CHAPTER PDE
Partial Differential Equations in Two Independent Variables

D.0 An Overview

Drawing on the Sturm-Liouville eigenvalue theory and the approximation of functions we are now ready to develop the spectral approach to the approximate solution of certain linear diffusion, wave and potential problems. All these problems have the same general structure and we shall outline the general solution process first before turning to an extensive discussion of specific problems.

We shall consider partial differential equations in two independent variables \((x, t)\) where usually \(x\) denotes a space coordinate and \(t\) denotes time. However, on occasion, as in potential problems, both variables may denote space coordinates.

All problems to be considered are of the form

\[(0.1) \quad \mathcal{L}u(x, t) = F(x, t)\]

where \(\mathcal{L}\) is a linear partial differential operator, with possibly variable coefficients, defined for \(x \in (0, L)\) and \(t \in (0, T)\). The equation \((0.1)\) is to be solved for a function \(u\) which satisfies boundary conditions at \(x = 0\) and \(x = L\) and initial conditions at \(t = 0\) or, as in the case of a potential problem, boundary conditions at \(t = 0\) and \(t = T\). For definiteness we shall assume now that \(u\) is to satisfy the initial condition

\[(0.2) \quad u(x, 0) = u_0(x)\]

where \(u_0\) is given.

In all our applications it is possible to subtract a known function \(v(x, t)\) from \(u(x, t)\) so that

\[w(x, t) = u(x, t) - v(x, t)\]

satisfies one of the boundary conditions at \(x = 0\) and \(x = L\) listed in Table xxx. In other words, \(w\) as a function of \(x\) belongs to one of the subspaces \(M\) described in Chapter 2. \(t\) in this instance is regarded simply as a parameter.

The problem can be restated for \(w\) as: Find a function \(w(x, t)\) which satisfies

\[\mathcal{L}w = \mathcal{L}u - \mathcal{L}v = F(x, t) - \mathcal{L}v(x, t) \equiv G(x, t),\]

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which belongs to $M$ for all $t$ and which satisfies the given conditions at $t = 0$ (and possibly at $t = T$), i.e. here

$$w(x, 0) = u_0(x) - v(x, 0) \equiv w_0(x).$$

We emphasize that $G$ and $w_0$ are known data functions.

We now make the two essential assumptions which lie at the heart of any separation of variables method:

I) The partial differential equation (0.1) can be written in the form

$$\mathcal{L} w(x, t) = \mathcal{L}_1(x) w + \mathcal{L}_2(t) w = G(x, t)$$

where

i) $\mathcal{L}_1$ denotes the terms involving functions of $x$ and derivatives with respect to $x$,

ii) $\mathcal{L}_2$ denotes the terms involving functions of $t$ and derivatives with respect to $t$.

II) The eigenvalue problem

$$\mathcal{L}_1(x) \phi = \mu \phi$$

has obtainable solutions $\{\mu_n, \phi_n\}_{n=1}^N$ in $M$.

The computation of an approximate solution of (0.1-2) is now automatic. We define

$$M_N = \text{span}\{\phi_1(x), \ldots, \phi_N(x)\}.$$ 

We compute the best approximations

$$P_N G(x, t) = \sum_{n=1}^{N} \beta_n(t) \phi_n(x)$$

$$P_N w_0(x) = \sum_{n=1}^{N} \hat{\alpha}_n \phi_n(x)$$

of the space dependent data functions (treating $t$ as a parameter) and solve the approximate problem

$$\mathcal{L} w_N = P_N G(x, t)$$

$$w_N(x, 0) = P_N w_0(x).$$
It turns out that the solution $w_N(x, t)$ has to belong to $M_N$ for all $t$ and thus has to have the form

$$w_N(x, t) = \sum_{n=1}^{N} \alpha_n(t)\phi_n(x).$$

Substitution into $Lw_N = P_NG$ shows that the coefficient functions $\{\alpha_n(t)\}$ must be chosen such that

$$\sum_{n=1}^{N} [\mu_n\alpha_n(t) + L_2(t)\alpha_n(t) - \beta_n(t)]\phi_n(x) = 0.$$

Since the eigenfunctions are linearly independent the term in the bracket must vanish. Hence each coefficient $\alpha_n(t)$ has to satisfy the ordinary differential equation

(0.3) \quad \mu_n\alpha_n(t) + L_2(t)\alpha_n(t) = \beta_n(t)

and the initial condition

$$\alpha_n(0) = \hat{\alpha}_n.$$

We go on the assumption that this ordinary differential equation is solvable so that $w_N(x, t)$ can be found. Thus $w_N(x, t)$ is an exact analytic solution of an approximation to the original problem. It is natural to ask how $w_N$ is related to the analytic solution $w(x, t)$ of the original problem. For most of the problems considered below we shall prove the following remarkable result:

$$w_N(x, t) = P_Nw(x, t)$$

Hence the computed solution is exactly the projection of the unknown analytic solution. In general one has a fair amount of information from the theory of partial differential equations about the smoothness properties of $w$. In particular, $w$ is nearly always square integrable. The general Sturm Liouville theory can then be invoked to conclude that, at least in the mean square sense, $w_N$ converges to $w$ as $N \to \infty$. This implies that when our finite sums are replaced by infinite series then the resulting function is, in a formal sense, the analytic solution $w(x, t)$. Some quantitative estimates for the quality of the approximation can be found for specific problems as outlined below.

D.1 The Diffusion Equation

The eigenfunction expansion method is easiest to apply to diffusion problems in one space dimension. We shall present the general solution method, illustrate it for a number
of worked examples of increasing complexity and then discuss the theoretical issues which arise when the original problem is replaced by a solvable approximation.

D.1.1 The Solution Technique

To make precise the steps required to find an eigenfunction solution of the diffusion equation we shall consider the following initial/boundary value problem for the heat equation:

\begin{align}
\mathcal{L}u &= u_{xx} - u_t = F(x, t), \quad x \in (0, L), t > 0 \\
u(0, t) &= A(t), \quad t > 0 \\
u(L, t) &= B(t), \quad t > 0 \\
u(x, 0) &= u_0(x), \quad x \in (0, L),
\end{align}

which models the temperature distribution \(u(x, t)\) in a slab of thickness \(L\) (or an insulated bar of length \(L\)). \(F(x, t)\) denotes an internal heat source or sink and \(A(t)\) and \(B(t)\) are prescribed (and generally time dependent) temperatures at the ends of the slab or bar. The initial temperature distribution is \(u_0(x)\). The first step in the solution process is always the reformulation of the problem for a function \(w\) which satisfies homogeneous boundary conditions. This is achieved by subtracting from \(u\) a function \(v(x, t)\) which satisfies exactly the same boundary conditions as \(u(x, t)\). For (1.1) a simple function \(v(x, t)\) which satisfies the same boundary conditions at \(x = 0\) and \(x = L\) is

\[v(x, t) = A(t)\frac{L - x}{x} + B(t)\frac{x}{L} .\]

Then

\[w(x, t) = u(x, t) - v(x, t)\]

solves

\[\mathcal{L}w = \mathcal{L}u - \mathcal{L}v = F(x, t) + v_t = F(x, t) + A'(t)\frac{L - x}{L} + B'(t)\frac{x}{L} \equiv G(x, t) .\]

\[w(0, t) = w(L, t) = 0\]

\[w(x, 0) = u_0(x) - v(x, 0) \equiv w_0(x) .\]
Here we have tacitly assumed that $A(t)$ and $B(t)$ are differentiable. Since

$$Lw = w_{xx} - w_t$$

we see that

$$L_1(x)w = w_{xx}, \quad L_2(t)w = -w_t.$$

The vector space $M$ is given by $M = \{ f \in C^2(0, L) : f(0) = f(L) = 0 \}$ and the eigenvalue problem is

$$\phi''(x) = \mu \phi(x)$$

$$\phi(0) = \phi(L) = 0.$$

The eigenvalues and eigenfunctions are available from Table xxxx as

$$\lambda_n = \frac{n\pi}{L}, \quad \mu_n = -\lambda_n^2, \quad \phi_n(x) = \sin \lambda_n x, \quad n = 1, 2, \ldots, N.$$

