Uncertainty Quantification (ACM41000)
Mini-project 2

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Instructions

- Assignment handed out: Monday, March 12th.
- Assignment due: Friday, April 6th.
- **Instructions for hand-in: Leave a hardcopy of the assignment in the homework box outside the School Office by 17:30 on Friday April 6th.**
- The report should be typeset in Latex. For maximum marks, the report should be clearly structured and the different steps in the calculations explained / summarized as appropriate. Diagrams should be included as required, and should be captioned and referred to in the text.
- The framework for marking this project is the 'UCD modular grades explained' document[1]
- Include all codes in an appendix – this can be done very quickly using the 'listings' package in Latex.

Background

The aim of this Project is to gain more familiarity with the properties of the heat / diffusion equation on an interval:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \qquad x \in (0, L), \qquad t > 0, \tag{1a}$$

subject to the initial condition

$$u(x, t = 0) = f(x), \tag{1b}$$

Here, L is the length of the interval and $D > 0$ is the diffusivity, with physical dimensions of [Length]^2/[Time]. We will examine the role of the boundary conditions on the properties of the solution; as such, the boundary conditions are left unspecified as yet.

[1] https://www.ucd.ie/registry/assessment/staff_info/modular%20grades%20explained%20staff.pdf

1 Mixed inhomogeneous boundary conditions

A pot on a stove has a handle of length L that can be modelled as a rod with diffusion constant D. The equation for the temperature is given in Equation (1b); now the following **mixed inhomogeneous** boundary conditions are specified:

$$u(x=0,t>0)=u_0, \qquad u_x(x=L,t>0)=0, \tag{2}$$

where u_0 is a constant. Furthermore, the initial condition in Equation (1b) is set to $f(x)=0$. Using only the first ($n=1$) term in the resulting Fourier series solution, find an estimate for the time at which the temperature of the end point $x=L$ is 99% of its final ($t\to\infty$) value. Leave the answer in terms of D and L.

Discussion

A homogeneous problem as zero as a possible solution; this is no longer the case for inhomogeneous problems. We saw this with ODEs – the same thing holds for PDEs. Non-zero boundary conditions are one way whereby inhomogeneity creeps into a problem. There is a generic method for dealing with such non-zero (or inhomogeneous) boundary conditions, which is exemplified below in the following set of suggested steps for solving the given problem:

1. Break up the solution:

   $$u(x,t)=u_{\mathrm{hom}}(x,t)+u_{\mathrm{PI}}(x). \tag{3}$$

   Here, $u_{\mathrm{hom}}(x,t)$ satisfies the PDE (1a) with homogeneous boundary conditions

   $$u(x=0,t>0)=0, \qquad u_x(x=L,t>0)=0, \tag{4}$$

   and $u_{\mathrm{PI}}(x)$ satisfies the PDE with the inhomogeneous boundary conditions (2). Since the PDE is linear, the sum in Equation (3) satisifes the PDE with the full boundary conditions (2), provided

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

   We will see that dealing with the inhomogeneous boundary conditions in this way greatly simplifies the problem.

2. The heat equation applied to $u_{\mathrm{PI}}(x)$ greatly simplifies – it is $\mathrm{d}^2u_{PI}/\mathrm{d}x^2=0$. The inhomogeneous boundary conditions are applied here: $u_{PI}(0)=u_0$, $u'_{PI}(L)=0$. Solve this problem to show that

   $$u_{PI}(x)=u_0.$$

3. Also, the heat equation applied to u_{hom} simplifies – the solution method is the same as the one developed in class. Attempt a separation-of-variables solution $u_{\mathrm{hom}}(x,t)=X(x)T(t)$ to obtain

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

Carry out the intermediate steps (paying particular attention to the boundary conditions) to show that the characteristic solution (similar to the one derived in class) is

$$u_n(x,t) = C_n \sin\left[\left(n+\tfrac{1}{2}\right)\frac{\pi x}{L}\right] \mathrm{e}^{-(n+1/2)^2\pi^2 Dt/L^2}, \qquad n = 0, 1, 2, \cdots .$$

4. Explain (in a few lines) why

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

5. Use the initial data

$$u_{\mathrm{hom}}(x,t=0) = \sum_{n=0}^{\infty} u_n(x,t=0) = -u_0,$$

and various orthogonality relations (to be found) for the **basis functions**

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

to find closed-form expressions for the C_n's.

