Solutions for Problems for The 1-D Heat Equation

18.303 Linear Partial Differential Equations

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1 Problem 2

Find the Fourier sine and cosine series of

$$f(x) = \frac{1}{2}(1-x), \qquad 0 < x < 1.$$

a. State a theorem which proves convergence of each series. Graph the functions to which they converge.

Solution: The sine series is

$$\hat{f}(x) = \sum_{n=1}^{\infty} B_n \sin(n\pi x)$$

where

$$\begin{aligned} B_n &= 2\int_0^1 f(x)\sin(n\pi x)\,dx = \int_0^1 (1-x)\sin(n\pi x)\,dx \\ &= \left[\frac{-(1-x)\cos n\pi x}{n\pi} - \frac{\sin n\pi x}{(n\pi)^2}\right]_{x=0}^1 \\ &= \frac{1}{n\pi} \end{aligned}$$

The cosine series is

$$\tilde{f}(x) = A_0 + \sum_{n=1}^{\infty} A_n \cos(n\pi x)$$

where

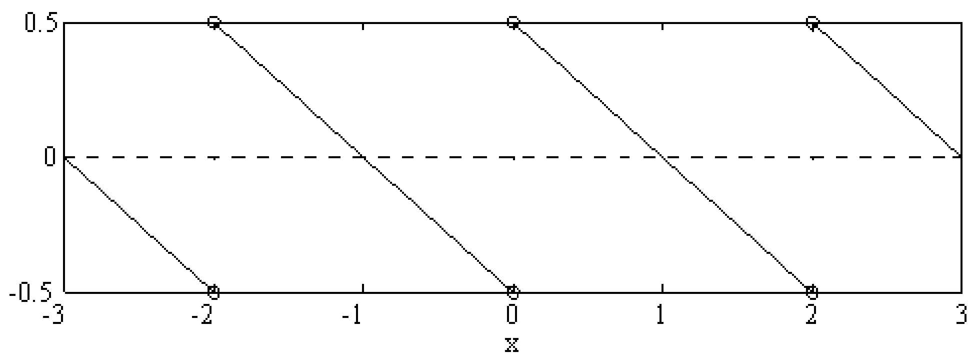
$$A_0 = \int_0^1 f(x)\,dx = \frac{1}{2}\int_0^1 (1-x)\,dx = \frac{1}{4}$$

$$
\begin{aligned}
A_n &= 2\int_0^1 f(x)\cos(n\pi x)\,dx = \int_0^1 (1-x)\cos(n\pi x)\,dx \\
&= \left[\frac{-(1-x)\sin n\pi x}{n\pi} - \frac{\cos n\pi x}{(n\pi)^2}\right]_{x=0}^{1} \\
&= \frac{1-\cos n\pi}{(n\pi)^2}
\end{aligned}
$$

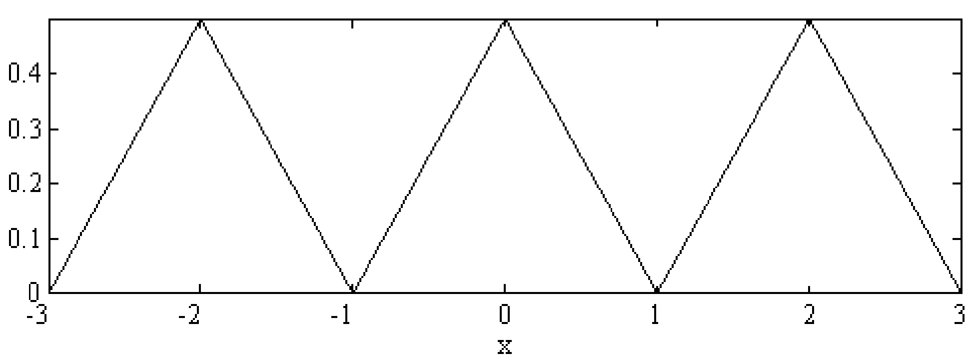
Thus $A_{2n} = 0$ and $A_{2n-1} = 2/\left((2n-1)^2\pi^2\right)$.

Both the sine and cosine series of $f(x)$ converge on the closed interval $[0,1]$ since $f(x)$ is piecewise continuous on $0 \le x \le 1$ and continuous on $0 < x < 1$, as required by the theorem in the notes.

The sine series is the odd periodic extension of $f(x)$, it is even, 2-periodic and discontinuous.



The cosine series is the even periodic extension of $f(x)$, it is even, 2-periodic and continuous.



b. Show that the Fourier sine series cannot be differentiated termwise (term-by-term). Show that the Fourier cosine series converges uniformly.

Solution: Differentiating $f(x)$ gives

$$\frac{df}{dx} = -\frac{1}{2}$$

Differentiating the sine series $\hat{f}(x)$ term-by-term gives

$$\frac{d\hat{f}}{dx} = \sum_{n=1}^{\infty} \cos(n\pi x)$$

This series does not converge because the summands do not approach zero as $n \to \infty$, for any x. For a series $\sum_n a_n$ to converge, the n'th summand a_n must approach zero as $n \to \infty$. An alternative method to show this series does not converge is to choose a single x where the series does not converge. Consider $x = 1/2$, then

$$\frac{d\hat{f}}{dx}\left(\frac{1}{2}\right) = \sum_{n=1}^{\infty} \cos\left(\frac{n\pi}{2}\right) = \sum_{,m=1}^{\infty} \cos(m\pi) = \sum_{,m=1}^{\infty} (-1)^m$$

where we let $m = 2n$. The partial sums

$$\sum_{,m=1}^{M} (-1)^m = \begin{cases} 0, & M \text{ even} \\ -1, & M \text{ odd} \end{cases}$$

do not converge, and hence the series at $x = 1/2$ does not converge. In particular, the term-by-term differentiated sine series does not converge, and hence the since series of $f(x)$, i.e. $\hat{f}(x)$ cannot be differentiated term-by-term.

