Ill-posed problems

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Spring 2011

Consider the initial value problem:

\[ \frac{\partial^2 f}{\partial t^2} = -\frac{\partial^2 f}{\partial x^2} \]

This is simply Laplace’s equation

\[ \frac{\partial^2 f}{\partial t^2} = \frac{\partial^2 f}{\partial x^2} = 0 \]

which has a solution if \( \partial f/\partial t \) or \( f \) are given on the boundaries.

Here, however, this equation appeared as an initial value problem, where the only boundary conditions available are at \( t = 0 \). Since this is a second order equation we will need two conditions, which we may assume are that \( f \) and \( \partial f/\partial x \) are specified at \( t = 0 \).

Look for solutions of the type:

\[ f(x,t) = \sum a_k(t)e^{ikx} \]

The general solution can be written as:

\[ f(x,t) = \sum a_k(t)e^{ikx} \]

where the \( a_k \)'s depend on the initial conditions.

Look for solutions of the type:

\[ f = a_k(t)e^{ikx} \]

Substitute into:

\[ \frac{\partial^2 f}{\partial t^2} = \frac{\partial^2 f}{\partial x^2} = 0 \]

to get:

\[ \frac{d^2 a_k}{dt^2} = k^2 a_k \]

Generally, both \( A \) and \( B \) are non-zero.

The general solution

\[ a_k(t) = Ae^{ikt} + Be^{-ikt} \]

\( A, B \) determined by initial conditions \( a(0), \ ika(0) \)

Generally, both \( A \) and \( B \) are non-zero.

Therefore: \( a(t) \to \infty \) as \( t \to \infty \)

Ill-posed Problem

Long wave with short wave perturbations
Similarly, it can be shown that the diffusion equation with a negative diffusion coefficient

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}; \quad D < 0$$

has solutions with unbounded growth rate for high wave number modes and is therefore an ill-posed problem.

Ill-posed problems generally appear when the initial or boundary data and the equation type do not match. Frequently arise because small but important higher order effects have been neglected. Ill-posedness generally manifests itself in the exponential growth of small perturbations so that the solution does not "depend continuously on the initial data". Inviscid vortex sheet rollup, multiphase flow models and some viscoelastic constitutive models are examples of problems that exhibit ill-posedness.

Classical Methods for Hyperbolic Equations

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The wave equation:

$$\frac{\partial^2 f}{\partial t^2} - c^2 \frac{\partial^2 f}{\partial x^2} = 0$$

Write as:

$$\frac{\partial u}{\partial t} - c \frac{\partial v}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} - \frac{\partial u}{\partial x} = 0$$

In general:

$$\frac{\partial u}{\partial t} + a_{11} \frac{\partial f}{\partial x} + a_{12} \frac{\partial g}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} + a_{21} \frac{\partial f}{\partial x} + a_{22} \frac{\partial g}{\partial x} = 0$$

Most of the issues involved can be addressed by examining:

$$\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = 0$$

Forward in Time, Centered in Space (FTCS) and Upwind

We will start by examining the linear advection equation:

$$\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = 0$$

The characteristic for this equation are:

$$\frac{dx}{dt} = U; \quad \frac{df}{dt} = 0,$$

Showing that the initial conditions are simply advected by a constant velocity \( U \).
Flow direction!

This restriction was first derived by Courant, Fredrik, and Levy in 1932, and is usually called the Courant condition, or the CFL condition.

Graphically:

\[ G = 1 - \lambda + \lambda e^{-\Delta t} \]

Stability condition: \( \lambda < 1 \)

\[ \frac{U \Delta t}{h} \leq 1 \]

Another scheme for

\[ \frac{df}{dt} + U \frac{df}{dx} = 0 \]

A simple forward in time, centered in space discretization yields

\[ f_{j}^{n+1} = f_{j}^{n} - \frac{\Delta t}{h} U (f_{j+1}^{n} - f_{j-1}^{n}) \]

This scheme is \( O(\Delta t, h) \) accurate.