2 Uniqueness of solutions for the Heat Equation

In class we studied Equation (1a) with homogeneous Dirichlet conditions. As it turns out, the smooth series solution so derived is unique. The same applies to the case with inhomogeneous Dirichlet conditions. The aim of this section is to prove this statement, with the following (suggested) sequence of steps. As such, Equation (1a) applies, with generic (inhomogeneous) Dirichlet boundary conditions

$$u(x=0,t) = b_L(t), \qquad u(x=L,t) = b_R(t), \qquad t > 0. \tag{5}$$

1. Suppose that $u_1(x,t)$ and $u_2(x,t)$ satisfy Equation (1a) with boundary conditions (5). Let $\phi(x,t) = u_2(x,t) - u_1(x,t)$. Since the PDE (1a) is linear, argue that $\phi(x,t)$ satisfies

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2}, \qquad x \in (0,L), \qquad t > 0, \tag{6}$$

with zero Dirichlet boundary conditions $\phi(x=0,t) = \phi(x=L,t) = 0$, for $t > 0$.

2. Multiply Equation (9) by $\phi(x,t)$ and integrate with respect to x. Apply integration by parts and the ϕ-boundary conditions to obtain

$$\tfrac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\phi\|_2^2 = -D\int_0^L \left(\frac{\partial \phi}{\partial x}\right)^2 \mathrm{d}x.$$

where $\|\phi\|_2^2(t)$ is the L^2 norm of ϕ:

$$\|\phi\|_2^2(t) = \int_0^L \left[\phi(x,t)\right]^2 \mathrm{d}x.$$

3. Argue that $\|\phi\|_2(T) \leq \|\phi\|_2(0) = 0$, hence $\|\phi\|_2(T) = 0$, for any $T > 0$. Conclude (with justification) that $\phi(x,t) = 0$ for all $x \in [0, L]$ and $t \geq 0$, hence $u_2 = u_1$ and the smooth solution is unique.

Solutions of Equation (1a) with homogeneous / inhomogeneous **Neumann** boundary conditions are not unique. However, we can get a handle on the non-uniqueness. We again start with Equation (1a) with generic Neumann boundary conditions

$$u_x(x = 0, t) = b_L(t), \qquad u_x(x = L, t) = b_R(t), \qquad t > 0. \tag{7}$$

1. Again, suppose that $u_1(x,t)$ and $u_2(x,t)$ satisfy Equation (1a) with boundary conditions (7). Let

$$\phi(x,t) = \frac{\partial}{\partial x}\left[u_2(x,t) - u_1(x,t)\right]. \tag{8}$$

   (Not a typo – notice the $\partial/\partial x$!). Since the PDE (1a) is linear, argue that $\phi(x,t)$ satisfies

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2}, \qquad x \in (0, L), \qquad t > 0, \tag{9}$$

   with zero **Dirichlet** boundary conditions $\phi(x = 0, t) = \phi(x = L, t) = 0$, for $t > 0$.

2. As before, show that $\phi = 0$, hence $u_2(x,t) - u_1(x,t) = \mathrm{Const.}$.

Thus, smooth solutions of the heat equation with Neumann boundary conditions are unique up to a constant.

Discussion

The heat equation is therefore a good physical model:

- It has a smooth solution – *no point in formulating a mathematical model if a solution doesn't exist.*
- The smooth solution is unique – *otherwise, which solution would we use?*

There is a third property as well, which is mentioned here but is not developed any further, for lack of time:

- The model is well posed: given two solutions of the heat equation where the boundary / initial data are slightly different (but 'close' in the appropriate sense), the difference between the two solutions remains close for all time – *continuous dependence on initial / boundary data*.

Mathematical models with all three of these properties are called **well posed**; the heat equation is one such model.