To show the cosine series $\tilde{f}(x)$ converges uniformly, we apply the Weirstrass M-Test:

$$\left|\sum_{n=1}^{\infty} A_n \cos(n\pi x)\right| \leq \sum_{n=1}^{\infty} |A_n \cos(n\pi x)| \leq \sum_{n=1}^{\infty} |A_n| = \sum_{n=1}^{\infty} \frac{2}{(2n-1)^2 \pi^2} \leq \frac{2}{\pi^2} \sum_{m=1}^{\infty} \frac{1}{m^2}$$

We know $\sum_{m=1}^{\infty} \frac{1}{m^2}$ converges from our class notes, and hence by the Weirstrass M-Test, the cosine series $\tilde{f}(x)$ converges uniformly.

2 Problem 3

A bar with initial temperature profile $f(x) > 0$, with ends held at 0^o C, will cool as $t \to \infty$, and approach a steady-state temperature 0^oC. However, whether or not all parts of the bar start cooling initially depends on the shape of the initial temperature profile. The following example may enable you to discover the relationship.

a. Find an initial temperature profile $f(x)$, $0 \leq x \leq 1$, which is a linear combination of $\sin \pi x$ and $\sin 3\pi x$, and satisfies $\frac{df}{dx}(0) = 0 = \frac{df}{dx}(1)$, $f\left(\frac{1}{2}\right) = 4$.

Solution: A linear combination of $\sin \pi x$ and $\sin 3\pi x$ is

$$f(x) = a \sin 3\pi x + b \sin \pi x$$

Imposing the conditions gives

$$\begin{aligned} 0 &= \frac{df}{dx}(0) = \pi(3a + b) \\ 0 &= \frac{df}{dx}(1) = -\pi(3a + b) \\ 4 &= f\left(\frac{1}{2}\right) = -a + b \end{aligned}$$

The first two equation are redundant. Solving for a, b gives

$$a = -1, \qquad b = 3.$$

Thus

$$f(x) = -\sin 3\pi x + 3 \sin \pi x \tag{1}$$

b. Solve the problem

$$u_t = u_{xx}; \qquad u(0,t) = 0 = u(1,t); \qquad u(x,0) = f(x).$$

This is easy, you can just write down the solution we had in class - but make sure you know how to get it.

Solution: This is the basic heat problem we considered in class, with solution

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin(n\pi x) e^{-n^2\pi^2 t} \tag{2}$$

where

$$B_n = 2 \int_0^1 f(x) \sin(n\pi x)\, dx \tag{3}$$

and $f(x)$ is given in (1). The form of (1) is already a sine series, with $B_1 = 3$, $B_3 = -1$ and $B_n = 0$ for all other n. You can check this for yourself by computing integrals in (3) for $f(x)$ given by (1), from the orthogonality of $\sin n\pi x$. Therefore,

$$u(x,t) = 3 \sin(\pi x) e^{-\pi^2 t} - \sin(3\pi x) e^{-9\pi^2 t} \tag{4}$$

c. Show that for some x, $0 \le x \le 1$, $u_t(x,0)$ is positive and for others it is negative. How is the sign of $u_t(x,0)$ related to the shape of the initial temperature profile? How is the sign of $u_t(x,t)$, $t > 0$, related to subsequent temperature profiles? Graph the temperature profile for $t = 0, 0.2, 0.5, 1$ on the same axis (you may use Matlab).

Differentiating $u(x,t)$ in time gives

$$u_t(x,t) = -\pi^2 \left(3 \sin(\pi x) e^{-\pi^2 t} - 9 \sin(3\pi x) e^{-9\pi^2 t}\right)$$

Setting $t = 0$ gives

$$u_t(x,0) = -3\pi^2 (\sin(\pi x) - 3 \sin(3\pi x))$$

Note that

$$u_t\left(\frac{1}{6}, 0\right) = \frac{15}{2}\pi^2 > 0, \qquad u_t\left(\frac{1}{2}, 0\right) = -12\pi^2 < 0$$

Thus at $x = 1/6$, u_t is positive and for $x = 1/2$, u_t is negative.

From the PDE,

$$u_t = u_{xx}$$

and hence the sign of u_t gives the concavity of the temperature profile $u(x,t_0)$, t_0 constant. Note that for $u_{xx}(x,t_0) > 0$, the profile $u(x,t_0)$ is concave up, and for $u_{xx}(x,t_0) < 0$, the profile $u(x,t_0)$ is concave down. At $t_0 = 0$, the sign of $u_t(x,0)$ give the concavity of the initial temperature profile $u(x,0) = f(x)$.

The plots of $u(x,t_0)$ for $t_0 = 0, 0.2, 0.5, 1$ are below.

3 Problem 4

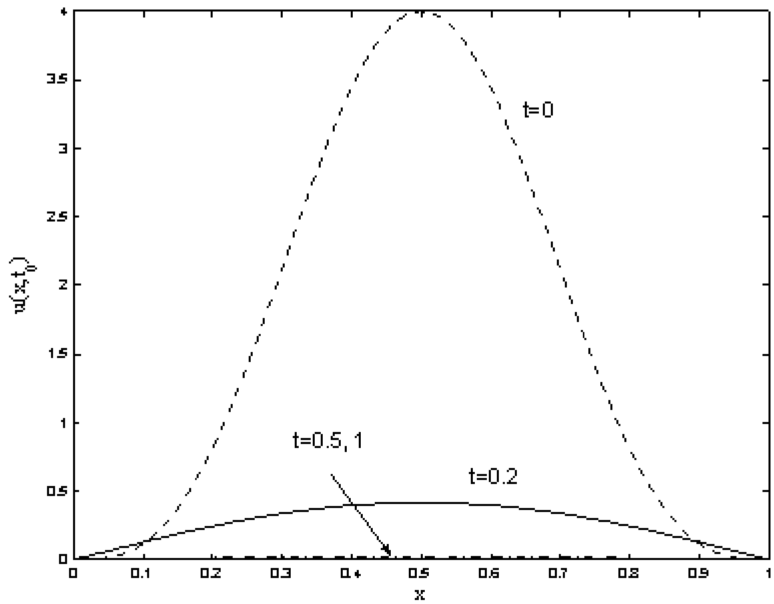
Solve the inhomogeneous heat problem with type I boundary conditions:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}; \qquad u(0,t) = 0 = u(1,t); \qquad u(x,0) = P_\varepsilon(x)$$

where $t > 0$, $0 \le x \le 1$, and

$$P_\varepsilon(x) = \begin{cases} 0 & \text{if } \left|x - \frac{1}{2}\right| > \frac{\varepsilon}{2} \\ \frac{u_0}{\varepsilon} & \text{if } \left|x - \frac{1}{2}\right| \le \frac{\varepsilon}{2} \end{cases} \tag{5}$$

Note: you already know the solution (just replace $P_\varepsilon(x)$ with $f(x)$ and write down the solution from class). Using symmetry of $P_\varepsilon(x)$ about $1/2$ can be used to simplify the calculation of the Fourier coefficients.



