

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:

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

- 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:

$$\frac{\partial}{\partial t} (X(x) \cdot T(t)) = \frac{\partial^2}{\partial x^2} (X(x) \cdot T(t))$$

$$\text{or } X(x) \cdot T_t(t) = T(t) \cdot X_{xx}(x)$$

- 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:

$$X_{xx}(x) + \lambda X(x) = 0 \quad X(0) = X(1) = 0, \quad (1)$$

$$T_t(t) + \lambda T(t) = 0 \quad (2)$$

- solve $X(x)$ -part:

$$X_k(x) = \sin(k\pi x) \quad \lambda_k = (k\pi)^2, k = 1, 2, \dots$$

- 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

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

solve the 1D heat equation PDE

- for the initial and boundary conditions:

$$u_k(0, t) = u_k(1, t) = 0, \quad t > 0$$

$$u_k(x, 0) = \sin(k\pi x), \quad x \in (0, 1).$$

- 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 :

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

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

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

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

An Explicit Scheme

- add initial and boundary conditions:

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

- 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”**

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

$$(u_k)_t = (u_k)_{xx}, \quad x \in (0, 1), t > 0$$

$$u_k(0, t) = u_k(1, t) = 0, \quad t > 0$$

$$u_k(x, 0) = f(x), \quad x \in (0, 1).$$

- 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)

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

Therefore:

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

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

Corollaries

- 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

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

$$w(0, t) = w(1, t) = 0$$

$$w(x, 0) = u_1(x, 0) - u_2(x, 0) = f_1(x) - f_2(x)$$

- 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!

Corollary 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:

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

- 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:

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

is **only correct, if**

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

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

- boundary conditions:

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

- initial conditions:

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

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 $j = 1, \dots, n-1$, 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 $A = \text{tridiag}(-1, 2, -1)$.
- 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:

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

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