". If so, read on. The solution of (3.2) can be deduced constructively, using Linear Algebra and numerics, and we will do just that in the next section.

One final note about the "failure" of the exponential guess. Guessing the exponential solution of the Heat Equation (with any boundary conditions) is, actually, not a bad move at all! Using linearity, it is entirely possible to deduce from (3.3) the textbook solutions of the Neumann problem for the Heat Equation. Give it a try—it is a great exercise. Even if you fail to make the right connections, it will help with understanding of what follows.

[8]The technical term is 'uncountably many'. Roughly speaking, it means that the elements of some infinite set cannot be indexed by integers or numbered.

4. Discretization

The class of analytically solvable ordinary differential equations is very small. For that reason ODE are usually solved numerically. The same can be said about partial differential equations. In fact, the situation with PDE is even more pronounced: they are usually solved numerically even when they can be solved analytically. Numerical solution of differential equations is a vast subject. In this section we will focus on the so-called *finite differences* and *semi*-discretization because that establishes an immediate connection between PDE and ODE .

4.1. **The calculus of finite differences.** Suppose we are given values of some differentiable function: $y_i = f(x_i)$ for $i = 1, \ldots, N$. Let us say we need the first derivative of that function. That is, we wish to compute $f'(x_i)$ for $i = 1, \ldots, N$. By definition,

$$f'(x_i) = \lim_{h \mapsto 0} \frac{f(x_i + h) - f(x_i)}{h}.$$

However, since our given data is discrete, we cannot compute the limit. What we can compute is the difference quotient when h equals the spacing between grid points. This suggests the approximation:

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}. \tag{4.1}$$

Equation (4.1) is said to be the approximation of the first derivative using *forward* differences.

Instead of using the "next" value at x_{i+1} to approximate the derivative at the "current" value x_i, we could also use the "previous" value:

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}. \tag{4.2}$$

As you may have guessed, this is called a *backward* difference approximation. Now, since we will always work with equispaced grids, we can think of both forward and backward differences in terms of one and the same operation:

$$\Delta_h(f) = f(x + h) - f(x). \tag{4.3}$$

Indeed, assuming that the spacing between the grid points is h, we can rewrite Equations (4.1) and (4.2) as $f'(x_i) \approx (\Delta_h f)(x_i)/h$ and $f'(x_i) \approx (\Delta_{-h} f)(x_i)/(-h)$, respectively. We will call the operation Δ_h simply a *difference operator*. Notice that it can be applied both to continuous functions and discrete sequences.

In order to approximate the solution of the Heat Equation, we will need to discretize the second derivative with respect to the spatial

variable x. One way to approximate the second derivative is simply to iterate Δ_h twice:

$$f''(x) \approx (\Delta_h^2 f)(x)/h^2 = \frac{f(x+2\,h) - 2\,f(x+h) + f(x)}{h^2}. \qquad (4.4)$$

Note that we dropped the subindex of the independent variable to emphasize that (4.4) applies to continuous functions and sequences alike. Iterated forward difference is a valid approximation of the second derivative, however, it is not the best. A much better approximation is:

$$f''(x) \approx \Delta_{-h}(\Delta_h f)(x)/(-h^2) = \frac{f(x+h) - 2\,f(x) + f(x-h)}{h^2}. \quad (4.5)$$

Equation (4.5) is called the *central difference* approximation of the second derivative. To see why it is superior to (4.4), let us expand both approximations into Taylor series with respect to h. The result, as you should verify, is:

$$\frac{f(x+2\,h) - 2\,f(x+h) + f(x)}{h^2} = f''(x) + f'''(x)\,h + \mathrm{O}(h^2)$$
$$\frac{f(x+h) - 2\,f(x) + f(x-h)}{h^2} = f''(x) + \frac{1}{12}\,f^{(4)}(x)\,h^2 + \mathrm{O}(h^3).$$

Evidently, in the limit as $h \to 0$, both approximations produce the second derivative. Yet for small but finite h the error of the central difference approximation decays quadratically whereas the error of the forward difference approximation decays only linearly. One says that the order of the central difference, which is two, is higher than the order of the forward difference, which is one. We will therefore use central difference to discretize the second derivative.

The Calculus of Finite Differences studies operations related to Δ_h. The above computation involving Taylor series is a typical but not representative result. Almost everything you know from continuous Calculus has finite difference analogues. We could therefore discuss the finite difference version of integration, the Fundamental Theorem of Calculus, various summation techniques, such as summation by parts, and so on. As fun as it would be, we have enough for our immediate needs and therefore proceed to the semi-discretization of the Heat Equation.

