Set 21: Ordinary Differential Equations: Runge Kutta Methods

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Sources

- U. Ascher and L. Petzold, Computer Methods for Ordinary Differential Equations and Differential-algebraic Equations, SIAM, 1998.
- J. D. Lambert, Numerical Methods for Ordinary Differential Systems, Wiley 1991, 1973.
- C. W. Gear, Numerical Initial Value Problems in Ordinary Differential Equations, Prentice Hall, 1973.
- R. Skeel, Numerical Differential Equations Class Notes, University of Illinois, 1979.

Motivation

Recall, for Adams methods the integral

$$y(t_n) = y(t_{n-1}) + \int_{t_{n-1}}^{t_n} f(t, y(t))dt$$

was approximated by interpolating f at previous steps at $t_{n-1}, \ldots, t_{n-k}$, i.e., outside the interval of integration for $k > 1$.

- Forward Euler approximated the area under the curve with $hy'(t_{n-1)}$, i.e., the height was taken at t_{n-1}.
- Backward Euler approximated the area under the curve with $hy'(t_n)$, i.e., the height was taken at t_n (which made it implicit via f).
- These are both first order one step methods.
- They are both first order one stage Runge Kutta methods.

One-step Multistage Methods: Runge Kutta Methods

- Quadrature methods applied to the interval $[t_{n-k}, t_n]$ when viewed as linear multistep methods are not satisfactory due to stability problems, e.g., $\rho(\xi) = \xi^k - 1$ which has all its roots on the unit circle – weak stability
- RK methods can often be derived from quadrature but the idea of steps changes to that of stages.
- one-step, multistage methods use multiple points **between** t_{n-1} and t_n to achieve higher order.
- **Only** $(t_n, \;\; y_n)$ is passed on to the next step to compute $(t_{n+1}, \;\; y_{n+1})$.

Implicit Midpoint Rule

Recall, using the midpoint in quadrature:

$$y(t_n) = y(t_{n-1}) + \int_{t_{n-1}}^{t_n} f(t, y(t))dt$$

$$y_n = y_{n-1} + hf(t_{n+1/2}, \frac{y_n + y_{n-1}}{2}),$$

where $t_{n+1/2} = t_{n-1} + h/2$.

- Implicit RK method.
- One-stage, one-step, second order

Explicit Midpoint Method

Converting the midpoint method to an explicit form starts to motivate the basic idea of stages.

First, construct an approximation of $y(t_{n+1/2})$ via forward Euler then apply the midpoint rule:

$$y_{n+1/2} = y_{n-1} + \frac{h}{2} f(t_{n-1}, y_{n-1})$$
$$y_n = y_{n-1} + h f(t_{n+1/2}, y_{n+1/2})$$

- explicit method
- one-step, two-stage, 2 evaluations of f.
- nonlinear in f
- second order

Trapezoidal Methods

Implicit Trapezoidal:

$$y_n = y_{n-1} + \frac{h}{2} f(t_n, y_n) + \frac{h}{2} f(t_{n-1}, y_{n-1})$$

Two-stage implicit RK of order 2.

Explicit Trapezoidal:

$$\begin{aligned} \hat{y}_1 &= y_{n-1} + h f(t_{n-1}, y_{n-1}) \\ y_n &= y_{n-1} + \frac{h}{2} f(t_n, \hat{y}_1) + \frac{h}{2} f(t_{n-1}, y_{n-1}) \end{aligned}$$

Two-stage explicit RK of order 2.

Classical 4-th Order Runge-Kutta

Simpson's rule: let $h = t_n - t_{n-1},\ t_{n+1/2} = t_{n-1} + h/2$

$$y(t_n) - y(t_{n-1}) \approx \frac{h}{6}\left(y'(t_{n-1}) + 4y'(t_{n+1/2}) + y'(t_n)\right)$$

One possible version is the classical explicit 4-stage RK method:

$$\begin{aligned}
\hat{y}_1 &= y_{n-1}, & f_1 &= f(t_{n-1}, \hat{y}_1) \\
\hat{y}_2 &= y_{n-1} + \frac{h}{2} f_1, & f_2 &= f(t_{n+1/2}, \hat{y}_2) \\
\hat{y}_3 &= y_{n-1} + \frac{h}{2} f_2, & f_3 &= f(t_{n+1/2}, \hat{y}_3) \\
\hat{y}_4 &= y_{n-1} + h f_3, & f_4 &= f(t_n, \hat{y}_4)
\end{aligned}$$

$$y_n = y_{n-1} + h\left(\frac{1}{6} f_1 + \frac{1}{3} f_2 + \frac{1}{3} f_3 + \frac{1}{6} f_4\right)$$

