Numerical Methods for Differential Equations

1.- Numerical Methods for ODEs

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Contents

- Numerical Methods for ODEs and DDEs (2 units, L. M. Abia)
  - Runge-Kutta and Multistep Methods.
  - Absolute Stability.
  - Numerical Methods for DDEs.
- Numerical Methods for Structured Population Models (2 units, O. Angulo)

The Problem

$$\mathbf{y}'(x) = \mathbf{f}(x, \mathbf{y}(x)), \quad a \le x \le b, \quad \mathbf{y}(a) = \mathbf{A},$$

$\mathbf{y}(x) = [y^1(x), \ldots, y^d(x)]^T \in \mathbb{R}^d$, $\quad \mathbf{f} : [a, b] \times I\!R^d \to I\!R^d$, $\quad \mathbf{f} = [f^1, \ldots, f^d]^T \in \mathbb{R}^d$.

SUCH THAT:

- $\mathbf{f} : [a, b] \times I\!R^d \to I\!R^d$ continuous
- f satisfies a Lipschitz condition with respect to $\mathbf{y}$

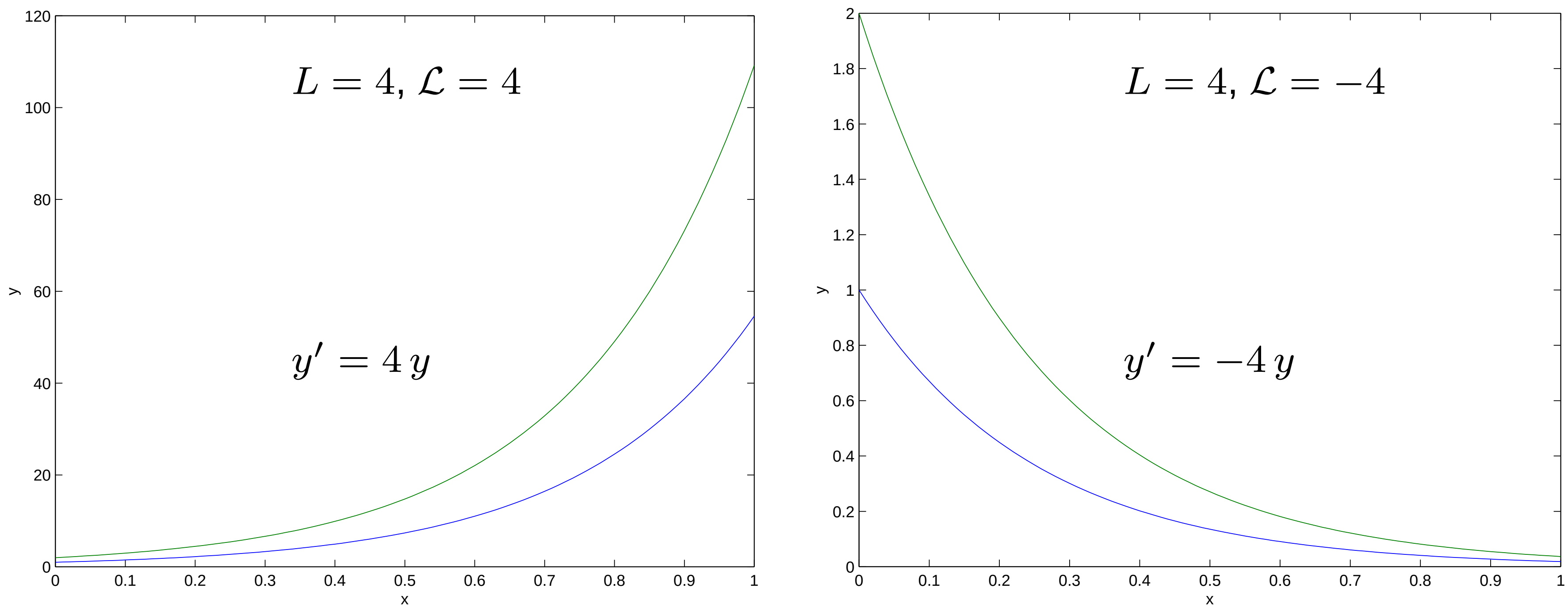
$$\|\mathbf{f}(x, \mathbf{y}_1) - \mathbf{f}(x, \mathbf{y}_2)\| \le L\, \|\mathbf{y}_1 - \mathbf{y}_2\|$$

for all $x \in [a, b]$, $\mathbf{y}_1$, $\mathbf{y}_2 \in \mathbb{R}^d$

$\Longrightarrow$ (Picard) Existence and uniqueness of a solution $\mathbf{y}(x)$ in $[a, b]$ and

$$\|\mathbf{y}_1(x) - \mathbf{y}_2(x)\| \le e^{L\,(x-a)}\, \|\mathbf{y}_1(a) - \mathbf{y}_2(a)\|, \quad x \in [a, b]$$

for any two solutions $\mathbf{y}_1(x)$,$\mathbf{y}_2(x)$.



- A more accurate estimate is obtained if $\mathbf{f}$ satisfies a one side Lipschitz condition with respect to $\mathbf{y}$

$$< \mathbf{f}(x,\mathbf{y}_1) - \mathbf{f}(x,\mathbf{y}_2), \mathbf{y}_1 - \mathbf{y}_2 > \leq \mathcal{L}\,\|\mathbf{y}_1 - \mathbf{y}_2\|^2 \quad \text{for all} \quad x \in [a,b], \mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^d.$$

Then

$$\|\mathbf{y}_1(x) - \mathbf{y}_2(x)\| \leq e^{\mathcal{L}\,(x-a)}\,\|\mathbf{y}_1(a) - \mathbf{y}_2(a)\|, \quad x \in [a,b]$$

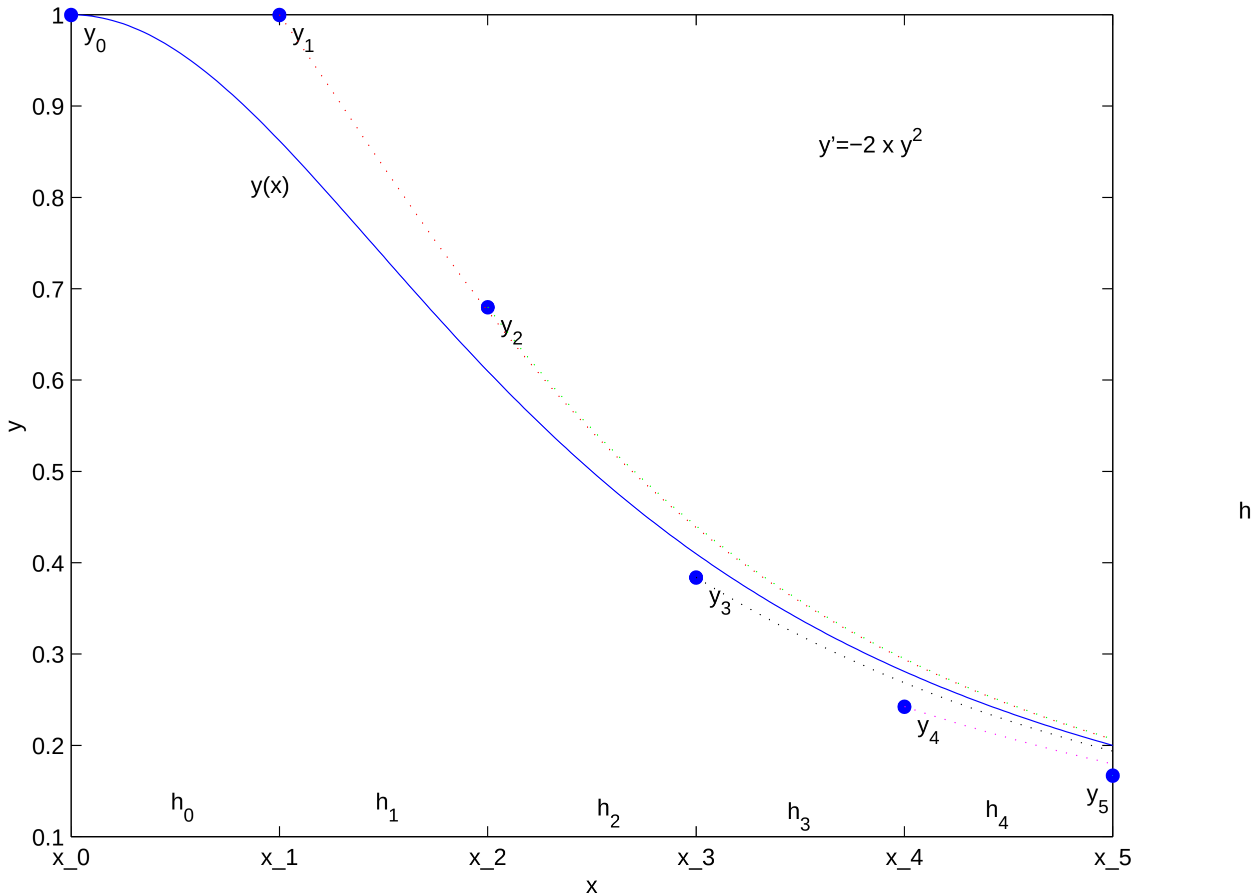
for any two solutions $\mathbf{y}_1(x)$,$\mathbf{y}_2(x)$.

