In search of stability: Runge–Kutta methods and Richardson extrapolation

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Outline

- Stability analysis of DIRK methods
  - 2-stage methods
  - 3-stage methods
- Richardson extrapolation
  - Richardson extrapolated Runge–Kutta methods
  - Stability analysis of Richardson extrapolated Runge–Kutta methods

Previously

Theorem

For a nonconfluent RK method the following implications hold:

$$\left\{\begin{array}{c}\text{Algebraic stability}\\ \Updownarrow \\ \text{BN-stability}\\ \Updownarrow \\ \text{AN-stability}\end{array}\right\} \Longrightarrow \text{B-stability} \Longrightarrow \text{A-stability}.$$

Theorem

For a genereal RK method the following implications hold:

$$\text{Algebraic stability} \Longrightarrow \left\{\begin{array}{ccc}\text{BN-stability} & \Rightarrow & \text{B-stability}\\ & & \Downarrow \\ \text{AN-stability} & \Rightarrow & \text{A-stability}\end{array}\right\}.$$

Stability analysis of DIRK methods

- We require implicit methods for good stability properties.
- We want to minimize the number of variables.

$$\Downarrow$$

- Ideal choice is DIRK methods.
- We use the theorem for nonconfluent methods:

$$\text{Algebraic stability} \iff \text{BN-stability} \iff \text{AN-stability.}$$

$$\Downarrow$$

We focus on nonconfluent DIRK methods.

First try

$$\begin{array}{c|cc} a_1 & a_1 & 0 \\ a_2+a_3 & a_2 & a_3 \\ \hline & b & 1-b \end{array}$$

Where $a_1 \neq a_2 + a_3$. The matrices B and M are

$$B = \begin{pmatrix} b & 0 \\ 0 & 1-b \end{pmatrix}$$

$$M = \begin{pmatrix} 2a_1 b - b^2 & (1-b)a_2 - b(1-b) \\ (1-b)a_2 - b(1-b) & 2a_3(1-b) - (1-b)^2 \end{pmatrix}$$

Simplifying conditions: $a_1 = a_3 := a$, $b = 1/2$, Then

$$M = \begin{pmatrix} a - \frac{1}{4} & \frac{1}{2}a_2 - \frac{1}{4} \\ \frac{1}{2}a_2 - \frac{1}{4} & a - \frac{1}{4} \end{pmatrix}.$$

First try

- Complete the square in the quadratic form
- introduce second order conditions

$$\Downarrow$$

$$a = \frac{1}{4}, \qquad a_2 = \frac{1}{2}$$

$$\begin{array}{c|cc} \frac{1}{4} & \frac{1}{4} & 0 \\ \frac{3}{4} & \frac{1}{2} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Qin and Zhang's method

Problems:

- Several assumptions
- Only one method derived

Pareschi and Russo

$$\begin{array}{c|cc} a & a & 0 \\ 1-a & 1-2a & a \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Second order, singly diagonal Runge–Kutta method (SDIRK)
Third order when $a^2 - a + \frac{1}{6} = 0$ holds.
The weights $b_{1,2} = 1/2 \Rightarrow$ the martix B is positive definite
The matrix M:

$$M = \begin{pmatrix} a - \frac{1}{4} & \frac{1}{4} - a \\ \frac{1}{4} - a & a - \frac{1}{4} \end{pmatrix}.$$

Eigenvalues: $\lambda_1 = 0$, $\lambda_2 = 2(a - \frac{1}{4})$

$$\text{Algebraically stable} \iff a \geq \frac{1}{4}$$

Pareschi and Russo, A-stability

Theorem

Let the stability function $R(z)$ be of the form $R(z) = \frac{N(z)}{D(z)}$ where N and D are polynomials of z and define the E-polynomial by

$$E(y) = D(iy)D(-iy) - N(iy)N(-iy).$$

A Runge–Kutta method with stability function $R(z)$ is A-stable if and only if all poles of R (that is all roots of D) are in the right half plane, and $E(y) \geq 0 \ \forall y \in \mathbb{R}$.

