Scientific Computing I

Module 6: The 1D Heat Equation

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Part I

Analytic Solutions of the 1D Heat Equation

The Heat Equation in 1D

- remember the heat equation:

$$T_t = \kappa \Delta T$$

- we examine the 1D case, and set $\kappa = 1$ to get:

$$u_t = u_{xx} \qquad \text{for} \quad x \in (0,1), t > 0$$

- using the following initial and boundary conditions:

$$\begin{aligned} u(x,0) &= f(x), \quad x \in (0,1) \\ u(0,t) &= u(1,t) = 0, \quad t > 0 \end{aligned}$$

Computing Analytic Solutions

First steps:

- try to find some solution of the PDE
- try to satisfy boundary conditions (but not the initial condition)

Ansatz: **Separation of Variables**

- assumption:

$$u(x,t) = X(x) \cdot T(t)$$

- insert this assumption into the heat equation

Separation of Variables

- insert $u(x,t) = X(x) \cdot T(t)$ into PDE:

$$\begin{aligned} \frac{\partial}{\partial t}\left(X(x) \cdot T(t)\right) &= \frac{\partial^2}{\partial x^2}\left(X(x) \cdot T(t)\right) \\ \text{or} \qquad X(x) \cdot T_t(t) &= T(t) \cdot X_{xx}(x) \end{aligned}$$

- divide by $X(x)T(t)$, and get:

$$\frac{T_t(t)}{T(t)} = \frac{X_{xx}(x)}{X(x)}$$

- true for all x and all t, only if:

$$\frac{T_t(t)}{T(t)} = \frac{X_{xx}(x)}{X(x)} = -\lambda$$

Transforming the PDE into two ODEs

- separation of variables leads to:

$$\frac{T_t(t)}{T(t)} = \frac{X_{xx}(x)}{X(x)} = -\lambda$$

- thus, we obtain two ODEs:

$$X_{xx}(x) + \lambda X(x) = 0 \qquad X(0) = X(1) = 0, \quad (1)$$
$$T_t(t) + \lambda T(t) = 0 \qquad (2)$$

- solve $X(x)$-part:

$$X_k(x) = \sin(k\pi x) \qquad \lambda_k = (k\pi)^2, k = 1, 2, \ldots$$

- solve $T(t)$-part (compare Model of Malthus):

$$T_k(t) = e^{-\lambda_k t} = e^{-(k\pi)^2 t}$$

Fourier's Method

- the functions

$$u_k(x,t) := T_k(t)X_k(x) = e^{-(k\pi)^2 t}\sin(k\pi x), \quad k = 1,2,\ldots,$$

  solve the 1D heat equation PDE
- for the initial and boundary conditions:

$$\begin{aligned} u_k(0,t) = u_k(1,t) &= 0, \quad t > 0 \\ u_k(x,0) &= \sin(k\pi x), \quad x \in (0,1). \end{aligned}$$

- use Fourier sine series for initial condition:

$$f(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x).$$

- and obtain solution for $u(x,0) = f(x)$:

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

Fourier's Method – A Recipe

1. Find coefficients c_k such that the initial condition $f(x)$ can be represented as
$$f(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x).$$
2. Verify that the solution candidate
$$u(x,t) := \sum_k c_k e^{-(k\pi)^2 t} \sin(k\pi x)$$
converges to a well-defined function u
3. Verify that u solves the differential equation $u_t = u_{xx}$
4. Verify that u satisfies the boundary conditions $u(0,t) = u(1,t) = 0$
5. Verify that u satisfies the initial condition $u(x,0) = f(x)$

Part II

Numerical Solutions of the 1D Heat Equation

Numerical Solution 1 – Discretisation

Discretisation similar to ODEs:

- compute approximations

$$v_j^{(m)} \approx u(x_j, t_m)$$

- at grid points x_j and time points t_m:

$$x_j := j \cdot h \qquad t_m := m \cdot \tau,$$

- approximate equation $u_t = u_{xx}$ by

$$\frac{v_j^{(m+1)} - v_j^{(m)}}{\tau} = \frac{v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)}}{h^2} \qquad (3)$$

for $j = 1, \ldots, n-1$, and $m \geq 0$.