Solution: This is the Heat Problem with Type I homogeneous BCs. The solution we derived in class is, with $f(x)$ replaced by $P_\varepsilon(x)$,

$$u(x,t) = \sum_{n=1}^{\infty} u_n(x,t) = \sum_{n=1}^{\infty} B_n \sin(n\pi x)\, e^{-n^2\pi^2 t} \tag{6}$$

where the B_n's are the Fourier coefficients of $f(x) = P_\varepsilon(x)$, given by

$$B_n = 2\int_0^1 P_\varepsilon(x)\sin(n\pi x)\,dx$$

Breaking the integral into three pieces and substituting for $P_\varepsilon(x)$ from (5) gives

$$\begin{aligned} B_n &= 2\int_0^{1/2-\varepsilon/2} P_\varepsilon(x)\sin(n\pi x)\,dx + 2\int_{1/2-\varepsilon/2}^{1/2+\varepsilon/2} P_\varepsilon(x)\sin(n\pi x)\,dx + 2\int_{1/2+\varepsilon/2}^{1} P_\varepsilon(x)\sin(n\pi x)\,dx \\ &= 0 + 2\int_{1/2-\varepsilon/2}^{1/2+\varepsilon/2} \frac{u_0}{\varepsilon}\sin(n\pi x)\,dx + 0 \\ &= \frac{2u_0}{\varepsilon}\left\{-\frac{\cos(n\pi x)}{n\pi}\right\}_{1/2-\varepsilon/2}^{1/2+\varepsilon/2} \\ &= u_0\frac{\cos\left(\frac{n\pi}{2}(1-\varepsilon)\right) - \cos\left(\frac{n\pi}{2}(1+\varepsilon)\right)}{\varepsilon n\pi/2} \end{aligned} \tag{7}$$

We apply the cosine rule

$$\cos(r-s) - \cos(r+s) = 2\sin r \sin s$$

with $r = n\pi/2$, $s = n\pi\varepsilon/2$ to Eq. (7),

$$B_n = \frac{4u_0}{\varepsilon n\pi} \sin\frac{n\pi}{2} \sin\frac{n\pi\varepsilon}{2}$$

When n is even (and nonzero), i.e. $n = 2m$ for some integer m,

$$B_{2m} = \frac{2u_0}{\varepsilon m\pi} \sin m\pi \sin m\pi\varepsilon = 0$$

When n is odd, i.e. $n = 2m-1$ for some integer m,

$$B_{2m-1} = 2u_0 (-1)^{m+1} \frac{\sin((2m-1)\pi\varepsilon/2)}{(2m-1)\pi\varepsilon/2}. \tag{8}$$

(a) The temperature at the midpoint of the rod, $x = 1/2$, at scaled time $t = 1/\pi^2$ is, from (6) and (8),

$$\begin{aligned} u(x,t) &= \sum_{m=1}^{\infty} 2u_0 (-1)^{m+1} \frac{\sin((2m-1)\pi\varepsilon/2)}{(2m-1)\pi\varepsilon/2} \sin\left((2m-1)\frac{\pi}{2}\right) e^{-(2m-1)^2} \\ &= \sum_{m=1}^{\infty} \frac{2u_0}{e^{(2m-1)^2}} \left(\frac{\sin((2m-1)\pi\varepsilon/2)}{(2m-1)\pi\varepsilon/2}\right). \end{aligned}$$

For $t \geq 1/\pi^2$, the first term gives a good approximation to $u(x,t)$,

$$u\left(\frac{1}{2}, \frac{1}{\pi^2}\right) \approx u_1\left(\frac{1}{2}, \frac{1}{\pi^2}\right) = \frac{2u_0}{e}\left(\frac{\sin(\pi\varepsilon/2)}{\pi\varepsilon/2}\right).$$

To distinguish between pulses with $\varepsilon = 1/1000$ and $\varepsilon = 1/2000$, note that $\lim_{\varepsilon\to 0} \frac{\sin \pi\varepsilon/2}{\pi\varepsilon/2} = 1$, and so for smaller and smaller ε, the corresponding temperature $u\left(\frac{1}{2}, \frac{1}{\pi^2}\right)$ gets closer and closer to $2u_0/e$,

$$u\left(\frac{1}{2}, \frac{1}{\pi^2}\right) \approx u_1\left(\frac{1}{2}, \frac{1}{\pi^2}\right) = \frac{2u_0}{e}\left(1 - \frac{\pi^2\varepsilon^2}{2\cdot 3!} + \cdots\right), \qquad \varepsilon \ll 1.$$

In particular,

$$\begin{aligned} u_1\left(\frac{1}{2}, \frac{1}{\pi^2}; \varepsilon = \frac{1}{1000}\right) - u_1\left(\frac{1}{2}, \frac{1}{\pi^2}; \varepsilon = \frac{1}{2000}\right) &= \frac{2u_0}{e}\left(\frac{\sin(\pi/2000)}{\pi/2000} - \frac{\sin(\pi/4000)}{\pi/4000}\right) \\ &\approx -\frac{2u_0}{e} \times 3.1 \times 10^{-7} \end{aligned}$$

Thus it is hard to distinguish these two temperature distributions, at least by measuring the temperature at the center of the rod at time $t = 1/\pi^2$. By this time, diffusion has smoothed out some of the details of the initial condition.