The best approximation in $M_N$ to $G$ and $w_0$ is readily found if we use the $L_2[0, L]$ norm and the associated inner product $\langle , \rangle$. Then $P_N G$ and $P_N w_0$ are the orthogonal projections

$$P_N G(x, t) = \sum_{n=1}^{N} \gamma_n(t) \phi_n(x)$$

$$P_N w_0(x) = \sum_{n=1}^{N} \alpha_n \phi_n(x)$$

where

$$\gamma(t) = \frac{\langle G(x, t), \phi_n(x) \rangle}{\langle \phi_n(x), \phi_n(x) \rangle}$$

$$= \frac{2}{L^2} \left[ A'(t) \langle L - x, \phi_n(x) \rangle + B'(t) \langle x, \phi_n(x) \rangle \right]$$

$$\alpha_n = \frac{2}{L} \langle w_0(x), \phi_n(x) \rangle.$$

The approximate solution can be expressed as

$$w_N(x, t) = \sum_{n=1}^{N} \alpha_n(t) \phi_n(x)$$

and substitution into

$$L w_N = P_N G(x, t)$$

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shows that

\[(1.3a)\]
\[-\lambda_n^2 \alpha_n(t) - \alpha_n'(t) = \gamma(t)\]

\[(1.3b)\]
\[\alpha_n(0) = \alpha_n.\]

This first order ordinary differential equation has the solution

\[(1.4)\]
\[\alpha_n(t) = \hat{\alpha}_n e^{-\lambda_n^2 t} - \int_0^t e^{-\lambda_n^2 (t-s)} \gamma_n(s) ds\]

so that

\[(1.5)\]
\[u_N(x, t) = \sum_{n=1}^{N} \alpha_n(t) \phi_n(x) + v(x, t).\]

The problem has a particularly simple solution if \(F \equiv 0\) and the boundary data are constant. Then \(\gamma_n(t) = 0\) and

\[u_N(x, t) = \sum_{n=1}^{N} \hat{\alpha}_n e^{-\lambda_n^2 t} \sin \lambda_n x + v(x)\]

where

\[\lambda_n = \frac{n\pi}{L}\]

and

\[\hat{\alpha}_n = \frac{2}{L} \langle u_0(x) - v(x), \phi_n(x) \rangle.\]

Note that \(u_N(x, t)\) decays to \(v(x)\) which is known as the steady state solution of this problem.

If instead of the simple boundary data (1.1b,c) the more general so-called reflection conditions

\[A_0 u(0, t) - A_1 u_x(0, t) = A_2(t)\]
\[B_0 u(L, t) + B_1 u_x(L, t) = B_2(t)\]

are given then the choice of \(v(x, t)\) is more complicated. One can fit a function of the form

\[v(x, t) = a(t)x + b(t)\]
by solving
\[
\begin{pmatrix}
-A_1 & A_0 \\
B_1L + B_0 & B_0
\end{pmatrix}
\begin{pmatrix}
a(t) \\
b(t)
\end{pmatrix}
= \begin{pmatrix}
A_2(t) \\
B_2(t)
\end{pmatrix}
\]
provided the matrix is non-singular. If it is singular then one can find a function of the form
\[v(x, t) = a(t)x^2 + b(t)x + c(t)\]
which satisfies the same boundary conditions as \(u(x, t)\). Once we have homogeneous boundary conditions we obtain the corresponding eigenvalues and eigenfunctions from Table xxxxxx and proceed exactly as above. Of course, the eigenvalues may be harder to compute and the projection of the data may require more complicated integrals to be evaluated, but the solution technique itself proceeds unchanged.

D.1.2 Applications
To illustrate and make concrete the eigenfunction expansion technique for the solution of diffusion problems we shall present a number of examples drawn primarily from the theory of heat conduction.

Examples with temperature data:

Example 1: Solve
\[
\mathcal{L}u \equiv u_{xx} - u_t = 0, \quad 0 < x < L, \quad t > 0
\]
\[u(0, t) = 1, \quad u(L, t) = 0, \quad t > 0\]
\[u(x, 0) = 0, \quad 0 < x < L.\]
This problem is fairly typical for thermal systems which are initially at a uniform temperature and which then are instantaneously heated at the boundary. The technical complication is that
\[
\lim_{t \to 0} u(0, t) \neq u(0, 0).
\]
The theory of partial differential equations assures that this problem has an infinitely differentiable solution \(u(x, t)\) for \(t > 0\) which assumes the given initial and boundary conditions except at \((0, 0)\) where it is discontinuous.

Answer: The problem is formally transformed to one with zero boundary data if we choose the steady state solution
\[v(x) = \left(1 - \frac{x}{L}\right)\]
and define
\[ w(x, t) = u(x, t) - v(x). \]

Then
\[ Lw \equiv w_{xx} - w_t = Lu - Lv = 0 \]
\[ w(0, t) = w(L, t) = 0 \]
\[ w(x, 0) = -v(x). \]

The associated eigenvalue problem is
\[ \phi'' = \mu \phi \]
\[ \phi(0) = \phi(L) = 0. \]

The eigenfunctions are \( \phi_n(x) = \sin \lambda_n x \) with \( \lambda_n = \frac{\pi n}{L} \). In this case the source term \( G \) is zero so that \( \gamma_n(t) = 0 \) and
\[ \hat{\alpha}_n = \frac{\langle -v(X), \phi_n(x) \rangle}{\langle \phi_n(x), \phi_n(x) \rangle} = -\frac{2}{L} \int_0^L \left( 1 - \frac{x}{L} \right) \sin \lambda_n x \, dx = -\frac{2}{n\pi}. \]

The approximate solution is
\[ u_N(x, t) = -\sum_{n=1}^{N} \frac{2}{n\pi} e^{-\lambda_n^2 t} \sin \lambda_n x + \left( 1 - \frac{x}{L} \right). \]

Fig. 1a shows \( u_N(x, 0) \) for \( N = 5 \). We can observe the Gibbs phenomenon near \( x = 0 \) due to approximating \( v(x) \) with a Fourier sine series. Fig. 1b shows the solution \( u_5(x, t) \) for a few values of \( t \). We observe a thermal wave moving from \( x = 0 \) into the medium.

**Example 2:** Solve
\[ Lu \equiv u_{xx} - u_t = 0 \]
\[ u(0, t) = 0, \quad u(L, t) = e^{-t} \]
\[ u(x, 0) = \frac{x}{L}. \]

Now the initial and boundary data are continuous but the boundary values are time dependent so that there is no steady state solution.
**Answer:** We obtain zero boundary conditions if we choose

\[ v(x, t) = \frac{x}{L} e^{-t}, \quad w(x, t) = u(x, t) - v(x, t). \]

Then

\[ \mathcal{L}w \equiv w_{xx} - w_t = \mathcal{L}u - \mathcal{L}v = \frac{-x}{L} e^{-t}, \]

\[ w(0, t) = w(L, t) = 0 \]

\[ w(x, 0) = 0. \]

The eigenfunctions are the same as in Example 1. We obtain

\[ \gamma_n(t) = \frac{\langle \phi_n(x), \phi_n(x) \rangle}{\langle \phi_n(x), \phi_n(x) \rangle} = \dot{\gamma}_n e^{-t} \]

where

\[ \dot{\gamma}_n = -\frac{2}{L} \int_0^L \frac{x}{L} \sin \lambda_n x \, dx = \frac{(-2)^n}{n\pi}. \]

Then

\[ \alpha'_n(t) = -\lambda_n^2 \alpha_n(t) - \dot{\gamma}_n e^{-t} \]

\[ \alpha_n(0) = 0, \]

so that

\[ \alpha_n(t) = -\int_0^t e^{-\lambda_n^2 (t-s)} \dot{\gamma}_n e^{-s} \, ds \]

\[ = \frac{n}{1 - \lambda_n^2} \left( e^{-t} - e^{-\lambda_n^2 t} \right) \]

and

\[ u_N(x, t) = \sum_{n=1}^N \alpha_n(t) \sin \lambda_n x + \frac{x}{L} e^{-t}. \]

Fig. 2 shows the solution \( u_N(x, t) \) at \( t = .01 \) for \( N = 1, 3, \) and 5.

The next application is meant to illustrate the value of an (approximate) analytic formula in determining the influence of physical parameters on the solution.

**Example 3:** A bar with uniform cross section \( A \) and length \( L \) and constant thermal parameter is perfectly insulated along its length. Initially it is at a uniform temperature \( T_0 > 0 \). At time \( t = 0 \) both ends of the bar are chilled to \( T = 0 \) and kept at \( T = 0 \). Find a
relationship between the data of the problem and the time it takes for the thermal energy stored in the bar to decrease to half its original value.