An Explicit Scheme

- add initial and boundary conditions:

$$\begin{aligned} v_0^{(m)} &= v_n^{(m)} = 0, \qquad \text{for all} \quad m \geq 0, \\ v_j^{(0)} &= f(x_j), \qquad \text{for} \quad j = 1, \dots, n-1. \end{aligned}$$

- and obtain an explicit scheme:

$$v_j^{(m+1)} = v_j^{(m)} + \frac{\tau}{h^2} \left(v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right)$$

- we can, step by step, compute all values $v_j^{(m)}$
  - for all time steps (m),
  - starting with the initial conditions $v_j^{(0)} = f(x_j)$.
- **"explicit time stepping scheme"**

Accuracy of the Explicit Scheme

Observations:

- first order accurate in τ:

$$u_t(x,t) = \frac{u(x,t+\tau) - u(x,t)}{\tau} + \mathcal{O}(\tau)$$

- second order accurate in h:

$$u_{xx}(x,t) = \frac{u(x-h,t) - 2u(x,t) + u(x+h,t)}{h^2} + \mathcal{O}(h^2)$$

- stability condition of the step size!
  (similar to ODE)

$\Rightarrow$ examine conservation of “energy”
or **Neumann Stability Analysis**

Solutions of the Explicit Scheme

- explicit scheme:

$$\frac{v_j^{(m+1)} - v_j^{(m)}}{\tau} = \frac{v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)}}{h^2}$$

- assumption: there are solutions of the form

$$u_j^{(m)} = (a_k)^m \sin(\pi k x_j), \qquad \text{where } x_j := jh. \quad (4)$$

- compare with exact solution:

$$u_k(x,t) = e^{-(k\pi)^2 t} \sin(k\pi x)$$

- $(a_k)^m \sim e^{-(k\pi)^2 t}$, thus $(a_k)^m$ should decrease
  $\Rightarrow |a_k| < 1$ necessary

Solutions of the Explicit Scheme (2)

- insert $u_j^{(m)} = (a_k)^m \sin(\pi k x_j)$ into

$$\frac{v_j^{(m+1)} - v_j^{(m)}}{\tau} = \frac{v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)}}{h^2}$$

- leads to condition (see separate worksheet)

$$a_k = 1 + \frac{\tau}{h^2}\left(2\cos(\pi k h) - 2\right) = 1 - \frac{4\tau}{h^2}\sin^2\left(\frac{\pi k h}{2}\right).$$

- for stability: $|a_k| < 1$ only if

$$\frac{4\tau}{h^2} < 2 \quad \text{or} \quad \tau < \frac{h^2}{2}.$$

Solutions of the Explicit Scheme (3)

- in practice: numerical solution is of the form

$$v_j^{(m)} := \sum_{k=1}^{n-1} c_k (a_k)^m \sin(\pi k x_j).$$

- stability, because $|a_k| < 1$ for all k
- the coefficients c_k result from a sine transform of the initial values f_j:

$$u_j^{(0)} = f_j = \sum_{k=1}^{n-1} c_k \sin(\pi k x_j).$$

Numerical Solution 2 – An Implicit Scheme

- apply implicit Euler:

$$\frac{v_j^{(m+1)} - v_j^{(m)}}{\tau} = \frac{v_{j-1}^{(m+1)} - 2v_j^{(m+1)} + v_{j+1}^{(m+1)}}{h^2}$$

  for $j = 1, \ldots, n-1$, and $m \geq 0$.
- boundary conditions:

$$v_0^{(m)} = v_n^{(m)} = 0, \qquad \text{for all} \quad m \geq 0,$$

- initial conditions:

$$v_j^{(0)} = f(x_j), \qquad \text{for} \quad j = 1, \ldots, n-1.$$

Implicit Time Stepping

- solve implicit scheme for $v_j^{(m+1)}$:

$$v_j^{(m+1)} - \frac{\tau}{h^2}\left(v_{j-1}^{(m+1)} - 2v_j^{(m+1)} + v_{j+1}^{(m+1)}\right) = v_j^{(m)}.$$