Discrete Variable Methods

$$a = x_0 < x_1 < x_2 < \ldots < x_N = b.$$

$$x_{n+1} = x_n + h_{n+1},\, n = 0, \ldots, N-1, \quad h = \text{máx}_{0 \le n \le N-1} h_{n+1}.$$

$\{\mathbf{y}_n\}_{n=0}^{N}$, Numerical Solution, $\quad y_n \approx y(x_n)$



$$y_0 = A,\, \mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\, \mathbf{f}(x_n, \mathbf{y}_n),\, n = 0, \ldots, N-1, \quad \text{(Euler Method)}$$

Discrete Variable Methods

- Methods can be **explicit** or **implicit**:
  - $\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\,\mathbf{f}(x_n, \mathbf{y}_n), n = 0, \ldots, N-1, \quad \mathbf{y}_0 \approx \mathbf{A}$ (Euler Method)
  - $\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\,\mathbf{f}(x_n, \mathbf{y}_{n+1}), n = 0, \ldots, N-1, \quad \mathbf{y}_0 \approx \mathbf{A}$ (Backward Euler)
- One-step methods

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}_n, \mathbf{y}_{n+1}; \mathbf{f}, h_{n+1}), \quad \mathbf{y}_0 \text{ dado .}$$

- Multistep methods

$$\mathbf{y}_{n+1} = \sum_{j=1}^{k} \alpha_j \mathbf{y}_{n+1-j} + h\mathbf{\Phi}(x_n, \mathbf{y}_{n+1}, \ldots, \mathbf{y}_{n+k-1}; \mathbf{f}, h),$$

or

$$\mathbf{y}_{n+1} = \sum_{j=1}^{k} \alpha_{n,j} \mathbf{y}_{n+1-j} + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}_{n+1}, \ldots, \mathbf{y}_{n+k-1}; \mathbf{f}, \Delta_n),$$

with $\Delta_n = \{x_{n+1}, \ldots, x_{n-k+1}\}$, and $\mathbf{y}_0, \ldots, \mathbf{y}_{k-1}$ dados .

- Others

One-Step Methods for ODEs

- Local solution at $x = x_n$,

$$\mathbf{u}' = \mathbf{f}(x, \mathbf{u}), \quad x > x_n, \quad \mathbf{u}(x_n) = \mathbf{y}_n.$$

- Local error at the step $x_n \to x_{n+1}$

$$\mathbf{le}_{n+1} := \mathbf{u}(x_{n+1}) - \mathbf{y}_{n+1}$$

- Example: Taylor Series Method (d=1 for simplicity):

$$u(x_{n+1}) \approx y_{n+1} = y_n + hu'(x_n) + \frac{h^2}{2}u''(x_n) + \frac{h^3}{6}u'''(x_n),$$

where

$$\begin{aligned} u'(x_n) &= f, \\ u''(x_n) &= f_x + f_y f, \\ u'''(x_n) &= f_{xx} + 2f_{xy}f + f_{yy}f^2 + f_y f_x + f_y^2 f, \end{aligned}$$

with all the functions evaluated at (x_n, y_n).

General Explicit Runge-Kutta Methods

- A general explicit s-stages Runge-Kutta method is given by the formulae

$$\begin{aligned} \mathbf{y}_{n+1} &= \mathbf{y}_n + h\sum_{i=1}^{s} b_i \mathbf{f}(x_n + c_i h, \mathbf{Y}_i), \\ \mathbf{Y}_i &= \mathbf{y}_n + h\sum_{j=1}^{i-1} a_{ij} \mathbf{f}(x_n + c_j h, \mathbf{Y}_j), \quad i = 1, \ldots, s, \end{aligned}$$

  The quantities $\mathbf{Y}_i, i = 1, \ldots, s$, are called inner stages of the method.

- The method is completely defined by the parameters

$$\begin{array}{c|ccccc} c_1 & 0 & & & \\ c_2 & a_{21} & 0 & & \\ \vdots & \vdots & \vdots & \ddots & \\ c_s & a_{s1} & a_{s2} & \cdots & 0 \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}, \qquad \begin{array}{c} \mathbf{c} = [c_1, \ldots, c_s]^T, (abscisae) \\ \mathbf{b} = [b_1, \ldots, b_s]^T, (weights) \\ A = (a_{ij}), \quad \sum_{j=1}^{s} a_{ij} = c_i, i = 1, \ldots, s \end{array}$$

One-step Methods for ODEs

- Classical low order Runge-Kutta Methods are easily obtained from

$$\mathbf{u}(x_n + h) = \mathbf{u}(x_n) + \int_{x_n}^{x_n+h} \mathbf{f}(x, \mathbf{u}(x))dx,$$

using quadrature rules. For example,

  - Modified Euler method

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\,\mathbf{f}(x_n + \frac{1}{2}h, \mathbf{y}_n + \frac{1}{2}h\mathbf{f}(x_n, \mathbf{y}_n)),$$

  - Improved Euler Method

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{h}{2}(\mathbf{f}(x_n, \mathbf{y}_n) + \mathbf{f}(x_n + h, \mathbf{y}_n + h\mathbf{f}(x_n, \mathbf{y}_n))$$

Other RK formulae

The general approach is to match up to a given order the terms in the Taylor serie expansions for $\mathbf{u}(x_n + h)$ and $\mathbf{y}_{n+1}(h)$. For example, for the scalar equation $y' = f(x, y)$ and for an explicit 3-stages RK-method

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

, we have

$$\begin{aligned} u(x_n + h) &= y_n + hf + \frac{1}{2}h^2(f_x + ff_y) \\ &+ \frac{1}{6}h^3(f_y(f_x + ff_y) + (f_{xx} + 2ff_{xy} + f^2 f_{yy})) + O(h^4), \end{aligned}$$

and

$$\begin{aligned} y_{n+1} &= y_n + h(b_1 + b_2 + b_3)f + h^2(b_2c_2 + b_3c_3)(f_x + ff_y) \\ &+ \frac{1}{2}h^3[2b_3c_2a_{32}(f_x + ff_y)f_y + (b_2c_2^2 + b_3c_3^2)(f_{xx} + 2ff_{xy} + f^2 f_{yy})] \\ &+ O(h^4). \end{aligned}$$

where $f_x, f_y, f_{xx}, \ldots$, are evaluated at $(x_n, \mathbf{y}_n)$.

- Explicit 2-stage RK methods ($b_3 = c_3 = a_{31} = a_{32} = 0$, $b_1, b_2, a_{21} = c_2$):

$$\begin{array}{l} b_1 + b_2 = 1, \\ b_2 c_2 = \frac{1}{2} \end{array}, \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ c/2 & c/2 & 0 \\ \hline & 1 - 1/c & 1/c \end{array}, \qquad \begin{array}{l} c = 2, \text{ Modified Euler} \\ c = 1, \text{ Improved Euler} \end{array}$$

- Explicit 3-stage RK methods ($b_1, b_2, b_3, c_3, a_{31}, a_{32}, a_{21}$)

$$\begin{array}{l} b_1 + b_2 + b_3 = 1, \\ b_2 c_2 + b_3 c_3 = \frac{1}{2} \\ b_2 c_2^2 + b_3 c_3^2 = \frac{1}{3} \\ b_3 c_2 a_{32} = \frac{1}{6} \end{array}, \qquad \begin{array}{c|ccc} 0 & & & \\ 1/3 & 1/3 & & \\ 2/3 & 0 & 2/3 & \\ \hline & 1/4 & 0 & 3/4 \end{array}, \qquad \begin{array}{c|ccc} 0 & & & \\ 1/2 & 1/2 & & \\ 1 & -1 & 2 & \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$$

4-Stages Classical RK-methods

- Order conditions

$$
\begin{aligned}
&b_1 + b_2 + b_3 + b_4 = 1, \\
&b_2 c_2 + b_3 c_3 + b_4 c_4 = 1/2, \\
&b_2 c_2^2 + b_3 c_3^2 + b_4 c_4^2 = 1/3, \\
&b_3 a_{32} c_2 + b_4 (a_{42} c_2 + a_{43} c_3) = 1/6, \\
&b_2 c_2^3 + b_3 c_3^3 + b_4 c_4^3 = 1/4, \\
&b_3 c_3 a_{32} c_2 + b_4 c_4 (a_{42} c_2 + a_{43} c_3) = 1/8, \\
&b_3 a_{32} c_2^2 + b_4 (a_{42} c_2^2 + a_{43} c_3^2) = 1/2, \\
&b_4 a_{43} a_{32} c_2 = 1/24
\end{aligned}
$$

$$
\begin{array}{c|cccc}
0 & & & & \\
1/2 & 1/2 & & & \\
1/2 & 0 & 1/2 & & \\
1 & 0 & 0 & 1 & \\
\hline
 & 1/6 & 2/6 & 2/6 & 1/6
\end{array}
\qquad
\begin{array}{c|cccc}
0 & & & & \\
1/3 & 1/3 & & & \\
2/3 & -1/3 & 1 & & \\
1 & 1 & -1 & 1 & \\
\hline
 & 1/8 & 3/8 & 3/8 & 1/8
\end{array}
.
$$

The algebraic theory of order for RK methods

$$\mathbf{y}' = \mathbf{f}(\mathbf{y}), \quad a \le x \le b, \qquad \mathbf{f} = [f^1, \dots, f^d].$$