**Answer:** The mathematical model for the temperature $T(x,t)$ in the bar (assuming heat flow along $x$ only) is given by

$$kT_{xx} - \rho c T_t = 0$$

$$T(0, t) = T(L, t) = 0$$

$$T(x, 0) = T_0.$$

Here the conductivity $k$, the density $\rho$ and the heat capacity $c$ are assumed constant. The thermal energy of the bar is by definition

$$E(t) = \int_0^L \rho c T(x, t) A \, dx.$$

The problem can be made dimensionless if we choose

$$y = \frac{x}{L}, \quad \tau = \frac{k}{\rho c L^2} t$$

and define

$$u(y, \tau) = \frac{T(Ly, \frac{\rho c L^2}{k} \tau)}{T_0}.$$

Then

$$\mathcal{L} u \equiv u_{yy} - u_\tau = 0, \quad \tau > 0, \quad 0 < y < 1$$

$$u(0, \tau) = u(1, \tau) = 0, \quad \tau > 0$$

$$u(y, 0) = 1, \quad 0 \leq y \leq 1.$$

The expression for the energy of the bar becomes

$$E(\tau) = \rho c \int_0^1 T \left( Ly, \frac{\rho c L^2}{k} \tau \right) AL \, dy = cT_0 AL \int_0^1 u(y, \tau) \, dy.$$

Since $E(0) = \rho c T_0 AL$ the question now is: Find $\hat{\tau}$ such that

$$\frac{E(\hat{\tau})}{E(0)} = \int_0^1 u(y, \hat{\tau}) \, dy = \frac{1}{2}.$$
Almost by inspection we see that an approximation to \( u(y, \tau) \) is given by

\[
u_N(y, \tau) = \sum_{n=1}^{N} \alpha_n e^{-\lambda_n^2 \tau} \sin \lambda_n y
\]

where \( \lambda_n = n\pi \) and

\[
\alpha_n = 2 \langle 1, \sin \lambda_n y \rangle = \frac{2}{n\pi} \left[ 1 - \cos n\pi \right] = \frac{2}{n\pi} \left[ 1 - (-1)^n \right].
\]

Hence we need to find \( \hat{\tau} \) such that

\[
\sum_{n=1}^{N} \alpha_n e^{-\lambda_n^2 \hat{\tau}} \int_0^1 \sin \lambda_n y \, dy
= \sum_{n=1}^{N} \frac{2}{(n\pi)^2 \left[ 1 - (-1)^n \right]^2 \pi^2 e^{-\pi^2 \hat{\tau}} n^2} = \frac{1}{2}
\]

If we define

\[
z = e^{-\pi^2 \hat{\tau}}
\]

then we have the polynomial problem

\[
P_N(z) = \frac{8}{\pi^2} \left[ \frac{z}{1} + \frac{z^9}{9} + \frac{z^{25}}{25} + \ldots \right] = \frac{1}{2}.
\]

By inspection we see that \( P_N(0) = 0 \) and \( P_N'(z) > 0 \) for \( z > 0 \). Hence there can be only one positive root \( z_N \) which, however, has to be found numerically. Of course, the function \( u_N(x, t) \) is only an approximate solution so the root \( z_N \) is only meaningful if it is reasonably independent of \( N \). To show the influence of the number of terms in the approximation we list below the computed value of \( z_N \) for a few \( N \).

<table>
<thead>
<tr>
<th>( N )</th>
<th>( z_N )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>.61685</td>
</tr>
<tr>
<td>3</td>
<td>.61544</td>
</tr>
<tr>
<td>5</td>
<td>.61544</td>
</tr>
<tr>
<td>7</td>
<td>.61544</td>
</tr>
</tbody>
</table>

As is usually the case, very few terms are required to obtain a stable approximate solution of the problem. Hence it follows that

\[
\hat{\tau} = \frac{-\ln .61544}{\pi^2}.
\]
The final answer is that the time $\hat{t}$ required for the thermal energy to decay to half its original value is given by

$$\hat{t} = \frac{\rho c L^2}{k}. $$

**Examples with flux data:**

**Example 4:**

Solve

$$L u = u_{xx} - u_t = 0$$

$$u(0, t) = 1, \quad u_x(L, t) = 0$$

$$u(x, 0) = 0$$

and find the time $\hat{t}$ such that $u(L, \hat{t}) = .5$.

**Answer:** The problem is transformed into a new problem with homogeneous boundary conditions if we choose

$$v(x, t) = 1$$

and set

$$w(x, t) = u(x, t) - v(x, t).$$

Then

$$L w = w_{xx} - w_t = L u - L v = 0$$

$$w(0, t) = w_x(L, t) = 0$$

$$w(x, 0) = -1.$$  

The associated eigenvalue problem is

$$\phi''(x) = \mu \phi(x)$$

$$\phi(0) = \phi'(L) = 0.$$
The eigenvalues and eigenfunctions are found from Table xxxx as

$$\lambda_n = \frac{(1 + 2n)\pi}{2L}, \quad \mu_n = -\lambda_n^2, \quad \phi_n(x) = \sin \lambda_n x$$

for \( n = 0, 1, \ldots \). If we write

$$w_N(x, t) = \sum_{n=0}^{N} \alpha_n(t)\phi_n(x)$$

then

$$-\lambda_n^2 \alpha_n(t) - \alpha_n'(t) = 0$$

$$\alpha_n(0) = \hat{\alpha}_n$$

where

$$\hat{\alpha}_n = \frac{\langle -1, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} = \frac{2}{L\lambda_n} \cos \lambda_n x \bigg|_0^L = \frac{-4}{(1 + 2n)\pi}.$$  

Hence the approximate solution is

$$u_N(x, t) = \sum_{n=0}^{N} \frac{-4}{(1 + 2n)\pi} e^{-\lambda_n^2 t} \sin \lambda_n x + 1.$$  

To find \( \hat{t} \) we need to solve the equation

$$\sum_{n=0}^{N} \frac{-4}{(1 + 2n)\pi} (\sin \lambda_n L) z^{(\pi/2 + n\pi)^2} = -.5$$

where

$$z = e^{-\frac{L}{\lambda} t}$$

and where

$$\sin \lambda_n L = (-1)^n.$$  

\( z \) can only be found numerically. The computer yields the following solutions for sums with \( N + 1 \) terms:

<table>
<thead>
<tr>
<th>( N )</th>
<th>( z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>.6847</td>
</tr>
<tr>
<td>1</td>
<td>.6847</td>
</tr>
<tr>
<td>2</td>
<td>.6847</td>
</tr>
</tbody>
</table>
Hence
\[ \hat{t} = L^2 |\ln 0.6847|. \]

**Example 5:** Let \( f(x) \) be a continuous function on \([0, L]\).

Find the behavior of the solution of
\[
\mathcal{L}u = u_{xx} - u_t = -t^2 f(x)
\]
\[ u_x(0, t) = u_x(L, t) = 0 \]
\[ u(x, 0) = 0 \]
as \( t \to \infty \).

**Answer:** The boundary data are already homogeneous and we can proceed with the eigenfunction expansion for \( u \). The associated eigenvalue problem is
\[
\phi''(x) = \mu \phi(x)
\]
\[ \phi(0) = \phi'(L) = 0. \]

The eigenvalues and eigenfunctions are obtained from Table xxxx as
\[ \lambda_n = \frac{n\pi}{L}, \quad \mu_n = -\lambda_n^2, \quad \phi_n(x) = \cos \lambda_n x \quad \text{for } n = 0, 1, \ldots, N. \]

The approximate solution is
\[
u_N(x, t) = \sum_{n=0}^{N} \alpha_n(t) \phi_n(x)
\]
where
\[ -\lambda_n^2 \alpha_n(t) - \alpha_n'(t) = \gamma_n(t) \]
\[ \alpha_n(0) = 0 \]
with
\[ \gamma_n(t) = -\hat{\gamma}_n t^2 \]
\[ \hat{\gamma}_n = \frac{\langle f(x), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle}. \]
We note that
\[ \hat{\gamma}_0 = \frac{\int_0^L f(x)dx}{L} \]
is by definition the average value \( \bar{f} \) of \( f \) on \([0, L]\).

The equation for \( \alpha_n(t) \) is readily integrated and yields
\[ \alpha_0(t) = \hat{\gamma}_0 \frac{t^3}{3} \]
\[ \alpha_n(t) = \hat{\gamma}_n \left( \frac{t^2}{\lambda_n^2} - \frac{2t}{\lambda_n^4} + \frac{2}{\lambda_n^6} \right) - \frac{2}{\lambda_n^6} \hat{\gamma}_n e^{-\lambda_n^2 t}, \quad n = 1, 2, \ldots, N \]
For large \( t \) the cubic term will dominate. Hence the solution \( u_N(x, t) \) approaches the uniform distribution
\[ u_0(x, t) = \bar{f} \frac{t^3}{3} \text{ as } t \to \infty \]
regardless of the actual form of \( f(x) \) provided only that \( \bar{f} \neq 0 \).