4.2. **Semi-discretization of the Heat Equation.** As we have already explained, our strategy is to discretize the spatial derivative $\partial^2 u/\partial x^2$ while leaving the time derivative alone; hence the term—*semi*-discretization. Later we will discretize all derivatives. However, as you will see, full discretization is much trickier than it sounds.

We commence the semi-discretization by replacing the continuous domain $[0, L]$ with an equispaced grid. Let N be a positive integer. Set $x_i = i\,L/N$ for $i = 0, \ldots, N$; we will often refer to the points x_i as *nodes*. On occasion, we will need to work with individual x_i's. Usually though we will apply operations on the entire grid at once. It will therefore be convenient to use vector notation $\mathbf{x}$ to denote the vector of nodes which will be a column vector by default. Having defined the grid, we can sample the unknown temperature on that grid: $u_i(t) = u(x_i, t)$; in vector notation, $\mathbf{u}(\mathbf{t}) = \mathbf{u}(\mathbf{x}, \mathbf{t})$. The vector $\mathbf{u}$ is an approximation of the continuous function u. In order to compare $\mathbf{u}$ with u, we agree to interpolate the components u_i linearly, the way MATLAB's `plot` command does.

As we have explained in Section 4.1, second derivatives should be approximated using central differences (4.5). We therefore set

$$\frac{du_i}{dt} = K\,\frac{u_{i+1} - 2\,u_i + u_{i-1}}{h^2}, \quad i = 1, \ldots, N-1.$$

where h is the spacing between nodes. Notice that central differences can only be applied at the *interior nodes*. The boundary nodes x_0 and x_N need to be treated separately using the boundary conditions.

4.3. **Treatment of boundary nodes.** Computationally, the easiest boundary conditions are Dirichlet. If the temperature at the boundary nodes is prescribed, then u_0 and u_N are simply set to their respective values. The number of unknowns therefore is equal to the number of interior nodes.

For Neumann boundary conditions one discretizes flux using boundary and interior nodes. At the zero-node, we must use the forward difference:

$$\frac{u_1 - u_0}{h} = 0.$$

Meanwhile, at the other endpoint:

$$\frac{u_N - u_{N-1}}{h} = 0.$$

It should now be clear how to deal with Robin-type boundary values which are linear combinations of Neumann and Dirichlet boundary values.

Periodic boundary conditions $u(0, t) = u(L, t)$ are, in a way, artificial because the circle has no boundary. Hence one can apply central differences at all nodes but using circular shift at the "end nodes", e.g.:

$$\frac{du_0}{dt} = K\,\frac{u_1 - 2\,u_0 + u_N}{h^2}.$$

Conceptually, the type of boundary conditions are not all that important at this point in our discussion. Therefore we will work with *periodic* boundary conditions leaving other types as exercises. The reason for the sudden shift from Neumann conditions to periodic conditions is purely technical: the eigen-decomposition of the matrix corresponding to periodic boundary conditions is slightly easier to investigate.

4.4. **Evolution of temperature on a circle.** In order to simplify matters, we will set $K = 1$ and $L = 2\pi$. Thus the version of the Heat Equation that we now consider is:

$$\begin{aligned} &\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 \le x < 2\,\pi, \quad t > 0, \\ &u(0,t) = u(2\pi,t), \\ &u(x,0) = f(x). \end{aligned} \tag{4.6}$$

The nature of the initial condition f will be clarified in due time. For now, think of $f(x)$ as a prescribed function which may or may not be periodic.

Figure 4.4 schematically illustrates the discretization. We have already explained how to think about discretization abstractly. However, it may be helpful to derive central differences using more intuitive approach. It will also help to review the derivation of the Heat Equation itself.

Imagine that we have a perfectly insulated metal ring with initial temperature distribution given by some known function $f(x)$, $0 \le x < 2\pi$. Divide the ring into N equal segments (elements) and number them counterclockwise; in the figure $N = 24$. Assuming that the segments are so small that their temperatures are uniform, we can speak of the temperature of the n-th segment u_n. Equivalently, we can think of u_n's as temperatures measured at midpoints which are marked with thick dots. Let x_n denote the coordinate of the n-th midpoint and let Δx be the distance between midpoints (which is the same as the length of the elements). At time zero, $u_n = f(x_n)$ in accordance with the initial condition. Thereafter, u_n's change at the rate governed by heat exchange with immediate neighbors.

