Numerical Solutions to PDEs

Lecture Notes #8
— Stability for Multistep Schemes —
Schur and von Neumann Polynomials

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1 Recap
   - In a previous episode of Math 693b...

2 Stability
   - “Proof” by Picture...
   - Beyond “Proof by Picture” — Building a Theoretical Toolbox

3 Schur and von Neumann Polynomials
   - Definitions and Theorems
   - Examples: Revisited with Theoretical Toolbox in Hand...
   - Algorithm for von Neumann / Schur Polynomials
Previously...

We looked at stability for multistep schemes. — First, we did a complete analysis of the stability picture for the leapfrog scheme,

\[
\frac{v_{m+1}^{n+1} - v_{m-1}^{n-1}}{2k} + a \frac{v_{m+1}^n - v_{m-1}^n}{2h} = 0
\]

in which we found bounds for the roots of

\[
g(\theta)^2 + \left[ 2ia\lambda \sin(\theta) \right] g(\theta) - 1 = 0
\]

so that \(|g_{\pm}(\theta)| \leq 1\) for simple roots and \(|g_{\pm}(\theta)| < 1\) for multiple roots.

The analysis for general multi-step scheme has the same “flavor,” but we postponed the development of a unified framework for that analysis until today.
Last time, we boldly stated that the scheme

\[
\frac{3v_{m+1}^n - 4v_m^n + v_{m-1}^n}{2k} + a \frac{v_{m+1}^{n+1} - v_{m-1}^{n+1}}{2h} = f_{m+1}^n
\]

with amplification polynomial

\[
\Phi(g, \theta) = \left[ \frac{3 + 2ia\lambda \sin(\theta)}{2} \right] g^2 - 2g + \frac{1}{2}
\]

is unconditionally stable, and order-(2,2) accurate.

Whereas pictures are not proof, the plots of the roots for various values of \(a\lambda\) and \(\theta \in [-\pi, \pi]\) shown on slide 7 seem to indicate that the stability is indeed unconditional.
Sure, we can take the amplification polynomial

\[ \Phi(g, \theta) = \left[ \frac{3 + 2ia\lambda \sin(\theta)}{2} \right] g^2 - 2g + \frac{1}{2} = 0 \]

and formally apply the quadratic formula

\[ g_{\pm}(\theta) = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{4 \pm \sqrt{2 - 4 \left[ \frac{3+2ia\lambda \sin(\theta)}{2} \right] \frac{1}{2}}}{2 \left[ \frac{3+2ia\lambda \sin(\theta)}{2} \right]} \]

\[ \leadsto g_{\pm}(\theta) = \frac{2 \pm \sqrt{1 - 2ia\lambda \sin(\theta)}}{3 + 2ia\lambda \sin(\theta)} \]
Example: Unnamed Scheme From Last Time

\[ g_{\pm}(\theta) = \frac{2 \pm \sqrt{1 - 2ia\lambda \sin(\theta)}}{3 + 2ia\lambda \sin(\theta)} \]

\[ \leadsto g_{\pm}(\theta) = \frac{(2 \pm \sqrt{1 - 2ia\lambda \sin(\theta)}) (3 - 2ia\lambda \sin(\theta))}{9 + 4(a\lambda)^2 \sin^2(\theta)} \]

Next, define an appropriate branch for the square-root in the complex plane; chase down the various cases... and there it is?!
Example: Unnamed Scheme From Last Time

- $a\lambda = 1$
- $a\lambda = 4$
- $a\lambda = 16$
- $a\lambda = 64$
Example #2: Another Second-Order Accurate Scheme

The second order accurate scheme

\[
\frac{7v_{n+1}^m - 8v_n^m + v_{n-1}^m}{6k} + a\delta_0 \left[ \frac{2v_{n+1}^m + v_n^m}{3} \right] = f_{m}^{n+2/3}
\]

has the amplification polynomial

\[
\Phi(g) = \left[ 7 + 4i\beta \right] g^2 - \left[ 8 - 2i\beta \right] g + 1
\]

where \( \beta = a\lambda \sin(\theta) \). Also seems to have pretty decent stability properties (see next slide).
Example #2: Root Plots

- For $a\lambda = 1$, the roots are all located within the unit circle.
- For $a\lambda = 4$, the roots are still within the unit circle but closer to the boundary.
- For $a\lambda = 16$, the roots are all located on the boundary of the unit circle.
- For $a\lambda = 64$, the roots are all located at the origin.

