Runge-Kutta stepping schemes

▼ Classical 4-step Runge-Kutta

To solve the equation

$$dy/dt = f(t, y)$$

we use the following scheme

$$
\begin{aligned}
k_1 &= \Delta t\, f(t, y) \\
k_2 &= \Delta t\, f(t + \Delta t/2,\ y + k_1/2) \\
k_3 &= \Delta t\, f(t + \Delta t/2,\ y + k_2/2) \\
k_4 &= \Delta t\, f(t + \Delta t,\ y + k_3) \\
y(t+\Delta t) &= y(t) + (\Delta t/6)(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}
$$

↳ 1) Method is order 4
(i.e. error is $O(\Delta t^5)$)

2) Does not require initialization

3) Requires 4 function evaluations.
(LMFs require only 1 function evaluation to attain any order)

Generalized Runge-Kutta schemes

An s-stage Runge-Kutta scheme has the form

$$\boxed{\begin{aligned} &K_a = \Delta t\, f\left(t + c_a \Delta t,\ y + \sum_{b=1}^{s} A_{ab} K_b\right), \\ &\forall a \in \{1, 2, \dots, s\} \\ &y(t+\Delta t) = y(t) + \sum_{a=1}^{s} b_a K_a \end{aligned}}$$

where we introduce the simplifying condition

$$\boxed{c_a = \sum_{b=1}^{s} A_{ab}}$$

→ Butcher tableau

$$\begin{array}{c|cccc} c_1 & A_{11} & A_{12} & \cdots & A_{1s} \\ c_2 & A_{21} & A_{22} & \cdots & A_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & A_{s1} & A_{s2} & \cdots & A_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

A brief way to represent a Runge-Kutta scheme

Explicit / Implicit classification

A Runge-Kutta scheme is

a) Explicit $\Leftrightarrow$ $A_{ab} = 0, \forall a,b : a \leq b$
b) Implicit $\Leftrightarrow$ not Explicit
(requires solution of non-linear equation)
c) Diagonally Implicit (DIRK) $\Leftrightarrow$ $A_{ab} = 0, \forall a,b : a < b$

d) Singly Diagonally Implicit (SDIRK) $\Leftrightarrow$

$$\begin{cases} \text{DIRK} \\ A_{11} = A_{22} = \cdots = A_{ss} \end{cases}$$ (diagonal elements are equal).

Typical RK schemes

① 1-stage RK

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

$k_1 = \Delta t f(t, y)$ Euler rule
$y_{n+1} = y_n + k_1$

(2) 2-stage RG

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1 & 0 \end{array}$$

(Euler)

$k_1 = f(t, y)$
$k_2 = f(t + \Delta t, y + \Delta t k_1)$
$y = y + \Delta t k_1$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 0 & 1 \end{array}$$

$y = y + \Delta t k_2$
(midpoint rule)*

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

$y = y + \Delta t \dfrac{(k_1 + k_2)}{2}$
(trapezoidal rule)*

* These are EXPLICIT, thus different from their LMF cousins

(3) 3-stage RK

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

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 1 & -1 & 2 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$$

④ 4-stage Runge-Kutta

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
1/2 & 1/2 & 0 & 0 & 0 \\
1/2 & 0 & 1/2 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & 1/6 & 1/3 & 1/3 & 1/6
\end{array}
$$

(classical Runge-Kutta)

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
1/4 & 1/4 & 0 & 0 & 0 \\
1/2 & 0 & 1/2 & 0 & 0 \\
1 & 1 & -2 & 2 & 0 \\
\hline
 & 1/6 & 0 & 2/3 & 1/6
\end{array}
$$

(another 4-stage RG).

Order Conditions for RG methods

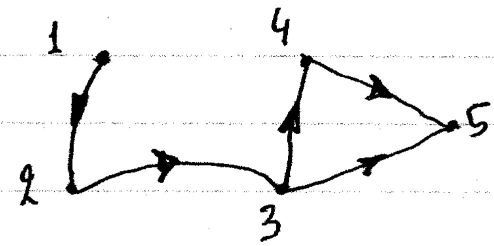
The construction of the order conditions is based on the theory of rooted trees

Review of rooted trees

Def: A *directed graph* $G = (V, E)$ consists of

a) V = a set of vertices
b) $E \subseteq V \times V$ = a set of edges

example



1,2 directly connected
1,3 connected.