General RK s-stage Form

$$f_i = f(t_{n-1} + \gamma_i h, \hat{y}_i) \quad 1 \le i \le s$$

$$\hat{y}_i = y_{n-1} + h \sum_{j=1}^{s} \alpha_{ij} f_j \quad 1 \le i \le s$$

$$y_n = y_{n-1} + h \sum_{j=1}^{s} \beta_j f_j$$

- $\gamma_i = \sum_{j=1}^{s} \alpha_{ij}$
- $\hat{y}_i \approx y(t_{n-1} + \gamma_i h)$ possibly to lower order
- explicit if and only if $\alpha_{ij} = 0$ for $j \ge i$
- other representations possible, e.g., in terms of intermediate f values

Matrix Form

General RK s-stage Method:

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cccc} \gamma_1 & \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1s} \\ \gamma_2 & \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \gamma_s & \alpha_{s1} & \alpha_{s2} & \cdots & \alpha_{ss} \\ \hline & \beta_1 & \beta_2 & \cdots & \beta_s \end{array}$$

- Explicit if and only if A is strictly lower triangular.
- $c = Ae$, $e = \begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix}^T$

Example

Forward Euler $s = 1$ and $p = 1$

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad y_n = y_{n-1} + h(1 * f_1)$$

$$\hat{y}_1 = y_{n-1} + h(0 * f_1), \quad f_1 = f(t_{n-1} + 0 * h, \hat{y}_1)$$

Example

Family of $s = 2$ and $p = 2$ with parameter μ

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

$\mu = 1$ is explicit trapezoidal and $\mu = 1/2$ is explicit midpoint.

Explicit Midpoint

$s = 2$ and $p = 2$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array} \qquad y_n = y_{n-1} + h(0 * f_1 + f_2)$$

$$\hat{y}_1 = y_{n-1} + 0 * f_1 + 0 * f_2, \quad f_1 = f(t_{n-1} + 0 * h, \;\; \hat{y}_1)$$

$$\hat{y}_2 = y_{n-1} + h(\frac{1}{2} f_1 + 0 * f_2), \quad f_2 = f(t_{n-1} + \frac{1}{2} h, \;\; \hat{y}_2),$$

Example

Family of explicit methods with $s = 3$ and $p = 3$ parameterized by μ

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

Classical Explicit 4-th order $s = 4$ and $p = 4$

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \qquad y_n = y_{n-1} + h\left(\frac{1}{6}f_1 + \frac{1}{3}f_2 + \frac{1}{3}f_3 + \frac{1}{6}f_4\right)$$

$$\hat{y}_1 = y_{n-1} + h(0f_1 + 0f_2 + 0f_3 + 0f_4), \quad f_1 = f(t_{n-1}, \hat{y}_1)$$

$$\hat{y}_2 = y_{n-1} + h(\frac{1}{2}f_1 + 0f_2 + 0f_3 + 0f_4), \quad f_2 = f(t_{n-1} + \frac{h}{2}, \hat{y}_2)$$

$$\hat{y}_3 = y_{n-1} + h(0f_1 + \frac{1}{2}f_2 + 0f_3 + 0f_4), \quad f_3 = f(t_{n-1} + \frac{h}{2}, \hat{y}_3)$$

$$\hat{y}_4 = y_{n-1} + h(0f_1 + 0f_2 + f_3 + 0f_4), \quad f_4 = f(t_n, \hat{y}_4)$$

Explicit Method Achievable Order

- For any RK method the order is determined by a series of algebraic conditions derived from Taylor expansions
- Not as simple in form as linear multistep methods.
- For explicit methods $p \leq s$.

