A-stability of Runge-Kutta Methods

Recall that our general R-K method had the form

$$\begin{cases} \vec{\xi}_j = \vec{y}_n + h \sum_{i=1}^{\nu} a_{j,i} \vec{f}(t_n + \tau_i h, \vec{\xi}_i) & j = 1, 2, \ldots, \nu \\ \vec{y}_{n+1} = \vec{y}_n + h \sum_{j=1}^{\nu} w_j \vec{f}(t_n + \tau_j h, \vec{\xi}_j) \\ A = \text{matrix with components } a_{j,i} & \begin{cases} \text{ERK strictly lower triang.} \\ \text{IRK full in general} \end{cases} \end{cases}$$

Applying this to the equation $y' = \lambda y$ gives

$$\begin{cases} \xi_j = y_n + h \sum_{i=1}^{\nu} a_{j,i} \lambda \xi_i & j = 1, 2, \ldots, \nu \\ y_{n+1} = y_n + h \sum_{j=1}^{\nu} w_j \lambda \xi_j \end{cases}$$

In Matrix form we have

$$\vec{\xi} = \mathbb{1}_\nu y_n + h\lambda A \vec{\xi}$$

where

$$\vec{\xi} = \begin{bmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \vdots \\ \xi_\nu \end{bmatrix} \qquad \mathbb{1}_\nu = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \in \mathbb{R}^\nu$$

So $$(I_\nu - h\lambda A)\vec{\xi} = 1_\nu y_n$$

where $I_\nu = \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}$ is the $\nu \times \nu$ identity matrix.

Then, assuming $I_\nu - h\lambda A$ is invertible (previously we've assume $1 - h\lambda \neq 0$ for example)

$$\boxed{\vec{\xi} = (I_\nu - h\lambda A)^{-1} 1_\nu y_n}$$

Then, inserting this into $y_{n+1} = y_n + h \sum_{j=1}^{\nu} w_j \lambda \xi_j$

gives

$$y_{n+1} = y_n + h\lambda \vec{w}^T \vec{\xi}$$ (i.e. $\vec{w}^T\vec{\xi}$ = inner product)

$$= y_n + h\lambda \vec{w}^T (I_\nu - h\lambda A)^{-1} 1_\nu y_n$$

$$\boxed{y_{n+1} = \left(1 + h\lambda \vec{w}^T (I_\nu - h\lambda A)^{-1} 1_\nu\right) y_n}$$ $n = 0, 1, 2, \ldots$

$$\boxed{y_n = \left(1 + h\lambda \vec{w}^T (I_\nu - h\lambda A)^{-1} 1_\nu\right)^n}$$ with $y_0 = 1$, $n = 0, 1, 2, \ldots$

In general, as before, we require

$$\left| 1 + h\lambda \vec{w}^T (I_\nu - h\lambda A)^{-1} 1_\nu \right| < 1$$

for stability. (i.e. to identify the linear stability domain).

Recall, the example

$$\begin{array}{c|cc} 0 & & \\ 1/2 & 1/2 & \\ \hline & 0 & 1 \end{array} \qquad \vec{c} = \begin{bmatrix} 0 \\ 1/2 \end{bmatrix} \quad \vec{w} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad A = \begin{bmatrix} 0 & 0 \\ 1/2 & 0 \end{bmatrix} \quad \nu = 2$$

(Euler/Midpoint Rule)

$$\vec{y}_{n+1} = \vec{y}_n + h \vec{f}\left(t_n + \tfrac{1}{2}h, \vec{y}_n + \tfrac{1}{2}h\vec{f}(t_n, \vec{y}_n)\right)$$