Let q_n be the energy content of the n-th segment: $q_n = c\,\rho\,A\,\Delta x\,u_n$. Taking the time derivative we get, on one hand:

$$\frac{dq_n}{dt} = c\,\rho\,A\,\Delta x\,\frac{du_n}{dt}.$$

On the other hand, discrete version of Fourier's Law gives:

$$\frac{dq_n}{dt} = -k\,\frac{u_{n-1} - u_n}{\Delta x}\,A - k\,\frac{u_n - u_{n+1}}{\Delta x}\,A, \quad n = 2, \ldots, N-1.$$

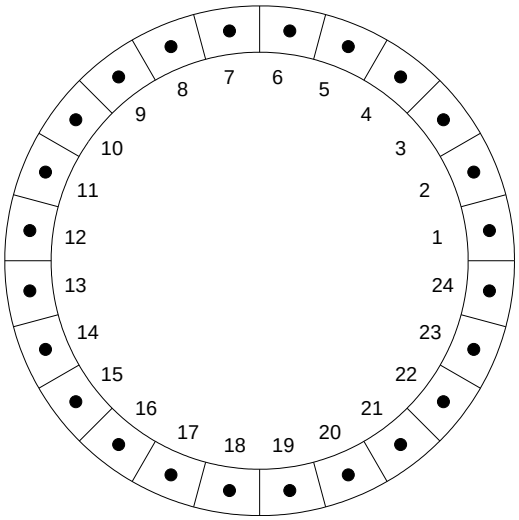

FIGURE 1. Discretization of a circle using 24 elements.

For $n = 1$ and $n = N$ the statement is slightly different, as is clear from Figure 4.4:

$$\begin{aligned} \frac{dq_1}{dt} &= -k\,\frac{u_N - u_1}{\Delta x}\,A - k\,\frac{u_1 - u_2}{\Delta x}\,A \\ \frac{dq_N}{dt} &= -k\,\frac{u_{N-1} - u_N}{\Delta x}\,A - k\,\frac{u_N - u_1}{\Delta x}\,A. \end{aligned}$$

Balancing the energy, and taking into account that thermal diffusivity $K = k/(c\,\rho) = 1$ by assumption, we arrive at the following system of linear ODE:

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

Let x be the column vector of midpoints and let u be the column vector of temperatures. Also, let A be the N-by-N matrix whose rows are obtained by cyclic permutations of $[-2, 1, 0, \ldots, 0, 1]$; such matrices are called *circulant*. The discretized version of Equation (4.6) can be

written in matrix-vector form as:

$$\frac{du}{dt} = \frac{1}{(\Delta x)^2} A\, u, \quad u(0) = f(x). \tag{4.7}$$

We now turn our attention to the task of solving this equation in MATLAB.

4.5. **Matlab implementation.** We begin by specifying the initial condition using the *function handle* construct:

```
f = @(x) 1 + cos(2*x);        % initial condition  (continuous)
```

It is advisable to start, as we do, with a very simple initial condition; that can be always changed later.

Next we discretize the ring using three lines of code.

```
% discretization of S^1:
N = 50;                       % number of elements
x = pi*(1:2:2*N)'/N;          % midpoints
dx = x(2)-x(1);               % size of each element
```

Notice that we use fifty elements whose midpoints are computed as a *column* vector.

Now comes the tricky part of setting up the ODE. The initial condition is simple to compute. However the computation of the matrix requires some now-how. We mentioned earlier that the matrix of the ODE is circulant. At this point, you may not find that very helpful. The more helpful tidbit is that the matrix is also *Toeplitz* because it is constant along rows. That is what the following snippet uses to construct it:

```
% Set up ODE:
u0 = f(x);                    % initial condition (discrete)
r = [-2 1 zeros(1,N-3) 1];
A = toeplitz(r',r);           % matrix of the system
```

Type `help toeplitz` at the command prompt for information about the use.