We shall continue our discussion of one dimensional diffusion by considering two problems which go beyond a simple model problem and are meant to indicate the advantage of combining analytic and numerical techniques to solve more realistic problems with little effort.

**Example 6:** Dynamic determination of a convective heat transfer coefficient from measured data.

An insulated bar is initially at the uniform ambient temperature \( T\infty \) and then heated at one end to \( T_0 > T\infty \) while it loses energy at the other end due to convective cooling. We may assume that after scaling space and time the non-dimensional temperature
\[ u(x, t) = \frac{T(x, t) - T\infty}{T_0 - T\infty} \]
satisfies the problem
\[ \mathcal{L}u \equiv u_{xx} - u_t = 0 \]
\[ u(0, t) = 1, \quad u_x(1, t) = -hu(1, t) \]
\[ u(x, 0) = 0 \]
where \( h \) is an unknown (scaled) heat transfer coefficient which is to be determined such that \( u(1, t) \) is consistent with measured data \((t_i, U(t_i))\), where \( U(t_i) \) is the temperature recorded at \( x = 1 \) at \( t = t_i \) for \( i = 1, \ldots, M \).
**Answer:** It is reasonable to suggest that $h$ should be computed such that $u(1, t_i)$ approximates $U(t_i)$ in the mean square sense. Hence we wish to find that value of $h$ which minimizes

$$E(h) = \sum_{i=1}^{M} (u(1, t_i, h) - U(t_i))^2 \dot{w}(t_i)$$

where $u(x, t, h)$ indicates that the analytic solution $u$ depends on $h$. $\dot{w}(t)$ is a weight function chosen to accentuate those data which are thought to be most relevant. The relationship between $u(x, t, h)$ and $h$ is quite implicit and nonlinear so that the tools of calculus for minimizing $E(h)$ are of little use. However, it is easy to calculate and plot $E(h)$ for a range of values for $h$ if we approximate $u$ by its eigenfunction expansion. To find $u_N(x, t)$ we write

$$w(x, t) = u(x, t, h) - v(x)$$

where

$$v(x) = 1 - \frac{h}{1 + h} x.$$  

Then

$$\mathcal{L} w \equiv w_{xx} - w_t = 0$$

$$w(0, t) = 0, \quad w_x(1, t) = -hw(1, t)$$

$$w(x, 0) = \frac{h}{1 + h} x - 1.$$  

The associated eigenvalue problem is

$$\phi'' = \mu \phi$$

$$\phi(0) = 0, \quad \phi'(1) = -h\phi(1).$$

The eigenfunctions are

$$\phi_n(x) = \sin \lambda_n x$$

where $\{\lambda_n(h)\}$ are the solutions of

$$f(\lambda, h) = \lambda \cos + h \sin \lambda = 0.$$  

For $h = 0$ the roots are $\lambda_n(0) = \frac{\pi}{2} + n\pi$ for $n = 1, 2, \ldots$. Newton’s method will yield the corresponding ($\lambda_n(h_k)$) for $h_k = h_{k-1} + \Delta h$ with $\Delta h$ sufficiently small when $\lambda_n(h_{k-1})$ is chosen as initial guess for the iteration. Table x below contains some representative results.
Table x: Roots of f(λ, h) = 0

<table>
<thead>
<tr>
<th>h</th>
<th>λ₁</th>
<th>λ₂</th>
<th>λ₃</th>
<th>λ₄</th>
<th>λ₅</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00000</td>
<td>1.57080</td>
<td>4.71239</td>
<td>7.85398</td>
<td>10.99557</td>
<td>14.13717</td>
</tr>
<tr>
<td>0.10000</td>
<td>1.63199</td>
<td>4.73351</td>
<td>7.86669</td>
<td>11.00466</td>
<td>14.14424</td>
</tr>
<tr>
<td>0.20000</td>
<td>1.68868</td>
<td>4.75443</td>
<td>7.87936</td>
<td>11.01373</td>
<td>14.15130</td>
</tr>
<tr>
<td>0.30000</td>
<td>1.74140</td>
<td>4.77513</td>
<td>7.89198</td>
<td>11.02278</td>
<td>14.15835</td>
</tr>
<tr>
<td>0.40000</td>
<td>1.79058</td>
<td>4.79561</td>
<td>7.90454</td>
<td>11.03182</td>
<td>14.16540</td>
</tr>
<tr>
<td>0.50000</td>
<td>1.83660</td>
<td>4.81584</td>
<td>7.91705</td>
<td>11.04083</td>
<td>14.17243</td>
</tr>
<tr>
<td>0.60000</td>
<td>1.87976</td>
<td>4.83583</td>
<td>7.92950</td>
<td>11.04982</td>
<td>14.17946</td>
</tr>
<tr>
<td>0.70000</td>
<td>1.92035</td>
<td>4.85557</td>
<td>7.94189</td>
<td>11.05879</td>
<td>14.18647</td>
</tr>
<tr>
<td>0.80000</td>
<td>1.95857</td>
<td>4.87504</td>
<td>7.95422</td>
<td>11.06773</td>
<td>14.19347</td>
</tr>
<tr>
<td>0.90000</td>
<td>1.99465</td>
<td>4.89425</td>
<td>7.96648</td>
<td>11.07665</td>
<td>14.20046</td>
</tr>
<tr>
<td>1.00000</td>
<td>2.02876</td>
<td>4.91318</td>
<td>7.97867</td>
<td>11.08554</td>
<td>14.20744</td>
</tr>
</tbody>
</table>

The eigenfunction expansion for w is

\[ w_N(x, t) = \sum_{n=1}^{N} \alpha_n(t) \phi_n(x) \]

where

\[
-\lambda_n^2 \alpha_n(t) - \alpha_n'(t) = 0
\]

\[ \alpha_n(0) = \frac{h}{1 + h} \frac{\langle x, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} - \frac{\langle 1, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle}. \]

A straightforward integration and the use of (2.1) show that

\[
\frac{h}{1 + h} \langle x, \phi_n \rangle = -\frac{1}{\lambda_n} \cos \lambda_n
\]

\[
\langle 1, \phi_n \rangle = \frac{1}{\lambda_n} (1 - \cos \lambda_n)
\]

\[
\langle \phi_n, \phi_n \rangle = \frac{1}{2} (1 + \frac{1}{h} \cos^2 \lambda_n)
\]

so that

\[ \alpha_n(t) = \frac{-2h}{\lambda_n(h + \cos \lambda_n)} e^{-\lambda_n^2 t}. \]

Hence for any numerical value of h the solution

\[ u_N(x, t, h) = w_N(x, t) + v(x) \]

is essentially given by formula so that the error \( E(h) \) is readily plotted. To give a numerical demonstration suppose that (the measured) \( U(t) \) is arbitrarily chosen as

\[ U(t) = \frac{(1 - e^{-t})^4}{2}. \]
Let the experiment be observed over the interval \([0, T]\) and data collected at 200 evenly spaced time intervals. When we compute \(E(h)\) for \(h = .1 \times i, \ i = 0, \ldots, 50\), with ten terms in the eigenfunction expansion, and then minimize \(E(h)\) the following results are obtained for the minimizer \(h^*\)

<table>
<thead>
<tr>
<th>(T)</th>
<th>(h^*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.6</td>
</tr>
<tr>
<td>2</td>
<td>1.5</td>
</tr>
<tr>
<td>4</td>
<td>1.2</td>
</tr>
<tr>
<td>8</td>
<td>1.1</td>
</tr>
<tr>
<td>16</td>
<td>1.1</td>
</tr>
<tr>
<td>32</td>
<td>1.0</td>
</tr>
</tbody>
</table>

These results indicate that the assumed boundary temperature \(U(t)\) is not consistent with any solution of the model problem for a constant \(h\). But they also show that as \(t \to \infty\) and \(U(t) \to 1/2\) the numerical results converge to the heat transfer coefficient \(h = 1\) consistent with the steady state solution

\[ v(x) = 1 - x/2. \]

This behavior of the computed sequence \(\{h^*\}\) simply reflects that more and more data are collected near the steady state as \(T \to \infty\).

