Classifying PDEs

Looking at the PDE
\[ Au_{xx} + 2Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu + .. = 0, \]
and its discriminant, \( B^2 - AC \), the equation is said to be:

- **Parabolic** if \( B^2 - AC = 0 \) - for example, the heat equation, \( u_t = u_{xx} \)
- **Hyperbolic** if \( B^2 - AC > 0 \) - for example, the second order wave equation, \( u_{tt} = u_{xx} \)
- **Elliptic** if \( B^2 - AC < 0 \) - for example, Laplace equation, \( u_{xx} + u_{yy} = 0 \)
This can be generalized to second order equations in $N$ dimensions via the positive definiteness of the second order operator involved:

$$(\nabla)^T \begin{pmatrix} A & B \\ B & C \end{pmatrix} (\nabla) \ u + \{\text{lower order terms}\} = 0$$
Heat equation

The simple parabolic PDE

\[
\frac{\partial u}{\partial t} = K \frac{\partial^2 u}{\partial^2 x}
\]

with the initial values

\[ u(0, x) = u_0(x) \]

and some boundary conditions is called the (one-dimensional) heat equation.
This equation describes the thermal energy transport in a 1D rod, where $u(t, x)$ describes the temperature at a point $x$ at time $t$ and $K$ denotes the thermal conductivity constant.

In 2D it describes the effect of defocusing on an image in optics.

The solution is given by convolution of the initial data with a Gaussian kernel:

$$u(x, t) = G(x, t) * u_0(x) = \int_{\mathbb{R}} G(\bar{x}, t) u_0(x - \bar{x}) d\bar{x}$$
Boundary conditions

Dirichlet:

\[ u(t, 0) = a \quad \quad u(t, 1) = b \]

Neumann:

\[ u_x(t, 0) = a \quad \quad u_x(t, 1) = b \]

Reflective - Neumann with \( a = b = 0 \).
Mixed boundary conditions:

\[ u(t, 0) = a, \quad u_x(t, 1) = b. \]

Periodic:

\[ u(t, 0^-) = u(t, 1^+) \]
Discretization of the heat equation

Replace the continuous system of coordinates \((t, x)\) by a discrete grid \((n, m) = (n\Delta t, m\Delta x)\), and the continuous function \(u(t, x)\) by a discrete version \(u^n_m = u(n\Delta t, m\Delta x)\).

![The grid](image)

**Figure**: The grid
Finite differences

1. Replace the first-order time derivative $u_t(t, x)$ by a forward finite difference in time

$$D_t^+ u^n_m = \frac{u_{m+1}^n - u_m^n}{\Delta t} \approx u_t(t).$$

2. Replace the second-order space derivative $u_{xx}(t, x)$ by a central difference in space

$$D_{xx}^0 u^n_m = \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{(\Delta x)^2} \approx u_{xx}(x).$$
Finite differences’ motivation

From the Taylor expansion,

\[ u(t + \Delta t) = u(t) + u_t(t)\Delta t + \frac{1}{2}u_{tt}(t)(\Delta t)^2 + \ldots \]

we obtain

\[ u_t(t) = \frac{u(t + \Delta t) - u(t)}{\Delta t} - \frac{1}{2}u_{tt}(t)\Delta t + \ldots \]

\[ = \frac{u(t + \Delta t) - u(t)}{\Delta t} + \mathcal{O}(\Delta t). \]

This first-order approximation of the first derivative is called the \textit{forward finite-difference approximation} and is denoted by \( D_t^+ u^n_m \).
Finite differences

Forward difference

\[ D_t^+ u_m^n = \frac{u_m^{n+1} - u_m^n}{\Delta t} \approx u_t(t) + O(\Delta t). \]

In the same manner, backward difference can be defined

\[ D_t^- u_m^n = \frac{u_m^n - u_m^{n-1}}{\Delta t} \approx u_t(t) + O(\Delta t). \]

To approximate a second-order derivative, use the central difference approximation

\[ D_{xx}^0 u_m^n = \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{(\Delta x)^2} \approx u_{xx}(x) + O((\Delta x)^2). \]