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Example #3: An Order-(3,4) Accurate Scheme

The (3,4)-order accurate scheme

$$\frac{23v_{m}^{n+1} - 21v_{m}^{n} - 3v_{m}^{n-1} + v_{m}^{n-2}}{24k} + \left[ 1 + \frac{h^2}{6} \delta^2 \right]^{-1} \cdot \left[ a \delta_0 \left( \frac{v_{m}^{n+1} + v_{m}^{n}}{2} \right) + \frac{k^2 a^2}{8} \delta^2 \left( \frac{v_{m}^{n+1} - v_{m}^{n}}{k} \right) \right] = f_{m}^{n+1/2},$$

has the amplification polynomial

$$\Phi(g) = \left[ 23 - 12\alpha + 12i\beta \right] g^3 - \left[ 21 - 12\alpha - 12i\beta \right] g^2 - 3g + 1,$$

where

$$\alpha = \frac{a^2 \lambda^2 \sin^2 \left( \frac{\theta}{2} \right)}{1 - \frac{2}{3} \sin^2 \left( \frac{\theta}{2} \right)}, \quad \beta = \frac{a \lambda \sin \left( \theta \right)}{1 - \frac{2}{3} \sin^2 \left( \frac{\theta}{2} \right)}.$$

Does not seem to be unconditionally stable...

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Example #3: Root Plots

- $a\lambda = 0.5$
- $a\lambda = 0.66667$
- $a\lambda = 0.75$
- $a\lambda = 0.8$

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Schur and von Neumann Polynomials
Example #4: An Order-(4,4) Accurate Scheme

The (4,4)-order accurate scheme

$$\frac{v_{n+2} - v_{n-2}}{4k} + a \left[ 1 + \frac{h^2}{6} \right]^{-1} \delta_0 \left( \frac{2v_{n+1}^n - v_n^m + 2n^{-1}}{3} \right)$$

has the amplification polynomial

$$\Phi(g) = g^4 + \frac{4}{3} i\beta \left( 2g^3 - g^2 + 2g \right) - 1,$$

where

$$\beta = \frac{a\lambda \sin (\theta)}{1 - \frac{2}{3} \sin^2 \left( \frac{\theta}{2} \right)}.$$

Does not seem to be unconditionally stable...
Example #4: Root Plots

- $a^\lambda = 0.2$
- $a^\lambda = 0.25$
- $a^\lambda = 0.3$
- $a^\lambda = 0.4$

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Moving Beyond “Proof By Picture”

Looking at the expressions and corresponding figures in the previous examples, it is quite clear that the analysis, *i.e.* the determination and bounding of the roots of these polynomials is quite a task.

The good news is that there is a well-developed theory and an algorithm for checking whether the roots of these polynomials satisfy the stability conditions: —

**Theorem (Stability of Multistep Schemes)**

*If the amplification polynomial \( \Phi(g, \theta) \) 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:*

(a)  \( |g_\nu(\theta)| \leq 1 \), and

(b)  *if \( |g_\nu(\theta)| = 1 \), then \( g_\nu(\theta) \) must be a simple root.*
Let \( \varphi_d(z) = a_d z^d + \cdots + a_0 = \sum_{\ell=0}^d a_\ell z^\ell \) be a polynomial of degree \( d \). If \( a_d \neq 0 \), then \( \varphi \) is of exact degree \( d \).

**Definition (Schur Polynomial)**

The polynomial \( \varphi \) is a Schur polynomial if all its roots, \( r_\nu \), satisfy \(|r_\nu| < 1\).

**Definition (von Neumann Polynomial)**

The polynomial \( \varphi \) is a von Neumann polynomial if all its roots, \( r_\nu \), satisfy \(|r_\nu| \leq 1\).
Let \( \varphi_d(z) = a_d z^d + \cdots + a_0 = \sum_{\ell=0}^{d} a_{\ell} z^{\ell} \) be a polynomial of degree \( d \). If \( a_d \neq 0 \), then \( \varphi \) is of exact degree \( d \).

**Definition (Simple von Neumann Polynomial)**

The polynomial \( \varphi \) is a simple von Neumann polynomial if \( \varphi \) is a von Neumann polynomial, and its roots on the unit circle are simple roots.

**Definition (Conservative Polynomial)**

The polynomial \( \varphi \) is a conservative polynomial if all its roots lie on the unit circle, i.e. \( |r_\nu| = 1 \).
For a polynomial of exact degree $d$, we define the polynomial

$$\varphi^*(z) = \sum_{\ell=0}^{d} \bar{a}_{d-\ell} z^\ell \equiv \varphi(1/\bar{z})z^d,$$

where $\bar{z}$ is the complex conjugate of $z$.