**Example 7:** Phase shift for a thermal wave.

Consider the problem

\[
\begin{align*}
    u_{xx} - u_t &= 0 \\
    u(0, t) &= \sin \omega t, \quad u_x(L, t) = 0 \\
    u(x, 0) &= 0.
\end{align*}
\]

It is reasonable to assume that \(u(L, t)\) will vary sinusoidally with frequency \(\omega\) as \(t \to \infty\). Find the phase shift of \(u(L, t)\) relative to \(u(0, t)\).

**Answer:** Let \(w(x, t) = u(x, t) - \sin \omega t\). Then

\[
\mathcal{L}w \equiv w_{xx} - w_t = \omega \cos \omega t
\]

\[w(0, t) = w_x(L, t) = 0\]

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\[ w(x, 0) = 0. \]

The eigenfunctions associated with this problem are

\[ \phi_n(x) = \sin \lambda_n x \quad \text{where} \quad \lambda_n = \frac{\left( \frac{\pi}{2} + n\pi \right)}{L}, \quad n = 0, 1, \ldots \]

Then

\[ P_N(\omega \cos \omega t) = \omega \cos \omega t \sum_{n=0}^{N} \hat{\gamma}_n \phi_n(x) \]

where

\[ \hat{\gamma}_n = \frac{\langle 1, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle}. \]

If

\[ w_N(x, t) = \sum_{n=0}^{N} \alpha_n(t) \phi_n(x) \]

then

\[-\lambda_n^2 \alpha_n(t) - \alpha_n'(t) = \hat{\gamma}_n \omega \cos \omega t.\]

It follows that

\[ \alpha_n(t) = c e^{-\lambda_n^2 t} + \alpha_{np}(t). \]

To find the particular integral we use the method of undetermined coefficients and try

\[ \alpha_{np}(t) = A_n \cos \omega t + B_n \sin \omega t. \]

Substituting into the differential equation and equating the coefficients of \( \sin \omega t \) and \( \cos \omega t \) we find that

\[-\lambda_n^2 A_n - \omega B_n = \hat{\gamma}_n \omega \]

\[-\lambda_n^2 B_n + \omega A_n = 0 \]

so that

\[ A_n = \frac{-\hat{\gamma}_n \omega \lambda_n^2}{\lambda_n^4 + \omega^2} \]

\[ B_n = \frac{-\hat{\gamma}_n \omega^2}{\lambda_n^4 + \omega^2}. \]
Assembling all the parts we find that

\[ u_N(x, t) = \sum_{n=0}^{N} \left[ A_n \left( \cos \omega t - e^{-\lambda_n^2 t} \right) + B_n \sin \omega t \right] \phi_n(x) + \sin \omega t. \]

To find the phase shift we make the following observation.

\[ \sin \omega t \sim \sum_{n=0}^{\infty} \sin \omega t \hat{\gamma}_n \phi_n(x) \]

is the Fourier series of the 4L periodic odd function which coincides with \( \sin \omega t \) on \((0, 2L)\). This series converges uniformly near \( x = L \). For \( t \gg 1 \) the exponential terms may be ignored so that we can write

\[ u_N(1, t) = \sum_{n=0}^{N} [A_n \cos \omega t + (B_n + \hat{\gamma}_n) \sin \omega t] \phi_n(1) \]

This expression can rearranged into

\[ u_N(1, t) = \sum_{n=0}^{N} \frac{\hat{\gamma}_n \lambda_n^2}{\sqrt{\lambda_n^4 + \omega^2}} \left[ -\frac{\omega}{\sqrt{\lambda_n^4 + \omega^2}} \cos \omega t + \frac{\lambda_n^2}{\sqrt{\lambda_n^4 + \omega^2}} \sin \omega t \right] \phi_n(1). \]

If we set

\[ \sin \psi_n = \frac{\omega}{\sqrt{\lambda_n^4 + \omega^2}} \]

then

\[ u_N(1, t) = \sum_{n=0}^{N} -\frac{\hat{\gamma}_n \lambda_n^2}{\sqrt{\lambda_n^4 + \omega^2}} \sin (\omega t - \psi_n) \phi_n(1). \]

Since \( \hat{\gamma}_n = \frac{2}{T \lambda_n} \), we see that the dominant term corresponds to \( n = 0 \) which yields a phase shift \( \psi_0 \) given by

\[ \sin \psi_0 = \frac{\omega}{\sqrt{(\pi T)^4 + \omega^2}}. \]

The next two examples deal with heat flow in a disk and sphere. In these geometries the eigenfunctions become considerably more complicated.

**Example 8:** Heat flow in a disk.

A disk of radius \( R \) is initially at a uniform temperature \( u_0 = 1 \). At time \( t = 0 \) the boundary is cooled instantaneously to and maintained at \( u(R, t) = 0 \). Find the time required for the temperature at the center of the disk to fall to \( u(0, t) = .5 \).
**Answer:** Since there is no angular dependence in the data, the temperature \( u(r, t) \) is given by the radial heat equation

\[
u_{rr} + \frac{1}{r} u_r - u_t = 0
\]

subject to the symmetry condition

\[u_r(0, t) = 0\]

and the initial and boundary data

\[u(R, t) = 0, \quad u(r, 0) = 1.\]

Since the boundary data already are homogeneous we see that the eigenvalue problem associated with the spatial part of the radial heat equation is

\[
\phi''(r) + \frac{1}{r} \phi'(r) = \mu \phi(r)
\]

\[\phi'(0) = 0, \quad \phi(R) = 0.\]

The equations can be transformed to standard form as described in Chapter ST

\[
(r \phi'(r))' = \mu r \phi(r)
\]

\[\phi'(0) = 0, \quad \phi(R) = 0.\]

Were this problem given on an annulus \( r_0 < r < R \) with \( r_0 > 0 \) then it would be a standard Sturm-Liouville problem with countably many eigenvalues and eigenfunctions, and with eigenfunctions for distinct eigenvalues orthogonal in \( L^2_{[r_0, R]} \).

The general theory does not apply because the coefficient of \( \phi''(r) \) vanishes at \( r = 0 \). This makes the problem a singular Sturm-Liouville problem. Fortunately, the conclusions of the general theory remain applicable. Equation (2.2) is a special form of the extensively studied Bessel’s equation. It has negative eigenvalues so that we can write

\[-\mu = \lambda^2\]

For arbitrary \( \lambda \) the solution of Bessel’s equation satisfying \( \phi'(0) = 0 \) is the so-called Bessel function of the first kind of order zero given by

\[
J_0(\lambda r) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!m!} \left( \frac{\lambda r}{2} \right)^{2m}
\]

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A plot of $J_0(x)$ vs. $x$ is shown below. Like $\cos \lambda r$ the Bessel function oscillates and the zero-crossings depend on $\lambda$. Different eigenfunctions are found if $\lambda_n$ is chosen such that

$$J_0(\lambda_n R) = 0.$$ 

It follows that there are countably many eigenvalues $0 < \lambda_1 < \lambda_2 < \cdots$ where

$$\lambda_n R = x_n$$

is the $n$th root of the Bessel function $J_0(x)$. These roots are tabulated in mathematical handbooks so that the $\{x_n\}$ may be considered known. Finally, since $J_0(0) = 1$ and $J_0'(0) = 0$ it is straightforward to verify as in the regular Sturm-Liouville case that

$$\int_0^R J_0(\lambda_m r) J_0(\lambda_n r) r \, dr = 0, \quad m \neq n,$$

i.e. that the eigenfunctions corresponding to distinct eigenvalues are orthogonal in $L_2[0, R, r]$.