- We introduce the notation (from tensorial calculus)

$$\frac{\partial f^i}{\partial y^j} = f^i_{,j}, \quad \frac{\partial^2 f^i}{\partial y^j \partial y^k} = f^i_{,j,k}, \qquad 1 \le i, j, k \le d.$$

and

- The convention that when an index is repeated in an expression then we assume that the expression is to be summed over all values of the index. For example,

$$(\mathbf{u}')^i(x_n) = f^i(\mathbf{y}_n), \quad i = 1, \dots, d,$$

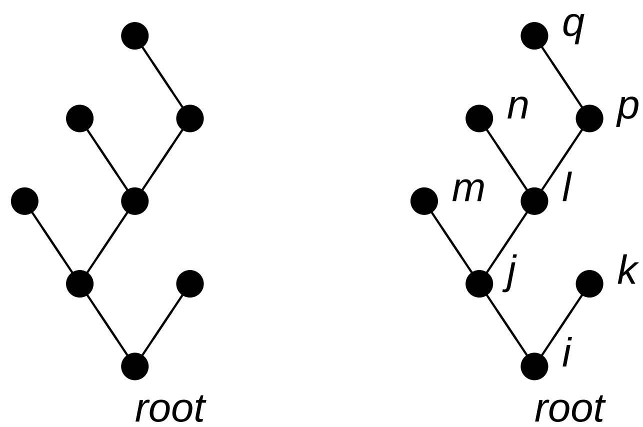
$$(\mathbf{u}'')^i(x_n) = \sum_{j=1}^{d} f^i_{,j}(\mathbf{y}_n) f^j(\mathbf{y}_n) = f^i_{,j}(\mathbf{y}_n) f^j(\mathbf{y}_n), \quad i = 1, \dots, d.$$

$$(\mathbf{u}''')^i(x_n) = f^i_{,j,k} f^j f^k + f^i_{,j} f^j_{,k} f^k,$$

$$(\mathbf{u}^{(4)})^i(x_n) = f^i_{,j,k,l} f^j f^k f^l + f^i_{,j,k} f^j_{,l} f^l f^k + f^i_{,j,k} f^j f^k_{,l} f^l$$

$$+ f^i_{,j,l} f^l f^j_{,k} f^k + f^i_{,j} f^j_{,k,l} f^k f^l + f^i_{,j} f^j_{,k} f^k_{,l} f^l,$$

Order Conditions for RK Methods



We associate an elementary differential of $\mathbf{f}$ to each monotone labelling of a rooted tree, as for example, in

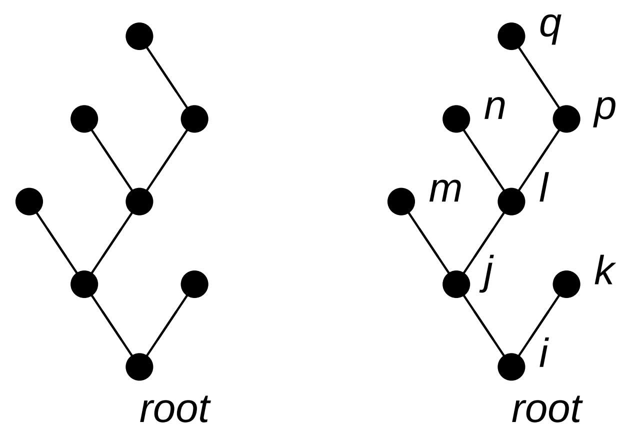
$$(\mathbf{F})^i(\lambda\tau) = \sum_{j,k,l,m,n,p,q=1}^{d} f^i_{,j,k} f^k f^j_{,l,m} f^m f^l_{,p,n} f^n f^p_{,q} f^q.$$

Then

$$\mathbf{u}^{(q)}(x_n + h) = \sum_{\tau \in T_q} \alpha(\tau)\mathbf{F}(\tau)(\mathbf{y}_n)$$

Here T_q is the set of all the rooted trees with order (number of nodes) q, and $\alpha(\tau)$ represents the number of different monotone labelling for the rooted tree τ.

Order Conditions for RK Methods



- For each monotone labelling $\lambda\tau$ of a rooted tree τ of order q with labels $j_1 < j_2 < \ldots < j_q$ we introduce the coefficients

$$\Psi^i(\tau) = \sum_{j,k,l,m,n,p,q=1}^{s} a_{ij}a_{ik}a_{jm}a_{jl}a_{ln}a_{lp}a_{pq} = \sum_{j,l,p} c_i a_{ij} c_j a_{jl} c_l a_{lp} c_p,$$

  and we put $\mathbf{\Psi}(\tau) = [\Psi^1(\lambda\tau), \ldots, \Psi^s(\lambda\tau)]$.

- We denote $\tau = [\tau_1, \tau_2, \ldots, \tau_M]$ if τ is obtained by connecting the roots of the rooted trees $\tau_1, \ldots, \tau_M$ to a new node that is going to become the root of the rooted tree τ. Then we define the density $\gamma(\tau)$ of τ, by recurrence,

$$\gamma(\tau) := \rho(\tau)\gamma(\tau_1)\gamma(\tau_2)\ldots\gamma(\tau_M), \quad \rho(\tau) = \text{number of nodes}$$

Order Conditions for RK methods

With the previous definitions we have that the q-derivatives of $\mathbf{y}_{n+1}(h)$ and $\mathbf{Y}_i(h), i = 1, 2, \ldots, s$ at $h = 0$ are given respectively by the expressions

$$\left.(\mathbf{Y}_i)^{(q)}\right|_{h=0} = \sum_{\tau \in T_q} \alpha(\tau)\gamma(\tau) \sum_{j=1}^{s} a_{ij} \Psi^j(\tau)\mathbf{F}(\tau)(\mathbf{y}_n)$$

$$\left.(\mathbf{y}_{n+1})^{(q)}\right|_{h=0} = \sum_{\tau \in T_q} \alpha(\tau)\gamma(\tau) \sum_{i=1}^{s} b_i \Psi^i(\tau)\mathbf{F}(\tau)(\mathbf{y}_n)$$

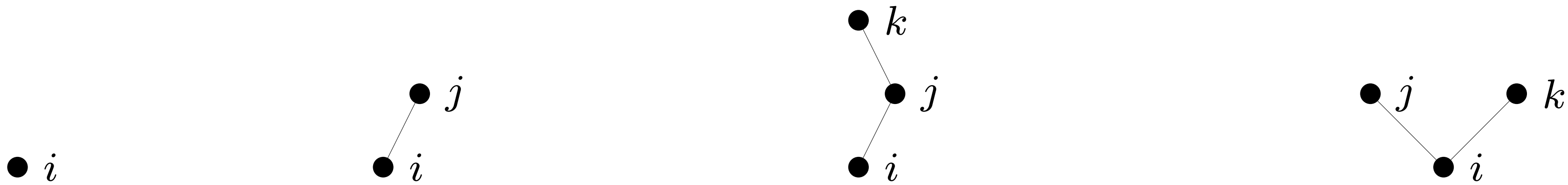
Then, a RK method of s stages has at least order p iff

$$\sum_{i=1}^{s} b_i \Psi^i(\tau) = \frac{1}{\gamma(\tau)}, \quad \forall \tau \text{ of order less than or equal } p, \quad \text{and}$$

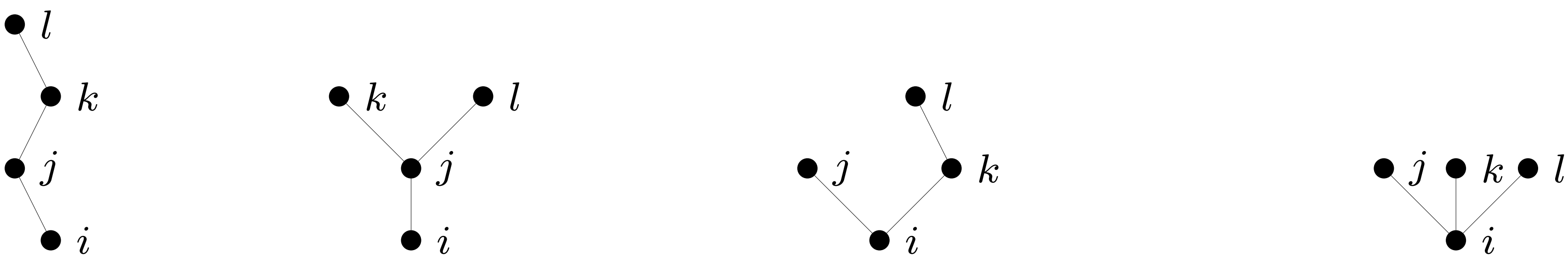
$$\mathbf{y}(x_n + h) - \mathbf{y}_{n+1} = \sum_{m=p+1}^{M} \left[\sum_{\tau \in T_m} \alpha(\tau) e(\tau) \mathbf{F}(\tau)(\mathbf{y}(x_n)) \right] \frac{h^m}{m!} + O(h^{M+1}).$$

where $e(\tau) = 1 - \gamma(\tau) \sum_{i=1}^{s} b_i \Psi^i(\tau)$.

Order Conditions for order 4



$\sum_i b_i = 1$ $\quad \sum_{ij} b_i a_{ij} = \frac{1}{2}$ $\quad \sum_{ijk} b_i a_{ij} a_{jk} = \frac{1}{6}$ $\quad \sum_{ijk} b_i a_{ij} a_{ik} = \frac{1}{3}$



$\sum_{ijkl} b_i a_{ij} a_{jk} a_{kl} = \frac{1}{24}$ $\quad \sum_{ijkl} b_i a_{ij} a_{ik} a_{kl} = \frac{1}{8}$ $\quad \sum_{ijkl} b_i a_{ij} a_{ik} a_{il} = \frac{1}{3}$

$\sum_{ijkl} b_i a_{ij} a_{jk} a_{jl} = \frac{1}{12}$

order p	1	2	3	4	5	6	7	8	9	10
n. order conditions	1	2	4	8	17	37	85	200	486	1205
n. of stages in explicit m.	1	2	3	4	6	7	9	11	≥ 11	

Convergence, Consistency and Stability

- We write down an explicit one-step method in the form

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}_n; \mathbf{f}, h_{n+1}), \quad \mathbf{y}_0 \text{ dado }, \quad n = 0, \ldots, N-1,$$

  ((i) $\Phi(x, \mathbf{y}; \mathbf{f}, h)$ Lipschitz with respect to $\mathbf{y}$, (ii) $\Phi(x, \mathbf{y}; 0, h) \equiv 0$)

- We introduce the **global errors** $\mathbf{e}_n := \mathbf{y}(x_n) - \mathbf{y}_n$, $n = 0, \ldots, N$, and we consider successive numerical integrations of the problem each time on finer discrete grids

$$a = x_0^h < x_1^h < \cdots < x_{N_h}^h = b, \quad h := \max_{1 \le n \le N_h} h_n := (x_n^h - x_{n-1}^h)$$

  with $\mathbf{y}_0^h \to \mathbf{A}$ and $N_h \to \infty$, $h \to 0$.

