Numerical Solutions to PDEs
Lecture Notes #14
— Second Order Equations —
Introduction; Finite Differences

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Outline

1 Recap
   - The ADI Method

2 Second-Order (Time) Equations
   - Examples: Wave-Equation
   - What’s in a name?! — “Hyperbolic” vs. “Parabolic”
   - The Euler-Bernoulli Beam Equation

3 Finite Differences
   - Stability for Second-Order Equations
   - Example: CTCS for the Wave Equation
   - Example: Order-(2,2) for the Euler-Bernoulli Equation

4 von Neumann Polynomials and Stability
The Alternating Direction Implicit (ADI) method allows us to solve (primarily) parabolic equations in multiple space dimension, by “slicing” higher-dimensional problems into one-dimensional sub-problems.

The “slicing” pushes the boundary of what size problem is computationally feasible.

A fully discretized ADI scheme based on a Crank-Nicolson iteration for $u_t = A_1 u + A_2 u = u_{xx} + u_{yy}$ is given by

$$\begin{bmatrix} I - \frac{k}{2} A_{1,h} \end{bmatrix} \begin{bmatrix} I - \frac{k}{2} A_{2,h} \end{bmatrix} v^{n+1} = \begin{bmatrix} I + \frac{k}{2} A_{1,h} \end{bmatrix} \begin{bmatrix} I + \frac{k}{2} A_{2,h} \end{bmatrix} v^n.$$

There are several approaches to solving this, including the Peaceman-Rachford, and D’Yakonov schemes.
We now turn our attention to PDEs with second order time derivatives, e.g.

\[ u_{tt} - a^2 u_{xx} = 0 \]  
\[ u_{tt} + b^2 u_{xxxx} = 0 \]  
\[ u_{tt} - c^2 u_{ttxx} + b^2 u_{xxxx} = 0 \]

The wave equation  
The Euler-Bernoulli (beam) equation  
The Rayleigh (beam) equation

Most of our previously developed methods and theory can be applied to these equations, with minor modifications.

Most prominently, the **definition of stability** must take the second order (time) derivative in time into account.
In one space-dimension, the second order wave equation is given by

\[ u_{tt} - a^2 u_{xx} = 0, \]

where \( a \) is a non-negative real value (the speed of propagation).

The initial value problem for this equation requires two initial conditions, typically given as

\[ u(0, x) = u_0(x), \quad u_t(0, x) = u_1(x). \]

With exact solutions given by

\[ u(t, x) = \frac{u_0(x - at) + u_0(x + at)}{2} + \frac{1}{2a} \int_{x-at}^{x+at} u_1(s) \, ds. \]
The exact solution shows that we have **two characteristic speeds** $\pm a$ associated with the second-order wave-equation.

In the Fourier domain, the solution is given by

\[
\hat{u}(t, \omega) = \hat{u}_0(\omega) \cos(a \omega t) + \hat{u}_1(\omega) \frac{\sin(a \omega t)}{a \omega}
\]

\[
= \hat{u}_+(\omega) e^{ia \omega t} + \hat{u}_-(\omega) e^{-ia \omega t}.
\]

All these expressions show that the general solution consists of two waves — one moving to the right, and one moving to the left.
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Another way of seeing this is to formally “split” the differential operator:

$$
\left[ \frac{\partial^2}{\partial t^2} - a^2 \frac{\partial^2}{\partial x^2} \right] u = \left[ \frac{\partial}{\partial t} - a \frac{\partial}{\partial x} \right] \left[ \frac{\partial}{\partial t} + a \frac{\partial}{\partial x} \right] u = 0.
$$
We fix $a = 1$, and use the following initial data

$$u_0(x) = \begin{cases} 
\cos(\pi x / 2) & |x| \leq 1, \\
0 & |x| > 1,
\end{cases} \quad u_1(x) = 0$$

The exact solution is given by

$$u(t, x) = \frac{1}{2} \left[ \cos \left( \frac{\pi (x - t)}{2} \right) + \cos \left( \frac{\pi (x + t)}{2} \right) \right].$$

**Figure:** Snapshots at $T = 0$, $T = 0.5$, and $T = 1.0$. See also the movie `wave01.mpg`
Second-Order (Time) Equations
Finite Differences
von Neumann Polynomials and Stability