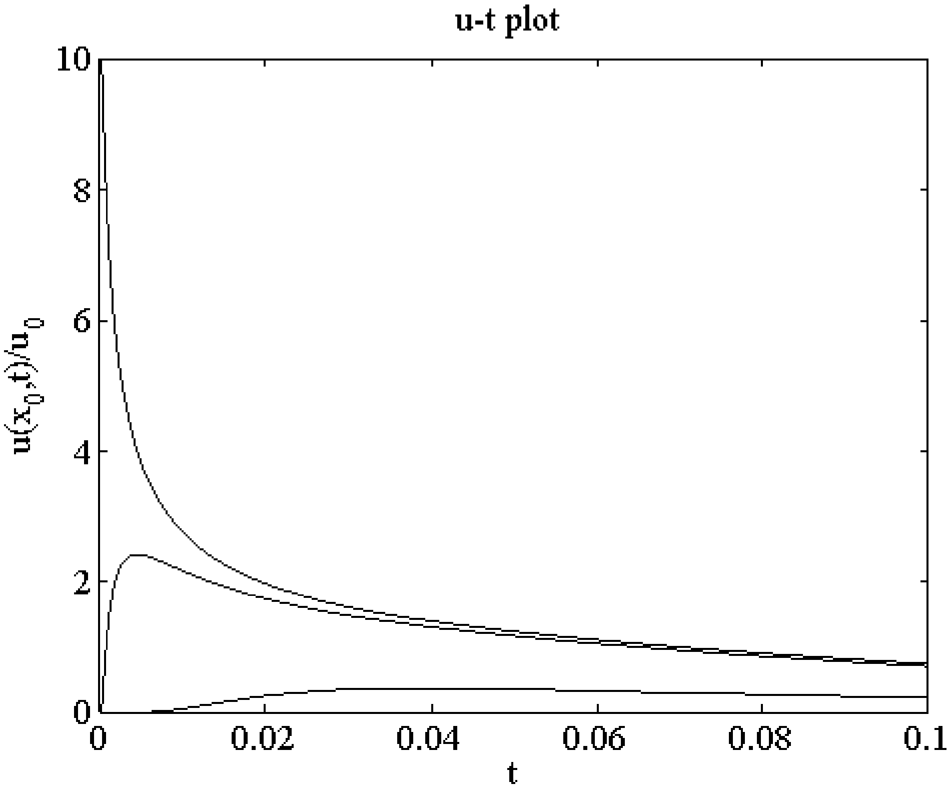


Figure 1: Time temperature profiles $u(x_0, t)$ at $x_0 = 0.5$, 0.4 and 0.1 (from top to bottom). The t-axis is the time profile corresponding to $x_0 = 0$, 1.

(b) Illustrate the solution qualitatively by sketching (i) some typical temperature profiles in the $u - t$ plane (i.e. $x =$ constant) and in the $u - x$ plane (i.e. $t =$ constant), and (ii) some typical level curves $u(x,t) =$ constant in the $x - t$ plane. At what points of the set $D = \{(x,t) : 0 \leq x \leq 1, t \geq 0\}$ is $u(x,t)$ discontinuous?

The solution $u(x,t)$ is discontinuous at $t = 0$ at the points $x = (1 \pm \varepsilon)/2$. That said, $u(x,t)$ is piecewise continuous on the entire interval $[0,1]$. Thus, the Fourier series for $u(x,0)$ converges everywhere on the interval and equals $u(x,0)$ at all points except $x = (1 \pm \varepsilon)/2$. The temperature profiles ($u - t$ plane, $u - x$ plane), 3D solution and level curves are shown.

4 Problem 5

Consider two iron rods (thermal diffusivity $\kappa = 0.15$ cm^2 sec^{-1}) each 20 cm long and with insulated sides, one at a temperature of 100^{o}C and the other at 0^{o}C throughout. The rods

