

Uncertainty Quantification (ACM41000)

Mini Project 2

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Abstract

Analytic and numerical analysis of the heat / diffusion equation.

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1 Introduction

2 Mixed Inhomogenous Boundary Conditions

Breaking up the equation into two parts

$$u(x, t) = u_{hom}(x, t) + u_{PI}(x, t) \quad (1)$$

2.1 $u_{hom}(x, t)$ solution with mixed homogenous boundary conditions

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \quad x \in (0, L) \quad (2)$$

Initial Conditions

$$u(x, t = 0) = f(x) \quad (3)$$

Mixed homogenous boundary conditions

$$u(x = 0, t > 0) = u(x = L, t > 0) = 0 \quad (4)$$

Using the separation of variables method $u(x, t) = X(x)T(t)$

$$\begin{aligned} \frac{\partial X(x)T(t)}{\partial t} &= D \frac{\partial^2 X(x)T(t)}{\partial x^2} \\ \frac{1}{T(t)} \frac{\partial T(t)}{\partial t} &= D \frac{1}{X(x)} \frac{\partial^2 X(x)}{\partial x^2} \end{aligned}$$

LHS is a function of $T(t)$ only and the RHS is a function of $X(x)$ only. This means LHS = RHS = Constants

$$\frac{1}{T(t)} \frac{\partial T(t)}{\partial t} = D \frac{1}{X(x)} \frac{\partial^2 X(x)}{\partial x^2} = -\lambda D$$

This produces the two following equations which can be solved separately and recombined for the final solution

$$\frac{1}{T(t)} \frac{\partial T(t)}{\partial t} = -\lambda D \quad (5)$$

$$D \frac{1}{X(x)} \frac{\partial^2 X(x)}{\partial x^2} = -\lambda D \quad (6)$$

2.1.1 Solve for $X(x)$

Rearranging equation 6

$$\cancel{D} \frac{\partial^2 X(x)}{\partial x^2} + \lambda X(x) \cancel{D} = 0$$

This is a second order linear homogenous ODE with constant coefficients. This can be seen as the solution of a quadratic of the form

$$\Psi^2 + \lambda \Psi = 0$$

Solutions to this quadratic are

$$\Psi = 0$$

$$\Psi = \lambda$$

Ignoring the $\Psi = 0$ solution and focusing on the $\Psi = \lambda$

- $\lambda = 0$:

$$X(x) = Ax + B$$

$$X'(x) = A$$

Applying boundary conditions

$$X(0) = 0 = A(0) + B$$

$$B = 0$$

Trivial Solution, no further analysis on this solution

- $\lambda < 0$:
Trivial Solution, no further analysis on this solution
- $\lambda > 0$:

The form of the solution is

$$X(x) = A \sin(\sqrt{\lambda}x) + B \cos(\sqrt{\lambda}x)$$

Applying boundary conditions

$$X(0) = A \sin(\sqrt{\lambda}0) + B \cos(\sqrt{\lambda}0) = 0$$

$$X(0) = A \sin(0) + B \cos(0) = 0$$

$$X(0) = A \cdot 0 + B \cdot 1 = 0$$

$$B = 0$$

$$X'(x) = A\sqrt{\lambda}\cos(\sqrt{\lambda}x) - B\sqrt{\lambda}\sin(\sqrt{\lambda}x) = 0$$

$$X'(L) = A\cos(\sqrt{\lambda}L) - 0 \cdot \sqrt{\lambda}\sin(\sqrt{\lambda}L) = 0$$