We recursively define the polynomial $\varphi_{d-1}$ of exact degree $d - 1$ by

$$\varphi_{d-1}(z) = \frac{\varphi^*(0)\varphi_d(z) - \varphi_d(0)\varphi^*_d(z)}{z} \equiv \frac{\bar{a}_d\varphi_d(z) - a_0\varphi^*_d(z)}{z}.$$

We are now ready to state theorems which provide tests for Schur and simple von Neumann polynomials.
Theorem (Schur Polynomial Test)

\( \varphi_d \) is a Schur polynomial of exact degree \( d \) if and only if \( \varphi_d - 1 \) is a Schur polynomial of exact degree \( d - 1 \) and \( |\varphi_d(0)| < |\varphi^*_d(0)| \).

Theorem (Simple von Neumann Polynomial Test)

\( \varphi_d \) is a simple von Neumann polynomial if and only if either

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

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

The (somewhat lengthy) proofs, which depend on Rouché’s theorem (complex analysis) are in Strikwerda pp. 110–114.
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 (Conservative Polynomial Test)

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

Theorem (Simple Conservative Polynomial Test)

\( \varphi_d \) is a simple conservative polynomial if and only if \( \varphi_{d-1} \) is identically zero and \( \varphi'_d \) is a Schur polynomial.
The scheme had the amplification polynomial

\[ \varphi_2(z) = \left[ \frac{3 + 2ia\lambda \sin(\theta)}{2} \right] z^2 - 2z + \frac{1}{2}. \]

It is stable exactly when \( \varphi_2(z) \) is a simple von Neumann polynomial. We make repeated use of the simple-von-Neumann-polynomial-test in order to check stability of the scheme.

We first test \( |\varphi_2(0)|^2 = \frac{1}{4} < \frac{1}{4} \left( 3^2 + 4a^2\lambda^2 \sin^2(\theta) \right) = |\varphi_2^*(0)|^2 \), then define, with \((c + di)\) being the coefficient in front of \(z^2\) in \(\varphi_2(z)\):

\[ \varphi_1(z) = \frac{1}{z} \left[ (c-di) \left( (c+di)z^2 - 2z + \frac{1}{2} \right) - \frac{1}{2} \left( (c-di) - 2z + \frac{1}{2}z^2 \right) \right] \]

\[ = \left( d^2 + c^2 - \frac{1}{4} \right) z + (1 - 2c + 2id) \]
Now, \( \varphi_1(z) \) is a simple von Neumann polynomial as long as

\[
\left(d^2 + c^2 - \frac{1}{4}\right)^2 \geq (1 - 2c)^2 + 4d^2 = 1 + 4c^2 + 4d^2 - 4c
\]

where \( c = \frac{3}{2} \), and \( d = a\lambda \sin(\theta) \).

Plugging in we must have

\[
a^4\lambda^4 \sin^4(\theta) + 4a^2\lambda^2 \sin^2(\theta) + 4 \geq 4a^2\lambda^2 \sin^2(\theta) + 4
\]

Which holds strictly for \( \sin(\theta) \neq 0 \), and with equality when \( \sin(\theta) = 0 \).

**Conclusion:** The scheme is unconditionally stable.
The scheme had the amplification polynomial

$$\varphi_2(z) = \left[7 + 4i\beta\right]z^2 - \left[8 - 2i\beta\right]z + 1$$

it is stable exactly when $\varphi_2(z)$ is a simple von Neumann polynomial. We make repeated use of the simple-von-Neumann-polynomial-test in order to check stability of the scheme.

With $\beta = a\lambda \sin(\theta)$, we first test $|\varphi_2^*(0)| = |7 - 4i\beta| > 1 = |\varphi_2(0)|$, then define

$$\varphi_1(z) = \frac{1}{z} \left( (7 - 4i\beta) \left( [7 + 4i\beta]z^2 - [8 - 2i\beta]z + 1 \right) \right.$$

$$\left. - 1 \left( [7 - 4i\beta] - [8 + 2i\beta]z + z^2 \right) \right)$$

$$= 4 \left( (12 + 4\beta^2)z + ((2\beta^2 - 12) + 12i\beta) \right).$$
$$\varphi_1(z) = 4 \left( (12 + 4\beta^2) z + (2\beta^2 - 12) + 12i\beta \right)$$

is a simple von Neumann polynomial if and only if

$$|\varphi_1(0)|^2 = |(2\beta^2 - 12) + 12i\beta|^2 = (12 - 2\beta^2)^2 + 12^2\beta^2$$

$$= 144 + 96\beta^2 + 4\beta^4 \leq |\varphi_1^*(0)|^2 = (12 + 4\beta^2)^2 = 144 + 96\beta^2 + 16\beta^4$$

The inequality holds strictly as long as $$\beta \neq 0$$, in which case we get equality.