We now find an approximate solution of the heat flow problem in the usual way. We solve

$$u_{rr} + \frac{1}{r} u_r - u_t = 0$$

$$u_r(0, t) = u(R, t) = 0$$

with the projected initial condition

$$P_N u(r, 0) = \sum_{n=1}^N \hat{\alpha}_n \phi_n(r)$$

where

$$\hat{\alpha}_n = \frac{\langle 1, \phi_n(r) \rangle}{\langle \phi_n, \phi_n \rangle}$$

In this case

$$\phi_n(r) = J_0(\lambda_n r) \quad \text{and} \quad \langle f(r), g(r) \rangle = \int_0^R f(r) g(r) r \, dr.$$ 

The solution of this problem is

$$u_N(r, t) = \sum_{n=1}^N \alpha_n(t) \phi_n(r)$$
where

\[-\lambda_n^2 \alpha(t) - \alpha'(t) = 0\]

\[\alpha_n(0) = \hat{\alpha}_n.\]

Hence

\[u_N(r, t) = \sum_{n=1}^{N} \hat{\alpha}_n e^{-\lambda_n^2 t} J_0(\lambda_n r).\]

The evaluation of the inner products involving Bessel functions is not quite as forbidding for this model problem as might appear from the series definition of the Bessel function. Numerous differential and integral identities are known for Bessel functions of various orders. For example, it can be shown that

\[\langle 1, J_0(\lambda_n r) \rangle = \frac{R^2}{x_n} J_1(x_n)\]

\[\langle J_0(\lambda_n r), J_0(\lambda_n r) \rangle = \frac{R^2}{2} J_1^2(x_n)\]

where \(x_n\) is the \(n\)th root of \(J_0(x) = 0\) and \(J_1(x)\) is the Bessel function of order 1 which also is tabulated or available from computer libraries. Using the values given in [ ] we find

<table>
<thead>
<tr>
<th>(n)</th>
<th>(x_n)</th>
<th>(J_1(x_n))</th>
<th>(n)</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>2.405</td>
<td>.5191</td>
<td>1.602</td>
</tr>
<tr>
<td>2</td>
<td>5.520</td>
<td>-.3403</td>
<td>-1.065</td>
</tr>
<tr>
<td>3</td>
<td>8.654</td>
<td>.2715</td>
<td>0.8512</td>
</tr>
<tr>
<td>4</td>
<td>11.792</td>
<td>-.2325</td>
<td>-0.7295</td>
</tr>
</tbody>
</table>

If we set

\[z = e^{-\frac{t}{R^2}}\]

then the approximate solution to our problem is that value of \(z\) which satisfies

\[.5 = \sum_{n=1}^{N} \hat{\alpha}_n z^{x_n^2}\]

For \(N = 2, 3\) and \(4\) the computer yields

\[z = .818\]
so that the temperature at the center of the disk is reduced to half its original value at time
\[ t = R^2 |\ln 0.818|. \]

We shall conclude our discussion of one-dimensional diffusion by considering radial diffusion in a sphere. As we shall see, this problem is simpler than the analogous problem of radial diffusion in a disk.

**Example 9.** A sphere of radius \( R \) is initially at a uniform temperature \( u = 1 \). At time \( t = 0 \) the boundary is cooled instantaneously to and maintained at \( u(R, t) = 0 \). Find the time required for the temperature at the center of the sphere to fall to \( u(0, t) = 0.5 \).

**Answer:** The temperature in the sphere is modeled by the radial heat equation
\[
\frac{u_{rr}}{r} + \frac{2}{r} u_r - u = 0
\]
subject to
\[
\begin{align*}
u_r(0, t) &= 0, \quad u(R, t) = 0 \\
u(r, 0) &= 1.
\end{align*}
\]

The only change compared to the formulation of Example 8 is the factor 2 in the heat equation. This problem already has homogeneous boundary conditions and needs no further transformation. The associated eigenvalue problem is
\[
\phi''(r) + \frac{2}{r} \phi'(r) = \mu \phi(r)
\]
\[
\phi'(0) = \phi(R) = 0.
\]

The key observation is that the differential equation can be rewritten as
\[
(r\phi(r))'' = \mu(r\phi(r))
\]
\[
(r\phi(r))(R) = 0.
\]

We do not have a boundary condition for \( r\phi(r) \) at \( r = 0 \) but if we make the reasonable assumption that \( \lim_{r \to 0} |\phi(r)| < \infty \) then we have another singular Sturm-Liouville problem and it is readily verified that
\[
\phi(r) = \sin \frac{\lambda r}{r}
\]
for $\mu = -\lambda^2$ satisfies the differential equation and the boundary conditions

$$\phi(0) = \lambda, \quad \phi'(0) = 0.$$  

The boundary condition at $r = R$ requires that

$$\sin \lambda R = 0$$

so that we have the eigenfunctions

$$\phi_n(r) = \frac{\sin \lambda_n r}{r}, \quad \lambda_n = \frac{n\pi}{R}, \quad n = 1, 2 \ldots$$

By inspection we find that the eigenfunctions $\{\phi_n(r)\}$ are orthogonal in $L_2[0, R, r^2]$. If we now write

$$u_N(r, t) = \sum_{n=1}^{N} \alpha_n(t) \phi_n(r)$$

and substitute it into the radial heat equation we obtain from

$$\sum_{n=1}^{N} \left[ -\lambda_n^2 \alpha_n(t) - \alpha_n'(t) \right] \phi_n(r) = 0$$

$$u_N(r, 0) = \sum_{n=1}^{N} \left( \frac{\langle 1, \phi_n(r) \rangle}{\langle \phi_n, \phi_n \rangle} \right) \phi_n(r)$$

that

$$u_N(r, t) = \sum_{n=1}^{N} \left( \frac{\langle 1, \phi_n(r) \rangle}{\langle \phi_n, \phi_n \rangle} \right) e^{-\lambda_n^2 t} \phi_n(r).$$

A straightforward calculation shows that

$$\langle 1, \phi_n \rangle = \int_{0}^{R} \sin \lambda_n r \, r \, dr = \frac{-R \cos \lambda_n R}{\lambda_n} = \frac{(-1)^{n+1} R}{\lambda_n}$$

$$\langle \phi_n, \phi_n \rangle = \frac{R}{2}$$

so that

$$u_N(r, t) = 2 \sum_{n=1}^{N} (-1)^{n+1} e^{-\lambda_n^2 t} \frac{\sin \lambda_n r}{\lambda_n r}.$$
We observe that
\[ u_N(0, 0) = 2 \sum_{n=1}^{N} (-1)^{n+1} = \begin{cases} 2 & \text{if } N \text{ is even} \\ 0 & \text{if } N \text{ is odd} \end{cases} \]

Hence the orthogonal projection \( u_N \) does not converge to the initial condition \( u_0(r) = 1 \) at \( r = 0 \) as \( N \to \infty \). The general theory lets us infer mean square convergence on \((0, R)\). For \( r > 0 \) and \( t = 0 \) we do have slow pointwise convergence and for \( t > 0 \) we have convergence for all \( r \in [0, R] \). These comments are illustrated by the data of Table xyxy computed for \( R = 1 \).

**Table xyxy: Numerical values of** \( u_N(r, t) \) **for radial heat flow on a sphere**

<table>
<thead>
<tr>
<th>( N )</th>
<th>( u_N(.001, 0) )</th>
<th>( u_N(.01, 1) )</th>
<th>( u_N(.001, .1) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>.000180</td>
<td>0.707100</td>
<td>.707099</td>
</tr>
<tr>
<td>100</td>
<td>.016531</td>
<td>0.707100</td>
<td>.707099</td>
</tr>
<tr>
<td>1000</td>
<td>1.000510</td>
<td>0.707100</td>
<td>.707099</td>
</tr>
<tr>
<td>10000</td>
<td>.999945</td>
<td>0.707100</td>
<td>.707099</td>
</tr>
</tbody>
</table>

To find the time \( \hat{t} \) when \( u(0, \hat{t}) = .5 \) we need to solve

\[
.5 = 2 \sum_{n=1}^{N} (-1)^{n+1} z^n
\]

where

\[
z = e^{-(\frac{\pi}{R})^2 \hat{t}}
\]

The numerical answer is found to be

\[
z \approx .25417
\]

for all \( N > 2 \). Hence

\[
\hat{t} \approx \frac{|\ln .25417|}{2} R^2 \approx .1388 R^2.
\]

**D.3 Theory**

**D.3.1 Convergence of** \( u_N(x, t) \) **to the analytic solution**

The dominant question for our approximation method has to be: How is the computed approximation \( u_N(x, t) \) related to the analytic solution \( u(x, t) \).

The answer depends strongly on the properties of the analytic solution \( u(x, t) \). For the initial/boundary value problem (1.1) the theory of partial differential equations gives
precise information on the existence, uniqueness and smoothness of the solution (see [], Chapter IV.9). In essence, if the data are sufficiently smooth and consistent then the analytic solution will also be a smooth bounded function. In this case we can relate easily the computed solution $u_N(x, t)$ to the analytic solution $u(x, t)$.