Example #2: The Second-Order Wave-Equation

We fix \( a = 1 \), and use the following initial data

\[
    u_0(x) = 0, \quad u_1(x) = \begin{cases} 
        1 & |x| \leq 1, \\
        0 & |x| > 1, 
    \end{cases}
\]

The exact solution is given by

\[
    u(t, x) = \frac{1}{2} \int_{x-t}^{x+t} u_1(s) \, ds = \frac{1}{2} \text{length}\left\{ [x - t, x + t] \cap [-1, 1] \right\}.
\]

Figure: Snapshots at \( T = 0 \), \( T = 0.5 \), and \( T = 1.0 \). See also the movie wave02.mpg
Example #3: The Second-Order Wave-Equation

We fix $a = 1$, and use the following initial data

$$u_0(x) = \begin{cases} 
-\cos(\pi x/2) & |x| \leq 1, \\
0 & |x| > 1, 
\end{cases} \quad u_1(x) = \begin{cases} 
1 & |x| \leq 1, \\
0 & |x| > 1, 
\end{cases}$$

The exact solution is given by

$$u(t, x) = \frac{-1}{2} \left[ -\cos \left( \frac{\pi(x - t)}{2} \right) + \cos \left( \frac{\pi(x + t)}{2} \right) \right] + \frac{1}{2} \text{length} \{ [x - t, x + t] \cap [-1, 1] \}. $$

Figure: Snapshots at $T = 0$, $T = 0.5$, and $T = 1.0$. See also the movie wave03.mpg
The names “hyperbolic” and “parabolic” are historical, and originate from the fact that the symbols of the second-order equations are similar to the equations for hyperbolas and parabolas.

Laplace transforming in time, and Fourier transforming in the spatial coordinates, and setting $\eta = i\xi$ gives:

For $u_{tt} - a^2u_{xx} = 0$, the symbol is given by $s^2 - a^2\eta^2$,
For $u_t - bu_{xx} = 0$, the symbol is given by $s - b\eta^2$.

The solutions to

$$s^2 - a^2\eta^2 = C_h, \quad s - b\eta^2 = C_p,$$

describe hyperbolas and parabolas, respectively.
“Hyperbolic” vs. “Parabolic”

The names are just based on this formal similarity, but are now fixtures in the language of PDEs. The key to hyperbolic systems is that the solution propagates with finite speed(s), and the key to parabolic systems is that the solution becomes smoother than its initial data.

Figure: [LEFT] The hyperbolas \( s^2 - a^2 \eta^2 = C_h \) in the \((\eta, s)\)-plane; and [RIGHT] the parabolas \( s - b^2 \eta^2 = C_p \) in the \((\eta, s)\)-plane.
The Euler-Bernoulli equation

\[ u_{tt} = -b^2 u_{xxxx}, \]

describes the vertical motion of a thin horizontal beam with small displacements from rest.

Using the Fourier transform, it is straightforward to write down the exact solution

\[
\begin{align*}
    u(t, x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega x} \left[ \hat{u}_0(\omega) \cos(b\omega^2 t) + \hat{u}_1(\omega) \frac{\sin(b\omega^2 t)}{b\omega^2} \right] d\omega \\
    &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega(x+b\omega t)} \hat{u}_+(\omega) + e^{i\omega(x-b\omega t)} \hat{u}_-(\omega) d\omega
\end{align*}
\]

The second formulas show that the propagation speed is \( \pm b\omega \), hence the equation is dispersive.
The Euler-Bernoulli equation does not have finite speed of propagation, $b \omega$ is unbounded; hence it is **not hyperbolic**. [DISPERSSIVE]

Further, there is no increased smoothness in the solution as time evolves, hence it is **not parabolic**. [NON-DISSIPATIVE]
Our definitions for convergence, consistency, and order of accuracy remain the same, however we must modify or definition of stability:

**Definition (Stability for Second Order Problems)**

A finite difference scheme \( P_{k,h}v^n_m = 0 \) for an equation that is second-order in \( t \) is stable in a stability region \( \Lambda \) if there is an integer \( J \) and for any positive time \( T \) there is a constant \( C_T \) such that

\[
h \sum_{m=-\infty}^{\infty} |v^n_m|^2 \leq (1 + n^2) C_T h \sum_{j=0}^{J} \sum_{m=-\infty}^{\infty} |v^j_m|^2
\]

for all solutions \( v^n_m \) and for \( 0 \leq nk \leq T \) with \( (k, h) \in \Lambda \).

