Scientific Computing I

Module 6: Analytical and Numerical Solutions of the 1D Heat Equation

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Winter 2015/2016

Part I: Analytical Solution

The Heat Equation in 1D

- remember the heat equation without heat sources:

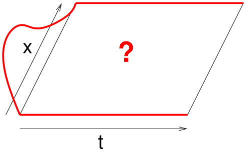
$$T_t = \kappa \Delta T$$

- 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:

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



Computing Analytical Solutions

We will, step by step, try to . . .

1. find *some* solution of the PDE
   (i.e., not necessarily *the* or *all* solutions)
2. that satisfy the boundary conditions
3. finally, satisfy initial conditions

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Ansatz: **Separation of Variables**

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

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

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

- can be true if (and only if!) neither left- nor right-hand side depend on x or t $\Rightarrow$ both terms need to be constant!

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:

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

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

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$$T_t(t) + \lambda T(t) = 0. \tag{2}$$

- solve $X(x)$-part:

$$X(x) = \sin\left(\sqrt{\lambda}x\right) \quad \text{or} \quad X(x) = \cos\left(\sqrt{\lambda}x\right),$$

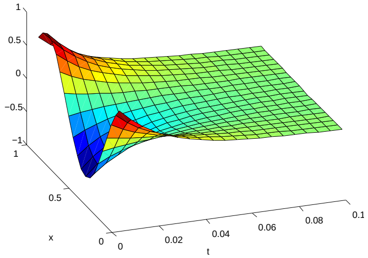
- solve $T(t)$-part:

$$T(t) = e^{-\lambda t}.$$

Ensuring the Boundary Conditions

- We have computed general solutions

$$u(x,t) = \sin\left(\sqrt{\lambda}x\right) e^{-\lambda t} \text{ or } u(x,t) = \cos\left(\sqrt{\lambda}x\right) e^{-\lambda t}.$$



The boundary conditions of our example are

$$u(0,t) = u(1,t) = 0 \text{ for all } t.$$

- Thus, we can reduce possible solutions to

$$u_k(x,t) = \sin(k\pi x)\, e^{-(k\pi)^2 t}, \qquad k = 1, 2, 3 \ldots$$

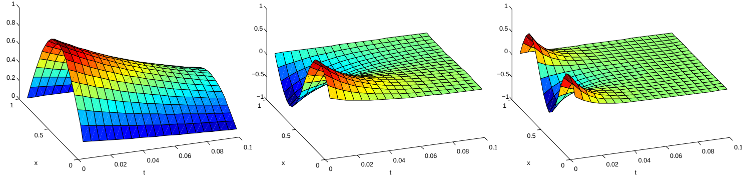
Ensuring the Initial Conditions – Fourier's Method

- The functions

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

solve the 1D heat equation PDE with correct boundary values and for the initial conditions:

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



- To ensure the initial conditions, we use the Fourier sine series:

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

Limits of Analytical Solutions

- For the 1D heat equation, we obtain an analytical solution

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

- Solutions for the heat equation with heat sources?
  Separation of variables yields

$$X(x) \cdot T_t(t) = T(t) \cdot X_{xx}(x) + f(x).$$

  $\Rightarrow$ No analytical solution computable for arbitrary f.

- similar: unit square as computational domain?

$\Rightarrow$ **need for numerical methods!**

Part II: Numerical Solution

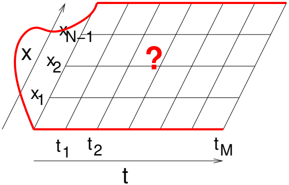
Numerical Solution 1 – An Explicit Scheme

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:

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



$$\text{approximate } u_{xx} \text{ at } (x_j, t_m) \quad \text{by} \quad \frac{v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)}}{h^2},$$

$$u_t \text{ at } (x_j, t_m) \quad \text{by} \quad \frac{v_j^{(m+1)} - v_j^{(m)}}{\tau}.$$

An Explicit Scheme

- This approximation results in the equations

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

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

- Add initial and boundary conditions:

$$\begin{aligned} v_0^{(m)} &= v_N^{(m)} = 0, \qquad \text{for all} \quad m \geq 0, \\ v_j^{(0)} &= g(x_j), \qquad \text{for} \quad j = 1, \ldots, N-1 \end{aligned}$$

- 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 $v_j^{(m)}$ starting with $v_j^{(0)} = g(x_j)$.

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- $\Rightarrow$ ipython notebook demo

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 of the Explicit Scheme

- exact solution:

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

- explicit scheme:

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

Is there a stability condition for τ as observed in the ODE case?

- assumption: there are solutions of the form

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

- compare with the exact solution $\Rightarrow$ $(a_k)^m$ should decrease
$\Rightarrow |a_k| < 1$ necessary

Stability of the Explicit Scheme (2)

- Inserting $v_j^{(m)} = (a_k)^m \sin(\pi k x_j)$ 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

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

- for stability: $|a_k| < 1$ for all k if

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

for detailed computation, see tutorials!

Stability of the Explicit Scheme (3)

- solution for general initial conditions:

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

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

- stability for $\tau < \frac{h^2}{2}$ because $|a_k| < 1$ for all k

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:

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

An Implicit Scheme

- implicit equations 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 $m \geq 0$.
- solution:

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

  where $A = \text{tridiag}(-1, 2, -1)$.
- Use a solver for linear system of equations to obtain $v_j^{(m+1)}$ in every step.

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Stability 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

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

- into the implicit scheme, and obtain (see tutorials):

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

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

$\Rightarrow$ unconditionally stable

Evaluation!

Part III

Energy Considerations

Energy of the Analytic Solution

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

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

Energy of the Analytic Solution

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- define an **"energy"** function of the solution (mathematical concept, not physical energy!):

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

Energy of the Analytic Solution

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- define an **"energy"** function of the solution (mathematical concept, not physical energy!):

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- for conservation of energy, analyse

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

Energy of the Analytic Solution (2)

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

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&= -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 $u(x,0) = g(x)$:

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

Corollaries

- assume: both $u_1(x,t)$ and $u_2(x,t)$ are solutions for initial conditions $g_1(x)$ and $g_2(x)$
- 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 $g_w(x) = g_1(x) - g_2(x)$

Corollary 1 – Uniqueness

- if $g_1 = g_2$, then $g_w(x) = 0$
- energy is decreasing:

$$\begin{aligned}\int_0^1 (u_1 - u_2)^2(x,t)\,dx &= \int_0^1 w^2(x,t)\,dx \\ &\leq \int_0^1 (g_1 - g_2)^2(x)\,dx = 0\end{aligned}$$

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- 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: $g_2 = g_1 + \epsilon$ (ϵ small), then

$$\int_0^1 w^2(x,t)\,dx \leq \int_0^1 (g_1 - g_2)^2(x)\,dx$$
$$= \int_0^1 \epsilon(x)^2\,dx$$

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- 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:

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

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

- 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

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

- change of energy in each time step (use $v^{(m+1)} = Mv^{(m)}$):

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

Energy for the Implicit Scheme (2)

- energy for the implicit scheme:

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

  with the iteration matrix $M = \left(I + \frac{\tau}{h^2} A \right)^{-1}$
- examine eigenvalues of matrix $M^T M - I$

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  with the iteration matrix $M = \left(I + \frac{\tau}{h^2} A \right)^{-1}$
- 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

for detailed computation, see separate worksheet!