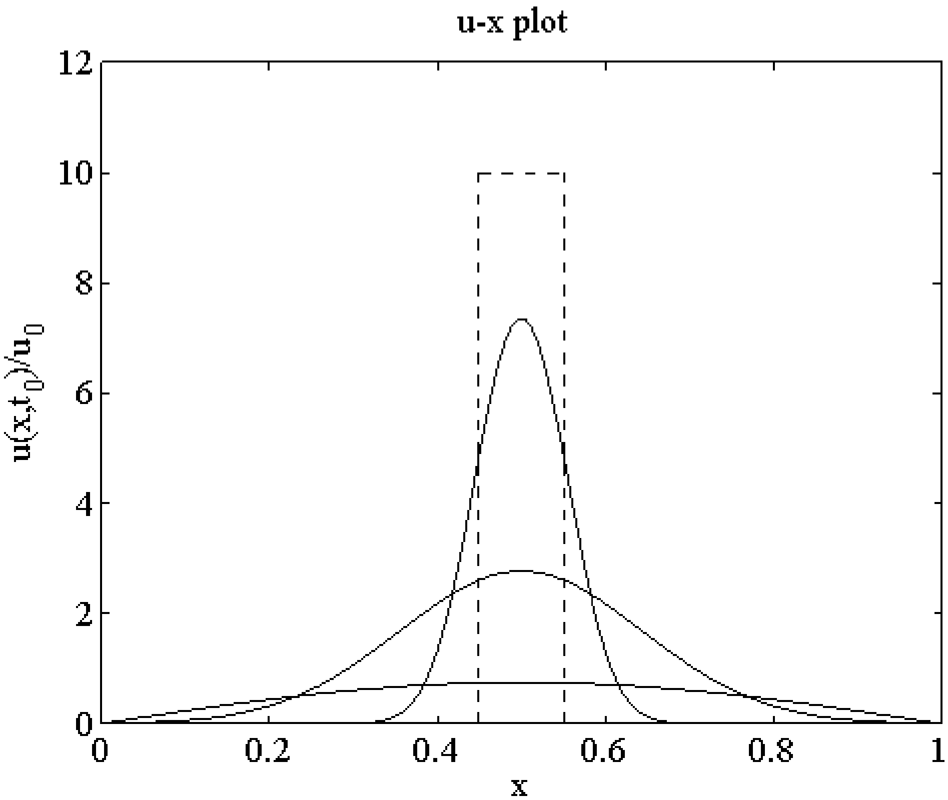
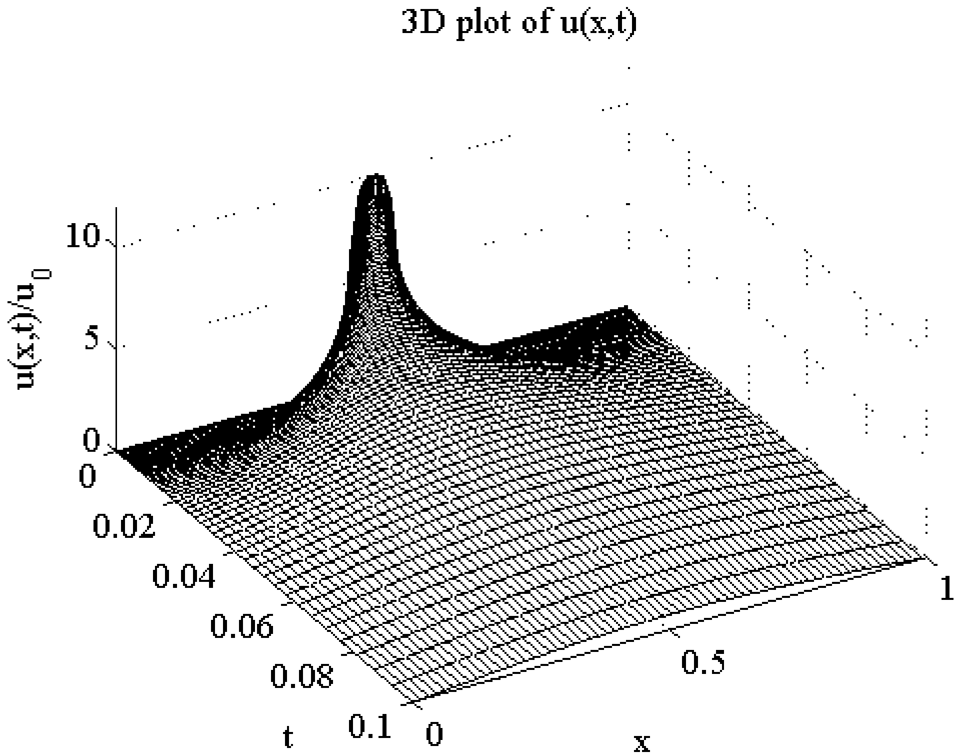


Figure 2: Spatial temperature profiles $u(x,t_0)$ at $t_0 = 0$ (dash), 0.001, 0.01, 0.1. The x-axis from 0 to 1 is the limiting temperature profile $u(x,t_0)$ as $t_0 \to \infty$.



are joined end to end in perfect thermal contact, and their free ends are kept at 0^oC. Show that the temperature at the interface 10 minutes after contact has been made approximately 36.5^oC. Find an upper bound for the error in your answer. Can this method be applied if the rods are made of glass (thermal diffusivity $\kappa = 0.006$ cm^2 sec^{-1})?

Solution: The rods are placed end-to-end and treated as one rod with length $l = 40$ cm. We define the dimensionless spatial coordinate $x = x'/l$. Let $u(x,t)$ be the temperature in the joined rods, for $x \in [0,1]$ and $t \geq 0$. The join is at $x = 1/2$. The initial temperature distribution in the joined rods is

$$u(x,0) = f(x) = \begin{cases} 100, & 0 \leq x \leq 1/2, \\ 0, & 1/2 \leq x \leq 1. \end{cases} \tag{9}$$

Since the ends of the rod are held at 0^o C, the boundary conditions are $u(0,t) = 0 = u(1,t)$. Since there are no sources in the rods, the homogeneous Heat Equation $u_t = u_{xx}$ governs the variation in temperature. The problem for $u(x,t)$ is thus the basic Heat Problem with Type I homogeneous BCs and IC $f(x)$. From the derivation in class, we found the solution to be

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin(n\pi x) \exp\left(-n^2\pi^2 t\right)$$

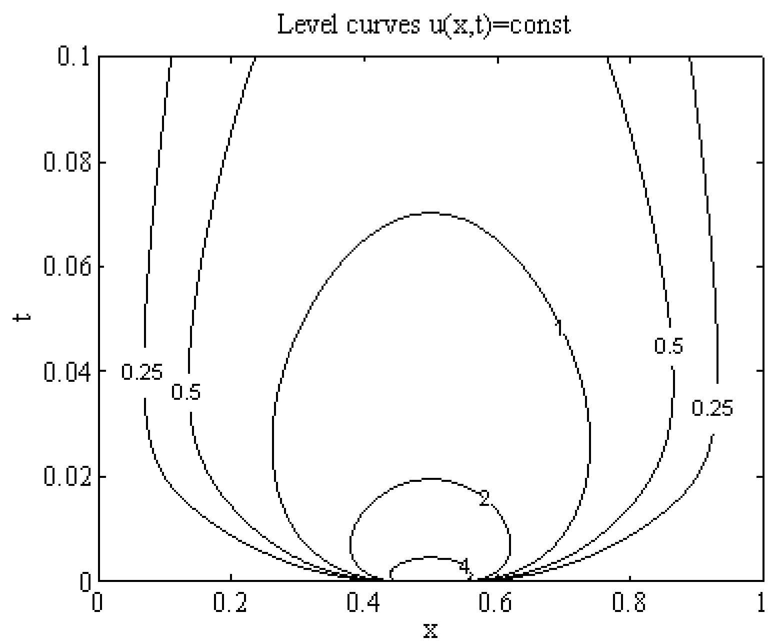


Figure 3: Level curves $u(x,t)/u_0 = C$ for various values of the constant C. Numbers adjacent to curves indicate the value of C. The line segment $(1-\varepsilon)/2 \leq x \leq (1+\varepsilon)/2$ at $t=0$ is the level curve with $C = 1/\varepsilon = 10$. The lines $x=0$ and $x=1$ are also level curves with $C=0$.