The factor \((1 + n^2)\) is new, and shows that we allow a linear growth in \( t \). \( J \) is almost always 1, since data must be given at two time-levels.
In the **von Neumann analysis** we must require that the (at least) two amplification factors satisfy

$$|g_\nu| \leq 1 + Kk$$

If there are **no lower order terms**, then the stability condition is $|g_\nu| \leq 1$ with **double roots** on the unit circle **allowed**.

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**Theorem (Stability for Second Order Problems)**

*If the amplification polynomial $\Phi(g, \theta)$ for a second-order time-dependent equation is explicitly independent of $h$ and $k$, then the necessary and sufficient condition for the finite difference scheme to be stable is that all roots, $g_\nu(\theta)$, satisfy the following conditions:*

1. $(a)$ $|g_\nu(\theta)| \leq 1$, and
2. $(b)$ if $|g_\nu(\theta)| = 1$, then $|g_\nu(\theta)|$ must be at most a double root.
The “standard” second order accurate scheme for \( u_{tt} = a^2 u_{xx} \) is:

\[
\frac{v_{m}^{n+1} - 2v_{m}^{n} + v_{m}^{n-1}}{k^2} = a^2 \frac{v_{m+1}^{n} - 2v_{m}^{n} + v_{m-1}^{n}}{h^2}
\]

As usual, we set \( v_{m}^{n} \sim g^n e^{im\theta} \) and factor out common terms, to get

\[
g - 2 - g^{-1} = -4a^2 \lambda^2 \sin^2 \left( \frac{\theta}{2} \right)
\]

\[
(g^{1/2} - g^{-1/2})^2 = (\pm 2ia\lambda \sin \left( \frac{\theta}{2} \right))^2
\]

\[
g^{1/2} - g^{-1/2} = \pm 2ia\lambda \sin \left( \frac{\theta}{2} \right)
\]

\[
g \pm 2ia\lambda \sin \left( \frac{\theta}{2} \right) \text{ } g^{1/2} - 1 = 0
\]

\[
g_{\pm}^{1/2} = \pm ia\lambda \sin \left( \frac{\theta}{2} \right) \pm \sqrt{1 - a^2 \lambda^2 \sin^2 \left( \frac{\theta}{2} \right)}
\]

\[
g_{\pm} = \left( \sqrt{1 - a^2 \lambda^2 \sin^2 \left( \frac{\theta}{2} \right)} \pm ia\lambda \sin \left( \frac{\theta}{2} \right) \right)^2
\]
We have

\[ g_{\pm} = \left( \sqrt{1 - a^2 \lambda^2 \sin^2 \left( \frac{\theta}{2} \right)} \pm i a \lambda \sin \left( \frac{\theta}{2} \right) \right)^2, \]

and it is clear that as long as \( a \lambda \leq 1 \), we have \( |g_{\pm}| \leq 1 \). At \( \theta = 0 \) \( g_+ = g_- \). The equality also occurs when \( a \lambda = 1 \), and \( \theta = \pi \).

Since we can allow two equal roots on the unit circle, we have shown that the scheme is stable if and only if \( a \lambda \leq 1 \).

**Note:** Usually we take \( a \lambda < 1 \) to avoid the linear growth of the wave with \( \phi = \pi \), where \( g_{\pm} = (\pm i)^2 = -1 \), even though this growth (formally) does not affect the stability of the scheme.
The simplest second-order accurate scheme is given by

\[
\frac{v_{m}^{n+1} - 2v_{m}^{n} + v_{m}^{n-1}}{k^2} = -b^2 \frac{v_{m+2}^{n} - 4v_{m+1}^{n} + 6v_{m}^{n} - 4v_{m-1}^{n} + v_{m-2}^{n}}{h^4}
\]

The amplification factors are given by the roots of

\[
g - 2 + g^{-1} = -16b^2 \mu^2 \sin^4 \left( \frac{\theta}{2} \right), \quad \mu = \frac{k}{h^2}
\]