Root of $D(z) = 1/a \implies a > 0$

$$E(y) = \frac{1}{4}(1-2a)^2(4a-1)y^4$$

Condition for A-stability: $a \geq \frac{1}{4}$.
No additional stable method found

First order, second stage DIRK method

a	a	0
1	$1-a$	a
	$1-a$	a

First order for any a, second order when $a^2 - 2a + \frac{1}{2} = 0$ holds
For algebraic stability: matrix B is positive semidefinite $\Leftrightarrow a \in [0,1]$

Matrix M:

$$M = \begin{pmatrix} -3a^2 + 4a - 1 & 0 \\ 0 & a^2 \end{pmatrix}.$$

Algebraically stable $\Longleftrightarrow$ $a \in \left[\frac{1}{3}, 1\right]$

Condition for A-stability: $\frac{2-\sqrt{2}}{2} \leq a \leq \frac{2+\sqrt{2}}{2}$

Crouzeix's 2-stage third order method

$$
\begin{array}{c|cc}
\dfrac{3\mu-1}{6\mu} & \dfrac{3\mu-1}{6\mu} & 0 \\
\dfrac{1+\mu}{2} & \mu & \dfrac{1-\mu}{2} \\
\hline
 & \dfrac{3\mu^2}{3\mu^2+1} & \dfrac{1}{3\mu^2+1}
\end{array}
$$

Third order for any $\mu \neq 0$

Algebraic stability:

- Weights are positive for any $\mu \neq 0 \implies B$ is positive definite
- Harder to check conditions for matrix M
- Idea: factor out $1/(3\mu^2+1)^2$

Crouzeix's 2-stage third order method

$$M = \frac{1}{(3\mu^2+1)^2}\widetilde{M}$$

$$\widetilde{M} = \begin{pmatrix} (3\mu^2-\mu)(3\mu^2+1)-9\mu^2 & \mu(3\mu^2+1)-3\mu^2 \\ \mu(3\mu^2+1)-3\mu^2 & (1-\mu)(3\mu^2+1)-1 \end{pmatrix}$$

By simplifying $\widetilde{M}$:

$$M = \frac{\mu(3\mu^2-3\mu+1)}{(3\mu^2+1)^2}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$$

Eigenvalues: $\lambda_1 = 0$, $\lambda_2 = -2$

Algebraically stable $\iff$ $\mu < 0$

Crouzeix's 3-stage fourt order method

$$
\begin{array}{c|ccc}
\frac{1+v}{2} & \frac{1+v}{2} & 0 & 0 \\
\frac{1}{2} & -\frac{v}{2} & \frac{1+v}{2} & 0 \\
\frac{1-v}{2} & 1+v & -1-2v & \frac{1+v}{2} \\
\hline
 & \frac{1}{6v^2} & 1-\frac{1}{3v^2} & \frac{1}{6v^2}
\end{array}
$$

Third order for any $v \neq 0$, fourth order when $3v^3 - 3v - 1 = 0$ holds.
We focus only on the fourth order case

Crouzeix's 3-stage fourt order method

We use the same idea as before to simplify M:

$$M = \frac{1}{36v^4}\widetilde{M}$$

$$\widetilde{M} = \begin{pmatrix} 6v^3 + 6v^2 - 1 & -18v^5 + 6v^3 - 6v^2 + 2 & 6v^3 + 6v^2 - 1 \\ -18v^5 + 6v^3 - 6v^2 + 2 & 36v^5 - 12v^3 + 12v^2 - 4 & -12v^3 - 12v^2 + 2 \\ 6v^3 + 6v^2 - 1 & -12v^3 - 12v^2 + 2 & 6v^3 + 6v^2 - 1 \end{pmatrix}$$

Crouzeix's 3-stage fourt order method

We use the fourth order condition $3v^3 - 3v - 1 = 0$ to eliminate higher order terms of $\widetilde{M}$

$$M = \frac{6v^2 + 6v + 1}{36v^4} \begin{pmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{pmatrix}$$

Eigenvalues: $\lambda_{1,2} = 0$, $\lambda_3 = 6$
Condition for algebraic stability: $6v^2 + 6v + 1 \geq 0$
Only the method with $v = \frac{2}{\sqrt{3}} \cos \frac{\pi}{18}$ will be algebraically stable

Richardson extrapolation

- Convergence acceleration method
- Used for numerical integration and for solving ODEs and PDEs
- Goals:
  - Stability analysis of Richardson extrapolated Runge–Kutta methods
  - Improve stability properties (if possible)

Richardson extrapolation

General method:

- Problem: $y'(t) = f(t, y(t))$,
- Equidistant grid with stepsize h,
- Suppose our RK method has order p,
- Suppose we have y_n

Then

- Take a step with h: $v_{n+1} \approx y(t_{n+1})$,
- Take two steps with $h/2$: $w_{n+1} \approx y(t_{n+1})$,
- Calculate y_{n+1} using $y_{n+1} = \dfrac{2^p w_{n+1} - v_{n+1}}{2^p - 1}$.