$$X(0) = A\cos(\sqrt{\lambda}L) = 0$$

Ignoring the trivial solution $A = 0$, yields the period solution

$$\cos(\sqrt{\lambda}L) = 0 = \cos((n + \frac{1}{2})\pi)$$

$$\sqrt{\lambda}L = (n + \frac{1}{2})\pi$$

$$\lambda_n = \frac{(n + \frac{1}{2})^2 \pi^2}{L^2}$$

Plugging this value back into $X(x)$ yields

$$X(x) = A_n \sin\left(\frac{(n + \frac{1}{2})\pi x}{L}\right) \quad (7)$$

where $n \in \mathbb{Z}_{\geq 0}$

2.1.2 Solve for $T(t)$

$$\frac{1}{T(t)} \frac{\partial T(t)}{\partial t} = -\lambda D \quad (8)$$

Using the periodic value of λ_n

$$\frac{1}{T_n(t)} \frac{\partial T_n(t)}{\partial t} = -\lambda_n D \quad (9)$$

Integrating both side with respect to t and solving for $T(t)$

$$\begin{aligned} \int \frac{1}{T_n(t)} \frac{\partial T_n(t)}{\partial t} dt &= - \int \lambda_n D dt \\ \log(T_n(t)) &= -\lambda_n D t + C \\ T_n(t) &= e^{-\lambda_n D t} e^C \\ T_n(0) &= e^C \\ T_n(t) &= T_n(0) e^{-\lambda_n D t} \end{aligned}$$

Plugging in the value of $\lambda_n = \frac{(n + \frac{1}{2})^2 \pi^2}{L^2}$ yields the solution

$$T_n(t) = T_n(0) e^{-\frac{(n + \frac{1}{2})^2 \pi^2}{L^2} D t} \quad (10)$$

2.1.3 Recombine $u(x, t) = X(x)T(t)$

Since we used the method of separation of variables to solve $u(x, t)$

$$\begin{aligned} u(x, t) &= X(x)T(t) \\ u_n(x, t) &= A_n \sin\left(\frac{(n + \frac{1}{2})\pi x}{L}\right) T_n(0) e^{-\frac{(n + \frac{1}{2})^2 \pi^2}{L^2} D t} \end{aligned}$$

Letting $C_n = A_n T_n(0)$ give final form of solution for $u_n(x, t)$

$$u_n(x, t) = C_n \sin\left(\frac{(n + \frac{1}{2})\pi x}{L}\right) e^{-\frac{(n + \frac{1}{2})^2 \pi^2}{L^2} D t} \quad (11)$$

2.1.4 Linearity of solutions $u_n(x, t), n \in \mathbb{Z}_{\geq 0}$

Each $u_n(x, t), n \in \mathbb{Z}_{\geq 0}$ is a solution to the PDE in Equation (2) with homogenous boundary conditions, $u_{hom}(x, t)$. The linearity property of homogenous PDE's states that if $u_1(x, t)$ and $u_2(x, t)$ are solutions of a linear homogenous PDE on some region $\mathcal{R} (= (0, L))$, then $u_*(x, t) = C_1 u_1(x, t) + C_2 u_2(x, t)$ is also a solution of $u_{hom}(x, t)$. Where $C_1, C_2 \in \mathbb{R}$ are constants.

This implies that any number of linear combinations of solutions to $u_{hom}(x, t)$ are also solutions.

$$u_{hom}(x, t) = \sum_{n=0}^{\infty} u_n(x, t) \quad (12)$$

2.1.5 Form of C_n 's

Since the PDE is linear and to solve we split it into homogenous and Inhomogenous equations under the condition that

$$u_{hom}(x, t=0) + u_{PI}(x) = 0$$

And we have found that $u_{PI}(x) = u_0$, therefore $u_{hom}(x, t=0) = -u_0$

Using the orthogonality property of the basis functions on $(0, L)$

$$\left\{ \sin \left[\frac{(n + \frac{1}{2})\pi x}{L} \right] \right\}_{n=0}^{\infty}$$

$$I_{n,m} = \int \sin \left[\frac{(n + \frac{1}{2})\pi x}{L} \right] \sin \left[\frac{(m + \frac{1}{2})\pi x}{L} \right] dx$$

where $y = \frac{\pi x}{L}$ and $dy = \frac{L}{\pi} = dx$

$$I_{n,m} = \frac{L}{\pi} \int_0^{\pi} \sin \left[(n + \frac{1}{2})y \right] \sin \left[(m + \frac{1}{2})y \right] dy$$

$$I_{n,m} = \frac{L}{\pi} \left[\frac{\sin((m-n)y)}{2(m-n)} - \frac{\sin((m+n)y)}{2(m+n+1)} \right]_0^{\pi}$$

$$I_{n,m} = \begin{cases} 0 & m \neq n \\ \frac{L}{2} & m = n \end{cases}$$

$$I_{n,m} = \frac{L}{2} \delta_{n,m}$$

where

$$\delta_{n,m} = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$$

From Equation (11-12) it can be seen and the initial condition derived above

$$u_{hom}(x, t = 0) = -u_0 = \sum_{n=0}^{\infty} C_n \sin\left[\frac{(n + \frac{1}{2})\pi x}{L}\right] = -u_0$$