It is stable if and only if

\[
2b\mu \sin^2 \left( \frac{\theta}{2} \right) \leq 1 \iff b\mu \leq \frac{1}{2}
\]
All schemes for second order (time) equations require some initialization of $\nu_m^1$. With

$$u(0, x) = u_0(x), \quad u_t(0, x) = u_1(x),$$

given, the simplest procedure is based on the Taylor expansion:

$$u(k, x) \sim u_0(x) + ku_1(x) + \frac{1}{2}k^2 u_{tt}(0, x) + O(k^3).$$

Using $u_{tt} = a^2 u_{xx}$, we get a second order accurate initialization from

$$\frac{\nu_m^1 - [u_0]_m}{k} = [u_1]_m + \frac{a^2 k \delta_x^2}{2} \nu_m^0.$$  

**Note:** The initialization should be of the same order of accuracy as the scheme in order not to degrade the overall method.
We can modify our previously defined algorithms for von Neumann and Schur polynomials, to test for the stability of second-order schemes.

First we extend

**Old Definition: von Neumann Polynomial**

The polynomial \( \varphi \) is a von Neumann polynomial if all its roots, \( r_\nu \), satisfy \( |r_\nu| \leq 1 \).

**Definition (von Neumann and Schur Polynomials)**

The polynomial \( \varphi \) is a von Neumann polynomial of order \( q \) if all its roots, \( r_\nu \), satisfy the following conditions:

(a) \( |r_\nu| \leq 1 \), and

(b) the roots with \( |r_\nu| = 1 \) have multiplicity at most \( q \).

A von Neumann polynomial of order 0 is defined to be a Schur polynomial.
Old Theorem (von Neumann Polynomial Test)

\( \varphi_d \) is a von Neumann polynomial of degree \( d \), if and only if either

(a) \(|\varphi_d(0)| < |\varphi^*_d(0)|\) and \( \varphi_{d-1} \) is a von Neumann polynomial of degree \( d - 1 \), or

(b) \( \varphi_{d-1} \) is identically zero and \( \varphi'_d \) is a von Neumann polynomial.

Theorem (von Neumann Polynomial Test)

A polynomial \( \varphi_d \) of exact degree \( d \) is a von Neumann polynomial of order \( q \), if and only if either

(a) \(|\varphi_d(0)| < |\varphi^*_d(0)|\) and \( \varphi_{d-1} \) is a von Neumann polynomial of degree \( d - 1 \) and order \( q \), or

(b) \( \varphi_{d-1} \) is identically zero and \( \varphi'_d \) is a von Neumann polynomial of order \( q - 1 \).
With this more general definition, we have that a simple von Neumann polynomial is a von Neumann of degree 1.

Also, these generalizations explain some of the parts of the algorithm:

**Algorithm**

Start with \( \varphi_d(z) \) of exact degree \( d \), and set NeumannOrder = 0.

while \( (d > 0) \) do

1. Construct \( \varphi_d^*(z) \)
2. Define \( c_d = |\varphi_d^*(0)|^2 - |\varphi_d(0)|^2 \). (*)
3. Construct the polynomial \( \psi(z) = \frac{1}{z}(\varphi_d^*(0)\varphi_d(z) - \varphi_d(0)\varphi_d^*(z)) \).
   4.1. If \( \psi(z) \equiv 0 \), then increase NeumannOrder by 1, and set \( \varphi_{d-1}(z) := \varphi_d'(z) \).
   4.2. Otherwise, if the coefficient of degree \( d - 1 \) in \( \psi(z) \) is 0, then the polynomial is not a von Neumann polynomial of any order, terminate algorithm.
   4.3. Otherwise, set \( \varphi_{d-1}(z) := \psi(z) \).

end-while (decrease \( d \) by 1)

(*) Enforce appropriate conditions on \( c_d \).
The new theorem (and the algorithm) can be used to analyze stability for second order equations.

If $\Phi(g, \theta)$ is the amplification polynomial of finite difference scheme for a second order equation for which the restricted condition $|g_\nu(\theta)| \leq 1$ can be used, then the scheme is stable if and only if $\Phi(g, \theta)$ is a von Neumann polynomial of order 2.

**Next time:** Boundary conditions; two and three spatial dimensions.