- Convergence (of order p) means

$$\max_{0 \le n \le N_h} \|\mathbf{y}(x_n) - \mathbf{y}_n\| \to 0, \quad (\text{ or } = O(h^p)), \quad (h \to 0).$$

  when $\mathbf{y}_0(h) \to \mathbf{y}(x_0)$, for each initial value problem (with $\mathbf{f} \in C^p$).

Consistency and Stability

- The **local truncation error** $\mathbf{t}_{n+1}$ at $x = x_{n+1}$, $n = 0, \ldots, N-1$, is defined by

$$\mathbf{y}(x_{n+1}) = \mathbf{y}(x_n) + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}(x_n), h_{n+1}) + \mathbf{t}_{n+1}, \quad n = 0, \ldots, N-1. \qquad (1)$$

  We also put $\mathbf{t}_0 := \mathbf{y}(x_0) - \mathbf{y}_0$.

- **Consistency** (of order p) means

$$\max_{n=0,\ldots,N-1} \frac{1}{h_{n+1}} \|\mathbf{t}_{n+1}\| \to 0, \quad (= O(h^p)), \quad (h \to 0).$$

  for each initial value problem (wiht $\mathbf{f} \in C^p$).

- **Stability** it is related with how does the solutions of respectively

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}_n, h_{n+1}), \quad n = 0, \ldots, N_h - 1, \quad \mathbf{y}_0 \approx \mathbf{A}$$
$$\mathbf{z}_{n+1} = \mathbf{z}_n + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{z}_n, h_{n+1}) + \mathbf{d}_{n+1}, \quad n = 0, \ldots, N_h - 1, \quad \mathbf{z}_0 = \mathbf{y}_0 + \mathbf{d}_0$$

  compare. The method it is said 0-stable if there are positive constants $S, \hat{h}$, such that if $h < \hat{h}$,

$$\max_{0 \le n \le N_h} \|\mathbf{y}_n - \mathbf{z}_n\| \le S \sum_{j=0}^{N_h} \|\mathbf{d}_j\|.$$

Convergence for one-step methods

- Consistency (of order p) + Stability $\Longrightarrow$ Convergence (of order p)
  We can compare now for $n = 0, \ldots, N_h - 1$,

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}_n, h_{n+1}), \quad \mathbf{y}_0 \approx \mathbf{A}$$
$$\mathbf{y}(x_{n+1}) = \mathbf{y}(x_n) + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}(x_n), h_{n+1}) + \mathbf{t}_{n+1}, \quad \mathbf{y}(x_0) = \mathbf{A}_0$$

  to obtain the convergence

$$\begin{aligned}
\max_{n=0,\ldots,N} \|\mathbf{y}(x_n) - \mathbf{y}_n\| &\leq S \sum_{n=0}^{N} \|\mathbf{t}_n\| \\
&\leq S \max(1, b-a) \max(\|\mathbf{t}_0\|, \max_{0 \leq n \leq N-1} \frac{\|\mathbf{t}_{n+1}\|}{h_{n+1}})) \\
&\leq O(h^p), \quad (h \to 0)..
\end{aligned}$$

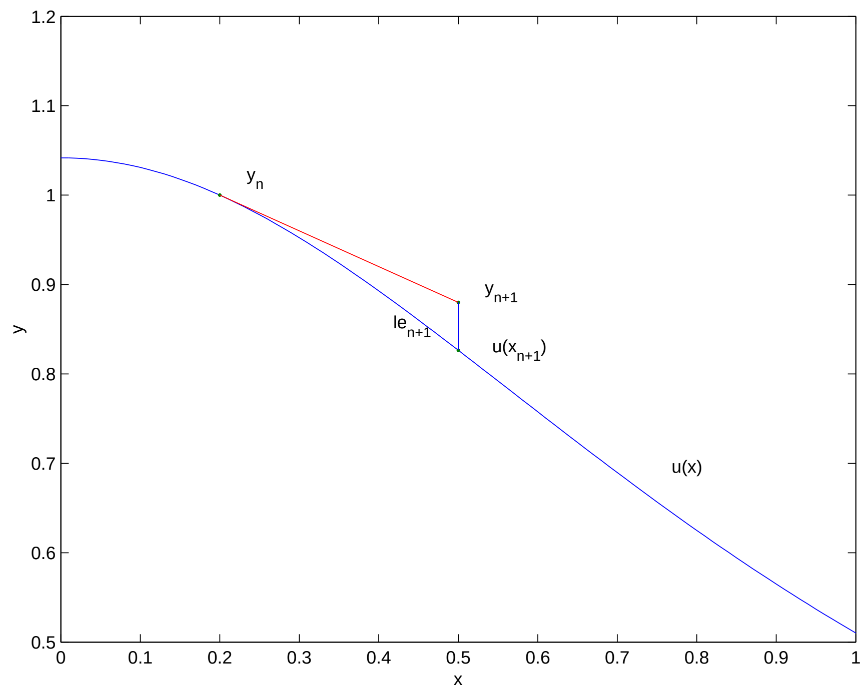
- The same ideas are valid for one-step implicit methods of the form

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}_n, \mathbf{y}_{n+1}; \mathbf{f}, h_{n+1}), \quad \mathbf{y}_0 \text{ dado }, \quad n = 0, \ldots, N-1,$$

  ((i) $\Phi(x, \mathbf{y}, \mathbf{z}; \mathbf{f}, h)$ Lipschitz with respect to $\mathbf{y}$ and $\mathbf{z}$, (ii) $\Phi(x, \mathbf{y}, \mathbf{z}; 0, h) \equiv 0$)

Step-size control in RK methods

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\mathbf{\Phi}(x_n, \mathbf{y}_n; \mathbf{f}, h_{n+1}),$$



$$\mathbf{le}_{n+1} = \mathbf{u}(x_{n+1}) - \mathbf{y}_{n+1} = h_{n+1}^{p+1}\mathbf{\Psi}(x_n, \mathbf{y}_n) + O(h_{n+1}^{p+2})$$

Some criterion for error (for a tolerance τ)

$\|\mathbf{le}_{n+1}\| \leq \tau$ (error per step) or $\|\mathbf{le}_{n+1}\| \leq \tau h_{n+1}$ (error per unit step)

Step-size control in RK methods

Assuming $\mathbf{est}_{n+1}$ is an estimate of $\mathbf{le}_{n+1}$,

$$\mathbf{est}_{n+1} \approx \mathbf{le}_{n+1} = \mathbf{u}(x_{n+1}) - \mathbf{y}_{n+1} = h_{n+1}^{p+1}\boldsymbol{\Psi}(x_n, \mathbf{y}_n) + O(h_{n+1}^{p+2})$$

- If step at $x = x_n$ is rejected ($\|\mathbf{est}_{n+1}\| > \tau($ tolerance$)$), from

  $$\mathbf{u}(x_n + h^*) - \mathbf{y}_{n+1}^* = (h^*)^{p+1}\boldsymbol{\Psi}(x_n, \mathbf{y}_n) + O((h^*)^{p+2}) \approx (h^*/h_{n+1})^{p+1}\mathbf{est}_{n+1},$$

  we obtain the optimal h^*

  $$h^* \approx h_{n+1}(\beta\tau/\|\mathbf{est}_{n+1}\|)^{1/(p+1)}, \quad \beta \text{ (fraction of tolerance, p.e. 0.9).}$$

- If step from $x = x_n$ is a success,

  $$\mathbf{le}_{n+2} = h_{n+1}^{p+1}\boldsymbol{\Psi}(x_{n+1}, \mathbf{y}_{n+1}) + O(h_{n+1}^{p+2}),$$

  and we use $\boldsymbol{\Psi}(x_{n+1}, \mathbf{y}_{n+1}) = \boldsymbol{\Psi}(x_n, \mathbf{y}_n) + O(h_{n+1})$, to predict a suitable h_{n+1} as

  $$h_{n+1} = h_{n+1}(\beta\tau/\|\mathbf{est}_{n+1}\|)^{1/(p+1)}.$$

- Usually, successive step-sizes are restricted to $c_0 \leq \frac{h_{n+1}}{h_n} \leq c_1$.

