Scientific Computing I

Module 6: The 1D Heat Equation

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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:

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

- 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:

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

- 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 Maltus):

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

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 $u_k(x,0) = f(x)$:

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

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

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
$$\frac{v_j^{(m+1)} - v_j^{(m)}}{\tau} = \frac{v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)}}{h^2} \tag{3}$$
for $j = 1, \ldots, n-1$, and $m \geq 0$.

An Explicit Scheme

- add initial and boundary conditions:
$$\begin{aligned} v_0^{(m)} &= v_n^{(m)} = 0, \qquad \text{for all} \quad m \geq 0, \\ v_j^{(0)} &= f(x_j), \qquad \text{for} \quad j = 1, \ldots, n-1. \end{aligned}$$
- 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"**

Solutions 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)

⇒ examine conservation of "energy"

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)

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

Therefore:

- $E(t) \leq E(0)$ (energy never increases)
- compare to initial condition $u(x,0) = f(x)$:
$$\int_0^1 u^2(x,t)\,dx = E(t) \leq E(0) = \int_0^1 f^2(x)\,dx$$

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 $f_w(x) = f_1(x) - f_2(x)$

Corollary 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

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

- 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 of the Numerical Solution (2)

- lengthy computation 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

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:

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

  with $M := (I + rA)^{-1}$, we get

$$v^{(m)} = M^m v^{(0)}$$

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