So

$$\vec{w}^T (I_\nu - h\lambda A)^{-1} 1_\nu = [0 \ 1] \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - h\lambda \begin{bmatrix} 0 & 0 \\ 1/2 & 0 \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$= [0 \ 1] \begin{bmatrix} 1 & 0 \\ -\frac{1}{2}h\lambda & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$= [0 \ 1] \begin{bmatrix} 1 & 0 \\ \frac{1}{2}h\lambda & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = [0 \ 1] \begin{bmatrix} 1 \\ 1 + 1/2 h\lambda \end{bmatrix} = 1 + \tfrac{1}{2}h\lambda$$

$$\left| 1 + h\lambda\left(1 + \tfrac{1}{2}h\lambda\right) \right| < 1 \quad \Leftarrow \text{Same as Heun's method...}$$

So ~~similar to Euler in terms of stability but~~

It turns out that the quantity

$$1 + h\lambda \vec{w}^T (I_\nu - h\lambda A)^{-1} 1_\nu$$

is a rational function of $z \equiv$ [redacted] $h\lambda$.

This result is stated in <u>Lemma 4.1</u> (Iserles p.60)

Lemma 4.1

For every Runge-Kutta method there exists a rational function $r \in \mathbb{P}_{\nu/\nu}$ such that

$$y_n = \left[r(h\lambda) \right]^n \qquad n = 0, 1, 2, \ldots$$

Moreover, if the RK method is explicit, then $r \in \mathbb{P}_\nu$.

Def: $\mathbb{P}_{\alpha/\beta}$: set of all rational functions $\hat{p}/\hat{q}$ where $\hat{p} \in \mathbb{P}_\alpha$ (polynomial of degree α) and $\hat{q} \in \mathbb{P}_\beta$ (" " " β).

Proof:

Basically, it is claimed that

$$r(z) = 1 + z w^T (I_\nu - zA)^{-1} 1_\nu$$

is a rational function of a particular variety.

This follows from a formula from linear algebra...

Matrix Inversion Formula (D.C. Lay, Linear Algebra + Applications, 3rd edition)

Let A be an invertible $n \times n$ matrix. Then

$$A^{-1} = \frac{\operatorname{adj} A}{\det A}$$

where ~~[illegible]~~ $\det A$ is the determinant of A

and $\operatorname{adj} A$ is the adjugate (or classical adjoint) of A defined as the matrix of cofactors...

$$\operatorname{adj} A = \begin{bmatrix} C_{11} & C_{21} & \cdots & C_{n1} \\ C_{12} & C_{22} & & \vdots \\ \vdots & & \ddots & \vdots \\ C_{1n} & \cdots & & C_{nn} \end{bmatrix}$$

where

$$C_{ji} = (-1)^{i+j} \det A_{ji}$$

where A_{ji} is the submatrix of A formed by deleting row j and column i of A.

Basically, think of applying Cramers rule to $\vec{e}_j$ (the j^{th} column of the identity)

EXAMPLE

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

solving $A\vec{x} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ gives the first column of A^{-1}.

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$x_1 = \frac{\det \begin{bmatrix} 1 & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \end{bmatrix}}{\det A} = \frac{(a_{22}a_{33} - a_{32}a_{23})}{\det A} = \frac{+\det A_{11}}{\det A} = \frac{C_{11}}{\det A}$$

$$x_2 = \frac{\det \begin{bmatrix} a_{11} & 1 & a_{13} \\ a_{21} & 0 & a_{23} \\ a_{31} & 0 & a_{33} \end{bmatrix}}{\det A} = \frac{-(a_{21}a_{33} - a_{31}a_{23})}{\det A} = \frac{-\det A_{12}}{\det A} = \frac{C_{12}}{\det A}$$

$$x_3 = \frac{\det \begin{bmatrix} a_{11} & a_{12} & 1 \\ a_{21} & a_{22} & 0 \\ a_{31} & a_{32} & 0 \end{bmatrix}}{\det A} = \frac{(a_{21}a_{32} - a_{31}a_{22})}{\det A} = \frac{+\det A_{13}}{\det A} = \frac{C_{13}}{\det A}$$