**Note:** Since $$\varphi_1(z)$$ only has one root, it is sufficient to bound that root by \( \leq 1 \) in order for $$\varphi_1(z)$$ to be a simple von Neumann polynomial.

**Conclusion:** The scheme is unconditionally stable.
Stability

Schur and von Neumann Polynomials

Definitions and Theorems

Examples: Revisited with Theoretical Toolbox in Hand...

Algorithm for von Neumann / Schur Polynomials

Example #3: Revisited

In this case the amplification polynomial is given by

\[ \varphi_3(z) = \left[ 23 - 12 \alpha + 12 i \beta \right] z^3 - \left[ 21 - 12 \alpha - 12 i \beta \right] z^2 - 3z + 1 \]

where

\[ \alpha = \frac{a^2 \lambda^2 \sin^2 \left( \frac{\theta}{2} \right)}{1 - \frac{2}{3} \sin^2 \left( \frac{\theta}{2} \right)} \in [0, 3a^2 \lambda^2], \quad \beta = \frac{a \lambda \sin \theta}{1 - \frac{2}{3} \sin^2 \left( \frac{\theta}{2} \right)} \in [-a \lambda \sqrt{3}, a \lambda \sqrt{3}] . \]

The first check \(|\varphi_3(0)| < |\varphi^*_3(0)|\) can be expressed as

\(|\varphi^*_3(0)|^2 - |\varphi_3(z)|^2 > 0, \) and we get

\[ |\varphi^*_3(0)|^2 - |\varphi_3(0)|^2 = 24(2 - \alpha)(11 - 6 \alpha) + 12^2 \beta^2 \]

we see that we must require \(0 \leq \alpha \leq \frac{11}{6}\) for stability.
The polynomial $\varphi_2(z)$ is (after division by the common factor 24)

$$
\varphi_2(z) = \left[ (11 - 6\alpha)(2 - \alpha) + 6\beta^2 \right] z^2
- 2 \left[ (2 - \alpha)(5 - 3\alpha) - 3\beta^2 - (11 - 6\alpha)i\beta \right] z - (2 - \alpha - 2i\beta),
$$

and

$$
|\varphi_2^*(0)|^2 - |\varphi_2(0)|^2 = 4(5 - 3\alpha) \left[ 3(2 - \alpha)^3 + \beta^2(13 - 6\alpha) \right] + 36\beta^4.
$$

This now requires that $0 \leq \alpha \leq \frac{5}{3} < \frac{11}{6}$ for stability.
Finally, the polynomial \( \varphi_1(z) \) is

\[
\varphi_1(z) = \left[ 120 - 252\alpha + 198\alpha^2 - 69\alpha^3 + 9\alpha^4(18\alpha^2 - 69\alpha + 65)\beta^2 + 9\beta^4 \right] z
\]

\[
+ 9\beta^4 + 6(5 - 3\alpha)i\beta^3 + (3\alpha - 5)\beta^2 - \left(18\alpha^3 + 102\alpha^2 + 192\alpha - 120\right)i\beta
\]

\[
- 9\alpha^4 + 69\alpha^3 - 198\alpha^2 + 252\alpha - 120
\]

The root-condition \( |\varphi_1^*(0)|^2 - |\varphi_1(0)|^2 > 0 \) translates to

\[
12\beta^4(5 - 3\alpha) \left[ 6\beta^2 + (11 - 6\alpha)(2 - \alpha) \right] > 0
\]

This holds in the range \( 0 \leq \alpha \leq \frac{5}{3} \); our strictest bound on \( \alpha \).
We now have that
\[
\alpha = |a\lambda|^2 \frac{\sin^2 \left( \frac{\theta}{2} \right)}{1 - \frac{2}{3} \sin^2 \left( \frac{\theta}{2} \right)} \leq \frac{5}{3}
\]
\[
\in [0, 3]
\]
and it follows that the scheme is stable if and only if
\[
|a\lambda| \leq \frac{\sqrt{5}}{3} \approx 0.7454 \ldots
\]
\[ \varphi_4(z) = z^4 + \frac{4}{3} i \beta \left( 2z^3 - z^2 + 2z \right) - 1, \quad \beta = \frac{a \lambda \sin(\theta)}{1 - \frac{2}{3} \sin^2 \left( \frac{\theta}{2} \right)} \in [-a \lambda \sqrt{3}, a \lambda \sqrt{3}] \]