$V = \{1, 2, 3, 4, 5\}$
$E = \{(1,2), (2,3), (3,4), (3,5), (4,5)\}$

Def: Let $a, b \in V$ be two vertices

a) a, b are directly connected iff $(a, b) \in E$ (notation $a \Rightarrow b$)

b) a, b are connected iff
$\exists \{x_1, x_2, \dots, x_n\} \subseteq V$ such that
$a = x_1 \wedge b = x_n \wedge$
$\wedge (\forall k \in [n-1] : (x_k, x_{k+1}) \in E)$

Def: A graph $G=(V,E)$ is a <u>rooted tree</u> with root $r \in V$ iff

1) If a vertex $a \in V$ is not the root, only one arrow goes to a.

$$\forall a \in V - \{r\} : \left((b_1,a),(b_2,a) \in E \Rightarrow b_1 = b_2 \right)$$
$$\forall a \in V - \{r\} : \exists b \in V : (b,a) \in E \land b \neq a$$

2) No arrow goes to the root

$$\forall (a,b) \in E : b \neq r$$

3) Every vertex $a \in V - \{r\}$ is connected to the root

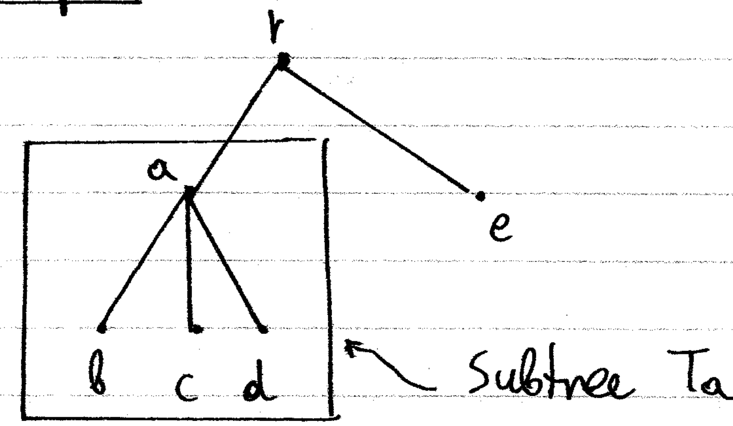
$$\forall a \in V - \{r\} : r \longrightarrow a$$

Def: If T is a rooted tree and $a \in V - \{r\}$ then a defines a <u>subtree</u> $T_a = (V_a, E_a)$

$$V_a = \{ x \in V : a \longrightarrow x \} \cup \{a\}$$
$$E_a = \{ (x,y) \in E : x,y \in V_a \}$$

with root a.

example

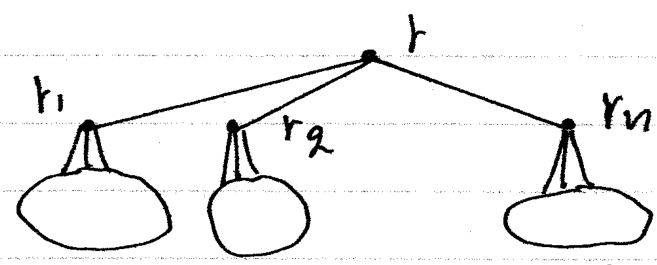


▶ Tree construction

Let τ be the unit tree with $V=\{r\}$ and $E=\emptyset$.
Assume we have constructed the rooted trees $T_1, T_2, \ldots, T_n$, with roots $r_1, r_2, \ldots, r_n$.
The tree

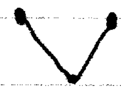
$$T = [T_1 T_2 \cdots T_n]$$

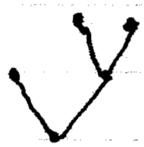
is defined as



Any rooted tree can be constructed recursively from τ with this operation:

example

 $= [\tau]$  $= [\tau^2]$

 $= [\tau[\tau^2]]$  $= [[\tau]]$

▶ Functions on trees

Let T be a rooted tree

1) The order $r(T)$ is $r(T) = |V| =$ number of vertices

2) The density $\gamma(T)$ is defined as

$$\boxed{\gamma(T) = \prod_{a \in V} r(T_a)}$$

where T_a is the subtree of T defined by the vertex a.