- with the ratio $r := \tau/h^2$, we can write it as

$$-rv_{j-1}^{(m+1)} + (1+2r)v_j^{(m+1)} - rv_{j+1}^{(m+1)} = v_j^{(m)}$$

  for $j = 1, \ldots, n-1$, and $m \geq 0$

- solve a system of linear equations to obtain $v_j^{(m+1)}$ in every step

System of Linear Equations:

- the matrix of the linear system of equations is given by $I + rA$, where $A = \mathrm{tridiag}(-1, 2, -1)$.
- system is **tridiagonal**, solving requires $\mathcal{O}(n)$ operations.
- solution:

$$v^{(m)} = (I + rA)^{-1} v^{(m-1)};$$

Solutions of the Implicit Scheme

- implicit scheme:

$$\frac{v_j^{(m+1)} - v_j^{(m)}}{\tau} = \frac{v_{j-1}^{(m+1)} - 2v_j^{(m+1)} + v_{j+1}^{(m+1)}}{h^2}$$

- again: insert assumed solutions

$$u_j^{(m)} = (a_k)^m \sin(\pi k x_j), \qquad \text{where } x_j := jh.$$

- into implicit scheme, and obtain:

$$\begin{aligned} a_k - 1 &= -\frac{4\tau}{h^2}\sin^2\left(\frac{\pi k h}{2}\right) a_k \\ a_k &= \left(1 + \frac{4\tau}{h^2}\sin^2\left(\frac{\pi k h}{2}\right)\right)^{-1}. \end{aligned}$$

Solutions of the Implicit Scheme (2)

- solutions of the implicit scheme:

$$v_j^{(m)} := \sum_{k=1}^{n-1} c_k (a_k)^m \sin(\pi k x_j).$$

- with

$$a_k = \left(1 + \frac{4\tau}{h^2} \sin^2\left(\frac{\pi k h}{2}\right)\right)^{-1}.$$

- $0 < a_k < 1$ independent of k and h

$\Rightarrow$ unconditionally stable

Part III

Energy Considerations (Additional Material – Not Compulsory)

Energy of the Analytic Solution

- $u(x,y)$ a solution of

$$\begin{aligned}(u_k)_t &= (u_k)_{xx}, \quad x \in (0,1), t > 0 \\ u_k(0,t) = u_k(1,t) &= 0, \quad t > 0 \\ u_k(x,0) &= f(x), \quad x \in (0,1).\end{aligned}$$

- define the **energy** of the solution:

$$E(t) := \int_0^1 u^2(x,t)\,dx$$

- for conservation of energy, analyse

$$E'(t) := \frac{d}{dt}\int_0^1 u^2(x,t)\,dx$$

Energy of the Analytic Solution (2)

$$
\begin{aligned}
E'(t) &= \int_0^1 \frac{\partial}{\partial t} u^2(x,t)\,dx = \int_0^1 2u(x,t)u_t(x,t)\,dx \\
&= 2\int_0^1 u(x,t)u_{xx}(x,t)\,dx \\
&= 2\left[u(x,t)u_x(x,t)\right]_0^1 - 2\int_0^1 \left(u_x(x,t)\right)^2\,dx \\
&= -2\int_0^1 \left(u_x(x,t)\right)^2\,dx \le 0
\end{aligned}
$$

Therefore:

- $E(t) \le E(0)$ (energy never increases)
- compare to initial condition $u(x,0) = f(x)$:

$$\int_0^1 u^2(x,t)\,dx = E(t) \le E(0) = \int_0^1 f^2(x)\,dx$$

Corrollaries

- assume: both $u_1(x,t)$ and $u_2(x,t)$ are solutions for initial conditions $f_1(x)$ and $f_2(x)$
- let $w(x,t) := u_1(x,t) - u_2(x,t)$, then

$$
\begin{aligned}
w_t(x,t) &= (u_1)_t(x,t) - (u_2)_t(x,t) \\
&= (u_1)_{xx}(x,t) - (u_2)_{xx}(x,t) = w_{xx}(x,t) \\
w(0,t) &= w(1,t) = 0 \\
w(x,0) &= u_1(x,0) - u_2(x,0) = f_1(x) - f_2(x)
\end{aligned}
$$