s	1	2	3	4	5	6	7	8	9	10
p	1	2	3	4	4	5	6	6	7	7

Discretization Error Determination

We need two basic sets of identities (suppressing arguments):

$$y' = f$$

$$y'' = f_t + f_y f$$

$$y''' = f_{tt} + 2f_{ty}f + f_y f_t + f_{yy}f^2 + f_y^2 f$$

$$\vdots$$

$$F(u + \Delta u, v + \Delta v) = F + [F_u \Delta u + F_v \Delta v]$$

$$+\frac{1}{2}\left[F_{uu}\Delta u^2 + 2F_{uv}\Delta u \Delta v + F_{vv}\Delta v^2\right] + \cdots + \frac{1}{n!}\ell^n F + \cdots ,$$

where

$$\ell^n F = \sum_{j=0}^{n} \binom{n}{j} \Delta u^j \Delta v^{n-j} \frac{\partial^n F}{\partial u^j \partial v^{n-j}}$$

Explicit Midpoint Rule Order

$$
\begin{aligned}
\hat{y}_1(t_{n-1}) &= y(t_{n-1}) + \frac{h}{2} f(t_{n-1}, y(t_{n-1})) \\
&= y(t_{n-1}) + \frac{h}{2} y'(t_{n-1})
\end{aligned}
$$

$$
\frac{y(t_n) - y(t_{n-1})}{h} = f(t_{n-1} + \frac{h}{2}, y(t_{n-1}) + \frac{h}{2} y'(t_{n-1}))
$$

Reducing the left side yields

$$
\begin{aligned}
\frac{y(t_n) - y(t_{n-1})}{h} &= y'(t_{n-1}) + \frac{h}{2} y''(t_{n-1}) + \frac{h^2}{6} y'''(t_{n-1}) + O(h^3) \\
&= y' + \frac{h}{2} y'' + \frac{h^2}{6} y''' + O(h^3)
\end{aligned}
$$

Explicit Midpoint Rule Order

Reducing the right side yields, $\Delta t = h/2$, $\Delta y = fh/2$,

$$f(t_{n-1} + \frac{h}{2}, y + \frac{h}{2}f) = f + \frac{h}{2}f_t + \frac{h}{2}f_y f$$

$$+\frac{1}{2}\Big[f_{tt}(\frac{h^2}{4}) + 2f_{ty}(\frac{h}{2} * \frac{h}{2}f) + f_{yy}(\frac{h^2}{4}f^2)\Big] + O(h^3)$$

$$= f + \frac{h}{2}(f_t + f_y f) + \frac{h^2}{8}\Big[f_{tt} + f_{yy}f^2 + 2f_{ty}f\Big] + O(h^3)$$

Explicit Midpoint Rule Order

The constant and $O(h)$ terms are 0 since

$$y' - f = 0 \quad \text{and} \quad y'' - (f_t + f_y f) = 0$$

The $O(h^2)$ terms are nonzero since terms are missing on the right side from the y''' expression and therefore

$$d_n = O(h^2)$$

Embeded RK Methods

For error estimation and stepsize control, we seek $\hat{y}_n$ of order p and y_n of order $p+1$ via two methods where one is embedded in the other, i.e., the order $p+1$ uses the evaluations of the order p method.

For example, Forward Euler and an explicit trapezoidal

$$\begin{array}{c|c} c & A \\ \hline & \hat{b}^T \\ \hline & b^T \end{array} = \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Fehlberg 4(5) pair and Dormand-Prince 4(5) pair are popular explicit embedded pairs. (see Ascher and Petzold for A, b, c)

Embeded RK Methods

Forward Euler and explicit Trapezoidal as an embedded pair,

$$\hat{y}_1 = y_{n-1} + h(0 * f_1 + 0 * f_2), \quad f_1 = f(t_{n-1},\ \hat{y}_1)$$

$$\hat{y}_2 = y_{n-1} + h(f_1 + 0 * f_2), \quad f_2 = f(t_{n-1} + h,\ \hat{y}_2)$$

$$y_{fe} = y_{n-1} + h(f_1 + 0 * f_2)$$

$$y_{et} = y_{n-1} + h(\frac{1}{2} f_1 + \frac{1}{2} f_2)$$

$$e_{fe} = y_{et} - y_{fe}$$

- The estimate is used for the less accurate of the two.
- Stepsize can be adjusted accordingly.
- For nonstiff problems, the more accurate, e.g., y_{et}, is often used as y_n.