where

$$B_n = 2\int_0^1 f(x)\sin(n\pi x)\,dx \tag{10}$$

To save time, we note that we only desire the solution at $x = 1/2$,

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi}{2}\right)\exp\left(-n^2\pi^2 t\right)$$

Since $\sin(n\pi/2)$ is zero for even n, the sum is over the odd terms,

$$\begin{aligned} u(x,t) &= \sum_{k=1}^{\infty} B_{2k-1}\sin\left(\frac{(2k-1)\pi}{2}\right)\exp\left(-(2k-1)^2\pi^2 t\right) \\ &= \sum_{k=1}^{\infty} B_{2k-1}(-1)^{k-1}\exp\left(-(2k-1)^2\pi^2 t\right). \end{aligned} \tag{11}$$

Substituting the IC (9) into (10) and setting $n = 2k-1$ gives

$$B_{2k-1} = 200\int_0^{1/2}\sin((2k-1)\pi x)\,dx = \frac{200}{(2k-1)\pi}\left(1-\cos\left(\frac{(2k-1)\pi}{2}\right)\right) = \frac{200}{(2k-1)\pi}. \tag{12}$$

Substituting the B_{2k-1} in (12) into the expression (11) for $u(1/2,t)$ gives

$$u\left(\frac{1}{2},t\right) = \frac{200}{\pi}\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{(2k-1)}\exp\left(-(2k-1)^2\pi^2 t\right). \tag{13}$$

We are asked to fine the temperature at $x = 1/2$ after $t' = 10$ minutes. This corresponds to a scaled time of

$$\begin{aligned} t_{10} &= \frac{\kappa}{l^2}\times 10 \text{ mins} \\ &= 0.15/40^2\times 10\times 60 \simeq 0.056 \qquad \text{for iron } (\kappa = 0.15 \text{ cm}^2/\text{s}) \\ &= 0.006/40^2\times 10\times 60 \simeq 0.002 \qquad \text{for glass } (\kappa = 0.006 \text{ cm}^2/\text{s}) \end{aligned}$$

Recall in the notes we made the first term approximation for $t \geq 1/\pi^2 \simeq 0.1$, and hence both these values fall under that. To see how the number of terms retained affects the sum, we compute $u(1/2,t)$ from (13) for various numbers of terms. For iron ($t = t_{10} = 0.056$), we obtain

$$\begin{aligned} u\left(\frac{1}{2},t_{10}\right) &\simeq 36.631 \text{ (1 term)} \\ &\simeq 36.484 \text{ (2 terms)} \\ &\simeq 36.484 \text{ (3 or more terms)} \end{aligned} \tag{14}$$

In this case, the first term $u_1(1/2, t_{10})$ does a good job of approximating the series for $u(1/2, t_{10})$. For glass ($t = t_{10} = 0.002$),

$$\begin{aligned} u\left(\frac{1}{2}, t_{10}\right) &\simeq 62.4 \text{ (1 term)} \\ &\simeq 44.7 \text{ (2 terms)} \\ &\simeq 52.4 \text{ (3 terms)} \\ &\simeq 49.0 \text{ (4 terms)} \\ &\simeq 50.4 \text{ (5 terms)} \\ &\simeq 49.9 \text{ (6 terms)} \\ &\simeq 50.04 \text{ (7 terms)} \end{aligned}$$

In this case, the convergence is much slower and the first term $u_1(1/2, t_{10})$ is a poor estimate of $u(1/2, t_{10})$.

The upper bound on the error was discussed in §6.2. The approximate error we derived in class is, since the series for $u(1/2, t)$ only has odd terms,

$$\left| u\left(\frac{1}{2}, t\right) - u_1\left(\frac{1}{2}, t\right) \right| \leq \frac{Be^{-3\pi^2 t}}{1 - e^{-2\pi^2 t}} \tag{15}$$

where B is the upper bound for B_{2k-1} for all $k = 2, 3, ...$ In the notes, we wrote

$$|B_n| \leq 2 \int_0^1 |f(x)|\, dx = 2 \cdot \frac{1}{2} \cdot 100 = 100$$

However, we can obtain a better approximation since we have the formula for B_n

$$|B_{2k-1}| = \left| \frac{200}{(2k-1)\pi} \right| \leq \frac{200}{3\pi} \qquad k = 2, 3, ...$$

Therefore, $B = 200/(3\pi)$ and from (15),

$$\left| u\left(\frac{1}{2}, t\right) - u_1\left(\frac{1}{2}, t\right) \right| \leq \frac{200}{3\pi} \frac{e^{-3\pi^2 t}}{1 - e^{-2\pi^2 t}} < 6.1 \text{ for } t \geq t_{10} = 0.056.$$

This error bound is still not very good - in (14) the error between $u(1/2, t_{10})$ (for iron, $t_{10} = 0.056$) and the first term $u_1(1/2, t_{10})$ is roughly 0.15, much less than 6.1. I have now added a much better estimate to §6.2. It turns out that, since the series $u(1/2, t)$ only has odd terms,

$$\left| u\left(\frac{1}{2}, t\right) - u_1\left(\frac{1}{2}, t\right) \right| \leq \frac{Be^{-9\pi^2 t}}{1 - e^{-6\pi^2 t}} = \frac{200}{3\pi} \frac{e^{-9\pi^2 t}}{1 - e^{-6\pi^2 t}}$$

Now the error for $t = t_{10} = 0.056$ is 0.152, which is more in line with (14).

5 Problem 7

Consider the heat flow problem with dimensionless position and time,

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2}; \qquad 0 < x < 1, \qquad t > 0 \\ u(0,t) &= 0 = \frac{\partial u}{\partial x}(1,t); \qquad t > 0 \\ u(x,0) &= f(x) \qquad\qquad 0 < x < 1. \end{aligned} \tag{16}$$

Solution:

(a) The physical significance of the condition $u_x(1,t) = 0$ is that the end of the rod at $x = 1$ is insulated, i.e. the heat flux (proportional to u_x by Fourier's law) is zero at $x = 1$.