Local Extrapolation

- Given an asymptotically correct estimate of the local error (for a method of order p)

$$\mathbf{est}_{n+1} = \mathbf{le}_{n+1} + O(h_{n+1}^{p+2}), \quad h_{n+1} \to 0$$

- Extrapolation is to define a new numerical approximation

$$\hat{\mathbf{y}}_{n+1} = \mathbf{y}_{n+1} + \mathbf{est}_{n+1},$$

  of order $p+1$,

$$u(x_n + h_{n+1}) - \hat{\mathbf{y}}_{n+1} = O(h_{n+1}^{p+2}), \quad (h_{n+1} \to 0).$$

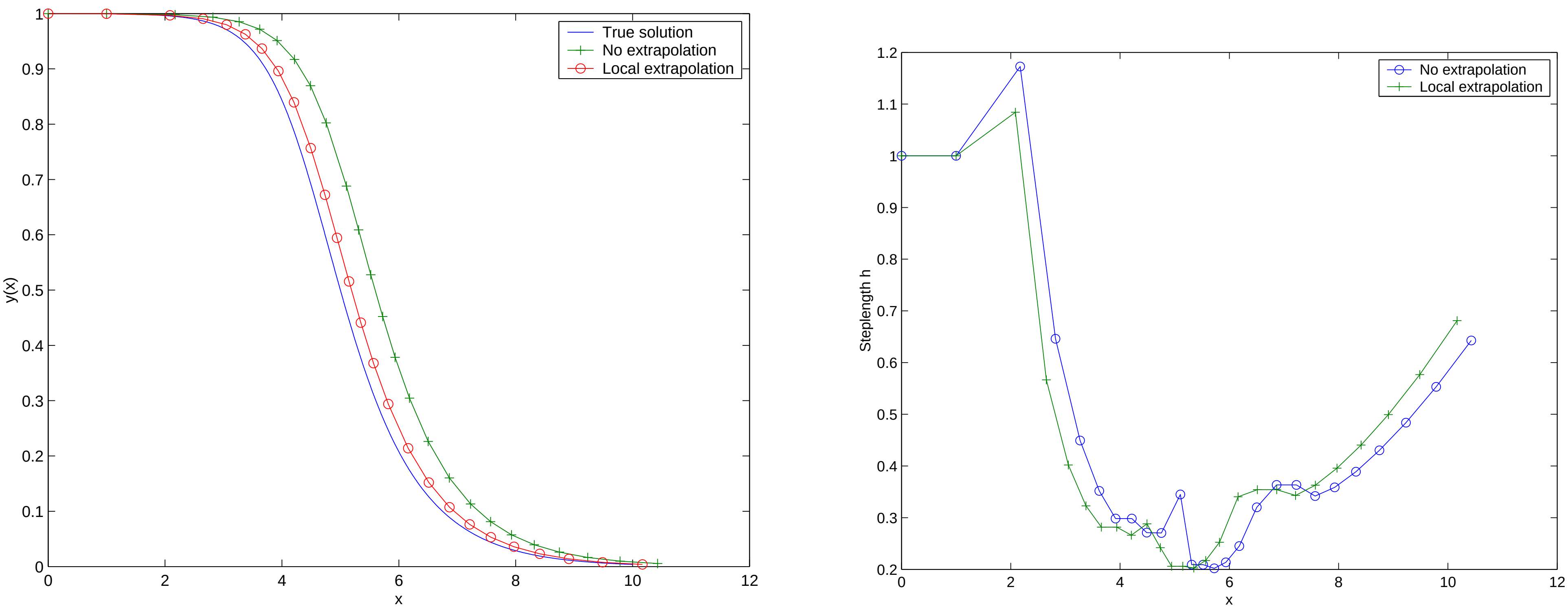
- Alternatively,

$$\mathbf{est}_{n+1} = \hat{\mathbf{y}}_{n+1} - \mathbf{y}_{n+1}.$$

  The estimator is obtained from two numerical approximations $\hat{\mathbf{y}}_{n+1}, \mathbf{y}_{n+1}$ of respectively order $p+1$ and p.

- Local extrapolation is to advance the numerical solution with the approximation of higher order $\hat{\mathbf{y}}_{n+1}$, although the estimate of the error is only asymptotically valid for the low order approximation $\mathbf{y}_{n+1}$

Local extrapolation vs No extrapolation



$$y' = y^3 - y, \quad y(0) = 1/\sqrt{1 + 3\exp(-10)}, \quad x \in [0, 10]$$

TOL = $1{,}0e - 3, \quad h_0 = 1{,}0$

Method: Taylor series Method 23

Richardson's extrapolation to the limit

From $x = x_n$ we compute aproximations $\mathbf{y}_{n+1}(h)$ with step size h and $\mathbf{y}_{n+1/2}(h/2), \mathbf{y}_{n+1}(h/2)$ with step size $h/2$

$$\begin{aligned}
\mathbf{u}(x_{n+1}) - \mathbf{y}_{n+1}(h) &= h^{p+1}\mathbf{\Psi}(x_n, \mathbf{y}_n) + O(h^{p+2}) \quad (= \mathbf{le}_{n+1}) \\
\mathbf{v}(x_{n+1}) - \mathbf{y}_{n+1}(h/2) &= \frac{h^{p+1}}{2^{p+1}}\mathbf{\Psi}(x_{n+1/2}, \mathbf{y}_{n+1/2}) + O(h^{p+2}) \\
&= \frac{h^{p+1}}{2^{p+1}}\mathbf{\Psi}(x_n, \mathbf{y}_n) + O(h^{p+2})
\end{aligned}$$

with $\mathbf{v}(x)$ the local solution at $x = x_{n+1/2}$. Hence, we obtain

$$(\mathbf{y}_{n+1}(h/2) - \mathbf{y}_{n+1}(h)) + \underbrace{(\mathbf{u}(x_{n+1/2}) - \mathbf{y}_{n+1/2}(h/2))(1 + O(h))}_{\frac{1}{2^{p+1}}\mathbf{le}_{n+1} + O(h^{p+2})} = (1 - \frac{1}{2^{p+1}})\mathbf{le}_{n+1} + O(h^{p+2})$$

from which

$$\mathbf{le}_{n+1} = \frac{2^p}{2^p - 1}(\mathbf{y}_{n+1}(h/2) - \mathbf{y}_{n+1}(h)) + O(h^{p+2})$$

Embedded RK pairs

- This approach is based in advancing the solution with simultaneously two RK methods of orders p and $p+1$ respectively.
- The key point is that both RK methods have in common the maximum number of inner stages.(Merson (1957),
- For example, for the explicit five stages RK method of order 4

$$
\begin{array}{c|ccccc}
0 & & & & & \\
\frac{1}{3} & \frac{1}{3} & & & & \\
\frac{1}{3} & \frac{1}{6} & \frac{1}{6} & & & \\
\frac{1}{2} & \frac{1}{8} & 0 & \frac{3}{8} & & \\
1 & \frac{1}{2} & 0 & -\frac{3}{2} & 2 & \\
\hline
 & \frac{1}{6} & 0 & 0 & \frac{2}{3} & \frac{1}{6}
\end{array}
,
\qquad
\begin{aligned}
\mathbf{Y}_1 &= \mathbf{y}_n, \\
\mathbf{Y}_2 &= \mathbf{y}_n + \tfrac{h_{n+1}}{3}\mathbf{f}_1, \\
\mathbf{Y}_3 &= \mathbf{y}_n + h_{n+1}(\tfrac{1}{6}\mathbf{f}_1 + \tfrac{1}{6}\mathbf{f}_2), \\
\mathbf{Y}_4 &= \mathbf{y}_n + h_{n+1}(\tfrac{1}{8}\mathbf{f}_1 + \tfrac{3}{8}\mathbf{f}_3), \\
\mathbf{Y}_5 &= \mathbf{y}_n + h_{n+1}(\tfrac{1}{2}\mathbf{f}_1 - \tfrac{3}{2}\mathbf{f}_3 + 2\mathbf{f}_4), \\
\mathbf{y}_{n+1} &= \mathbf{y}_n + h_{n+1}(\tfrac{1}{6}\mathbf{f}_1 + \tfrac{2}{3}\mathbf{f}_4 + \tfrac{1}{6}\mathbf{f}_5) \\
\mathbf{est}_{n+1} &= h_{n+1}(-\frac{1}{15}\mathbf{f}_1 + \frac{3}{10}\mathbf{f}_3 - \frac{4}{15}\mathbf{f}_4 + \frac{1}{30}\mathbf{f}_5) \\
\mathbf{f}_i &= \mathbf{f}(x_n + c_i h_{n+1}, \mathbf{Y}_i), \quad i = 1, \ldots, 5.
\end{aligned}
$$

the error estimate is asimptotically correct to the fourth order.