Multiplying both sides by $\sin\left[\frac{(m + \frac{1}{2})\pi x}{L}\right]$ and integrating

$$\begin{aligned} - \int_0^L u_0 \sin\left[\frac{(m + \frac{1}{2})\pi x}{L}\right] dx &= \int_0^L \sum_{n=0}^{\infty} C_n \sin\left[\frac{(n + \frac{1}{2})\pi x}{L}\right] \sin\left[\frac{(m + \frac{1}{2})\pi x}{L}\right] dx \\ - \int_0^L u_0 \sin\left[\frac{(m + \frac{1}{2})\pi x}{L}\right] dx &= \sum_{n=0}^{\infty} C_n \int_0^L \sin\left[\frac{(n + \frac{1}{2})\pi x}{L}\right] \sin\left[\frac{(m + \frac{1}{2})\pi x}{L}\right] dx \end{aligned}$$

Using the orthogonality property this simplifies to

$$\begin{aligned} - \int_0^L u_0 \sin\left[\frac{(m + \frac{1}{2})\pi x}{L}\right] dx &= \sum_{n=0}^{\infty} C_n \frac{L}{2} \delta_{n,m} \\ - \int_0^L u_0 \sin\left[\frac{(m + \frac{1}{2})\pi x}{L}\right] dx &= C_n \frac{L}{2} \end{aligned}$$

Solving for C_n

$$C_n = -\frac{2}{L} \int_0^L u_0 \sin\left[\frac{(m + \frac{1}{2})\pi x}{L}\right] dx \quad (13)$$

Plugging the expression for C_n in Equation (12)

$$u_{hom}(x, t) = \sum_{n=0}^{\infty} -\frac{2u_0}{L} \int_0^L u_0 \sin\left[\frac{(m + \frac{1}{2})\pi \phi}{L}\right] d\phi \sin\left(\frac{(n + \frac{1}{2})\pi x}{L}\right) e^{-\frac{(n + \frac{1}{2})^2 \pi^2}{L^2} Dt} \quad (14)$$

2.2 $u_{PI}(x)$ Inhomogenous boundary conditions

$$\frac{d^2 u_{PI}}{dx^2} = 0 \quad (15)$$

Inhomogenous boundary conditions

$$\begin{aligned} u_{PI}(x = 0) &= u_0 \\ u'_{PI}(x = L) &= 0 \end{aligned}$$

Solving for u_{PI}

$$\begin{aligned} \int \int \frac{d^2 u_{PI}}{dx^2} dx dx &= 0 \\ \int \left[\frac{du_{PI}}{dx} + A \right] dx &= 0 \\ u_{PI}(x) + Ax + B &= 0 \end{aligned}$$

Using the boundary conditions

$$\begin{aligned} u'_{PI}(L) + A &= 0 \\ 0 + A &= 0 \\ A &= 0 \end{aligned}$$

$$\begin{aligned} u_{PI}(0) + A(0) + B &= 0 \\ u_0 + (0)(0) + B &= 0 \\ B &= -u_0 \end{aligned}$$

Yields the expected solution

$$u_{PI}(x) - u_0 = 0 \quad (16)$$

$$u_{PI}(x) = u_0 \quad (17)$$

2.3 Full solution $u(x, t) = u_{hom}(x, t) + u_{PI}(x)$ at $t \rightarrow \infty$

Using only the first term in the series

$$\begin{aligned} u(x, t) &= u_{hom}(x, t) + u_{PI}(x) \\ &= -\frac{2u_0}{L} \int_0^L u_0 \sin\left[\frac{\pi\phi}{2L}\right] d\phi \sin\left(\frac{\pi x}{2L}\right) e^{-\frac{\pi^2}{4L^2}Dt} - u_0 \\ &= -\frac{2u_0}{L} \left[\frac{2L}{\pi} \cos\left[\frac{\pi\phi}{2L}\right]_0^L \right] \sin\left(\frac{\pi x}{2L}\right) e^{-\frac{\pi^2}{4L^2}Dt} - u_0 \end{aligned}$$