To examine the stability we use the von Neumann’s method:

The evolution of the error is governed by:

\[ \frac{e_{j}^{n+1} - e_{j}^{n}}{\Delta t} + \frac{U}{h} (e_{j}^{n+1} - e_{j}^{n}) = 0 \]

Write the error as:

\[ e_{j}^{n+1} = e_{j}^{n} e^{\Delta t \lambda} \]

Amplification factor

\[ G = \frac{e^{\Delta t \lambda}}{e^{\Delta t}} = 1 - \lambda (1 - e^{-\Delta t}) \]

Or:

\[ G = 1 - \lambda + \lambda e^{-\Delta t} \]

Need to find when \( |G| < 1 \)

Another way: Find the absolute value of the amplification factor

\[ G = 1 - \lambda + \lambda e^{-\Delta t} = 1 - \lambda + \lambda \cos kh - i \lambda \sin kh \]

\[ |G| = \sqrt{ (1 - \lambda)^2 + 2(1 - \lambda) \lambda \cos kh + \lambda^2 \cos^2 kh + \lambda^2 \sin^2 kh } \]

\[ = \sqrt{ (1 - \lambda)^2 + 2(1 - \lambda) \lambda \cos kh + \lambda^2 ( (1 + 2 \lambda) \cos kh + \lambda^2 \sin^2 kh ) } \]

\[ = \sqrt{ (1 - \lambda)^2 + 2(1 - \lambda) \lambda \cos kh + \lambda^2 (1 - 2 \lambda + 2 - 2(1 - \lambda) \cos kh) } \]

\[ |G| = 1 - 2 \lambda (1 - \lambda) \quad \text{if } \cos kh = 0 \]

\[ |G| = 1 \quad \text{if } \cos kh = 1 \]

\[ |G| = 1 - \lambda (4 - 3 \lambda) \quad \text{if } \cos kh = -1 \]

\[ |G| \leq 1 \quad \text{if } \lambda \leq 1 \]
The CFL condition implies that a signal has to travel less than one grid spacing in one time step.

\[ U \Delta t \leq h \]

**The Upwind Scheme**

For the linear advection equation:

\[ \frac{df}{dt} + U \frac{df}{dx} = 0 \]

\[ f_j^{n+1} = f_j^n - \frac{\Delta t}{h} U (f_j^n - f_{j-1}^n) \]

**Finite Volume point of view:**

\[ dt = 0.25h \]

Although the upwind method is exceptionally robust, its low accuracy in space and time makes it unsuitable for most serious computations.

**Generalized Upwind Scheme (for both \( U > 0 \) and \( U < 0 \))**

\[ f_j^{n+1} = f_j^n - \frac{\Delta t}{h} U (f_j^n - f_{j+1}^n), \quad U > 0 \]

\[ f_j^{n+1} = f_j^n - \frac{\Delta t}{h} U (f_j^n - f_{j-1}^n), \quad U < 0 \]

Define: \( U^+ = \frac{1}{2} (U + |U|) \), \( U^- = \frac{1}{2} (U - |U|) \)

The two cases can be combined into a single expression:

\[ f_j^{n+1} = f_j^n - \frac{\Delta t}{h} \left(U^+ (f_j^n - f_{j+1}^n) + U^- (f_j^n - f_{j-1}^n)\right) \]

Or, substituting \( U^+ = \frac{2U}{2h}(f_j^n + f_{j+1}^n) \)

\[ D_{num} = \frac{|U|}{2h} \]

**Other First Order Schemes**
**Implicit (Backward Euler) Method**

\[
\frac{f_i^{n+1} - f_i^n}{\Delta t} + U \frac{f_i^{n+1} - f_{i-1}^{n+1}}{\Delta x} = 0
\]

- Unconditionally stable
- 1st order in time, 2nd order in space
- Forms a tri-diagonal matrix (Thomas algorithm)

\[
\frac{U}{\Delta x} f_i^{n+1} + \frac{1}{\Delta x} f_i^{n+1} - \frac{U}{\Delta x} f_{i-1}^{n+1} = \frac{1}{\Delta x} f_i^n
\]

\[a_i f_i^{n+1} + d_i f_i^{n+1} + b_i f_i^n = C_i\]