So

$$A^{-1} = \begin{bmatrix} \frac{C_{11}}{\det A} & \cdot & \cdot \\ \frac{C_{12}}{\det A} & \cdot & \cdot \\ \frac{C_{13}}{\det A} & \cdot & \cdot \end{bmatrix} = \frac{1}{\det A} \begin{bmatrix} C_{11} & \cdot & \cdot \\ C_{12} & \cdot & \cdot \\ C_{13} & \cdot & \cdot \end{bmatrix}$$

Note: the cofactors have one less power of z than $\det A$. That is,

$$r(z) = 1 + z\, w^T (I_\nu - zA)^{-1} 1_\nu$$

with

$$(I_\nu - zA)^{-1} = \frac{\operatorname{adj}(I_\nu - zA) \;\in \mathbb{P}_{\nu-1}}{\det(I_\nu - zA) \;\in \mathbb{P}_\nu}$$

so with the extra factor of z in $r(z)$ we have

$r(z) \in P_{\nu/\nu}$.

* For the case of an Explicit R-K (ERK) scheme A is strictly lower triangular and $I - zA$ [redacted] is triangular with ones on the diagonal, so $\det(I - zA) = 1$. Then, $r(z) \in \mathbb{P}_\nu$ using what we know about $\operatorname{adj}(I_\nu - zA)$

Comments: for RK methods $y_n = [r(h\lambda)]^n$ with

- $r(z) \equiv 1 + z\vec{w}^T (I_\nu - zA)^{-1} 1_\nu \in \begin{cases} P_{\nu/\nu} & \text{implicit} \\ P_\nu & \text{explicit} \end{cases}$

- In the ERK case note that $r(0) = 1$ ~~(in particular $|r(0)| \not< 1$.)~~ So no ERK method is A-stable (Corollary to Lemma 4.1/4.2)

- IRK methods can be A-stable

EXAMPLES: (Iserles, p. 61)

$$\begin{array}{c|cc} 0 & 1/4 & -1/4 \\ 2/3 & 1/4 & 5/12 \\ \hline & 1/4 & 3/4 \end{array} \qquad \vec{c} = \begin{array}{c|cc} 1/3 & 5/12 & -1/12 \\ 1 & 3/4 & 1/4 \\ \hline & 3/4 & 1/4 \end{array} \begin{array}{l} = A \\ \\ = \vec{w}^T \end{array}$$

these are A-stable

both lead to

$$r(z) = \frac{1 + \frac{1}{3}z}{1 - \frac{2}{3}z + \frac{1}{6}z^2}$$

... verify that $|r(z)| < 1$ ... see book for calculations

Some further general results ...

Lemma 4.3 (Iserles, p. 61)

Let r be an arbitrary rational function that is not constant. Then $|r(z)| < 1$ for all $z \in \mathbb{C}^-$ if and only if all the poles of r have positive real parts and $|r(it)| \le 1$ for all $t \in \mathbb{R}$.

Comments:

- this result tells us that we can assess a method with

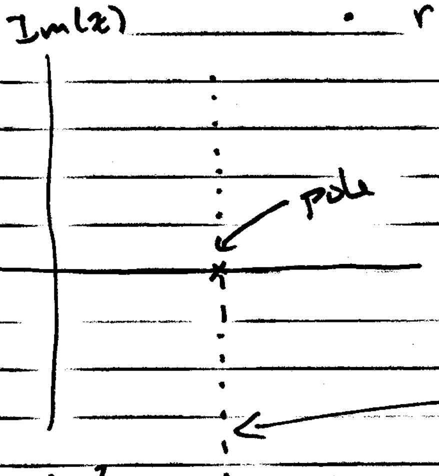
$$y_n = [r(h\lambda)]^n$$

as A-stable (or not) by examining the poles of r and checking $|r(it)|$.

EXAMPLE (Backward Euler)

$$r(z) = \frac{1}{1-z}$$

- pole: $z = 1$
- $r(it) = \dfrac{1}{1-it}$ so $|r(it)| \le 1$



So by Lemma 4.3 Backward Euler is A-stable

And Lemma 4.2

$y_n = [r(h\lambda)]^n \Rightarrow D = \{z \in \mathbb{C} \mid |r(z)| < 1\}$

note: $1-it$ so $|1-it| \ge 1 \Rightarrow \dfrac{1}{|1-it|} \le 1$.

