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Numerical Techniques 2022–2023

1. Discretization and stability

Daan Degrauwe

daan.degrauwe@meteo.be

Postgraduate Studies in Weather and Climate Modeling

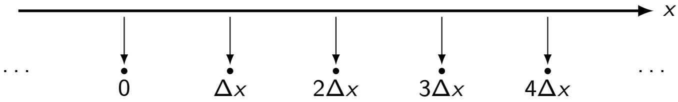
Ghent University

Content

- Discretization
- A prototype system: the 1D advection equation
- An example of a numerical scheme: the upstream scheme
- Accuracy and consistency
- Convergence
- Stability

Discretization

- Meteorological fields (temperature, wind, pressure, humidity, ...) are continuous in time and space.
- On a computer you cannot represent a continuous field; you would need an infinity of points.
- So a field will be *discretized*, i.e. it is represented by the values in a set of discrete points:



  replacing the continuous coordinate x by discrete points $i\Delta x$ labeled by i. Note that i is variable, and Δx is constant!
- similarly in 2D: $i\Delta x, j\Delta y$
- discretizing time: $n\Delta t$

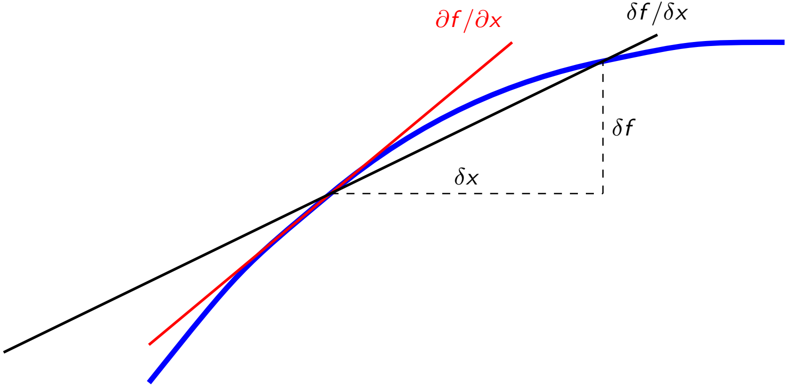
Discretization of derivatives: finite differences

- Many physical laws are differential equations
- Some definition of the derivative in x:

$$\frac{df}{dx}(x_0) = \lim_{\delta x \to 0} \frac{f(x_0 + \delta x) - f(x_0)}{\delta x}$$
$$\frac{df}{dx}(x_0) = \lim_{\delta x \to 0} \frac{f(x_0) - f(x_0 - \delta x)}{\delta x}$$
$$\frac{df}{dx}(x_0) = \lim_{\delta x \to 0} \frac{f(x_0 + \delta x) - f(x_0 - \delta x)}{2\delta x}$$

- On our discrete grid we can't take the limit $\delta x \to 0$, so the derivative is computed with a finite value $\delta x \to \Delta x$ (i.e. the grid distance).

- The limit is then better approximated by increasing the resolution



We will now consider the 1D advection equation with constant advection

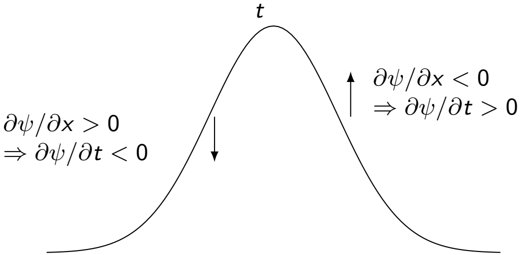
$$\frac{\partial \psi}{\partial t} + c\frac{\partial \psi}{\partial x} = 0$$

Why?

- hyperbolic systems can be decomposed into decoupled equations of this type
- most systems studied with atmospheric models are hyperbolic.