**Lax-Friedrichs method**

\[
f_i^{n+1} - \frac{b_i}{h} (f_{i+1}^n - f_i^n) + \frac{U}{2h} (f_i^n - f_{i-1}^n) = 0
\]

- Stable for \(\lambda < 1\)
- 1st order in time, 1st order in space
- Conditionally consistent

**Leap Frog Method**

The simplest stable second-order accurate (in time) method:

\[
\frac{\partial f}{\partial t} = \frac{f^{n+1} - f^n}{\Delta t} + O(\Delta t^2)
\]

\[
f_i^{n+1} = f_i^n - \frac{U}{h} \left( (\lambda - 1) f_i^n + \ldots \right)
\]

- Stable for \(|\lambda| < 1\)
- Dispersive (no dissipation) – error will not damp out
- Initial conditions at two time levels
- Oscillatory solution in time (alternating)

**Lax-Wendroff’s Method (LW-I)**

First expand the solution in time

\[
f(t + \Delta t) = f(t) + \frac{\partial f}{\partial t} \Delta t + \frac{\partial^2 f}{\partial t^2} \frac{\Delta t^2}{2} + \frac{\partial^3 f}{\partial t^3} \frac{\Delta t^3}{6} + \ldots
\]

Then use the original equation to rewrite the time derivatives

\[
\frac{\partial f}{\partial t} = -U \frac{\partial f}{\partial x}
\]

\[
\frac{\partial^2 f}{\partial t^2} = -\frac{\partial}{\partial t} \left( U \frac{\partial f}{\partial x} \right) = -U \frac{\partial}{\partial t} \frac{\partial f}{\partial x} = U^2 \frac{\partial^2 f}{\partial x^2}
\]

**Substituting**

\[
f(t + \Delta t) = f(t) - U \frac{\partial f}{\partial t} \Delta t + U^2 \frac{\partial^2 f}{\partial x^2} \frac{\Delta t^2}{2} + O(\Delta t^3)
\]

Using central differences for the spatial derivatives

\[
f_i^{n+1} = f_i^n - \frac{U h}{2 \Delta t} (f_{i+1}^n - f_i^n) + \frac{U^2 h^2}{2 \Delta t^2} (f_{i+1}^n - 2f_i^n + f_{i-1}^n)
\]

2nd order accurate in space and time

Stable for \( \frac{U h}{\Delta t} < 1 \)
Two-Step Lax-Wendroff’s Method (LW-II)

LW-I into two steps:

\[ \frac{f_{j+2}^{n+1} - (f_j^0 + f_{j+2}^0)}{2\Delta t} + U \left( \frac{f_j^{n+1} - f_j^n}{\Delta x} \right) = 0 \]  
Step 1 (Lax)

\[ \frac{f_j^{n+1} - f_j^n}{\Delta t} + U \left( \frac{f_{j+1}^{n+1} - f_{j+1}^n}{\Delta x} \right) = 0 \]  
Step 2 (Leapfrog)

- Stable for \( U\Delta t / h < 1 \)
- Second order accurate in time and space

For the linear equations, LW-II is identical to LW-I

MacCormack Method

Similar to LW-II, without \( j+1/2, j-1/2 \)

\[ f_j' = f_j^0 - U \frac{\Delta t}{h} (f_j^0 - f_j^1) \]  
Predictor

\[ f_j'' = \frac{1}{2} \left( f_j' + f_j - U \frac{\Delta t}{h} (f_j^0 - f_j^1) \right) \]  
Corrector

- A fractional step method
- Predictor: forward differencing
- Corrector: backward differencing
- For linear problems, accuracy and stability properties are identical to LW-I.

Second-Order Upwind Method

Warming and Beam (1975) – Upwind for both steps

\[ f_j' = f_j^0 - U \frac{\Delta t}{h} (f_j^0 - f_{j+1}^0) \]  
Predictor

\[ f_j'' = \frac{1}{2} \left( f_j' + f_j - U \frac{\Delta t}{h} (f_j^0 - f_{j+1}^0) - U \frac{\Delta t}{h} (f_j^0 - 2f_{j+1}^0 + f_{j+2}^0) \right) \]  
Corrector

Combining the two:

\[ f_j'' = f_j' - \lambda (f_j^0 - f_{j+1}^0) + \frac{1}{2} \lambda (\lambda - 1) (f_j^0 - 2f_{j+1}^0 + f_{j+2}^0) \]

- Stable if \( 0 \leq \lambda \leq 2 \)
- Second-order accurate in time and space

The one-step Lax-Wendroff is not easily extended to non-linear or multi-dimensional problems. The split version is.