Embedded RK pairs

- RK-Fehlberg Pairs (4(5) (6 stages), 5(6), 7(8), 8(9))

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{4} & \frac{1}{4} & & & & & \\
\frac{3}{8} & \frac{3}{32} & \frac{9}{32} & & & & \\
\frac{12}{13} & \frac{1932}{2197} & -\frac{7200}{2197} & \frac{7296}{2197} & & & \\
1 & \frac{439}{216} & -8 & \frac{3680}{513} & -\frac{845}{4104} & & \\
\frac{1}{2} & -\frac{8}{27} & 2 & -\frac{3544}{2565} & \frac{1859}{4104} & -\frac{11}{40} & \\
\hline
 & \frac{25}{216} & 0 & \frac{1408}{2565} & \frac{2197}{4104} & -\frac{1}{5} & 0 \\
 & \frac{16}{135} & 0 & \frac{6656}{12825} & \frac{28561}{56430} & -\frac{9}{50} & \frac{2}{55} \\
\hline
 & -\frac{1}{360} & 0 & -\frac{128}{4275} & -\frac{2197}{75240} & \frac{1}{50} & \frac{2}{55}
\end{array}
$$

Embedded RK pairs

- DOPRI (DOrmand and PRInce) Pairs (5(4) (7 stages), 8(7) (13 stages))

$$
\begin{array}{c|ccccccc}
0 & & & & & & & \\
\frac{1}{5} & \frac{1}{5} & & & & & & \\
\frac{3}{10} & \frac{3}{40} & \frac{9}{40} & & & & & \\
\frac{4}{5} & \frac{44}{45} & -\frac{56}{15} & \frac{32}{9} & & & & \\
\frac{8}{9} & \frac{19372}{6561} & -\frac{25360}{2187} & \frac{64448}{6561} & -\frac{212}{729} & & & \\
1 & \frac{9017}{3168} & -\frac{355}{33} & \frac{46732}{5247} & \frac{49}{176} & -\frac{5103}{18656} & & \\
1 & \frac{35}{384} & 0 & \frac{500}{1113} & \frac{125}{192} & -\frac{2187}{6784} & \frac{11}{84} & \\
\hline
 & \frac{5179}{57600} & 0 & \frac{7571}{16695} & \frac{393}{640} & -\frac{92097}{339200} & \frac{187}{2100} & \frac{1}{40} \\
 & \frac{35}{384} & 0 & \frac{500}{1113} & \frac{125}{192} & -\frac{2187}{6784} & \frac{11}{84} & 0 \\
\hline
 & \frac{71}{57600} & 0 & -\frac{71}{16695} & \frac{71}{1920} & -\frac{17253}{339200} & \frac{22}{525} & -\frac{1}{40}
\end{array}
$$

The RK pair in ODE23

- $$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & \\ 1/2 & 1/2 & 0 & 0 & \\ 3/4 & 0 & 3/4 & 0 & \\ \hline & 2/9 & 1/3 & 4/9 & \\ & 11/72 & 5/12 & 5/9 & -1/8 \\ \hline & -5/72 & 1/12 & 1/9 & -1/8 \end{array},$$
- RK pair (2,3) by Bogacki and Shampine.
- Use an interpolant or order 3.
- Implemented in MatLab.

The class of Linear Multistep Methods

- A k-step formula take the general form (with step size h constant)

$$\sum_{j=0}^{k} \alpha_j \mathbf{y}_{n+j} = h \sum_{j=0}^{k} \beta_j \mathbf{f}_{n+j}, \quad \alpha_k = 1, \quad |\alpha_0| + |\beta_0| \neq 0$$

  where

$$\mathbf{f}_{n+j} = \mathbf{f}(x_{n+j}, \mathbf{y}_{n+j}), \quad x_{n+j} = x_n + jh, \quad j = 0, \ldots, k$$

- With $\mathbf{y}_0 \approx \mathbf{A}$, we need a starting procedure to obtain $\mathbf{y}_1, \ldots, \mathbf{y}_{k-1}$,

$$[\mathbf{y}_{n+k-1}, \ldots, \mathbf{y}_n] \longrightarrow [\mathbf{y}_{n+k}, \ldots, \mathbf{y}_{n+1}],$$
$$[\mathbf{f}_{n+k-1}, \ldots, \mathbf{f}_n] \longrightarrow [\mathbf{f}_{n+k}, \ldots, \mathbf{f}_{n+1}]$$

- If $\beta_k \neq 0$, the formula is implicit, and we must solve

$$\mathbf{y}_{n+k} = h\beta_k \mathbf{f}(x_{n+k}, \mathbf{y}_{n+k}) + \mathbf{g},$$

  Typically, a fixed point iteration converges if $h\beta_k L < 1$,

$$\mathbf{y}_{n+k}^{[\nu+1]} = h\beta_k \mathbf{f}(x_{n+k}, \mathbf{y}_{n+k}^{[\nu]}) + \mathbf{g}, \quad \nu = 0, 1, \ldots \quad \mathbf{y}_{n+k}^{[0]} \text{ arbitrary}$$

- Characteristic Polynomials: $\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j, \sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^k$

An example

$$\mathbf{y}_{n+1} = -4\mathbf{y}_n + 5\mathbf{y}_{n-1} + h(4\mathbf{f}_n + 2\mathbf{f}_{n-1}).$$

1. Given $\mathbf{y}_0$, we evaluate $\mathbf{f}_0$ and we compute $\mathbf{y}_1$ with other method (p.e. a one-step method)
2. We evaluate $\mathbf{f}_1$ and we obtain $\mathbf{y}_2$ from the formula.
3. We discard $\mathbf{y}_0, \mathbf{f}_0$.
4. We evaluate $\mathbf{f}_2$ and we obtain $\mathbf{y}_3$ from the formula.
5. We discard $\mathbf{y}_1, \mathbf{f}_1$.
6. $\cdots$

We can evaluate the accuracy (order) of the method by expanding the residual in a Taylor series at $x = x_n$

$$\begin{aligned} t_{n+1} &:= y(x_{n+1}) + 4y(x_n) - 5y(x_{n-1}) - h(4y'(x_n) + 2y'(x_{n-1})) \\ &= -\frac{1}{6}h^4 y^{(4)}(x_n) + O(h^5), \quad (h \rightarrow 0) \end{aligned}$$

Order conditions for Linear Multistep Methods

- We introduce **the local truncation error** at $x = x_{n+k}$

$$\mathbf{t}_{n+k} := \sum_{j=0}^{k} \alpha_j \mathbf{y}(x_{n+j}) - h \sum_{j=0}^{k} \beta_j \mathbf{f}(x_{n+j}, \mathbf{y}(x_{n+j})).$$

To determine the order of consistence we do a Taylor series expansion in the step h

$$\begin{aligned} \mathcal{L}[\mathbf{w}(x), h] \quad &:= \quad \sum_{j=0}^{k} \alpha_j \mathbf{w}(x + jh) - h \sum_{j=0}^{k} \beta_j \mathbf{w}'(x + jh) \\ &= \quad C_0 \mathbf{w}(x) + C_1 h \mathbf{w}'(x) + \cdots + C_q h^q \mathbf{w}^{(q)}(x) + \cdots \end{aligned}$$

with

$$C_0 = \sum_{j=0}^{k} \alpha_j \equiv \rho(1), \quad C_1 = \sum_{j=0}^{k} (j\alpha_j - \beta_j) \equiv \rho'(1) - \sigma(1)$$

$$C_q = \frac{1}{q!} \sum_{j=0}^{k} j^q \alpha_j - \frac{1}{(q-1)!} \sum_{j=0}^{k} j^{q-1} \beta_j, \quad q = 2, 3, \ldots$$

- Order p : $C_0 = C_1 = \cdots = C_p = 0$, $C_{p+1} \neq 0$

The class of Adams Methods

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f(x, y(x))dx,$$

- Adams-Bashforth formulae:

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} P_{k-1}^{*}(x)dx, \quad P_{k-1}^{*}(x_{n-j}) = f(x_{n-j}, y_{n-j}), \quad j = 0, \ldots, k-1$$

In terms of the backward differences, $\nabla^0 f_n = f_n, \nabla^{j+1} f_n = \nabla^j f_n - \nabla^j f_{n-1}$,

$$P_{k-1}^{\star}(x) = \sum_{j=0}^{k-1} \frac{1}{j!h^j}(x - x_n) \cdots (x - x_{n+1-j})\nabla^j f_n,$$

Hence,

$$y_{n+1} = y_n + h(f_n + \frac{1}{2}\nabla f_n + \frac{5}{12}\nabla^2 f_n + \frac{3}{8}\nabla^3 f_n + \frac{251}{720}\nabla^4 f_n + \cdots).$$

The class of Adams Methods

$$y_{n+1} = y_n + h(f_n + \frac{1}{2}\nabla f_n + \frac{5}{12}\nabla^2 f_n + \frac{3}{8}\nabla^3 f_n + \frac{251}{720}\nabla^4 f_n + \cdots).$$

Expanding the backward differences in terms of function values, we obtain the standard k-step Adams-Bashforth methods for $k = 1, 2, 3, 4$ respectively

$$\begin{aligned}
y_{n+1} - y_n &= hf_n, \\
y_{n+1} - y_n &= \frac{h}{2}(3f_n - f_{n-1}), \\
y_{n+1} - y_n &= \frac{h}{12}(23f_n - 16f_{n-1} + 5f_{n-2}), \\
y_{n+1} - y_n &= \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}).
\end{aligned}$$

- Adams-Moulton formulae:

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} P_k(x)dx, \quad P_k(x_{n+1-j}) = f(x_{n+1-j}, y_{n+1-j}), \quad j = 0, \ldots, k$$

$$P_k(x) = \sum_{j=0}^{k} \frac{1}{j!h^j}(x - x_{n+1}) \cdots (x - x_{n+2-j})\nabla^j f_{n+1},$$

$$y_{n+1} = y_n + h(f_{n+1} - \frac{1}{2}\nabla f_{n+1} - \frac{1}{12}\nabla^2 f_{n+1} - \frac{1}{24}\nabla^3 f_{n+1} - \frac{19}{720}\nabla^4 f_{n+1} + \cdots)$$

If we expand the backward differences in terms of ordinates, we obtain for k=1,2,3,4 respectively

$$\begin{aligned}
y_{n+1} - y_n &= \frac{h}{2}(f_{n+1} + f_n), \\
y_{n+1} - y_n &= \frac{h}{12}(5f_{n+1} + 8f_n - f_{n-1}), \\
y_{n+1} - y_n &= \frac{h}{24}(9f_{n+1} + 19f_n - 5f_{n-1} + f_{n-2}), \\
y_{n+1} - y_n &= \frac{h}{720}(251f_{n+1} + 646f_n - 264f_{n-1} + 106f_{n-2} - 19f_{n-3}).
\end{aligned}$$