Implicit RK Methods Based on Collocation

Collocation: require the equations that define the problem to be satisfied at a set of predetermined points by a function from a selected class.

Let $t_i = t_{n-1} + \gamma_i h$ for $0 \leq \gamma_1 < \gamma_2 < \cdots < \gamma_s \leq 1$ and define the polynomial via collocating conditions:

$$P(t_{n-1}) = y_{n-1}$$
$$P'(t_i) = f(t_i, P(t_i)) = f_i \quad 1 \leq i \leq s$$

$P(t_n) = y_n$ defines an s-step implicit RK method.

Implicit RK Methods Based on Collocation

Specifically, using quadrature we have

$$P(t_n) - P(t_{n-1}) = h \sum_{j=1}^{s} \left(\int_0^1 L_j(\tau) d\tau \right) f_j = h \sum_{j=1}^{s} \beta_j f_j$$

$$L_j(t_{n-1} + \tau h) = \prod_{i=1, i \neq j}^{s} \frac{(\tau - \gamma_i)}{(\gamma_j - \gamma_i)}, \quad 0 \leq \gamma_i \leq 1$$

The $f_j = f(t_j, P(t_j))$ have unknowns $P(t_j)$

Implicit RK Methods Based on Collocation

s additional equations needed.

$$
\begin{aligned}
P(t_i) - P(t_{n-1}) &= h \sum_{j=1}^{s} \left(\int_0^{\gamma_i} L_j(\tau) d\tau \right) f_j \\
&= h \sum_{j=1}^{s} \alpha_{ij} f_j
\end{aligned}
$$

The method is defined by taking $\hat{y}_j = P(t_j)$.

Implicit RK Methods Based on Collocation

Gauss Methods: $p = 2s$ (maximal order) based on Gauss Legendre quadrature. Include implicit midpoint.

$$s = 1, \qquad \begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

$$s = 2, \qquad \begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{3-2\sqrt{3}}{12} \\ \frac{3+\sqrt{3}}{6} & \frac{3+2\sqrt{3}}{12} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Derivation of Gauss RK Methods

For s stage method, points are the roots of the degree s Legendre polynomial, $P_s(z)$, $-1 \leq z \leq 1$.

Care must be taken with the changes of variables. We have $-1 \leq z \leq 1$, $t_{n-1} \leq t \leq t_n$ and $0 \leq \tau \leq 1$.

For $s = 1$ we have

$$P_1(z) = z \rightarrow z_1 = 0$$

$$t = z\frac{h}{2} + \frac{t_n + t_{n-1}}{2} \rightarrow t_1 = \frac{t_n + t_{n-1}}{2}$$

$$\therefore \gamma_1 = \frac{1}{2}$$

Derivation of Gauss RK Methods

Since $s = 1$

$$L_1(t_{n-1} + \tau h) = \prod_{i=1, i\neq j}^{s} \frac{(\tau - \gamma_i)}{(\gamma_j - \gamma_i)} = 1$$

$$\beta_1 = \int_0^1 1 d\tau = 1$$

We also have

$$\alpha_{11} = \int_0^{\gamma_1} 1 d\tau = \frac{1}{2}$$

Derivation of Gauss RK Methods

The method is therefore given by

$$\hat{y}_1 = y_{n-1} + h\alpha_{11} f_1 = y_{n-1} + \frac{h}{2} f_1$$
$$f_1 = f(t_{n-1} + \gamma_1 h, \hat{y}_1) = f(t_{n-1} + \frac{1}{2}h, \hat{y}_1)$$
$$y_n = y_{n-1} + h\beta_1 f_1 = y_{n-1} + hf_1$$

i.e., the implicit midpoint rule.