Note: We can also write

\[ D_{xx}^0 u_m^n = D_x^- D_x^+ u_m^n. \]
Finite differences

Proving the order of convergence – by writing a fourth order Taylor series and canceling out terms,

\[
\frac{u^n_{m+1} - 2u^n_m + u^n_{m-1}}{(\Delta x)^2} =
\]

\[
= \frac{u^n_m + (u_x^n)_m \Delta x + \frac{1}{2} (u_{xx}^n)_m (\Delta x)^2 + \frac{1}{3!} (u_{xxx}^n)_m (\Delta x)^3 + \frac{1}{4!} (u_{xxxx}^n)_m (\Delta x)^4 - 2u^n_m + u^n_m - (u_x^n)_m \Delta x + \frac{1}{2} (u_{xx}^n)_m (\Delta x)^2 + \frac{1}{3!} (u_{xxx}^n)_m (\Delta x)^3 + \frac{1}{4!} (u_{xxxx}^n)_m (\Delta x)^4}{(\Delta x)^2} =
\]

\[
= \frac{\frac{1}{2} (u_{xx}^n)_m (\Delta x)^2 + \frac{1}{4!} (u_{xxxx}^n)_m (\Delta x)^4 + \frac{1}{2} (u_{xx}^n)_m (\Delta x)^2 + \frac{1}{4!} (u_{xxxx}^n)_m (\Delta x)^4}{(\Delta x)^2}
\]
Finite differences

\[ u_{xx} + \frac{1}{12} (u_{xxxx})^n_m (\Delta x)^2 = u_{xx} + O ((\Delta x)^2) \]
The discrete heat equation

The continuous equation $u_t(t, x) = Ku_{xx}(t, x)$ is replaced by

$$\frac{u_{m}^{n+1} - u_{m}^{n}}{\Delta t} = K \frac{u_{m+1}^{n} - 2u_{m}^{n} + u_{m-1}^{n}}{(\Delta x)^2}$$

or

$$u_{m}^{n+1} = u_{m}^{n} + \frac{\Delta t}{(\Delta x)^2} K \left( u_{m+1}^{n} - 2u_{m}^{n} + u_{m-1}^{n} \right),$$

This scheme is explicit (called also Euler scheme) and very simple to implement.
We denote the continuous solution by $U = u(t,x)$ and the discrete solution by $u = u^n_m$.

We denote the continuous PDE operator $\mathcal{L} = \partial_t - K \partial_{xx}$.

We denote the discrete operator $\mathcal{L}_{\Delta t, \Delta x} = D_t^+ - KD_{xx}^0$. 
Stability and Convergence

1. **Convergence**: the discrete solution converges to the continuous solution

   \[
   \lim_{\Delta t, \Delta x \to 0} \| u - U \|.
   \]

   in some norm.

2. **Consistency**: the discrete difference operator converges to the continuous

   \[
   \lim_{\Delta t, \Delta x \to 0} \| \mathcal{L}(u) - \mathcal{L}_{\Delta t, \Delta x}(u) \| = 0
   \]

   for every bounded \( u \).
3. **Numerical stability**: noise from initial conditions, numerical errors, etc. is not amplified.

The numerical scheme is $u^{n+1} = \mathcal{N} u^n$

Formally, stability means

$$\forall N > 0 \quad \exists C(N) > 0 \quad \text{s.t.} \quad \forall n \leq N \quad \|\mathcal{N}^n\| \leq C(N).$$

If $C$ is a constant for all $N$, this is known as unconditional stability.

**Lax’s equivalence theorem:** Given a well-posed initial value problem and a finite-difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence.

**consistency: stability $\Leftrightarrow$ convergence**
The CFL condition for the wave equation

- The (Courant-Friedrichs-Lewy (CFL) condition) is a necessary condition for advection problems limiting the maximum time step allowed in the difference equations.

- Specifically, this condition states that the domain of dependence of the differential equation must be included in the domain of dependence of the difference equation.

- Note: This does not apply to equations where information flows "instantly" such as the heat equation – but the term CFL condition is often still used to denote stability limitations on step size in these cases.
A condition for stability of the discrete heat equation

Denote $r = K \frac{\Delta t}{(\Delta x)^2}$. The finite difference scheme is

$$u^{n+1}_m = u^n_m + r (u^n_{m+1} - 2u^n_m + u^n_{m-1})$$

$$= (1 - 2r)u^n_m + ru^n_{m+1} + ru^n_{m-1}$$

If $1 - 2r > 0$, we can write:

$$u^{n+1}_m \leq (1 - 2r) \max_m u^n_m + r \max_m u^n_m + r \max_m u^n_m$$

Then

$$u^{n+1}_m \leq \max_m u^n_m (1 - 2r + 2r) = \max_m u^n_m.$$  

(maximum principle property)
Observation: Maximum principle implies stability of the scheme.