For the unit tree: $r(\tau) = 1$ and $\gamma(\tau) = 1$.

For a tree T given by

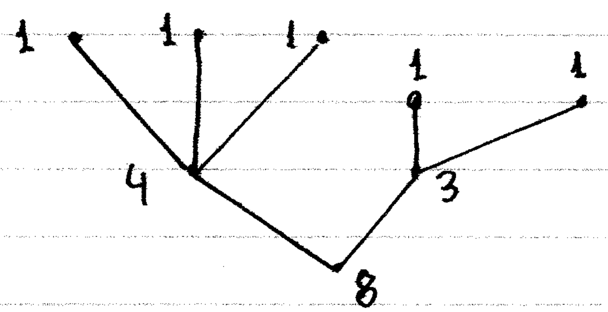
$$T = [T_1^{m_1} T_2^{m_2} \dots T_n^{m_n}]$$

$$\boxed{\begin{aligned} r(T) &= 1 + \sum_{a=1}^{n} m_a r(T_a) \\ \gamma(T) &= r(T) \prod_{a=1}^{n} [\gamma(T_a)]^{m_a} \end{aligned}}$$

$\longleftarrow$ order

$\longleftarrow$ density.

<u>example</u>



$\longleftarrow$ label order of each subtree.

$$\gamma(T) = 1 \cdot 1 \cdot 1 \cdot 4 \cdot 1 \cdot 1 \cdot 3 \cdot 8$$
$$= 4 \cdot 3 \cdot 8 = 96$$
$$r(T) = 8$$

Order conditions for RG

Consider an RG with tableau

$$\begin{array}{c|c} c_a & A_{ab} \\ \hline & b_a \end{array}, \text{ and } s \text{ steps.}$$

and let T be a rooted tree. $\mathbb{T}$ = set of all rooted trees
We define recursively:

$$(\Phi_a D)(\tau) = 1 \,, \forall a \in [s]$$

$$\Phi_a(T) = \sum_{b=1}^{s} A_{ab} (\Phi_b D)(T) \,, \forall a \in [s] \,, \forall T \in \mathbb{T}$$

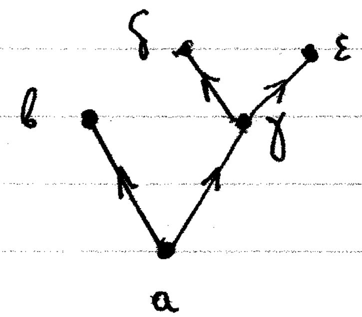
$$(\Phi_a D)([T_1 T_2 \cdots T_m]) = \prod_{b=1}^{m} \Phi_a(T_b)$$

$$\Phi(T) = \sum_{a=1}^{s} b_a (\Phi_a D)(T)$$

We call $\Phi(T)$ = elementary weight of T.
The necessary and sufficient conditions for order p are

$$\boxed{\begin{array}{l} 1)\ \displaystyle\sum_{b=1}^{s} A_{ab} = c_a \quad \text{(simplifying cond.)} \\ 2)\ \forall T \in \mathbb{T} : \left(r(T) \leq p \Rightarrow \Phi(T) = \dfrac{1}{\gamma(T)} \right) \end{array}}$$

example



The vertices b, δ, ε are called "leafs" bc they have no outgoing arrow.

$$\Phi(t) = \sum_{ab\gamma\delta\varepsilon} b_a A_{ab} A_{a\gamma} A_{\gamma\delta} A_{\gamma\varepsilon}$$

$$= \sum_{a\gamma} b_a A_{a\gamma} \left[\left(\sum_{b} A_{ab} \right) \left(\sum_{\delta} A_{\gamma\delta} \right) \left(\sum_{\varepsilon} A_{\gamma\varepsilon} \right) \right]$$

$$= \sum_{a\gamma} b_a A_{a\gamma} c_a c_\gamma c_\gamma$$

$$= \sum_{a\gamma} b_a A_{a\gamma} c_a c_\gamma^2$$

→ •1 The root contributes b_a

•2 Each arrow ab contributes a factor A_{ab}.

•3 The factors contributed by the leafs can be simplified via the simplifying condition.