Derivation of Gauss RK Methods

For $s = 2$ we have

$$P_2(z) = \frac{3}{2}z^2 - \frac{1}{2} \rightarrow z_\pm = \pm\frac{1}{\sqrt{3}}$$

$$t = z\frac{h}{2} + \frac{t_n + t_{n-1}}{2} \rightarrow t_\pm = t_{n+1/2} \pm \frac{1}{\sqrt{3}}h$$

$$t_{n-1} + \frac{h}{2} \pm \frac{h}{\sqrt{3}} = t_{n-1} + h\left(\frac{\sqrt{3} \pm 1}{2\sqrt{3}}\right)$$

$$\therefore \gamma_1 = \frac{3 - \sqrt{3}}{6}, \quad \gamma_2 = \frac{3 + \sqrt{3}}{6}$$

Derivation of Gauss RK Methods

$$\gamma_1 = \frac{3-\sqrt{3}}{6}, \quad \gamma_2 = \frac{3+\sqrt{3}}{6}$$

$$L_1(\tau) = \frac{(\tau-\gamma_2)}{(\gamma_1-\gamma_2)}, \quad L_2(\tau) = \frac{(\tau-\gamma_1)}{(\gamma_2-\gamma_1)}, \quad \gamma_2-\gamma_1 = \frac{\sqrt{3}}{3}$$

$$\alpha_{11} = \int_0^{\gamma_1} L_1(\tau)d\tau = -\frac{3}{\sqrt{3}}\left[(\tau-\gamma_2)^2\right]_0^{\gamma_1} = \frac{1}{4}$$

$$\alpha_{22} = \int_0^{\gamma_2} L_2(\tau)d\tau = \frac{3}{\sqrt{3}}\left[(\tau-\gamma_1)^2\right]_0^{\gamma_2} = \frac{1}{4}$$

Derivation of Gauss RK Methods

$$\alpha_{12} = \int_0^{\gamma_1} L_2(\tau)d\tau = \frac{3}{\sqrt{3}}\left[(\tau-\gamma_1)^2\right]_0^{\gamma_1} = \frac{1}{4} - \frac{1}{2\sqrt{3}} = \frac{3-2\sqrt{3}}{12}$$

$$\alpha_{21} = \int_0^{\gamma_2} L_1(\tau)d\tau = -\frac{3}{\sqrt{3}}\left[(\tau-\gamma_2)^2\right]_0^{\gamma_2} = \frac{1}{4} + \frac{1}{2\sqrt{3}} = \frac{3+2\sqrt{3}}{12}$$

$$\beta_1 = \int_0^{1} L_1(\tau)d\tau = -\frac{3}{2\sqrt{3}}\left[1-2\gamma_2\right] = \frac{1}{2}$$

$$\beta_2 = \int_0^{1} L_2(\tau)d\tau = \frac{3}{2\sqrt{3}}\left[1-2\gamma_1\right] = \frac{1}{2}$$

Implicit RK Methods Based on Collocation

Lobatto Methods: quadrature includes two ends of the interval, extends the trapezoidal rule, $p = 2s - 2$

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\
1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

Implicit RK Methods Based on Collocation

Radau Methods: quadrature includes t_n, extends the backward Euler

$p = 2s - 1$

$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

Stability

- All one-step methods, $y_n = y_{n-1} + h\Psi(t_{n-1}, y_{n-1}, h)$, are 0-stable for Lipschitz Ψ.
- $y' = \lambda y \to y_n = R(z) y_{n-1}$ with $z = h\lambda$, $e = \begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix}^T$ and
$$R(z) = 1 + z b^T (I - zA)^{-1} e$$
- $R(z)$ is a polynomial for explicit methods and for those with $p = s \leq 4$
$$R(z) = 1 + h\lambda + \cdots + \frac{(h\lambda)^p}{p!}$$
and all p-stage order p explicit methods have the same absolute stability region. (see figure from Ascher and Petzold on following slide)
- Explicit RK methods cannot be A-stable.

