Numerical solutions of differential equations

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Lecture 3

The Heat Equation - Part 2

Fully-discrete approximation of the heat equation

- Time discretization
- Stability

Time discretization

Space discretization of heat equation leads to

linear system of ordinary differential equations for $Q_j(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{Q}(t) = \mathbf{A}(t)\mathbf{Q}(t) + \mathbf{S}(t) =: \mathbf{F}(t, \mathbf{Q}(t))$$

Can be solved with standard ODE methods.

For instance: θ-schemes (family of simple methods) with $0 \le \theta \le 1$.

With step size $\triangle t > 0$ the approximations are given by:

$$\mathbf{Q}(t^{n+1}) \approx \mathbf{Q}^{n+1} = \mathbf{Q}^n + \triangle t\left(\theta\,\mathbf{F}(t^{n+1}, \mathbf{Q}^{n+1}) + (1-\theta)\,\mathbf{F}(t^n, \mathbf{Q}^n)\right)$$

θ yields convex combination of $\mathbf{F}(t^n, \mathbf{Q}^n)$ and $\mathbf{F}(t^{n+1}, \mathbf{Q}^{n+1})$.

- $\theta = 0$ fully explicit method
- $\theta = 1$ fully implicit method

Time discretization

For $0 \leq \theta \leq 1$ and step size $\triangle t > 0$:

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n + \triangle t \left(\theta\, \mathbf{F}(t^{n+1}, \mathbf{Q}^{n+1}) + (1-\theta)\, \mathbf{F}(t^n, \mathbf{Q}^n) \right)$$

- $\theta = 0$: Explicit Euler Method
  - also called Forward Euler Method
  - $\mathbf{Q}^{n+1} = \mathbf{Q}^n + \triangle t\, \mathbf{F}(t^n, \mathbf{Q}^n)$.
  - derived with forward difference quotient

$$\partial_t \mathbf{Q}(t^n) \approx \frac{\mathbf{Q}(t^{n+1}) - \mathbf{Q}(t^n)}{\triangle t} = \mathbf{F}(t^n, \mathbf{Q}^n).$$

  - order of accuracy is 1, i.e. $\mathcal{O}(\triangle t)$.

Time discretization

For $0 \leq \theta \leq 1$ and step size $\triangle t > 0$:

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n + \triangle t \left(\theta\, \mathbf{F}(t^{n+1}, \mathbf{Q}^{n+1}) + (1-\theta)\, \mathbf{F}(t^n, \mathbf{Q}^n)\right)$$

- $\theta = 1$: Implicit Euler Method
  - also called Backward Euler Method
  - $\mathbf{Q}^{n+1} = \mathbf{Q}^n + \triangle t\, \mathbf{F}(t^{n+1}, \mathbf{Q}^{n+1})$.
  - derived with backward difference quotient

$$\partial_t \mathbf{Q}(t^{n+1}) \approx \frac{\mathbf{Q}(t^{n+1}) - \mathbf{Q}(t^n)}{\triangle t} = \mathbf{F}(t^{n+1}, \mathbf{Q}^{n+1}).$$

  - order of accuracy is 1, i.e. $\mathcal{O}(\triangle t)$.
  - unconditionally stable.

Time discretization

For $0 \leq \theta \leq 1$ and step size $\triangle t > 0$:

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n + \triangle t \left(\theta\, \mathbf{F}(t^{n+1}, \mathbf{Q}^{n+1}) + (1-\theta)\, \mathbf{F}(t^n, \mathbf{Q}^n)\right)$$

- $\theta = \frac{1}{2}$: Crank-Nicolson
  - $\mathbf{Q}^{n+1} = \mathbf{Q}^n + \triangle t \frac{\mathbf{F}(t^{n+1},\mathbf{Q}^{n+1}) + \mathbf{F}(t^n,\mathbf{Q}^n)}{2}$.
  - derived with central difference quotient

$$\partial_t \mathbf{Q}(t^{n+\frac{1}{2}}) \approx \frac{\mathbf{Q}(t^{n+1}) - \mathbf{Q}(t^n)}{\triangle t} = \frac{\mathbf{F}(t^{n+1}, \mathbf{Q}^{n+1}) + \mathbf{F}(t^n, \mathbf{Q}^n)}{2}.$$

  - order of accuracy is 2, i.e. $\mathcal{O}(\triangle t^2)$.
  - unconditionally stable.