Order conditions for 2-stage RK

$$
\begin{array}{c|cc}
c_1 & 0 & 0 \\
c_2 & a_{21} & 0 \\
\hline
 & b_1 & b_2
\end{array}
$$

$$
\begin{cases}
\left.\begin{array}{l} c_1 = 0 \\ c_2 = a_{21} \end{array}\right] \longrightarrow \text{simplifying conditions} \\
b_1 + b_2 = 1 \\
b_1 c_1 + b_2 c_2 = 1/2
\end{cases}
$$

5 unknowns ; 4 equations ; 1 degree of freedom

Order conditions for 3-stage RK

$$
\begin{array}{cccc}
c_1 & 0 & 0 & 0 \\
c_2 & a_{21} & 0 & 0 \\
c_3 & a_{31} & a_{32} & 0 \\
 & b_1 & b_2 & b_3
\end{array}
\qquad
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
c_2 & a_{21} & 0 & 0 \\
c_3 & a_{31} & a_{32} & 0 \\
\hline
 & b_1 & b_2 & b_3
\end{array}
$$

Order conditions for 3-stage

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
c_2 & a_{21} & 0 & 0 \\
c_3 & a_{31} & a_{32} & 0 \\
\hline
 & b_1 & b_2 & b_3
\end{array}
$$

$$
\begin{cases}
c_2 = a_{21} \\
c_3 = a_{31} + a_{32} \\
b_1 + b_2 + b_3 = 1 \\
b_2 c_2 + b_3 c_3 = 1/2 \\
b_2 c_2^2 + b_3 c_3^2 = 1/3 \\
b_3 a_{32} c_2 = 1/6
\end{cases}
$$

8 unknowns ; 6 equations.
2 degrees of freedom
Use c_2, c_3 as parameters.

Order condition for 4-stage RG

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
c_2 & a_{21} & 0 & 0 & 0 \\
c_3 & a_{31} & a_{32} & 0 & 0 \\
c_4 & a_{41} & a_{42} & a_{43} & 0 \\
\hline
 & b_1 & b_2 & b_3 & b_4
\end{array}
$$

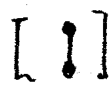
$$c_2 = a_{21}$$

$$c_3 = a_{31} + a_{32}$$

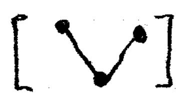
$$c_4 = a_{41} + a_{42} + a_{43}$$

$$b_1 + b_2 + b_3 + b_4 = 1 \qquad [\bullet]$$

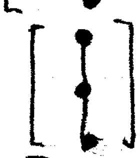
$$b_2 c_2 + b_3 c_3 + b_4 c_4 = 1/2$$



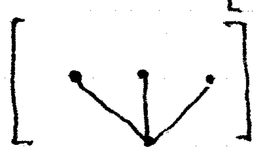
$$b_2 c_2^2 + b_3 c_3^2 + b_4 c_4^2 = 1/3$$



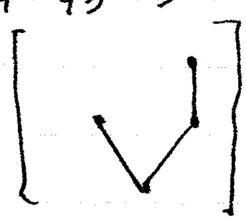
$$b_3 a_{32} c_2 + b_4 a_{42} c_2 + b_4 a_{43} c_3 = 1/6$$



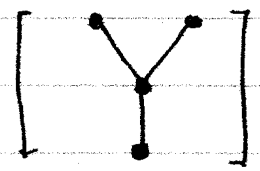
$$b_2 c_2^3 + b_3 c_3^3 + b_4 c_4^3 = 1/4$$



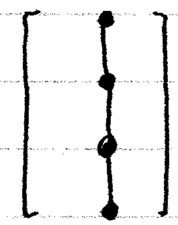
$$b_3 c_3 a_{32} c_2 + b_4 c_4 a_{42} c_2 + b_4 c_4 a_{43} c_3 = 1/8$$



$$b_3 a_{32} c_2^2 + b_4 a_{42} c_2^2 + b_4 a_{43} c_3^2 = 1/12$$



$$b_4 a_{43} a_{32} c_2 = 1/24$$



13 unknowns ; 11 equations
2 degrees of freedom

▶ It can be shown that
all possible solutions satisfy $c_4 = 1$
One may use c_2, c_3 as parameters.

Higher-order ERG

An explicit RG method of order p requires the following minimum number of s stages:

Order p	Minimum s
1, 2, 3, 4	1, 2, 3, 4 (respectively)
5	6
6	7
7	9
8	11
9	12–17 *
10	13–17 *

(*) Precise minimum unknown.