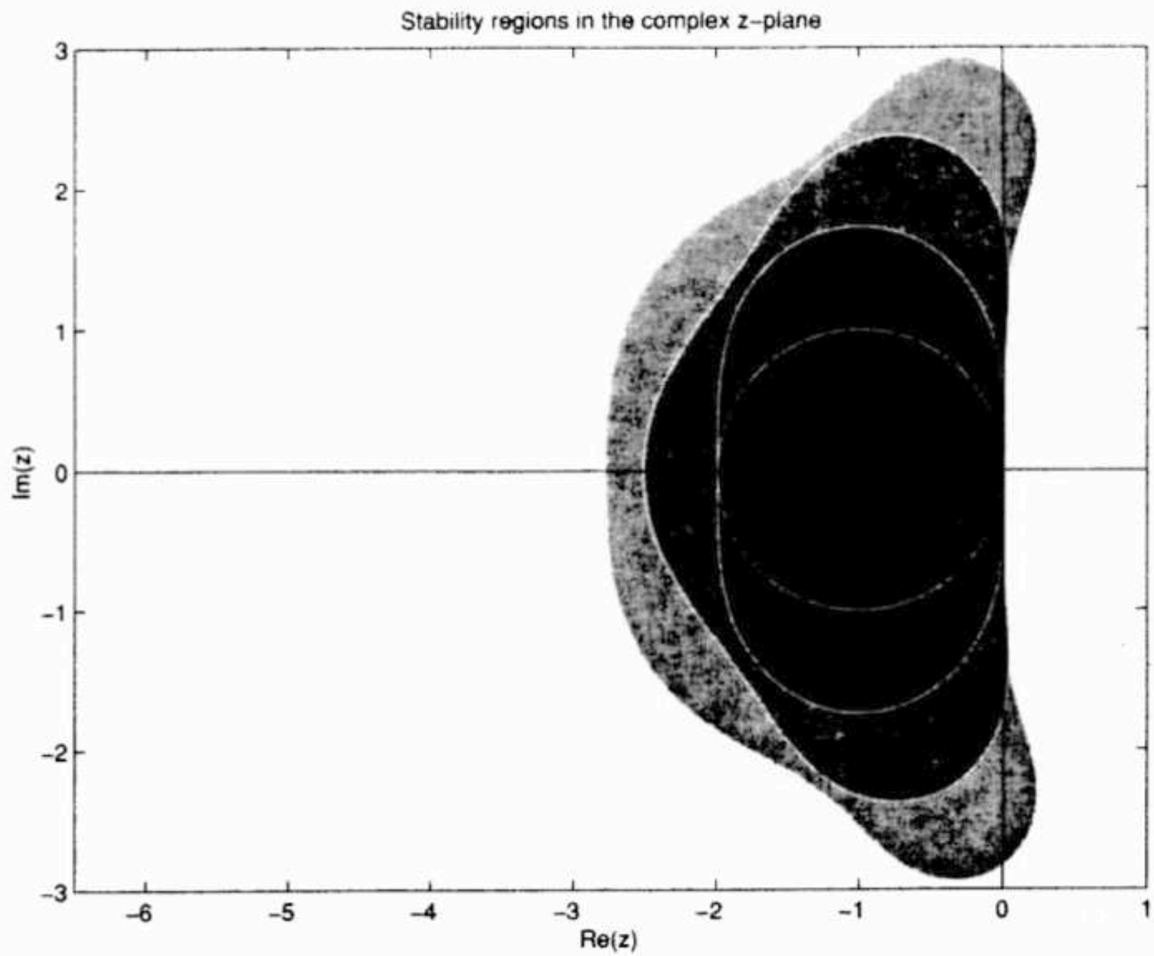

Figure 4.4: *Stability regions for p-stage explicit Runge–Kutta methods of order p, $p = 1, 2, 3, 4$. The inner circle corresponds to forward Euler, $p = 1$. The larger p is, the larger the stability region. Note the "ear lobes" of the fourth-order method protruding into the right half-plane.*

Stability

- For implicit RK methods $R(z)$ is rational
$$R(z) = \frac{P(z)}{Q(z)}$$
- A-stable methods are plentiful.
- If A is nonsingular and $b^T = e_s^T A$ the RK method is called stiffly accurate $\rightarrow$ has stiff decay. (but not vice versa)
- Gauss and Lobatto methods do not have stiff decay but they are A-stable
- Gauss and Lobatto methods are symmetric methods and are useful for boundary value problems but not for stiff problems
- Radau methods have stiff decay and are very good for stiff problems.

Efficiency and Explicit RK Methods

- When comparing the efficiency of different methods remember:
  - a single method may allow multiple implementations with different efficiencies
  - work per step must be viewed relative to different stepsize profiles
  - one step with multiple stages vs. multiple steps of an LMS
  - computation (or time) per unit accuracy
- Methods with a dense strict lower triangular A must have storage proportional to sm where m is the size of the system of ODEs. (similar to both implicit and explicit LMS methods)
- If A is also banded then storage can be very efficient,e.g., classical RK4: vector for y_n, vector for y_{n-1}, one y work vector, one f work vector each of size m .