**Theorem:** Let $w(x, t)$ be the analytic solution of (1.1) with homogeneous boundary data. If for $t > 0$ the derivatives $w_{xx}$ and $w_t \in L_2(0, L)$ then

$$w_N(x, t) = P_N w(x, t).$$

**Proof:** Since

$$w_{xx}(x, t) - w_t(x, t) = G(x, t)$$

$$w(0, t) = w(L, t) = 0$$

$$w(x, 0) = w_0(x)$$

we see that

$$P_N(w_{xx} - w_t) = P_N G$$

$$P_Nw(x, 0) = P_Nw_0(x).$$

Writing out the projections we obtain for each $n$

$$\langle w_{xx}, \phi_n \rangle - \langle w_t, \phi_n \rangle = \langle G, \phi_n \rangle.$$

Integration by parts shows that

$$\langle w_{xx}, \phi_n \rangle = -\lambda_n^2 \langle w, \phi_n \rangle,$$

and of course

$$\langle w_t, \phi_n \rangle = \frac{d}{dt} \langle w, \phi_n \rangle.$$}

Hence the term $\langle \frac{w, \phi_n}{\phi_n, \phi_n} \rangle$ satisfies the initial value problem (1.3a,b). Since its solution is unique it follows that $\alpha_n(t) \equiv \langle \frac{w, \phi_n}{\phi_n, \phi_n} \rangle$ and hence that

$$w_N(x, t) = P_N w(x, t).$$
For non-homogeneous boundary data we accept as approximate solution
\[ u_N(x, t) = w_N(x, t) + v(x, t). \]

Of course, \( u_N(x, t) \neq P_N u(x, t) \) because \( P_N u(x, t) \) does not usually satisfy the correct boundary conditions; instead we interpret \( u_N(x, t) \) as the best approximation to \( u(x, t) \) in the affine space \( \mathcal{M}_N + v \).

Since we have assumed that \( w_{xx}(x, t) \) for fixed \( t \) belongs to \( L_2(0, L) \) it follows that \( w \) itself belongs to \( L_2[0, L] \). The convergence result for eigenfunctions of Sturm-Liouville problems then assures that \( w_N(x, t) \to w(x, t) \) as \( N \to \infty \), at least in the mean square sense. Stronger results can be inferred for Fourier series expansions as described in Chapter 2. Of course, we cannot conclude that this convergence is uniform in \( t \). However, in general \( w(x, t) \) becomes a very smooth function as \( t \) increases so that one may expect that \( w_N(x, t) \) in fact converges uniformly. Computed results invariably show very rapid convergence as we move away from any discontinuity of the initial/boundary data. As the next results show the rate of convergence can in fact be quantified a priori by how well we can approximate the source term and initial data.

### D.3.2 An error bound for the approximate solution

The general Sturm-Liouville theory assures that the orthogonal projection of a function into the span of \( N \) eigenfunctions converges in the mean square sense as \( N \to \infty \). It is the aim of this section to compute how fast the approximate solution \( w_N \) of the diffusion problem with projected initial data and source terms converges in the mean square sense to the analytic solution of the original problem.

As before \( w(x, t) \) will denote the true solution of
\[
\mathcal{L} w \equiv w_{xx} - w_t = G(x, t)
\]
\[
w(0, t) = w(L, t) = 0
\]
\[
w(x, 0) = w_0(x).
\]

We shall assume again on theoretical grounds that the solution exists. The computable approximate solution \( w_N \) solves
\[
\mathcal{L} w \equiv w_{xx} - w_t = P_N G(x, t)
\]
\[ w(0, t) = w(L, t) = 0 \]
\[ w(x, 0) = P_N w_0(x) \]

where
\[ P_N G(x, t) = \sum_{n=1}^{N} \gamma_n(t) \phi_n(x) \]

and
\[ P_N w_0(x) = \sum_{n=1}^{N} \hat{\alpha}_n \phi_n(x). \]

Let
\[ e(x, t) = w(x, t) - w_N(x, t) \]

denote the error of the approximation. Then \( e(x, t) \) is the solution of

\[ \mathcal{L} e \equiv e_{xx} - e_t = G(x, t) - P_N G(x, t) \]
\[ e(0, t) = e(L, t) = 0 \]
\[ e(x, 0) = w_0(x) - P_N w_0(x). \]

If we multiply the differential equation by \( e(x, t) \) and integrate with respect to \( x \) we obtain
\[ \int_0^L (e_{xx} - e_t) e \, dx = \int_0^L [G - P_N G] e \, dx \]

After integrating the first term by parts and rewriting the time derivative the following equation results:
\[ \frac{1}{2} \frac{d}{dt} \int_0^L e^2(x, t) dx = - \int_0^L e_x(x, t)^2 dx - \int_0^L [G - P_N G] e(x, t) dx \]

It can be shown that any function vanishing at \( x = 0 \) and \( x = L \) and with a square integrable derivative (like \( e(x, t) \)) satisfies the inequality
\[ \int_0^L e(x, t)^2 dx \leq \left( \frac{L}{\pi} \right)^2 \int_0^L e_x(x, t)^2 dx. \]

This inequality allows the following estimate for the error at time \( t \):

\[ \frac{d}{dt} E(t) \leq -2 \left( \frac{\pi}{L} \right)^2 E(t) + 2 \int_0^L |G(x, t) - P_N G(x, t)| |e(x, t)| dx \]
where for convenience we have set

\[ E(t) = \int_0^L e(x, t)^2 \, dx. \]

Applying the algebraic-geometric mean inequality

\[ 2 \left( \frac{\sqrt{a^2}}{\sqrt{\epsilon}} \right) \leq \frac{a^2}{\epsilon} + \epsilon b^2 \]

with \( \epsilon = \left( \frac{1}{T} \right)^2 \) we can obtain the estimate

\[ \int_0^L [G(x, t) - P_N G(x, t)] e(x, t) \, dx \leq \left( \frac{L}{\pi} \right)^2 \int_0^L [G(x, t) - P_N G(x, t)]^2 \, dx + \left( \frac{\pi}{L} \right)^2 E(t). \]

With this estimate for (e.2) we have the following error bound

\[ E'(t) \leq - \left( \frac{\pi}{L} \right)^2 E(t) + \left( \frac{L}{\pi} \right)^2 \| G - P_N G \|_2^2 \]

\[ E(0) = \| w_0 - P_N w_0 \|_2^2 \]

where \( \| \cdot \|_2 \) is the usual norm of \( L_2[0, L] \). Inequalities like (3.3) occur frequently in the qualitative study of ordinary differential equations. If we express it as an equality

\[ E'(t) = - \left( \frac{\pi}{L} \right)^2 E(t) + \left( \frac{L}{\pi} \right)^2 \| G - P_N G \|_2^2 - g(t) \]

for some non-negative (but unknown) function \( g(t) \) then this equation has the solution

\[ E(t) = \| w_0 - P_N w_0 \|_2^2 e^{-\frac{(\pi/L)^2 t}{2}} + \int_0^t e^{-\frac{(\pi/L)^2 (t-s)}{2}} \left[ \left( \frac{L}{\pi} \right)^2 \| G(x, s) - P_N G(x, s) \|_2^2 - g(s) \right] \, ds \]

or finally,

\[ E(t) \leq \| w_0 - P_N w_0 \|_2^2 e^{-\frac{(\pi/L)^2 t}{2}} + \int_0^t e^{-\frac{(\pi/L)^2 (t-s)}{2}} \| G(x, s) - P_N G(x, s) \|_2^2 \, ds. \]

This inequality is known as Gronwall’s inequality for (3.3). Thus the error due to projecting the initial condition depends entirely on how well \( w_0 \) can be approximated in \( \text{span}\{\phi_n\}_{n=1}^N \) and can be made as small as desirable by taking sufficiently many eigenfunctions. In addition, this contribution to the overall error decays rapidly with time. The approximation of the source term \( G \) also converges in the mean square sense. If we can assert that
\[ \|G(x, t) - P_N G(x, t)\|_2 \to 0 \text{ uniformly in } t \text{ then we can conclude that } E(t) \to 0 \text{ uniformly in } t \text{ as } N \to \infty. \]  

As an illustration consider

\[ \mathcal{L}w \equiv w_{xx} - w_t = 0 \]

\[ w(0, t) = w(L, t) = 0 \]

\[ w(x, 0) = 1. \]

It is straightforward to compute that

\[ P_N(1) = \frac{4}{\pi} \sum_{n=0}^{N} \frac{1}{2n+1} \sin \left( \frac{2n+1}{L} \pi x \right). \]

Then it follows from the discussion of the Gibbs phenomenon in Chapter Fourier that

\[ \max_x |1 - P_N(1)| \cong .089. \]

This expression implies that \( w_N \) cannot converge uniformly for all \( t \) to the solution \( w \). It also implies that

\[ \|1 - P_N(1)\|_2^2 < .089^2 L \]

so that

\[ E(t) \leq .089^2 Le^{-\left(\pi/L\right)^2 t}. \]

While this error bound decreases to zero with time it does not improve with the number of terms in the approximation. It simply implies that the initial condition does not influence a long-term solution.