Lemma
(Maximum principle)
If $K \frac{\Delta t}{(\Delta x)^2} \leq 1/2$, then

$$\min_m u_m^0 \leq u_m^n \leq \max_m u_m^0.$$
Figure: Computation of the discrete heat equation with Neumann boundary conditions. ($h = 0.1$) Top left: Initial data. Top right: stable solution of the heat equation conditions $\Delta t = 0.0008$. Bottom left: stable solution of the heat equation for $\Delta t = 0.004$. Bottom right: unstable solution ($\Delta t = 0.006$).
The 2D heat equation. Numerical scheme.

\[ u_t = K(u_{xx} + u_{yy}) \]

\[ u_{m,p}^{n+1} = u_{m,p}^n + K\left(\frac{\Delta t}{(\Delta x)^2}(u_{m+1,p}^n - 2u_{m,p}^n + u_{m-1,p}^n) + \frac{\Delta t}{(\Delta y)^2}(u_{m,p+1}^n - 2u_{m,p}^n + u_{m,p-1}^n)\right). \]

A stability condition suggested by Courant, Friedrichs and Lewy:

\[ K\left(\frac{\Delta t}{(\Delta x)^2} + \frac{\Delta t}{(\Delta y)^2}\right) \leq \frac{1}{2}. \]

If \( \Delta x = \Delta y \), then the condition is:

\[ K \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{4}. \]
Stability condition by Fourier analysis.

Another way to check the stability of a numerical scheme is by Fourier analysis. Looking again at the heat equation:

\[ u_t = u_{xx} \]

using the linearity of the equation we assume a solution of the form \( u_m^n = \lambda^n e^{i\xi m\Delta x} \), where for stability we would like \( \|\lambda\| < 1 \).

For the usual explicit scheme, we obtain:

\[
\frac{u_{m+1}^n - u_m^n}{\Delta t} = \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{(\Delta x)^2} \rightarrow \\
\lambda^n(\lambda - 1)e^{i\xi m\Delta x} = \frac{\Delta t}{(\Delta x)^2} \lambda^n(e^{i\xi \Delta x} + e^{-i\xi \Delta x} - 2)e^{i\xi m\Delta x} \rightarrow \\
\lambda = 1 + \frac{\Delta t}{(\Delta x)^2}(e^{i\xi \Delta x} + e^{-i\xi \Delta x} - 2)\
\]
Stability condition by Fourier analysis.

finally arriving at

$$\|\lambda\| = \|1 + \frac{\Delta t}{(\Delta x)^2}(2\cos(\xi \Delta x) - 2)\| \leq 1.$$ 

Again we see that the condition $$\frac{\Delta t}{(\Delta x)^2} < \frac{1}{2}$$ guarantees stability. The same method extends to higher dimensions. In the case of a finite time interval $$T$$, we can settle for a weaker form of stability, by demanding merely

$$\|\lambda\| < 1 + \tilde{K}T$$

This condition is known as the von-Neumann condition. The analysis is often referred to as von-Neumann analysis.
The 2D heat equation. Numerical example

Figure: Application of the heat eq. on a gray-scale image.
Implicit finite difference schemes for the heat equation

\[
\frac{u_{m+1}^n - u_{m}^n}{\Delta t} = K \frac{u_{m+1}^{n+1} - 2u_{m}^{n+1} + u_{m-1}^{n+1}}{(\Delta x)^2}
\]

- Main advantage of implicit schemes: are unconditionally stable (i.e. stable for all time-steps and thus we can take large step times).
  
  \[(I - \Delta t A) U^{n+1} = U^n.\]

- Requires solving a linear system of equations. The matrix \((I - \Delta t A)\) is tridiagonal and can to be inverted using the Thomas algorithm (we will describe it in detail later on).

- Note: Assuring stability does not prevent the accuracy from deteriorating.