From this point on, things are straightforward: we solve the ODE using eigendecomposition and plot the solution.

```
% Solve ODE:
t = 1;                        % the value of time
[V,D] = eig(A);               % eigenvectors and eigenvalues of A
lambda = diag(D)/dx^2;        % eigenvalues of Equation (10)
v0 = V'*u0;                   % same as inv(V)*u0 in this case!
u = V*(exp(t*lambda).*v0);    % solution at t=1
```

```
% Plot results
figure
plot(x,u,'b-',x,u,'bo')
xlabel('x')
ylabel('u')
xlim([0 2*pi])
title(sprintf('Solution at t=%1.2f',t))
```

The output of the code is shown in Figure 4.5. Your homework is to experiment with this code further with the view of understanding how to solve the continuous Heat Equation.

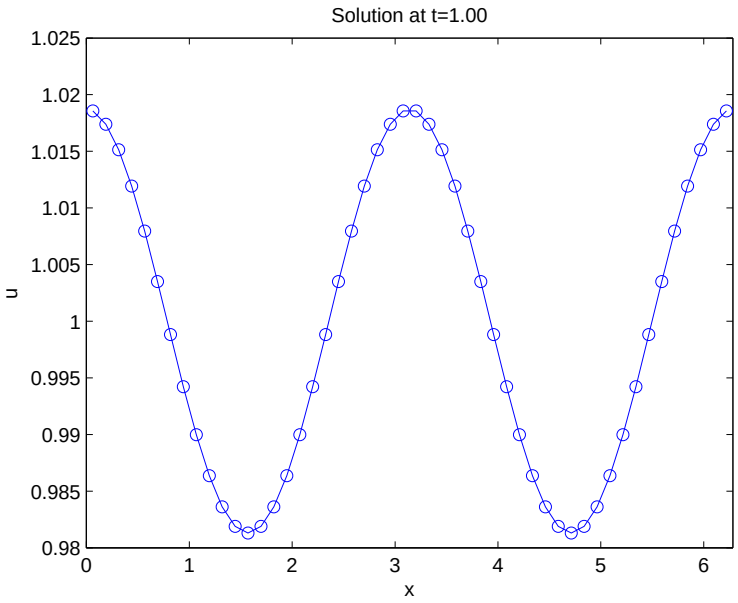

FIGURE 2. Solution of Equation (4.7) for $t = 1$ with $N = 50$; the initial condition is generated using $f(x) = 1 + \cos(2\,x)$.

HOMEWORK

(1) Consider the following ODE:

$$\frac{d^2y}{dt^2} + y = f(t).$$

It is linear but not homogeneous, unless $f(t) = 0$. Explain how one solves this ODE using linear algebra. Illustrate your explanation with a specific example.

(2) We showed that all purely exponential solutions of the Heat Equation with Neumann boundary conditions were trivial (constant). Suppose we choose Dirichlet or periodic boundary conditions. Can we find nontrivial exponential solutions then? Explain your answers.

(3) Consider the code given at the end of this handout. Explain the following two lines:

```
lambda = diag(D)/dx^2;          % eigenvalues of Equation (10)
v0 = V'*u0;                     % same as inv(V)*u0 in this case!
```

Specifically, why do we have to divide the eigenvalues of A by $(\Delta x)^2$ and why is the product $V' u_0$ the same as $V^{-1} u_0$?

(4) What does Figure 4.5 suggest about the solution of Equation (4.6) with initial condition $f(x) = 1 + \cos(2\,x)$? Formulate a conjecture. Then write code that confirms or disproves it. Attach both the code and the output.

(5) Examine the eigenvalues and eigenvectors of the matrix A for $N = 50$. What do you notice? Present plots of the eigenvectors (with eigenvalues put in the titles) that support your observations.

(6) What happens to the eigenvalues and eigenvectors of A as $N \to \infty$? Make a conjecture and produce numerical evidence supporting ti. Attach code and its output.

(7) Examine the solution of Equation (4.7) with initial conditions corresponding to the following choices of f in Equation (4.6):
   (a) $f(x) = \cos(nx)$, $n = 3, 4, 5$.
   (b) $f(x) = \cos(\omega\, x)$ with $\omega = \sqrt{2}$.
   (c) $f(x) = 1 + \sum_{n=1}^{10} a_n \cos(n\,x) + b_n \sin(n\,x)$ where a_n's and b_n's are any nonzero numbers of your choice.

   In each case, use the solutions of the discretized problem to guess the solutions of the continuous problems. Generate evidence supporting your guesswork.

(8) Examine the solution of Equation (4.7) with initial condition corresponding to $f = 1 + \text{sign}(x - \pi)$ in Equation (4.6). Make any observations that you think may be helpful for solving Equation (4.6) with this initial temperature.