In the Lax-Wendroff and the MacCormack methods the spatial and the temporal discretization are not independent.

Other methods have been developed where the time integration is independent of the spatial discretization, such as the Beam-Warming and various Runge-Kutta methods.
Beam-Warming

Stable for \( 0 < \lambda < 2 \)

Quick

Stable for \( \lambda < 1 \)

And Many More!

A large number of (conditionally) stable and accurate methods exist for hyperbolic equations with smooth solutions.

**Computational Fluid Dynamics**

**Summary**

\[ f_{j+1} + Uf_{j} = 0 \]

\[ \frac{3}{8} \left( f_{j} + f_{j+1} \right) + \frac{1}{8} \left( f_{j+1} - f_{j-1} \right) \]

\[ \Delta t \quad \lambda \quad \Delta x \]

**Stability in terms of Fluxes**

Consider the following initial conditions:

\[ U = 1 \]

\[ \Delta t = 1.5 \cdot U = 1.5 \]

\[ f_{j-1} = f_{j} = f_{j+1} \]

\[ F_{j+1/2} = Uf_{j} = 0 \]

\[ F_{j-1/2} = Uf_{j-1} = 1 \]

During one time step, \( U\Delta t \) of flow into cell \( j \), increasing the average value of \( f \) by \( U\Delta t / \Delta x \).

**Consider the following initial conditions:**

\[ F_{j+1/2} = Uf_{j+1/2} = U \]

\[ F_{j-1/2} = Uf_{j-1/2} = 0 \]

\[ f_{j} = f_{j+1} - \frac{\Delta t}{\Delta x} (Uf_{j+1/2} - f_{j-1/2}) = 0 - 1.5 (0 - 1) = 1.5 \]

**Computational Fluid Dynamics**

**Stability in terms of Fluxes**

Consider the following initial conditions:

\[ F_{j+1/2} = Uf_{j+1/2} = 1.5U \]

\[ F_{j-1/2} = Uf_{j-1/2} = 0.75U \]

\[ F_{j+1/2} = Uf_{j+1/2} = 2.25U \]

\[ \Delta t = 0.75 \cdot U = 0.75 \]

\[ f_{j+1} = f_{j} = f_{j+1} \]

\[ f_{j+1} = f_{j-1} - \frac{\Delta t}{\Delta x} (Uf_{j+1/2} - f_{j-1/2}) = 0 - 1.5 (0 - 1) = 2.25 \]

Taking a third step will result in an even larger positive value, and so on until the compute encounters a NaN (Not a Number).
If $\Delta t/h > 1$, the average value of $f$ in cell $j$ will be larger than in cell $j-1$. In the next step, $f$ will flow out of cell $j$ in both directions, creating a larger negative value of $f$. Taking a third step will result in an even larger positive value, and so on until the compute encounters a NaN (Not a Number).

By considering the fluxes, it is easy to see why the centered difference approximation is always unstable.

Consider the following initial conditions:

$$F_{j+\frac{1}{2}} - \frac{U}{2} (f_{j+1}^n + f_j^n) = 1.0$$

$$F_{j-\frac{1}{2}} - \frac{U}{2} (f_j^n + f_{j-1}^n) = 0.5$$

So cell $j$ will overflow immediately!

Modify the program described in class by adding a solution to the energy equation. The temperature feeds back on the flow solution by creating convective currents due to temperature differences. To account for this we use the Boussinesq approximation and add a body force term to the incompressible Navier-Stokes equations. The full equations to be solved are therefore

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = \alpha \nabla^2 T$$

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\frac{1}{\rho} \nabla p + \nu \nabla^2 u + \beta g (T - T_0)$$

where $T_0$ is the initial temperature.