Efficiency and Explicit RK Methods

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \qquad y_n = y_{n-1} + h\left(\frac{1}{6}f_1 + \frac{1}{3}f_2 + \frac{1}{3}f_3 + \frac{1}{6}f_4\right)$$

$$\begin{aligned}
\hat{y}_1 &= y_{n-1} + h(0f_1 + 0f_2 + 0f_3 + 0f_4), \quad f_1 = f(t_{n-1}, \hat{y}_1) \\
\hat{y}_2 &= y_{n-1} + h(\frac{1}{2}f_1 + 0f_2 + 0f_3 + 0f_4), \quad f_2 = f(t_{n-1} + \frac{h}{2}, \hat{y}_2) \\
\hat{y}_3 &= y_{n-1} + h(0f_1 + \frac{1}{2}f_2 + 0f_3 + 0f_4), \quad f_3 = f(t_{n-1} + \frac{h}{2}, \hat{y}_3) \\
\hat{y}_4 &= y_{n-1} + h(0f_1 + 0f_2 + f_3 + 0f_4), \quad f_4 = f(t_n, \hat{y}_4)
\end{aligned}$$

Efficiency and Implicit RK Methods

- Implict methods with a dense A require the solution of a system of sm nonlinear equations giving the $\hat{y}_i$ with a Jacobian matrix and a linear system of the form

$$\begin{bmatrix} I_m - h\alpha_{11}J_1 & -h\alpha_{12}J_2 & \cdots & -h\alpha_{1s}J_s \\ \vdots & & & \vdots \\ -h\alpha_{s1}J_1 & -h\alpha_{s2}J_2 & \cdots & I_m - h\alpha_{ss}J_s \end{bmatrix} \begin{bmatrix} d_1 \\ \vdots \\ d_s \end{bmatrix} = \begin{bmatrix} r_1 \\ \vdots \\ r_s \end{bmatrix}$$

  where $J_i = f_y(\hat{y}_i^{(k)})$ on the $k-$th Newton iteration.

- Such an expense is prohibitive in general and significantly increased compared to implicit LMS methods.

Efficiency and Implicit RK Methods

- Approximate Newton often used $J_i \approx f_y(y_{n-1})$ for all i and all iterations of Newton.
- Different α_{ij} still yields multiple matrices to evaluate before factoring $sm \times sm$ Jacobian (or to compute a preconditioner if iterative methods used).
- Collocation-based methods tend to have dense A, i.e., not many 0 elements.
- s kept small in most cases due to these problems.

Efficiency and (S)DIRK Methods

- Diagonally implicit RK methods have A lower triangular
- Implicitness is only present in stage i with respect to $\hat{y}_i$
- Solve s systems of m nonlinear equations.
- If the elements α_{ii} all equal to some constant then they are called Singly Diagonally implicit RK methods.
- Combined with approximation $J_i \approx f_y(y_{n-1})$ only one evaluation and factorization of $I - h\alpha f_y(y_{n-1})$ per time step.
- Less work for DIRK but lower achievable order: $p = s + 1$

DIRK and Stiffness

- If stiff decay is required then achievable order for a DIRK method is $p = s$
- DIRK methods with stiff decay are competitive with BDFs if the problem is not too stiff.
- DIRK methods drop to order 1 convergence in very stiff limit.
- Order of convergence reduction as $\mathcal{R}(\lambda) \to -\infty$ is seen for collocation methods.

DIRK Examples (Ascher and Petzold)

$$s = p = 1, \quad \text{backward Euler}$$

$$s = p = 2, \quad \begin{array}{c|cc} \gamma & \gamma & 0 \\ 1 & 1-\gamma & \gamma \\ \hline & 1-\gamma & \gamma \end{array}, \quad \gamma = \frac{2-\sqrt{2}}{2}$$

DIRK Examples (Ascher and Petzold)

$$s = p = 3$$

$$\begin{array}{c|ccc}
.4358665215 & .4358665215 & 0 & 0 \\
.7179332608 & .2820667392 & .4358665215 & 0 \\
1 & 1.208496649 & -.644363171 & .4358665215 \\
\hline
 & 1.208496649 & -.644363171 & .4358665215
\end{array}$$