Implicit RG

More degrees of freedom in order conditions.
Current research.
Excellent stability properties.

Stability of Runge-kutta schemes

- We have no issues with zero-stability.
- We are interested in absolute stability.

The stability ~~polyno~~ function

Consider the performance of an RK method on the equation

$$\frac{dy}{dt} = q y(t) \quad \text{with} \quad q \in \mathbb{C}, \ \mathrm{Re}\, q < 0$$

We use $f(t, y) = qy$. The stages are given by

$$k_a = \Delta t \, f\Big(t + c_a \Delta t, \, y + \sum_{b=1}^{s} A_{ab} k_b \Big)$$

$$= q \Delta t \Big(y + \sum_{b=1}^{s} (A_{ab} k_b) \Big) \Leftrightarrow$$

$$\Leftrightarrow \sum_{b=1}^{s} \big(\delta_{ab} - q \Delta t \, A_{ab} \big) k_b = (q \Delta t) y$$

$$\Leftrightarrow \ (I - q \Delta t A) k = (q \Delta t) y \vec{1}$$

with $k \in \mathbb{R}^s$ a vector and $\vec{1} = (1, 1, 1, \dots, 1) \in \mathbb{R}^s$.

This gives

$$K = (I - q\Delta t\, A)^{-1} q \Delta t\, y\, \vec{1}$$

and

$$y(t+\Delta t) \approx y(t) + \sum_{a=1}^{s} b_a k_a$$

$$= y + b^T K =$$

$$= y + b^T (I - q\Delta t\, A)^{-1} q\Delta t\, y\, \vec{1}$$

$$= \left[1 + b^T (I - q\Delta t A)^{-1} (q\Delta t\, \vec{1})\right] y$$

Let $z = q\Delta t$. Then $y(t+\Delta t) = R(z)\, y(t)$ with

$$\boxed{R(z) = 1 + b^T (I - zA)^{-1} (z\vec{1})}$$

↳ stability function.

Stability Region

Def: The stability region $\mathcal{S}$ of an RG scheme is defined as

$$\mathcal{S} = \{ z \in \mathbb{C} \mid |R(z)| \leq 1 \}$$

Def: An RG scheme is

a) A-stable $\Leftrightarrow$ $\{ z \in \mathbb{C} \mid Re(z) \leq 0 \} \subseteq \mathcal{S}$
b) $A(\alpha)$-stable $\Leftrightarrow$ $\{ z \in \mathbb{C} \mid |Arg(z) - \pi| < \alpha \} \subseteq \mathcal{S}$
c) $A(0)$-stable $\Leftrightarrow$ $\exists\, \alpha \in (0, \pi/2)$: $A(\alpha)$-stable

Def: An RG scheme is

$$\text{L-stable} \Leftrightarrow \text{A-stable} \wedge \lim_{\substack{z \to \infty \\ Re(z) < 0}} R(z) = 0$$

↳ An L-stable scheme is even more robust for a very stiff problem than an A-stable scheme.

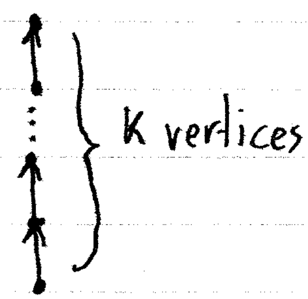
↳ ~~An~~ For a nonlinear problem, as before, we need $a \Delta t \in \mathcal{S}$ for all the eigenvalues a of the Jacobian $J(t)$.

Stability function for explicit RG

For an s-stage explicit RG with order $p \leq s$ we note that

a) The matrix A is nilpotent with $A^s = \mathbf{0}$

b) Rooted trees of the form

$t_k =$ 

give $\gamma(t_k) = k!$ and

$$\Phi = \sum b_1 A_{12} A_{23} \cdots A_{k-1,k} = b^T A^{k-1} \vec{1}$$

so from the order p condition we have

$$\boxed{b^T A^{k-1} \vec{1} = \frac{1}{k!}}, \ \forall k \in \{1, 2, \dots, p\}$$