Consistency and Convergence

- Convergence:
  The method is said convergent (of order p) if we have for any initial value problem

$$\max_{k\leq n\leq N_h} \|\mathbf{y}(x_n)-\mathbf{y}_n\| \to 0, \quad (= O(h^p)), \quad (h\to 0)$$

for all starting values $\mathbf{y}_n(h), n=0,1,\dots,k-1$ such that they satisfy

$$\|\mathbf{y}(x_0)-\mathbf{y}_n\| \to 0, \quad (= O(h^p)), \quad (h\to 0), \quad n=0,1,\dots,k-1,.$$

- Consistency: ($\rho(1)=0, \rho'(1)=\sigma(1)$)

$$\mathbf{t}_j := \mathbf{y}_j(h)-\mathbf{y}(x_j), j=0,\dots,k-1,$$

$$\mathbf{t}_{n+k} := \sum_{j=0}^{k}\alpha_j\mathbf{y}(x_{n+j}) - h\sum_{j=0}^{k}\beta_j\mathbf{f}(x_{n+j},\mathbf{y}(x_{n+j})), n\geq 0..$$

The method is consistent (of order p) if for all initial value problem ($\mathbf{f}\in C^p$)

$$\max_{0\leq n\leq N_h} \|\frac{\mathbf{t}_n}{h}\| \to 0, \quad (= O(h^p)),$$

Stability

- The method is 0-stable if positive constants S and h_0 exists such that for all $h \in (0, h_0]$, the numerical solutions of

$$\mathbf{Y}_{k-1} = \mathbf{s}(h),$$
$$\mathbf{Y}_{n+1} = A\mathbf{Y}_n + h\mathbf{e}_1\Phi(x_n, \mathbf{Y}_{n+1}, \mathbf{Y}_n, h)$$

and

$$\hat{\mathbf{Y}}_{k-1} = \mathbf{s}(h) + \mathbf{d}_{k-1},$$
$$\hat{\mathbf{Y}}_{n+1} = A\hat{\mathbf{Y}}_n + h\mathbf{e}_1\Phi(x_n, \hat{\mathbf{Y}}_{n+1}, \hat{\mathbf{Y}}_n, h) + \mathbf{d}_{n+1}$$

exist and satisfy

$$\max_{k-1 \leq n \leq N_h} \|\tilde{\mathbf{Y}}_n - \mathbf{Y}_n\| \leq S \sum_{j=k-1}^{n} \|\mathbf{d}_j\|$$

for all arbitrary perturbations $\mathbf{d}_j$, $j = k-1, \ldots, N-1$.

Stability and the Root Condition

For the problem $y' = 0$, a k steps linear multistep method reads

$$\alpha_k y_{n+k} + \cdots + \alpha_1 y_{n+1} + \alpha_0 y_n = 0.$$

We assume that $\xi_1, \ldots, \xi_\ell$ are roots of $\rho(\xi)$ of respective multiplicity $m_1, \ldots, m_\ell$.
The general solution of this linear difference equation is

$$y_n = c_1(n)\xi_1^n + \cdots + c_\ell(n)\xi_\ell^n,$$

where the coefficients $c_j(n), j = 1, \ldots, \ell$ are polynomials of degree $m_j - 1$.
Any perturbation of the null solution is bounded only if (the **root condition**)

(i) $|\xi_j| \leq 1, \quad j = 1, \ldots, k,$ (ii) If $|\xi_j| = 1,$ then ξ_j es simple.

Stability and the Root Condition

The root condition is also sufficient for the stability of the method, writen below as a one-step method ($d = 1$)

$$\mathbf{Y}_{k-1} = \mathbf{s}(h),$$
$$\mathbf{Y}_{n+1} = A\mathbf{Y}_n + h\mathbf{e}_1\Phi(x_n, \mathbf{Y}_{n+1}, \mathbf{Y}_n; \mathbf{f}, h)$$

with $\mathbf{Y}_n = [y_n, \ldots, y_{n-k+1}], \mathbf{s}(h) = [y_{k-1}, \ldots, y_0]$, and

$$A = \begin{bmatrix} -\alpha'_{k-1} & -\alpha'_{k-2} & \cdots & -\alpha'_1 & -\alpha'_0 \\ 1 & 0 & \cdots & 0 & 0 \\ & \ddots & \ddots & & \\ & & & 0 & 0 \\ & & & 1 & 0 \end{bmatrix}, \quad \alpha'_i = -\frac{\alpha_i}{\alpha_k}, \quad i = 0, \ldots, k-1.$$

$$\Phi(x_n, \mathbf{Y}_{n+1}, \mathbf{Y}_n; \mathbf{f}, h) = \sum_{j=0}^{k} \beta_{k-j}\mathbf{f}_{n-j}.$$

Theorem of Dahlquist

- Theorem of Dahlquist (1959): The method is convergent if and only if is consistent and 0-estable.
- If the method is convergent and consistent of order p, then

$$\max_{k \leq n \leq N_h} \|\mathbf{y}(x_n) - \mathbf{y}_n\| \to 0, \quad (= O(h^p)), \quad (h \to 0)$$

- First Barrier of Dahlquist: A linear k step method 0-estable has at most order $k+2$ if k is even, order $k+1$ if k is odd and order k if $\beta_k/\alpha_k \leq 0$.

Absolute Stability

We start considering the system

$$\mathbf{y}' = J\mathbf{y} + \mathbf{g}(x), \quad J \text{ diagonalizable constant real matrix } d \times d$$

The difference $\mathbf{e}(x)$ of two solutions $\mathbf{y}(x), \mathbf{z}(x)$, con $\mathbf{y}(a) = \mathbf{A}$, $\mathbf{z}(a) = \mathbf{A} + \delta_0$, satisfy

$$\mathbf{e}' = J\mathbf{e}, \quad a \leq x \leq b, \quad \mathbf{e}(a) = \delta_0.$$

If $Q^{-1}JQ = \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_d)$, $Q := [\mathbf{v}_1, \ldots, \mathbf{v}_d]$, we can do the change of variables $\mathbf{e}(x) = Q\eta$, to obtain

$$(\eta^r)' = \lambda_r \eta^r, \quad r = 1, \ldots, d.$$

$\Re\lambda_r > 0$ (exponential growth), $\Re\lambda_r \leq 0$, (bounded solution), $\Re\lambda_r < 0$ (exponential decreasing to zero).

Absolute Stability

If we consider the application of a linear multistep method

$$\sum_{j=0}^{k} \alpha_j \mathbf{y}_{n+j} = h \sum_{j=0}^{k} \beta_j \mathbf{f}_{n+j}, \quad |\alpha_0| + |\beta_0| \neq 0$$

to the system $\mathbf{y}' = J\mathbf{y} + \mathbf{g}(x)$, the difference $\{\mathbf{e}_n\}$ between two numerical solutions $\{\mathbf{y}_n\}$ and $\{\mathbf{z}_n\}$ satisfy

$$\sum_{j=0}^{k} (\alpha_j I - h\beta_j J)\mathbf{e}_{n+j} = \mathbf{0},$$

Now the change of variables $\mathbf{e}_n = Q\eta_n$, uncouples the equations and we have

$$\sum_{j=0}^{k} (\alpha_j - h\beta_j \lambda_r)\eta^r_{n+j} = 0, \quad r = 1, \ldots, d.$$

Absolute Stability

The general solution of this kind of equation is given by

$$\eta_n^r = \sum_{m=1}^{k} \chi_{rm} (\zeta_m^r)^n, \quad r = 1, 2, \ldots, d$$

where χ_{rm} are arbitrary complex constants and for r, $\zeta_1^r, \ldots, \zeta_k^r$ denote the roots of the characteristic polynomial of the difference equation (**stability polynomial of the linear multistep method**)

$$\pi(\zeta, \hat{h}) = \rho(\zeta) - \hat{h}\sigma(\zeta) = 0, \quad \hat{h} := \lambda_r h$$

The set

$$\mathcal{R}_A := \{\hat{h} \in \mathbb{C} : \pi(\zeta, \hat{h}) \text{satisface la condición de la raíz}\}$$

is called absolute stability domain of the method.
The boundary of this region is a subset of the graph $\gamma([-\pi, \pi])$, with

$$\gamma(\theta) = \rho(e^{i\theta})/\sigma(e^{i\theta}), \quad \theta \in [-\pi, \pi], \quad \text{(boundary locus method)}$$

Some examples

$$y' = \lambda y, \quad \Re\lambda < 0$$

- $y_{n+1} = y_n + hf(x_n, y_n)$, (Euler explicit)

$$y_{n+1} = (1 + \lambda h) y_n, \quad \Longrightarrow y_n \text{ bounded} \quad \text{iff} \quad |1 + \lambda h| \leq 1$$

- $y_{n+1} = y_n + hf(x_n, y_{n+1})$, (Backward implicit Euler)

$$y_{n+1} = y_n + \lambda h y_{n+1}, \quad \Longrightarrow y_{n+1} = \frac{1}{1 + \lambda h} y_n$$