- therefore, $w(x,t)$ is a solution of the heat equation for initial condition $f_w(x) = f_1(x) - f_2(x)$

Corrollary 1 – Uniqueness

- if $f_1 = f_2$, then $f_w(x) = 0$
- energy is decreasing:

$$\begin{aligned} \int_0^1 (u_1 - u_2)^2(x,t)\,dx &= \int_0^1 w^2(x,t)\,dx \\ &\leq \int_0^1 (f_1 - f_2)^2(x)\,dx = 0 \end{aligned}$$

- therefore:

$$\int_0^1 w^2(x,t)\,dx \leq 0 \quad \Leftrightarrow \quad w = 0 \quad \Leftrightarrow \quad u_1 = u_2.$$

- proof of uniqueness of the solution!

Corrollary 2 – Stability

- now: $f_2 = f_1 + \varepsilon$ (ε small), then

$$\int_0^1 w^2(x,t)\,dx \;\leq\; \int_0^1 (f_1 - f_2)^2(x)\,dx$$
$$= \int_0^1 \varepsilon(x)\,dx \leq \|\varepsilon\| \cdot 1$$

- therefore:
  - if ε is small, the difference between u_1 and u_2 also has got to be small, i.e.
  - small perturbations in the initial conditions lead to small perturbations in the solution.
- **stability estimate** for the solution!

Energy of the Numerical Solution

- we introduce the discrete energy:

$$E^{(m)} := h \sum_{j=1}^{n-1} \left(v_j^{(m)} \right)^2 .$$

- we would like to show that:

$$E^{(m+1)} \leq E^{(m)} \qquad \text{for} \quad m \geq 0.$$

- thus, we will compute $\Delta E^{(m)} := E^{(m+1)} - E^{(m)}$:

$$\Delta E^{(m)} = h \sum_{j=1}^{n-1} \left(\left(v_j^{(m+1)} \right)^2 - \left(v_j^{(m)} \right)^2 \right)$$

Energy in the Explicit Scheme

- lengthy computation (see separate worksheet) leads to stability condition:

$$\left(E^{(m+1)} - E^{(m)}\right) \leq 0, \qquad \text{or} \quad E^{(m+1)} \leq E^{(m)}$$

  is **only correct, if**

$$\frac{\tau}{h^2} \leq \frac{1}{2} \qquad \text{or} \quad \tau \leq \frac{h^2}{2}.$$

- otherwise:
  increasing energy (physically incorrect), leads to large oscillations in the solution

Energy for the Implicit Scheme

- analyse discrete energy

$$E^{(m)} := h \sum_{j=1}^{n-1} \left(v_j^{(m)}\right)^2 = h \left(v_j^{(m)}\right)^T v_j^{(m)}.$$

- change of energy in each time step:

$$\begin{aligned}
\Delta E^{(m)} &= h\left(\left(v^{(m+1)}\right)^T v^{(m+1)} - \left(v^{(m)}\right)^T v^{(m)}\right) \\
&= h\left(\left(Mv^{(m)}\right)^T Mv^{(m)} - \left(v^{(m)}\right)^T v^{(m)}\right) \\
&= h\left(\left(v^{(m)}\right)^T M^T M v^{(m)} - \left(v^{(m)}\right)^T v^{(m)}\right) \\
&= h\left(v^{(m)}\right)^T \left(M^T M - I\right) v^{(m)}
\end{aligned}$$

Energy for the Implicit Scheme (2)

- energy for the implicit scheme:

$$\Delta E^{(m)} = h \left(v^{(m)} \right)^T \left(M^T M - I \right) v^{(m)}$$

- examine eigenvalues of matrix $M^T M - I$
- result:
  - all eigenvalues < 0
  - therefore $\Delta E^{(m)} \leq 0$
  - implicit scheme stable for any τ and h