Time discretization - Stability

Let us assume that

- $k(x,t) = k \quad \Rightarrow \quad \mathbf{A}(t) = \mathbf{A}.$

Space-discrete heat equation:

$$\frac{d}{dt}\mathbf{Q}(t) = \mathbf{A}(t)\mathbf{Q}(t) + \mathbf{S}(t)$$

Space-time-discrete heat equation:

$$\mathbf{Q}^{n+1} = \mathbf{Q}^{n} + \triangle t\mathbf{A}\left(\theta\,\mathbf{Q}^{n+1} + (1-\theta)\,\mathbf{Q}^{n}\right) + \triangle t\left(\theta\,\mathbf{S}(t^{n+1})\right) + (1-\theta)\,\mathbf{S}(t^{n})\big)$$

Stability:

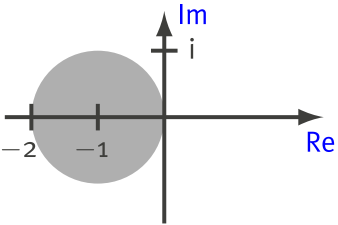
- In many cases restriction on $\triangle t$ for the method to be stable;
- Recall: To verify stability we need to investigate the eigenvalues of $\mathbf{A}$;
- For stability we must have

$$\triangle t\lambda_k \in D \qquad \text{for all eigenvalues } \lambda_k \text{ of } \mathbf{A}.$$

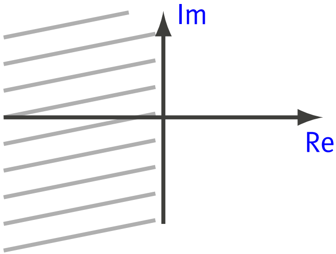
  Here D is the stability region of the ODE solver.

Time discretization - Stability

Examples of stability regions:



Explicit Euler



Implicit Euler

For stability we require $\triangle t \lambda_k \in D$ for all eigenvalues of $\mathbf{A}$.

- Explicit Euler: if λ_k is real $\Rightarrow -2 < \triangle t \lambda_k < 0 \Rightarrow -\triangle t \lambda_k \leq 2$.
- Implicit Euler: if λ_k is real $\Rightarrow \triangle t \lambda_k < 0 \Rightarrow$ easily fulfilled.

Time discretization - Stability

It remains to check the eigenvalues of $\mathbf{A}$ in our case, i.e

- Heat equation in 1d: $\partial_t u = \partial_x(\alpha \partial_x u) + S$
- $k(x,t) =: \alpha = \text{const.}$
- Neumann boundary condition $\partial_x u(0,t) = \partial_x u(1,t) = 0.$

Recall from last lecture ($\mathbf{A}$ is real, symmetric and invertible):

$$\mathbf{A} = \frac{\alpha}{h^2}\begin{pmatrix} -1 & 1 & 0 & \dots & \dots & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ & & & \ddots & & & 0 \\ & & & & 1 & -2 & 1 \\ 0 & \dots & \dots & \dots & 0 & 1 & -1 \end{pmatrix}.$$

Hence, the eigenvalues $\lambda_1, \cdots, \lambda_M$ are <u>real</u> and <u>nonzero</u>.

Let $\mathbf{v}^k$ denote corresponding eigenvectors with

$$\mathbf{A}\mathbf{v}^k = \lambda_k \mathbf{v}^k \qquad \text{with } 1 \le k \le M.$$

Time discretization - Stability

Recall from last lecture ($\mathbf{A}$ is real, symmetric and invertible):

$$\mathbf{A} = \frac{\alpha}{h^2}\begin{pmatrix} -1 & 1 & 0 & \dots & \dots & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ & & & \ddots & & & \\ & & & & & & 0 \\ & & & & 1 & -2 & 1 \\ 0 & \dots & \dots & \dots & 0 & 1 & -1 \end{pmatrix}.$$

Let $\mathbf{v}^k$ denote eigenvectors with $\mathbf{A}\mathbf{v}^k = \lambda_k \mathbf{v}^k$ with $1 \leq k \leq M$.