Physical interpretation of the advection equation:

- ψ is any (meteorological) field: temperature, pressure, humidity, pollutant concentration, ...
- c is the wind speed.
- time evolution: the field is *transported* with speed c:



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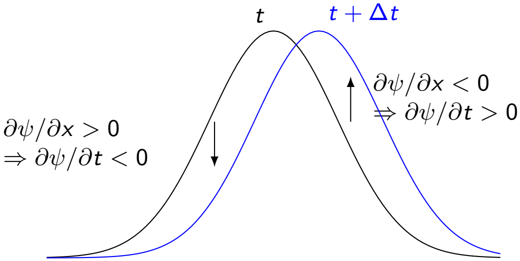

The exact solution of the advection equation

$$\frac{\partial \psi}{\partial t} + c\frac{\partial \psi}{\partial x} = 0$$

is given by

$$\psi(x, t) = \psi(x - ct, t = 0)$$

The upstream scheme

Let us call ϕ_j^n the solution of the discretized system at time $n\Delta t$ and at grid point $j\Delta x$.

We replace the derivatives by,

$$\frac{\partial \psi}{\partial t} \to \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t}$$
$$\frac{\partial \psi}{\partial x} \to \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x}$$

in the advection equation:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c\,\frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0$$

This is called the *upstream scheme*.

This equation can be solved w.r.t. ϕ_j^{n+1}:

$$\phi_j^{n+1} = (1-\mu)\phi_j^n + \mu\phi_{j-1}^n$$

with $\mu = c\Delta t/\Delta x$.

So if the solution is known at time $t = n\Delta t$,
then it can be calculated at $t = (n+1)\Delta t$.

- But we see that increasing the spatial resolution doesn't necessarily improve the solution !?

  We say that the discretized system becomes *unstable*.

- Stability is a central concept in this course. This lesson will (try to) explain why.

- For this we need additional concepts: accuracy, consistency and convergence.

Accuracy

Using a Taylor expansion

$$f(x_0 + \Delta x) = f(x_0) + \Delta x \frac{df}{dx}(x_0) + \frac{\Delta x^2}{2}\frac{d^2 f}{dx^2}(x_0) + \frac{\Delta x^3}{6}\frac{d^3 f}{dx^3}(x_0) + \ldots$$

the error in the approximation of the derivative is

$$\frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} - \frac{df}{dx}(x_0) = \frac{\Delta x}{2}\frac{d^2 f}{dx^2}(x_0) + \frac{\Delta x^2}{6}\frac{d^3 f}{dx^3}(x_0) + \ldots$$

The leading term is proportional to Δx, so this is called a first-order accurate method.

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Considering the centered finite-difference approximation

$$\frac{f(x_0+\Delta x) - f(x_0-\Delta x)}{2\Delta x} - \frac{df}{dx}(x_0) = \frac{\Delta x^2}{6}\frac{d^3 f}{dx^3}(x_0) + \frac{\Delta x^4}{120}\frac{d^5 f}{dx^5}(x_0) + \dots$$

we see that it is second-order accurate.

By using more information (more gridpoints), it is possible to obtain a more accurate approximation for the derivative:

$$\begin{aligned}\frac{df}{dx}(x_0) =&\frac{4}{3}\left(\frac{f(x_0+\Delta x)-f(x_0-\Delta x)}{2\Delta x}\right)\\&-\frac{1}{3}\left(\frac{f(x_0+2\Delta x)-f(x_0-2\Delta x)}{4\Delta x}\right)+O[\Delta x^4]\end{aligned}$$

A scheme is called *consistent* if the truncation error converges to zero when $\Delta x \to 0$ and $\Delta t \to 0$.

For example, the truncation error for the upstream scheme is:

$$\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} + c\frac{\psi_j^n - \psi_{j-1}^n}{\Delta x} = \frac{\Delta t}{2}\frac{\partial^2 \psi}{\partial t^2} - c\frac{\Delta x}{2}\frac{\partial^2 \psi}{\partial x^2} + \ldots$$

where ψ denotes the exact solution.

A finite-difference scheme is called *convergent* of order (p, q) if in the limit $\Delta t, \Delta x \to 0$, the numerical solution ϕ_j^n satisfies

$$\|\psi(n\Delta t, j\Delta x) - \phi_j^n\| = O[\Delta t^p] + O[\Delta x^q]$$

Convergence vs. consistence

Consistency tells you something about the equations, convergence tells you about the solution.