$$\cos\left[\frac{\pi x}{2L}\right]_0^L = \cos\left[\frac{\pi L}{2L}\right] - \cos(0) = -1$$

$$\begin{aligned} &= -\frac{2u_0}{L} \left[-\frac{2L}{\pi} \right] \sin\left(\frac{\pi x}{2L}\right) e^{-\frac{\pi^2}{4L^2}Dt} - u_0 \\ &= \frac{4u_0}{\pi} \sin\left(\frac{\pi x}{2L}\right) e^{-\frac{\pi^2}{4L^2}Dt} - u_0 \\ &= u_0 \left[\frac{4}{\pi} \sin\left(\frac{\pi x}{2L}\right) e^{-\frac{\pi^2}{4L^2}Dt} - 1 \right] \end{aligned}$$

Using the first term of the series

$$u(x, t) = u_0 \left[\frac{4}{\pi} \sin\left(\frac{\pi x}{2L}\right) e^{-\frac{\pi^2}{4L^2}Dt} - 1 \right] \quad (18)$$

Finding an estimate for the time at which the temperature at the end of the bar $x = L$ is 99% of its final value.

At $t \rightarrow \infty$ and $x = L$

$$\sin\left(\frac{\pi x}{2L}\right) = \sin\left(\frac{\pi}{2}\right) = 1$$

Equation (18) simplifies to

$$u(x = L, t = \infty) = u_0 \left[\frac{4}{\pi} e^{-\frac{\pi^2}{4L^2} Dt} - 1 \right] \quad (19)$$

The final temperature at the point L as $t \rightarrow \infty$ will be approximately u_0 , therefore

$$\begin{aligned} u_0 &= u_0 \left[\frac{4}{\pi} e^{-\frac{\pi^2}{4L^2} Dt} - 1 \right] \\ 1 &= \frac{4}{\pi} e^{-\frac{\pi^2}{4L^2} Dt} - 1 \\ \frac{4}{\pi} e^{-\frac{\pi^2}{4L^2} Dt} &= 2 \\ -\frac{\pi^2}{4L^2} Dt &= \log\left(\frac{2}{\pi}\right) \\ -\frac{\pi^2 D}{4L^2} t &= \log\left(\frac{2}{\pi}\right) \\ t &= -\frac{4L^2}{\pi^2 D} \log\left(\frac{2}{\pi}\right) \end{aligned}$$

The time at which the point L on the bar is close to its final value is

$$t \approx \frac{4L^2}{5\pi^2 D} \quad (20)$$

3 Uniqueness of Solutions for the Heat Equation

Let $u_1(x, t)$ and $u_2(x, t)$ be two solutions to Equation (2) that are subject to the Inhomogenous Dirichlet boundary conditions

$$\begin{aligned} u(x = 0, t) &= b_L(t) \\ u(x = L, t) &= b_R(t) \end{aligned}$$

Using the linearity property then $\phi(x, t) = u_1(x, t) - u_2(x, t)$ is also a solution to Equation (2)

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2} \quad x \in (0, L) \quad (21)$$

Initial Conditions

$$\phi(x, t = 0) = f(x) \quad (22)$$

Homogenous boundary conditions

$$\phi(x = 0, t > 0) = \phi(x = L, t > 0) = 0 \quad (23)$$

$$\begin{aligned}
\frac{\partial \phi}{\partial t} &= \frac{\partial(u_1 - u_2)}{\partial t} \\
&= \frac{\partial u_1}{\partial t} - \frac{\partial u_2}{\partial t} \\
&= D \frac{\partial^2 u_1}{\partial x^2} - D \frac{\partial^2 u_2}{\partial x^2} \\
&= \frac{\partial^2 u_1 - u_2}{\partial x^2} \\
&= \frac{\partial^2 \phi}{\partial x^2}
\end{aligned}$$

and the difference of the initial and boundary conditions

$$\begin{aligned}
u_1(x=0, t) - u_2(x=0, t) &= b_L(t) - b_L(t) = 0 \\
u_1(x=L, t) - u_2(x=L, t) &= b_R(t) - b_R(t) = 0 \\
u_1(x, t=0) - u_2(x, t=0) &= 0 - 0 = 0
\end{aligned}$$