(b) Showing that $\bar{u}(t) = \int_0^1 u^2(x,t)\,dx$ is non-increasing in time follows from the derivation in §8.1 of the lecture notes and noting that $uu_x = 0$ at $x = 0, 1$ since $u = 0$ at $x = 0$ and $u_x = 0$ at $x = 1$.

(c) Proving that (16) has at most one solution follows the derivation in class. Take two solutions u_1, u_2 of (16) and define $v(x,t) = u_1 - u_2$. Then show that the function $\bar{v}(t) = \int_0^1 v^2(x,t)\,dx$ is non-increasing as in part (b).

(d) To find a series solution for $f(x) = u_0$, u_0 a constant, we use separation of variables,

$$u(x,t) = X(x)\,T(t) \tag{17}$$

The PDE in (16) gives the usual

$$\frac{X''}{X} = \frac{T'}{T} = -\lambda$$

where λ is constant since the left hand side is a function of x only and the middle is a function of t only. Substituting (17) into the BCs in (16) gives

$$X(0) = \frac{dX}{dx}(1) = 0$$

The Sturm-Liouville boundary value problem for $X(x)$ is thus

$$X'' + \lambda X = 0; \qquad X(0) = \frac{dX}{dx}(1) = 0 \tag{18}$$

Let us try $\lambda < 0$. Then the solutions are

$$X(x) = c_1 e^{-\sqrt{|\lambda|}x} + c_2 e^{\sqrt{|\lambda|}x}$$

and imposing the BCs gives $c_1 = c_2 = 0$, i.e. $X(x)$ must be the trivial solution. For $\lambda = 0$, $X(x) = c_1 x + c_2$ and, again, imposing the BCs gives $c_1 = c_2 = 0$ and $X(x)$ is the trivial solution. Thus, in order to have a nontrivial solution, λ must be taken positive. In this case,

$$X = c_1 \sin \sqrt{\lambda} x + c_2 \cos \sqrt{\lambda} x$$

The BC $X(0) = 0$ implies $c_2 = 0$. The other BC implies

$$0 = \frac{dX}{dx}(1) = c_1 \sqrt{\lambda} \cos \sqrt{\lambda}$$

For a non-trivial solution, c_1 must be nonzero. Since $\lambda > 0$ then we must have $\cos \sqrt{\lambda} = 0$, which implies the eigenvalues are

$$\lambda_n = \frac{(2n-1)^2}{4} \pi^2, \qquad n = 1, 2, 3, ...$$

and the eigenfunctions are

$$X_n(x) = \sin\left(\frac{(2n-1)}{2} \pi x\right)$$

For each n, the solution for $T(t)$ is $T_n(t) = e^{-\lambda_n t}$. Hence the series solution for $u(x,t)$ is

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{(2n-1)}{2} \pi x\right) \exp\left(-\frac{(2n-1)^2}{4} \pi^2 t\right) \tag{19}$$

At $t = 0$,

$$f(x) = u(x,0) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{(2n-1)}{2} \pi x\right) \tag{20}$$

The orthogonality conditions are found using the identity

$$2 \sin\left(\frac{(2n-1)}{2} \pi x\right) \sin\left(\frac{(2m-1)}{2} \pi x\right) = \cos((m-n)\pi x) - \cos((1-m-n)\pi x)$$

Note also that for $m, n = 1, 2, 3...$, we have

$$\int_0^1 \cos((m-n)\pi x)\, dx = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases}$$

$$\int_0^1 \cos((1-m-n)\pi x)\, dx = 0$$

The last integral follows since $1 - m - n$ cannot be zero for any positive integers m, n. Thus, the orthogonality conditions are

$$\int_0^1 \sin\left(\frac{(2n-1)}{2} \pi x\right) \sin\left(\frac{(2m-1)}{2} \pi x\right) dx = \begin{cases} 1/2 & m = n \\ 0 & m \neq n \end{cases} \tag{21}$$

Multiplying each side of (20) by $\sin((2m-1)\pi x/2)$, integrating from $x = 0$ to 1, and applying the orthogonality condition (21) gives

$$B_n = 2\int_0^1 \sin\left(\frac{(2n-1)}{2}\pi x\right) f(x)\,dx \tag{22}$$

Substituting $f(x) = u_0$ into (22) gives

$$B_n = 2u_0 \int_0^1 \sin\left(\frac{(2n-1)}{2}\pi x\right) dx = \frac{4u_0}{(2n-1)\pi}\left(1 - \cos\left(\frac{(2n-1)}{2}\pi\right)\right) = \frac{4u_0}{(2n-1)\pi} \tag{23}$$

Thus, the series solution is

$$u(x,t) = \frac{4u_0}{\pi}\sum_{n=1}^{\infty} \frac{1}{(2n-1)} \sin\left(\frac{(2n-1)}{2}\pi x\right) \exp\left(-\frac{(2n-1)^2}{4}\pi^2 t\right).$$

An approximate solution valid for large times is the first term,

$$u(x,t) \approx u_1(x,t) = \frac{4u_0}{\pi} \sin\left(\frac{\pi x}{2}\right) \exp\left(-\frac{\pi^2 t}{4}\right).$$

Similar upper bounds on error can be derived as in the notes. Temperature profiles (u vs. x) are plotted below for different times.

6 Problem 8

Suppose a chemical is dissolved in water, in some long thin reaction container and let ϕ (moles/cm^3) indicate its concentration. Fick's Law in chemistry states that the rate of diffusion of a solute is proportional to the negative gradient of the solute concentration. Assume that the chemical is created, due to a chemical reaction, at a rate $g(x,t)$ (moles/cm^3 sec).

(a) Derive a PDE describing the distribution of ϕ. Formulate appropriate BCs and IC and state all assumptions.

(b) Show that the solution to the initial boundary value problem derived in (a) is unique.

Solution: The derivation is analogous to that of the Heat Equation with a source. Mass conservation of the reactant is used in place of energy conservation, and Fick's Law is used in place of Fourier's Law.