The upstream scheme example shows that these two are not identical: it is consistent but not convergent.

There's a problem with the usability of convergence: it relies on the exact solution, which is unknown in most cases.

The Lax equivalence theorem says that:

If a finite-difference scheme is linear, stable, and consistent, then it is convergent

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Importance: in practice we never know the true solution, but we can check if the scheme is *consistent* and *stable*.

But when is a scheme stable?

A sufficient condition for stability is that

$$\|\phi^n\| \leq \|\phi^0\| \quad \text{for all timesteps} \quad n > 0$$

Again, we don't need to know the true solution for this!

- It is difficult to check the evolution of $\|\phi^n\|$ in general.

- Von Neumann proposed to check stability by considering harmonic functions:

$$\phi(x) = \exp(ikx) = \cos(kx) + i\sin(kx)$$

If a scheme is stable for all harmonic functions (i.e. all values of k), then it is also stable for all (non-harmonic) functions.

- Because harmonic functions are eigenfunctions of the differential operator, one can express their time evolution as a multiplication with an *amplification factor* A_k:

$$\phi^n = A_k \phi^{n-1} = (A_k)^n \phi^0$$

- So stability requires $\|A_k\| \leq 1$, for all k.

Example: stability of the upstream scheme

Let us consider again the upstream scheme for the advection equation:

$$\phi_j^{n+1} = (1-\mu)\phi_j^n + \mu\phi_{j-1}^n$$

with $\mu = c\Delta t/\Delta x$.

What is the amplification factor?

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What is the amplification factor?

First, assume that $\phi_j^n = (A_k)^n e^{ikj\Delta x}$, so

$$(A_k)^{n+1} e^{ikj\Delta x} = (A_k)^n (1-\mu) e^{ikj\Delta x} + (A_k)^n \mu e^{ik(j-1)\Delta x}$$

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The amplification factor A_k then becomes

$$\begin{aligned} A_k &= 1 - \mu + \mu e^{-ik\Delta x} \\ &= (1 - \mu + \mu \cos k\Delta x) - i\mu \sin k\Delta x \end{aligned}$$

Example: stability of the upstream scheme

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The modulus of the complex number A_k is given by

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The modulus of the complex number A_k is given by

$$|A_k|^2 = 1 - 2\mu\left(1-\mu\right)\left(1-\cos k\Delta x\right)$$

This will be ≤ 1 for all values of k if

$$\mu\left(1-\mu\right) \geq 0$$

i.e. if

$$0 \leq \frac{c\Delta t}{\Delta x} \leq 1$$

Example: stability of the upstream scheme

- So the upstream scheme is *conditionally stable*, i.e. stability depends on the values of c, Δx and Δt.

- In general,
  - higher spatial resolution is less stable
  - smaller timesteps is more stable
  - higher velocity is less stable

- $\mu = \frac{c\Delta t}{\Delta x}$ is called the Courant number.

- The condition $\mu \leq 1$ is called the Courant-Fredrichs-Lewy (CFL) criterion.

Workflow

Starting from a discretized equation:

1. Check if the scheme is linear and consistent
2. Fill in a harmonic solution $\phi_j^n = (A_k)^n e^{i\,kj\Delta x}$ in the discretized equation
3. Calculate (the modulus of) the amplification factor A_k
4. If $|A_k| \leq 1$, the scheme is stable
5. If the scheme is stable and consistent, it is convergent
6. If the scheme is convergent, the *error on the solution* can be reduced by increasing the resolution

Summary

- *Discretization* of a continuous function on a grid
- Approximation of derivatives with *finite differences*
- *Accuracy* and *Consistency* of a scheme (error on equations)
- *Convergence* of a scheme (error on solution)
- *Stability* of a scheme: Von Neumann analysis, Courant number and CFL criterion
- Applied to the upstream scheme to solve the 1D advection equation