Proof of Lemma 4.3 (see Iserles, p. 61)

Lemma 4.4:

Suppose that the sequence $\{y_n\}$ $(n=0,1,2,\dots)$, produced by applying a <u>method of order p</u> to the linear equation $y' = \lambda y$; $y(0)=1$ with constant step size, obeys

$$y_n = \left[r(\lambda h) \right]^n \qquad n = 0,1,2,\dots$$

(i.e. $y_{n+1} = r(\lambda h)\, y_n$). Then

$$r(z) = e^z + O(z^{p+1}) \qquad z \to 0$$

This is then referred to as a function of order p.

Proof: i.e. $r(z)$ approximates e^z at least as well as the order of the method

let $Q \equiv y(t_{n+1}) - r(\lambda h)\, y(t_n)$ (see def. p. 8)

By our assumption, the method $y_{n+1} = r(\lambda h) y_n$ is order p so...

$$Q = y(t_{n+1}) - r(\lambda h)\, y(t_n) = O(h^{p+1})$$

so

$$r(\lambda h) = \frac{y(t_{n+1})}{y(t_n)} + \frac{1}{y(t_n)} \cdot O(h^{p+1})$$

but the exact solution has

$$y(t) = e^{\lambda t}$$

so

$$y(t_{n+1}) = e^{\lambda t_{n+1}} = e^{\lambda(t_n + h)} = e^{\lambda h} e^{\lambda t_n} = e^z\, y(t_n)$$

so

$$r(z) = e^{z} + \frac{1}{e^{\lambda t_n}} O(h^{p+1})$$

$z = h\lambda$

$$= e^{z} + \frac{1}{\lambda^{p+1} e^{\lambda t_n}} O(z^{p+1})$$

So

$$\underline{r(z) = e^{z} + O(z^{p+1})}$$

recall $y' = \lambda y$

$y_n = [r(h\lambda)]^n$

$\Downarrow$

$y_n = [e^{h\lambda} + O(h\lambda)^{p+1}]^n$

$= e^{hn\lambda} + O(h\lambda)^{p+1}$

$= e^{\lambda t_n} + O(h\lambda)^{p+1}$

Comments

- A rational function r that originates in an A-stable method is called A-acceptable (i.e. r is A-acceptable, the corresponding scheme is A-stable) (Iserles, p. 61)

- A function r that satisfies $r(z) = e^{z} + O(z^{p+1})$ is called "of order p".

  - note: the order of the numerical method is not ~~necessarily the same as the order of r~~

    - $r(z)$ is associated with application to a linear equation $y' = \lambda y$.

    - the order of r could be higher than the order of the method.

Note: $e^z = 1 + z + \frac{1}{2!}z^2 + \frac{1}{3!}z^3 + O(z^4)$

Let's revisit some $r(z)$ functions we've seen already...

- Euler: (first order method)

$$r(z) = 1 + z = e^z + O(z^2): \quad \underline{r \text{ is order } 1}$$

- Backward Euler: (first ~~order method~~)

$$r(z) = \frac{1}{1-z} = 1 + z + z^2 + O(z^3) = e^z + O(z^2)$$

$$: \quad \underline{r \text{ is order } 1}$$

- Trapezoid / Implicit Midpoint: (2^{nd} order methods ... see Ch. 1)

$$r(z) = \frac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z} = \left(1 + \tfrac{1}{2}z\right)\left(1 + \tfrac{1}{2}z + \tfrac{1}{4}z^2 + \tfrac{1}{8}z^3 + O(z^4)\right)$$

$$= 1 + z + \tfrac{1}{2}z^2 + \left(\tfrac{1}{8} + \tfrac{1}{8}\right)z^3 + O(z^4)$$

$$= e^z + O(z^3) \quad : \quad \underline{r \text{ is order } 2}$$