3 Numerical methods for the heat equation

Lastly, we are going to look at numerical methods to solve the heat equation. For want of time, there is no way to do this comprehensively, instead, the aim is to 'kill two birds with the one stone', and introduce **periodic boundary conditions** and **numerical spectral methods** simultaneously.

Periodic boundary conditions are not realistic of very many physical systems but are used as a convenient computational model when the system extent L is very large. As such, the boundary conditions read

$$u(x=0,t) = u(x=L,t), \qquad t>0;$$

spatial derivatives of $u(x,t)$ are also assumed to match accordingly. In this scenario, it is possible to construct the solution $u(x,t)$ as a Fourier series:

$$u(x,t) = \sum_{k=-\infty}^{\infty} \widehat{u_k}(t)\mathrm{e}^{\mathrm{i}(2\pi/L)kx},$$

where

$$\widehat{u_k}(t) = \frac{1}{L}\int_0^L \mathrm{e}^{-\mathrm{i}(2\pi/L)kx}u(x,t), \qquad k\in\mathbb{Z}.$$

The reality of the solution means that $(\widehat{u_k})^* = \widehat{u}{-k}$, where the star denotes complex conjugation. As such,

$$\widehat{u_0}(t) = \frac{1}{L}\int_0^L u(x,t)\in\mathbb{R}$$

corresponds to the spatial average of $u(x,t)$.

By multiplying both sides of Equation (1a) by $\mathrm{e}^{-\mathrm{i}(2\pi/L)kx}$ and integrating with respect to x, it is possible to derive an ordinary differential equation for the **Fourier coefficients** $\widehat{u_k}$:

$$\frac{\mathrm{d}\widehat{u_k}}{\mathrm{d}t} = -Dk^2\widehat{u_k}, \qquad t>0, \qquad k\in\mathbb{Z}.$$

This equation can be solved analytically; in the present context it is more instructive to solve it numerically with a very numerically stable **backward Euler method**:

$$\frac{\widehat{u_k}^{n+1}-\widehat{u_k}^{n}}{\Delta t} = -Dk^2\widehat{u_k}^{n+1}, \qquad n=0,1,2,\cdots,$$

where the superscript n now labels discrete time steps, with

$$\widehat{u_k}^{n} = \widehat{u_k}(t_n), \qquad t_n = n\Delta t, \qquad n=0,1,2,\cdots,$$

where Δt is the (small) timestep.

Using the Fast Fourier Transform (FFT) avaialble in numerical software such as Matlab or Python, these numerical steps are readily coded up as an algorithm (the pseudocode below uses Matlab-style syntax):

1. Create a vector `u0` of length `N` – for the initial conditions in real space. Also, create a vector of k-values. Be careful – the natural order for the vector of wavenumbers is

```
k_vec=(2*pi/L)*( -(N/2):1:(N/2)-1 );
```

where N is the length of u0 – also equal to the number of Fourier modes in the numerical approximation. This should be an even number but also a power of two for FFT to be most efficient.

2. Construct the vector uhat= $\widehat{u}_k^1$ using FFT. When k has the natural order indicated above, FFT should be used in combination with FFTSHIFT – at least in Matlab:

```
uhat=fftshift(fft(u0));
```

3. Update:

```
uhat_new=u_hat./(1+D*Delta_t*k_vec.*k_vec);
uhat=uhat_new;
```

4. Repeat Step 3 for the necessary number of timesteps.

5. Visualize the data at the final time (or at intermediate times) with un= $u(x, t_n)$, where

```
un=ifft(ifftshift(uhat));
```

Using this algorithm, solve the heat equation (periodic boundary conditions) numerically for $x \in [0, L]$ and $t \in [0, 10]$ with $L = D = 1$ and the given initial condition

$$u(x, t = 0) = \begin{cases} 0, & \text{if } x < 1/4, \\ 1, & \text{if } 1/4 \leq x \leq 3/4, \\ 0, & \text{if } x > 3/4. \end{cases}$$

Provide and appropriate graphical description of the spacetime evolution of the solution.