Consider a thin segment from x to $x + \Delta x$ of the reaction container, of cross-sectional area A. Let $\phi(x,t)$ be the concentration of the reactant at position x along the container

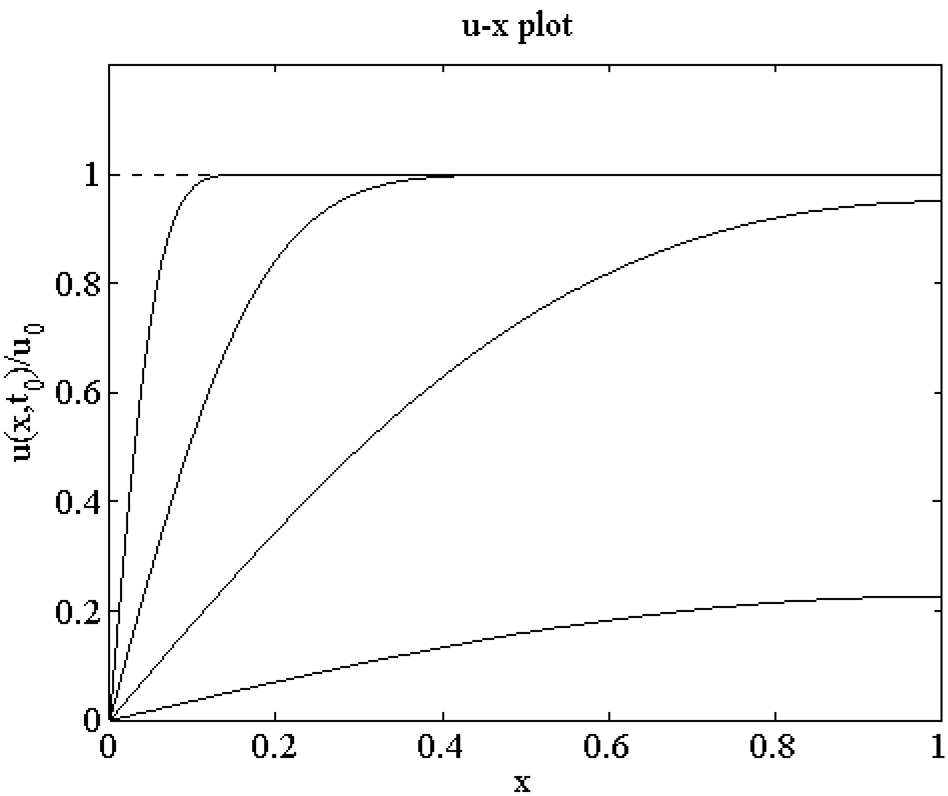


Figure 4: Temperature profiles $u\,(x, t_0)$ at various times $t_0 = 0.001$, 0.01, 0.1 and 0.7 (from left to right). Dashed line indicates the initial condition. The x-axis is the limit of the solution as $t \to \infty$.

and at time t. Analogous to the derivation of the heat equation, conservation of mass gives

$$\begin{array}{c}\text{change of}\\ \text{concentration } \phi\\ \text{in segment in time } \Delta t\end{array} = \begin{array}{c}\text{reactant in from}\\ \text{left boundary}\end{array} - \begin{array}{c}\text{reactant out from}\\ \text{right boundary}\end{array} + \begin{array}{c}\text{reactant}\\ \text{generated}\\ \text{in segment}\end{array}. \quad (24)$$

The last term in the mass balance equation is just $gA\Delta x\Delta t$. Fick's Law states that the reactant in and out from the left and right boundaries is, respectively,

$$\Delta tA\left(-F_0\frac{\partial\phi}{\partial x}\right)_x, \qquad -\Delta tA\left(-F_0\frac{\partial\phi}{\partial x}\right)_{x+\Delta x}$$

where F_0 is the chemical diffusivity. Therefore, (24) becomes

$$A\Delta x\phi\left(x,t+\Delta t\right) - A\Delta x\phi\left(x,t\right) = \Delta tA\left(-F_0\frac{\partial\phi}{\partial x}\right)_x - \Delta tA\left(-F_0\frac{\partial\phi}{\partial x}\right)_{x+\Delta x} + gA\Delta x\Delta t$$

Dividing by $A\Delta x\Delta t$ and rearranging yields

$$\frac{\phi\left(x,t+\Delta t\right)-\phi\left(x,t\right)}{\Delta t} = F_0\left(\frac{\left(\frac{\partial\phi}{\partial x}\right)_{x+\Delta x}-\left(\frac{\partial\phi}{\partial x}\right)_x}{\Delta x}\right) + g.$$

Taking the limit $\Delta t, \Delta x \to 0$ gives the chemical diffusion equation with a source,

$$\frac{\partial\phi}{\partial t} = F_0\frac{\partial^2\phi}{\partial x^2} + g \tag{25}$$

We assume the concentration ϕ is smooth.

For BCs, the ends of the reaction container are closed, so that $\phi_x = 0$ at $x = 0, l$ (Type II homogeneous BCs). Alternatively, we could be supplying or removing reactant at the ends, keeping the concentration fixed: $\phi = \phi_0$ at $x = 0, l$ (Type I inhomogeneous BCs). The IC is $\phi\left(x,0\right) = f\left(x\right)$ where $f\left(x\right)$ is the initial distribution of reactant. If the container is well mixed, then $f\left(x\right) = u_0$. If there is no reactant initially in the container, then $\phi\left(x,0\right) = 0$. Whatever the IC, we assume it is smooth.

To show uniqueness, we note that given two solutions u_1, u_2, we define the difference $v\left(x,t\right) = u_1 - u_2$, which satisfies the homogeneous diffusion equation

$$\phi_t = F_0\phi_{xx}$$

Similarly, for either Type II homogeneous or Type I inhomogeneous BCs on u_1 and u_2, the BCs on $v\left(x,t\right)$ are homogeneous Type I or II. In either case, we define the mean concentration as

$$\bar{v}\left(t\right) = \int_0^1 v^2\left(x,t\right)dx$$

and follow the derivation in the lecture notes.