Multiplying Equation (21) by $\phi(x, t)$ and integrating with respect to x

$$\begin{aligned}
\int_0^L \phi(x, t) \frac{\partial \phi}{\partial t} dx &= D \int_0^L \phi(x, t) \frac{\partial^2 \phi}{\partial x^2} dx \\
\frac{1}{2} \frac{d}{dt} \int_0^L [\phi(x, t)]^2 dx &= D \int_0^L \phi(x, t) \frac{\partial^2 \phi}{\partial x^2} dx \\
&= D \int_0^L \left[\frac{\partial}{\partial x} \left(\phi(x, t) \frac{\partial \phi}{\partial x} \right) - \left(\frac{\partial \phi}{\partial x} \right)^2 \right] dx \\
&= D \left[\phi(x) \frac{\partial \phi}{\partial x} \right]_{x=0}^{x=L} - D \int_0^L \left(\frac{\partial \phi}{\partial x} \right)^2 dx \\
&= D \left[\phi(L) \frac{\partial \phi}{\partial x}(L) - \phi(0) \frac{\partial \phi}{\partial x}(0) \right] - D \int_0^L \left(\frac{\partial \phi}{\partial x} \right)^2 dx
\end{aligned}$$

From the boundary conditions $\phi(x=0, t) = \phi(x=L, t) = 0$, so

$$\frac{1}{2} \frac{d}{dt} \int_0^L [\phi(x, t)]^2 dx = -D \int_0^L \left(\frac{\partial \phi}{\partial x} \right)^2 dx$$

Defining the L^2 norm of ϕ

$$\begin{aligned}
\| \phi \|_2^2 &= \int_0^L [\phi(x, t)]^2 dx \\
\frac{1}{2} \frac{d}{dt} \| \phi \|_2^2 &= -D \int_0^L \left(\frac{\partial \phi}{\partial x} \right)^2 dx
\end{aligned} \tag{24}$$

Equation (24) can be integrated with respect to t

$$\begin{aligned}\int_0^t \frac{1}{2} \frac{d}{dt} \|\phi\|_2^2 dt &= -D \int_0^t \int_0^L \left(\frac{\partial \phi}{\partial x} \right)^2 dx dt \\ \|\phi\|_2^2 \Big|_0^t &= -2D \int_0^t \|\phi\|_2^2(s) ds \\ \|\phi\|_2^2(t) &= \|\phi\|_2^2(0) - 2D \int_0^t \|\phi\|_2^2(s) ds\end{aligned}$$

$2D \int_0^t \|\phi\|_2^2(s) ds \geq 0$, therefore

$$\|\phi\|_2^2(t) \leq \|\phi\|_2^2(0) = 0 \implies \|\phi\|_2^2(t) = 0$$

SO $\phi(x, t) = 0 = u_1(x, t) - u_2(x, t)$, therefore $u_1(x, t) - u_2(x, t)$, the solution to the PDE is unique on $(0, L)$

4 Numerical Methods for the Heat Equation

The code in appendix A is a python class which solves the heat equation , with parameters $L, D, N, u0, t_{min}, t_{max}$

The class **HeatEquation1DFFTSolve** has three methods

- `solve` ; solves the PDE using python numpy methods numpy fast fourier transform methods
- `plot_solution` ; plots the distribution of heat over time
- `animate_solution` ; animation of the distribution evolve over time

Figure (1) shows the distribution of heat over time. Initially it starts as a box shaped function but as time progresses, the heat flows from areas of higher temperature to areas of lower temperature.