We use these results to calculate $R(z)$ as follows:

$$R(z) = 1 + z b^T (I - zA)^{-1} \vec{1}$$

$$= 1 + z b^T \left[\sum_{k=0}^{+\infty} (zA)^k \right] \vec{1}$$

$$= 1 + z b^T \left[\sum_{k=0}^{s-1} (zA)^k \right] \vec{1}$$

(use nilpotent $A^s = 0$)

$$= 1 + z + \sum_{k=1}^{p-1} \left[b^T A^k \vec{1} \right] z^{k+1} + z b^T \left[\sum_{k=p}^{s} (zA)^k \right] \vec{1}$$

$$= 1 + z + \sum_{k=2}^{p} \frac{z^k}{k!} + \sum_{k=p+1}^{s} C_k z^k$$

thus:

$$\boxed{R(z) = \sum_{k=0}^{p} \frac{z^k}{k!} + \sum_{k=p+1}^{s} C_k z^k \quad \text{with } C_k = b^T A^{k-1} \vec{1}}$$

We see that

a) For $s \leq 4$, we have $p = s$ and thus $R(z)$ is <u>universal</u> (i.e. independent of the choice of a specific RG scheme)

Specifically:

$$R(z) = \begin{cases} 1+z & , p=1 \\ 1+z+z^2/2 & , p=2 \\ 1+z+z^2/2+z^3/6 & , p=3 \\ 1+z+z^2/2+z^3/6+z^4/24 & , p=4 \end{cases}$$

for ALL explicit RG schemes with order $p \leq 4$.

b) For $p=5$, we need $s=6$ and

$$R(z) = 1+z+\frac{z^2}{2}+\frac{z^3}{6}+\frac{z^4}{24}+\frac{z^5}{120}+Cz^6$$

Here C is dependent on our choice of a particular RG scheme.

c) The stability regions of explicit RG are bounded blobs which <u>expand</u> with increasing p. This is opposite behaviour from LMF (both explicit/implicit) where the stability region <u>contracts</u> with increasing order p.

d) See next page for plot of stability regions.

Stability Function for Implicit RG

Thm: The stability function can be rewritten

$$R(z) = \frac{N(z)}{D(z)}$$

with $N(z), D(z)$ polynomials given by

$$N(z) = \det\left(I + z\left(\vec{1}\, b^T - A\right)\right)$$
$$D(z) = \det(I - zA)$$

Def: The polynomial

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

is the E-polynomial of the RG method

Thm: An RG scheme is A-stable iff.

a) All the zeroes of $D(z)$ are on $\{z \in \mathbb{C} \mid Re(z) > 0\}$
b) $E(y) \geq 0$, $\forall y \in \mathbb{R}$.

Thm: An RG scheme is L-stable iff

a) It is A-stable
b) $\deg N(z) < \deg D(z)$.

$\hookrightarrow$ To confirm the condition

$$E(y) \geq 0 \ , \ \forall y \in \mathbb{R}$$

numerically,

- 1 Find the real roots of $E(y)$
- 2 Check the sign of $E(y)$ for one point in each interval defined by the real roots!

Construction of Implicit RG schemes

① Gaussian Implicit RG schemes

These are s-stage schemes with
order of accuracy $p = 2s$ (!)
are A-stable
with tableau

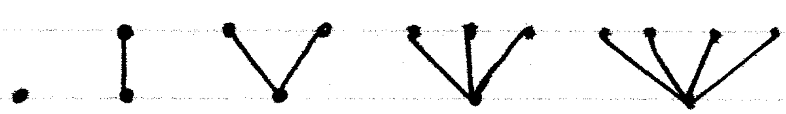
$$\begin{array}{c|c} c & A \\ \hline & b \end{array}$$

constructed as follows

- 1 Choose $c_1, c_2, \ldots, c_s$ to be the zeroes of the Legendre polynomial $P_s(x)$ (Recall my notes on Gaussian Quadrature)
- 1 Choose $b_1, b_2, \ldots, b_s$ such that they satisfy the linear system

$$\sum_{a=1}^{s} b_a c_a^{k-1} = \frac{1}{k}, \quad \forall k \in \{1, 2, \ldots, s\}$$

which corresponds to the trees:



, etc.

• 3 Choose A_{ab} to satisfy

$$\sum_{b=1}^{s} A_{ab} c_b = \frac{1}{2} c_a^2 \quad , \forall a \in \{1,2,3,\dots,s\}$$

It can be proved that the resulting RG scheme will indeed

a) Be A-stable

b) Have order of accuracy $p = 2s$.