Here, \(|\varphi_4(0)| = |\varphi^*_4(0)| = 1\). But \(\varphi_3(z) \equiv 0\), hence there is still hope, for \(\varphi_4(z)\) being a simple von Neumann polynomial. We must test whether \(\psi_3(z) = \frac{3}{4} \varphi_4'(z) = 3z^3 + i \beta (6z^2 - 2z + 2)\) is a Schur polynomial.

\[ |\psi^*_3(0)| - |\psi_3(0)| = 3 - |2\beta| > 0, \text{ as long as } |\beta| < \frac{3}{2}. \]

We form

\[ \psi_2(z) = (9 - 4\beta^2)z^2 + (4\beta^2 + 18i\beta)z - 12\beta^2 - 6i\beta \]

\[ |\psi^*_2(0)|^2 - |\psi_2(0)|^2 > 0 \text{ if and only if } (9 - 4\beta^2)^2 > (12\beta^2)^2 + (6\beta)^2, \]

which gives \(\beta^2 < \frac{9}{64} \left[ \sqrt{41} - 3 \right] < \frac{9}{4}\).
Next, we form

$$\psi_1(z) = \left( 81 - 108\beta^2 - 128\beta^4 \right)z + \left( [32\beta^4 + 144\beta^2] - i [264\beta^3 - 162\beta] \right)$$

The one root is inside the unit circle only if

$$\left( 81 - 108\beta^2 - 128\beta^4 \right)^2 - \left( [32\beta^4 + 144\beta^2]^2 + [264\beta^3 - 162\beta]^2 \right) \geq 0.$$  

This expression can be factored as

$$3\left( 9 - 4\beta^2 \right) \left( 3 - 16\beta^2 \right) \left( \beta^2 (80\beta^2 - 72) + 81 \right) \geq 0.$$  

Hence, $\psi_1(z)$ is a Schur polynomial for

$$\beta^2 < \frac{3}{16} < \frac{9}{64} [\sqrt{41} - 3].$$
Hence, our final stability condition is

$$|\beta| = \frac{|a\lambda \sin(\theta)|}{1 - \frac{2}{3} \sin^2 \left(\frac{\theta}{2}\right)} < \frac{\sqrt{3}}{4}.$$ 

The maximum occurs when \(\cos(\theta) = -1/2\), and the scheme is stable when \(|a\lambda| < \frac{1}{4}\).

Note that even though the scheme is implicit, it is not unconditionally stable.
Algorithm for von Neumann / Schur Polynomials

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

\begin{algorithm}
\textbf{while} \( (d > 0) \) \textbf{do}
\begin{enumerate}
\item Construct \( \varphi_d^*(z) \)
\item Define \( c_d = |\varphi_d^*(0)|^2 - |\varphi_d(0)|^2 \). (*)
\item Construct the polynomial \( \psi(z) = \frac{1}{z}(\varphi_d^*(0)\varphi_d(z) - \varphi_d(0)\varphi_d^*(z)) \).
\item.1 If \( \psi(z) \equiv 0 \), then increase NeumannOrder by 1, and set \( \varphi_{d-1}(z) := \varphi'_d(z) \).
\item.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, \textbf{terminate algorithm}.
\item.3 Otherwise, set \( \varphi_{d-1}(z) := \psi(z) \).
\end{enumerate}
\textbf{end-while} (decrease \( d \) by 1)
\end{algorithm}

(*) Enforce appropriate conditions on \( c_d \).
Comments on the Algorithm

At the end of the algorithm, if the polynomial has not been rejected by 4.2 —

- The polynomial is a von Neumann polynomial of the resulting order (NeumannOrder) provided that all the parameters $c_d$ satisfy the appropriate inequalities. — These inequalities provide the stability conditions.

- For first-order PDEs, the amplification polynomial must be a von Neumann polynomial of order 1 for the scheme to be stable.

- For second-order PDEs, the amplification polynomial must be a von Neumann polynomial of order 2 for the scheme to be stable.

- Schur polynomials are von Neumann polynomials of order 0.

This analysis can be automated using a symbolic toolbox. — Again, we have reduced something complicated to a deterministic “recipe.”