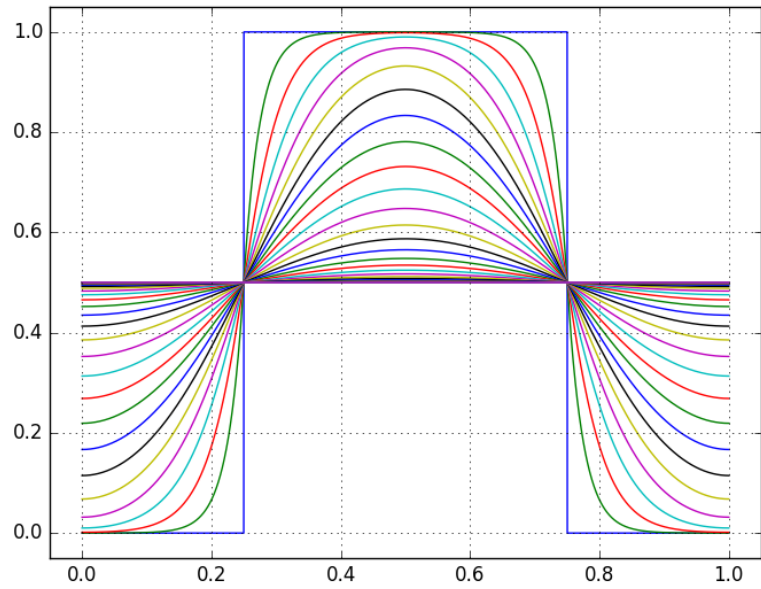


Figure 1: Distribution of heat over time

Appendices

A Python Code

Python solve Heat Equation PDE (1)

```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.animation as animation

class HeatEquation1DFFTSolve:

    def __init__(self, L, D, N, u0, t_min, t_max):
        self.L = L
        self.D = D
        self.N = N
        self.u0 = u0
        self.t_min = t_min
        self.t_max = t_max
        self.x_vec = np.arange(0, L, float(L)/N)
        self.delta_t = float(t_max) / N
        self.k_vec = (2*np.pi/L) * np.arange(-N/2, N/2)
        self.un = [self.u0]
        self.solution_epsilon = 0.000001

    def solve(self):
        uhat = np.fft.fftshift(np.fft.fft(self.u0))
        for i in range(1, self.N+1):
            uhat_new = uhat/(1+self.D*(i*self.delta_t)*self.
                k_vec*self.k_vec)
            uhat = uhat_new
            self.un.append(np.fft.ifft(np.fft.ifftshift(uhat)))

    def plot_solution(self):
        plt.axes().set_xlim(-0.05, self.L +.05)
        plt.axes().set_ylim(-0.05, self.L +.05)
        plt.axes().grid()
        for i in range(0, len(self.un)):
            plt.plot(self.x_vec, self.un[i])
            if (max(abs(self.un[i]))-min(abs(self.un[i]))) <
                self.solution_epsilon:
                break

    def animate_solution(self):
        fig, ax = plt.subplots()
        line, = ax.plot(self.x_vec, self.u0, lw=2)
        ax.grid()
        xdata, ydata = [], []
        time_label = ax.text(0.05, 0.90, 'time = 0.0', transform
            =ax.transAxes) # initialize the time label for the
            graph

    def solution_data():
        for i in range(0, len(self.un)):
            yield i*self.delta_t, self.x_vec, self.un[i]

    def init():
        ax.set_ylim(-0.05, self.L+.05)
        ax.set_xlim(-0.05, self.L+.05)
        del xdata[:]
        del ydata[:]
```

```

        line.set_data(xdata, ydata)
        return line,

def run(data):
    t, x, u = data
    time_label.set_text('time = %.3f' % t) # Display the
        current time to the accuracy of your liking.
    line.set_data(x, u)
    return line, time_label

ani = animation.FuncAnimation(
    fig,
    run,
    solution_data,
    blit=False,
    interval=1000,
    repeat=True,
    init_func=init)
return ani

#####
#####
##Init class
#####
#####

NN=2**14
he = HeatEquation1DFFTSolve(
    L = 1,
    D = 1,
    N = NN,
    u0 = np.array([1 if float(i)/NN >= .25 and float(i)/NN <=
        .75 else 0 for i in range(0,NN) ]),
    t_min = 0,
    t_max = 10)

#####
#Solve
#####
he.solve()

#####
#Solution Plot
#####
he.plot_solution()

#####
#Solution Animation
#####
he_ani = he.animate_solution()

```