<u>examples</u>

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$p = 2, \ s = 4$

$$
\begin{array}{c|ccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{\sqrt{15}}{15} & \frac{5}{36}-\frac{\sqrt{15}}{30} \\
\frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{24} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{\sqrt{15}}{30} & \frac{2}{9}+\frac{\sqrt{15}}{15} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

$p=3$, $s=6$

→ We can sacrifice order of accuracy p to attain L-stable implicit RG schemes

② Radau Implicit RG

- 1 Choose c_a as the roots of $P_s(x)+P_{s-1}(x)$ with $P_n(x)$ the Legendre polynomial
- 2 Choose b_a, A_{ab} same as above

▶ The resulting method is L-stable with $p=2s-1$

example

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 2/3 & 1/3 & 1/3 \\ \hline & 1/4 & 3/4 \end{array} \qquad \begin{array}{l} s=2 \\ p=3 \end{array}$$

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ (6-\sqrt{6})/10 & (9+\sqrt{6})/75 & (24+\sqrt{6})/120 & (168-73\sqrt{6})/600 \\ (6+\sqrt{6})/10 & (9-\sqrt{6})/75 & (168+73\sqrt{6})/600 & (24-\sqrt{6})/120 \\ \hline & 1/9 & (16+\sqrt{6})/36 & (16-\sqrt{6})/36 \end{array}$$

$s=3$, $p=5$

③ Lobatto Implicit RG

- 1 Choose c_a zeroes of $P_s(x) - P_{s-2}(x)$ where $P_n(x)$ is the Legendre polygonomial
- 2 Choose b_a, A_{ab} same as before.

example :

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/4 & 1/4 & 0 \\ 1 & 0 & 1 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array} \qquad \begin{array}{l} s=3 \\ p=4 \end{array}$$

- The resulting method is L-stable with $p = 2s - 2$

④ Diagonally Implicit RK (DIRK)

We sacrifice more order to obtain <u>faster</u> algorithm.

2-stage DIRK

$$
\begin{array}{c|cc}
\lambda & \lambda & 0 \\
c_2 & c_2 - \lambda & \lambda \\
\hline
 & b_1 & b_2
\end{array}
\qquad \text{with} \quad
\begin{cases}
b_1 + b_2 = 1 \\
b_1 \lambda + b_2 c_2 = 1/2
\end{cases}
$$

$$
p = 2 \; ; \quad
\begin{aligned}
&\text{A-stable} \iff \lambda \geq 1/4 \\
&\text{L-stable} \iff \lambda = 1 \pm (1/2)\sqrt{2}
\end{aligned}
$$

3-stage DIRK

$$
\begin{array}{c|ccc}
\lambda & \lambda & 0 & 0 \\
(1/2)(\lambda+1) & (1/2)(1-\lambda) & \lambda & 0 \\
1 & (1/4)(-6\lambda^2+16\lambda-1) & (1/4)(6\lambda^2-20\lambda+5) & \lambda \\
\hline
 & (1/4)(-6\lambda^2+16\lambda-1) & (1/4)(6\lambda^2-20\lambda+5) & \lambda
\end{array}
$$

$p = 3$

A-stable $\Leftrightarrow \lambda \in [1/3, a]$
L-stable $\Leftrightarrow \lambda = b$

with $a \approx 1.068$ the root of
$$2x^3 - 3x^2 + x - 1/12 = 0$$
and $b \approx 0.4358$ the root of
$$x^3 - 3x^2 + (3/2)x - 1/6 = 0$$

The advantage of DIRK is that each stage is decoupled from subsequent stages, and can be done by solving 1 nonlinear equation instead of advancing all stages simultaneously by solving a system of s equations!

Comparison Chart

LMF	Runge-Kutta
Efficient; one evaluation of f	Less efficient Multiple stages
Difficult to adjust Δt	Easy to adjust Δt
Order Barrier $p \leqslant s+2$ for convergence Order Barrier $p \leqslant 2$ for A-stability	No order barriers. A-stability can be achieved for $p = 2s$ and L-stability for $p = 2s-1$
Explicit LMF Stability region contracts when $p \nearrow$	Explicit RK Stability region expands when $p \nearrow$