The matrix encodes the relation

$$\frac{\alpha}{h^2}\left(\mathbf{v}^k_{j+1} - 2\mathbf{v}^k_j + \mathbf{v}^k_{j-1}\right) = \lambda_k \mathbf{v}^k_j \qquad \text{for } 1 \leq j \leq N-2,$$

where (from the Neumann condition) $\mathbf{v}^k_0 := \mathbf{v}^k_1$ and $\mathbf{v}^k_{N-1} := \mathbf{v}^k_{N-2}$.

Ansatz for eigenvectors inspired by Lecture 2 (solution admits cosine transform):

$$\mathbf{v}^k \in \mathbb{R}^N \qquad \text{with} \quad \mathbf{v}^k_j = \cos(k\pi x_j). \qquad \text{(satisfies boundary condition!)}$$

Time discretization - Stability

Next, we compute the eigenvectors to

$$\mathbf{v}^k \in \mathbb{R}^N \qquad \text{with} \quad \mathbf{v}_j^k = \cos(k\pi x_j),$$

where we use the relation

$$\frac{\alpha}{h^2}\left(\mathbf{v}_{j+1}^k - 2\mathbf{v}_j^k + \mathbf{v}_{j-1}^k\right) = \lambda_k \mathbf{v}_j^k \qquad \text{for } 1 \le j \le N-2.$$

Time discretization - Stability

We obtain:

$$
\begin{aligned}
&\frac{\alpha}{h^2}\left(\mathbf{v}_{j+1}^k - 2\mathbf{v}_j^k + \mathbf{v}_{j-1}^k\right) \\
&= \frac{\alpha}{h^2}\left[\underbrace{\cos(k\pi(x_j+h)) + \cos(k\pi(x_j-h))}_{=2\cos(k\pi x_j)\cos(k\pi h)} - 2\cos(k\pi x_j)\right] \\
&= \frac{2\alpha}{h^2}\left[\cos(k\pi x_j)\cos(k\pi h) - \cos(k\pi x_j)\right] \\
&= \frac{2\alpha}{h^2}\cos(k\pi x_j)\left[\underbrace{\cos(k\pi h) - 1}_{-2\sin^2(\frac{k\pi h}{2})}\right] \\
&= \underbrace{-\frac{4\alpha}{h^2}\sin^2\left(\frac{k\pi h}{2}\right)}_{=\lambda_k}\underbrace{\cos(k\pi x_j)}_{=\mathbf{v}_j^k}.
\end{aligned}
$$

Time discretization - Stability

Hence, the eigenvalues of **A** are given by

$$\lambda_k = -\frac{4\alpha}{h^2}\sin^2\left(\frac{k\pi h}{2}\right).$$

Since $0 \leq \sin^2(\frac{k\pi h}{2}) \leq 1$ we have

$\lambda_k \sim -\frac{4\alpha}{h^2}$ which depends on the discretization through h.

Stability for the heat equation.

Explicit Euler. Condition $-2 < \lambda_k \Delta t < 0$. Hence:

$$-2 \leq -\frac{4\alpha}{h^2}\Delta t \quad \Rightarrow \quad 4\alpha\frac{\Delta t}{h^2} \leq 2 \quad \Rightarrow \quad \alpha\frac{\Delta t}{h^2} \leq \frac{1}{2}.$$

Bad condition! The finer the mesh, the smaller the time steps!

Time discretization - Stability

Generally for the θ-scheme for the heat equation & Finite Volume Method:

$$\alpha\frac{\triangle t}{h^2} \leq \begin{cases} \frac{1}{2(1-2\theta)} & \text{for } \theta < \frac{1}{2}, \\ \infty & \text{for } \frac{1}{2} \leq \theta \leq 1 \end{cases} \qquad \text{Unconditionally stable.}$$

Hence, for $\frac{1}{2} \leq \theta \leq 1$ we can pick $\triangle t$ as large as we want.

However, the accuracy of the approximations still depends on $\triangle t$.