A sharper result is obtained if we apply Parseval’s identity

\[ L = \|1\|_0^2 = L \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \]

to estimate

\[ \|1 - P_N(1)\|_2^2 = L \left( 1 - \frac{8}{\pi^2} \sum_{n=0}^{N} \frac{1}{(2n+1)^2} \right) = L \frac{8}{\pi^2} \sum_{n=N+1}^{\infty} \frac{1}{(2n+1)^2} \leq \frac{8L}{\pi^2(4N + 6)} \]
where the last inequality follows from the integral test

$$\sum_{n=N+1}^{\infty} \frac{1}{(2n+1)^2} \leq \int_{N+1}^{\infty} \frac{dx}{(2x+1)^2} = \frac{1}{4N+6}$$

Now the mean square error decays with $N$ and time.

In general we cannot expect much more from our approximate solution because initial and boundary data may not be consistent so that the Gibbs phenomenon precludes a uniform convergence of $w_N$ to $w$. However, as we saw in Chapter Fourier, when the data are smooth then their Fourier series will converge uniformly. In this case it is possible to establish uniform convergence with the so-called maximum principle for the heat equation. Hence let us assume that $w_0(x)$ and $G(x,t)$ are such that

$$\max_x |w_0(x) - P_N w_0(x)| \to 0 \quad \text{for } x \in [0, L]$$

and

$$\max_{x,t} |G(x,t) - P_N G(x,t)| \to 0 \quad \text{for } (x,t) \in [0, L] \times [0, T]$$

as $N \to \infty$. Here $T$ is considered arbitrary but fixed. Then the error $e(x,t)$ satisfies (3.1) with continuous initial/boundary data and a smooth source term. Let $M$ be a constant given by

$$M = \max_{x,t} |G(x,t) - P_N G(x,t)| + \epsilon$$

for $(x,t) \in [0, L] \times [0, T]$ and arbitrary $\epsilon > 0$. If we define

$$\psi_\pm(x,t) = M \frac{x^2}{2} \pm e(x,t)$$

then

$$\mathcal{L} \psi_\pm = M \pm [G(x,t) - P_N G(x,t)] > 0$$

The functions $\psi_\pm$ must assume their maxima at $x = 0$, $x = L$ or $t = 0$ because if $\psi_\pm$ had a maximum at some point $(x^*, t^*) \in (0, L) \times (0, T]$ then necessarily

$$\psi_{x,xx}(x^*, t^*) \leq 0 \quad \text{and} \quad \psi_{x,t}(x^*, t^*) \geq 0.$$ 

These inequalities are inconsistent with $\mathcal{L} \psi_\pm(x,t) > 0$. 

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It follows that $\psi_{\pm}(x,t)$ assume their maxima on the boundary $x = 0$ or $x = L$ or $t = 0$
so that for all $\epsilon > 0$

$$\pm \epsilon(x,t) \leq \psi_{\pm}(x,t) \leq ML^2 + \max_x |w_0(x) - P_N w_0(x)|$$
or finally, that

$$|e(x,t)| \leq K \max_{x,t} |G(x,t) - P_N G(x,t)| + \max_x |w_0(x) - P_N w_0(x, t)|$$

where the constant $K$ depends on the length of the interval. In other words, if the orthogonal
projections converge uniformly to the data functions then the approximate solution likewise
will converge uniformly to the true solution on the computational domain $[0, L] \times [0, T]$.

D.3.3 Influence of the boundary conditions and Duhamel’s solution

The formulas derived for the solution of (1.1) involve the function $v$ used to zero out
the boundary conditions. Since there are many $v$ which may be used, and since the analytic
solution is uniquely determined by the boundary data and is independent of $v$ it may be
instructive to see how $v$ actually enters the computational solution. We recall, the original
problem is transformed into

$$\mathcal{L}w = w_{xx} - w_t = \mathcal{L}u - \mathcal{L}v = F - (v_{xx} - v_t)$$

$$w(0, t) = w(L, t) = 0$$

$$w(x, 0) = u_0(x) - v(x, 0).$$

Let us write the approximate solution $w_N(x,t)$ in the form

$$w_N(x,t) = w^1_N(x,t) + w^2_N(x,t)$$

where

$$\mathcal{L}w^1_N = P_N F(x,t)$$

$$w^1_N(x,0) = 0$$
and where $w^2_N$ accounts for the influence of the initial and boundary conditions

$$Lw^2_N = \sum_{n=1}^{N} \frac{\langle v_{xx} - v_t, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} \phi_n(x)$$

$$w^2_N(x, 0) = \sum_{n=1}^{N} \frac{\langle u_0(x) - v(x, 0), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} \phi_n(x).$$

The above discussion of the Dirichlet problem shows that

$$w^1_N(x, t) = -\sum_{n=1}^{N} \int_0^t e^{-\lambda_n^2(t-s)} \gamma_n(s) ds \phi_n(x)$$

where

$$\gamma_n(t) = \frac{\langle F(x, t), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle}.$$ 

We remark that $w^1_N(x, t)$ is identical to the solution obtained with Duhamel’s principle since by inspection the function

$$W_N(x, t, s) = e^{-\lambda_n^2(t-s)} \gamma_n(s) \phi_n(x)$$

solves the problem

$$W_{xx} - W_t = 0$$

$$W(0, t, s) = W(L, t, s) = 0$$

$$W(x, s, s) = -\frac{\langle F(x, s), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle}$$

so that

$$\sum_{n=1}^{N} W_n(x, s, s) = -P_N F(x, s)$$

and

$$w^1_N(x, t) = \int_0^t \sum_{n=1}^{N} W_n(x, t, s) ds.$$

We shall now compute $w^2_N$. Integration by parts shows that

$$\langle v_{xx}, \phi_n \rangle = \left[ v_x(x, t)\phi_n(x) - v(x, t)\phi'_n(x) \right]_0^L + \langle v, \phi''_n \rangle = C_n(t) - \lambda_n^2 \langle v, \phi_n \rangle$$

where for the data of (1.1)

$$C_n(t) = \lambda_n [A(t) - B(t) \cos \lambda_n L].$$
\(C_n(t)\) is independent of the choice of \(v\) since only the boundary data appear. If we write

\[ w^2_N(x, t) = \sum_{n=1}^{N} \alpha_n(t)\phi_n(x) \]

then

\[-\lambda_n^2 \alpha_n(t) - \alpha'(t) = \frac{1}{\langle \phi_n, \phi_n \rangle} \left[ -C_n(t) + \frac{d}{dt} \langle v, \phi_n \rangle + \lambda_n^2 \langle v, \phi_n \rangle \right].\]

It follows that

\[-\lambda_n^2 \left[ \alpha_n(t) + \frac{\langle v(x, t), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} \right] - \frac{d}{dt} \left[ \alpha_n(t) + \frac{\langle v(x, t), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} \right] = \frac{C_n(t)}{\langle \phi_n, \phi_n \rangle} \]

\[\alpha_n(0) + \frac{\langle v(x, 0), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} = \frac{\langle u_0(x), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle}\]

so that

\[\alpha_n(t) + \frac{\langle v(x, t), \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} = \frac{\langle u_0, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} e^{-\lambda_n^2 t} + \int_{0}^{t} e^{-\lambda_n^2 (t-s)} \frac{C_n(s)}{\langle \phi_n, \phi_n \rangle} ds.\]

Thus

\[u_N(x, t) = w^1_N(x, t) + \sum_{n=1}^{N} D_n(t)\phi_n(x) + [v(x, t) - P_N v(x, t)]\]

where

\[D_n(t) = \frac{\langle u_0, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} e^{-\lambda_n^2 t} \int_{0}^{t} -\lambda_n^2 (t-s) \frac{C_n(s)}{\langle \phi_n, \phi_n \rangle} ds\]

is again independent of the choice of \(v\).

Hence the solution \(u_N(x, t)\) at time \(t\) depends on the data of the original problem and on the difference between \(v\) and its orthogonal projection. While this difference will vary with the choice of \(v\) all choices of \(v\) lead to the same Gibbs phenomenon with an overshoot of \(0.089|A(t)|\) at \(x = 0\) and \(0.089|B(t)|\) at \(x = L\). Hence in a practical sense the particular \(v\) does not matter much. We note in closing that the final answer for \(u_N\) involves \(A(t)\) and \(B(t)\) only and not their derivatives.