Richardson extrapolation

Questions to answer:

- When should we use the new method?
  - The new method takes 3 times more steps
  - $h_{\text{new}} > 3h_{\text{old}}$
- Will we use y_{n+1} to calculate the next improved approximation?
  - No: Passive Richardson extrapolation
  - Yes: Active Richardson extrapolation

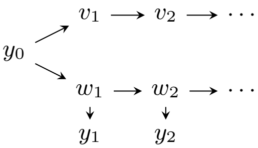

Figure: Passive implementation of Richardson extrapolation

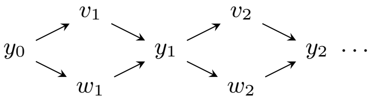

Figure: Active implementation of Richardson extrapolation

RE + RK methods

Suppose our RK method is of order p, with the stability function $R(z)$

$$v_{n+1} = R(z)y_n,$$
$$w_{n+1} = R^2\left(\frac{z}{2}\right)y_n.$$

Thus,

$$y_{n+1} = \frac{2^p w_{n+1} - z_{n+1}}{2^p - 1} y_n = \frac{2^p R^2\left(\frac{z}{2}\right) - R(z)}{2^p - 1} y_n.$$

Stability function of the Richardson extrapolated method will take the form:

$$R_{RE}(z) = \frac{2^p R^2\left(\frac{z}{2}\right) - R(z)}{2^p - 1}$$

RE + explicit RK methods

Theorem

For any explicit Runge–Kutta method with $s = p$, $p = 1, 2, 3, 4$ orders and stages, the stability region of the Richardson extrapolated method is greater than the stability region of the underlying Runge–Kutta method.

RE + explicit RK methods

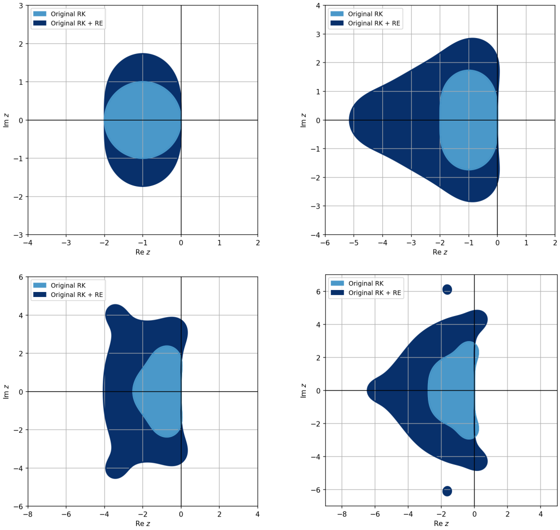

Figure: $s = p = 1, 2, 3, 4$ explicit Runge–Kutta and their Richardson extrapolated methods' stability regions

RE + explicit RK methods

New idea: Let $s \neq p$, then,

$$R(z) = 1 + z + \ldots + \frac{z^p}{p!} + \frac{z^{p+1}}{\gamma_{p+1}^{(s,p)}(p+1)!} + \ldots + \frac{z^s}{\gamma_s^{(s,p)} s!}$$

When $s = 4$, $p = 3 \Longrightarrow 1$ free parameter: $\gamma_4^{(3,4)}$

- Iterate $\gamma_4^{(3,4)}$ on the interval $[1, 5]$ with stepsize 0.01
- We require:
  - $[-6, 0] \subset S$
  - $[-4i, 4i] \subset S$

$\Longrightarrow \gamma_4^{(3,4)} \approx 2.4$ is a good candidate

RE + explicit RK methods

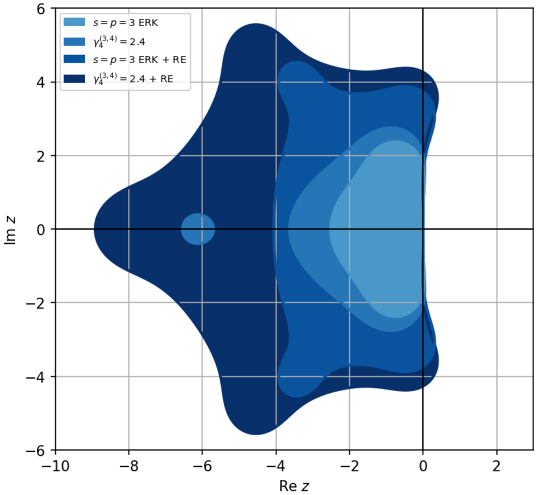

Figure: Stability function of $\gamma_4^{(3,4)} = 2.4$ compared with other stability regions

RE + explicit RK methods

Conjecture

The application of Richardson extrapolation to any explicit Runge–Kutta method leads to a new numerical method which has a larger stability region.

Thank you for your attention!

AI usage

I, Temesvári Ádám, declare that I used ChatGPT-4o for styling and writing parts of the LaTeX code for this presentation.