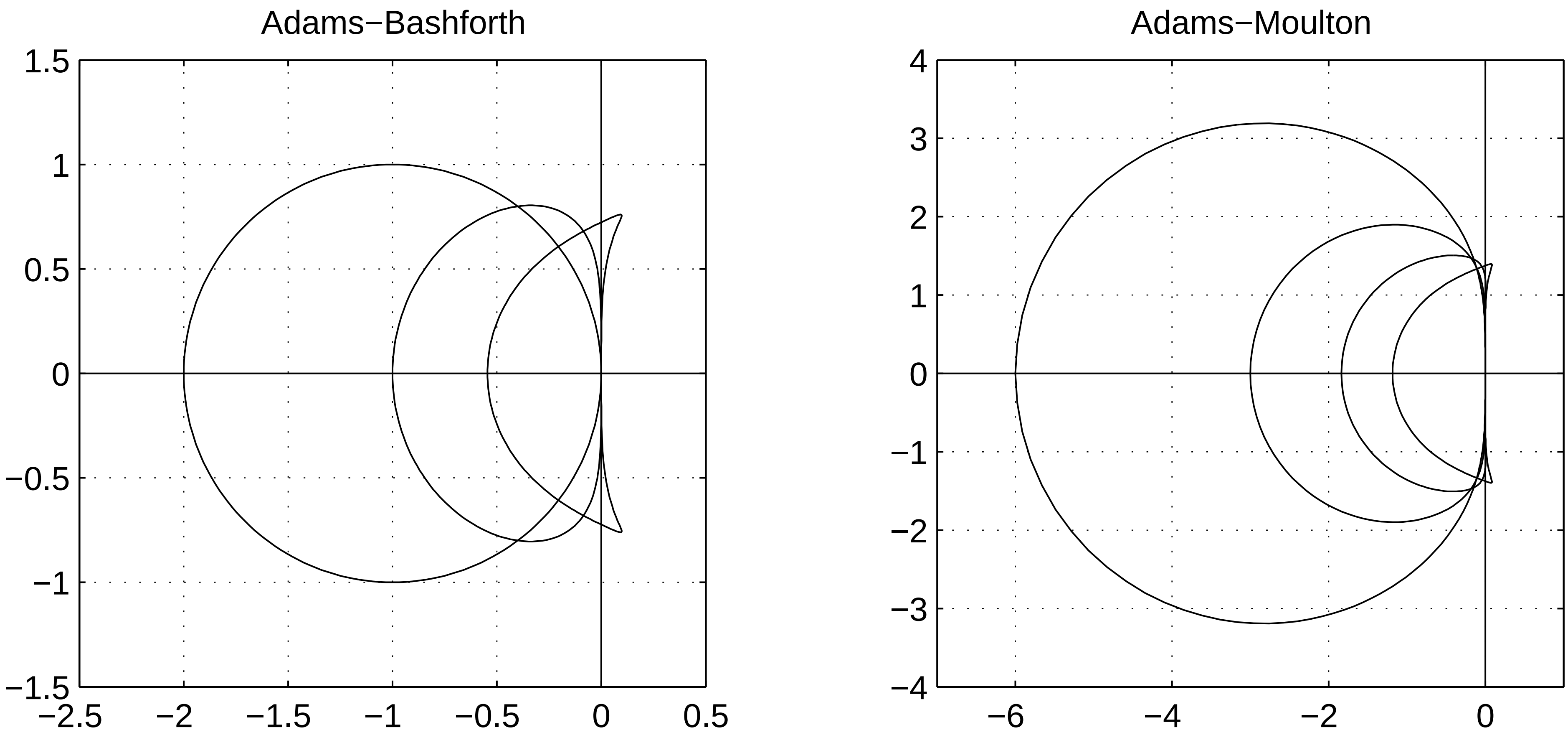
and $\{y_n\}$ bounded iff $|1 + \lambda h| \geq 1$.

- $y_{n+1} - y_n = \frac{1}{12} h(5f_{n+1} + 8f_n - f_{n-1})$, ($2$ step Adams-Moulton method)

$$(1 - \frac{5}{12}\hat{h}) y_{n+1} - (1 + \frac{2}{3}\hat{h}) y_n + \frac{1}{12}\hat{h} y_{n-1} = 0, \quad \hat{h} := \lambda h,$$

$\{y_n\}$ bounded iff $(1 - \frac{5}{12}\hat{h})\zeta^2 - (1 + \frac{2}{3}\hat{h})\zeta + \frac{1}{12}$ satisfies the root condition

Stability Regions for ADAMS Methods



A-Stability

- When $\mathbb{C}^- = \{z \in \mathbb{C} : \Re z < 0\} \subset \mathcal{R}_A$, the method is called A-stable.
- No explicit linear multistep method can be A-stable.
- In the class of Linear Multistep Methods, the trapezoidal rule is the A-stable methods with the highest order (second barrier of Dahlquist)

The Backward Derivative Formulae (BDF)

We construct the interpolation polynomial of degre k, $Q_k(x)$, with data

$$Q_k(x_{n+1-j}) = y_{n+1-j}, \quad j = 0, 1, \ldots, k.$$

and we impose that $Q_k(x)$ satisfies the ODE at $x = x_{n+1}$. Then results

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+1} = h f_{n+1}.$$

Only the BDF formulae con $1 \le k \le 6$ are stable:

$$y_{n+1} - y_n = h f_{n+1}$$

$$\frac{3}{2} y_{n+1} - 2 y_n + \frac{1}{2} y_{n-1} = h f_{n+1}$$

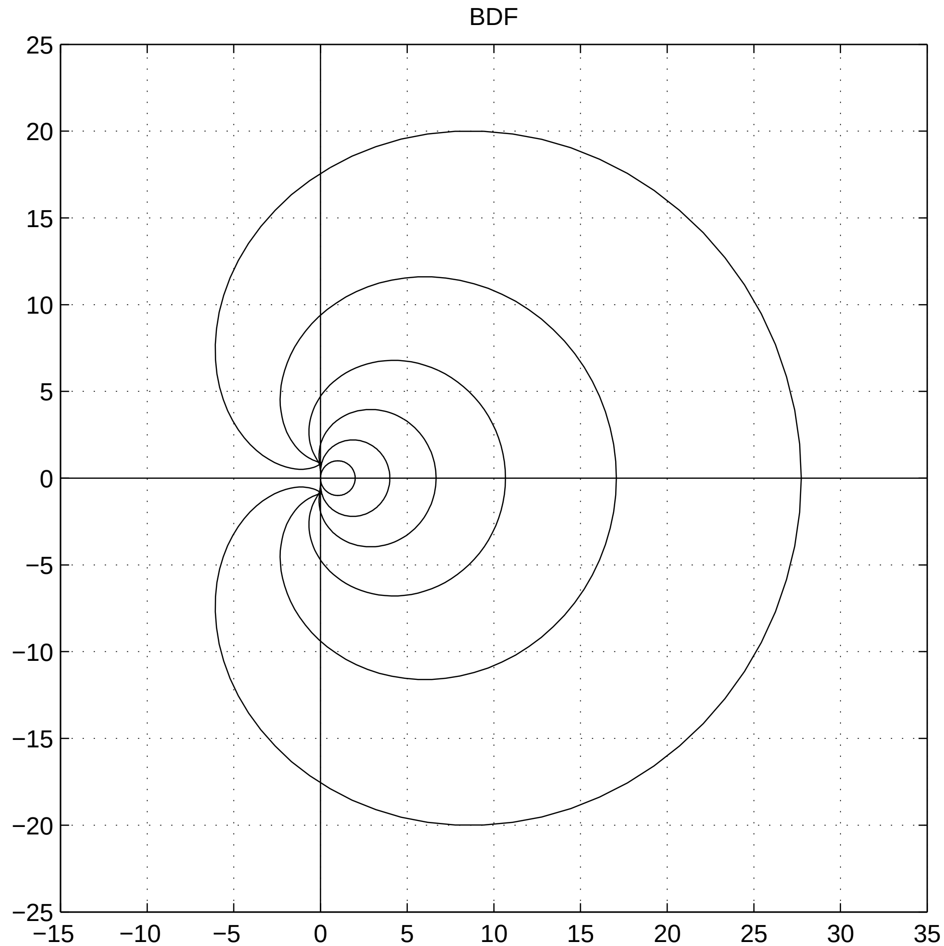
$$\frac{11}{6} y_{n+1} - 3 y_n + \frac{3}{2} y_{n-1} - \frac{1}{3} y_{n-2} = h f_{n+1},$$

$$\frac{25}{12} y_{n+1} - 4 y_n + 3 y_{n-1} - \frac{4}{3} y_{n-2} + \frac{1}{4} y_{n-3} = h f_{n+1},$$

$$\frac{137}{60} y_{n+1} - 5 y_n + 5 y_{n-1} - \frac{10}{3} y_{n-2} + \frac{5}{4} y_{n-3} - \frac{1}{5} y_{n-4} = h f_{n+1},$$

$$\frac{147}{60} y_{n+1} - 6 y_n + \frac{15}{2} y_{n-1} - \frac{20}{3} y_{n-2} + \frac{15}{4} y_{n-3} - \frac{6}{5} y_{n-4} + \frac{1}{6} y_{n-5} = h f_{n+1},$$

Absolute Stability of BDF



Absolute Stability of RK methods

We apply the RK method

$$
\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\
c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\
\hline
 & b_1 & b_2 & \cdots & b_s,
\end{array}
, \quad
\begin{array}{l}
\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^{s} b_i \mathbf{f}(x_n + c_i h, \mathbf{Y}_i) \\
\mathbf{Y}_i = \mathbf{y}_n + h \sum_{j=1}^{s} a_{ij} \mathbf{f}(x_n + c_j h, \mathbf{Y}_j), \quad i = 1, \ldots, s,
\end{array}
$$

to the linear test problem

$$y' = \lambda y, \quad \lambda \mathbb{C}, \quad \Re\lambda \leq 0.$$

We obtain

$$y_{n+1} = R(\hat{h}) y_n, \quad \hat{h} := \lambda h, \quad R(\hat{h}) = 1 + \hat{h} \mathbf{b}^T (I - \hat{h} A)^{-1} \mathbf{e}.$$

The set

$$\mathcal{R}_A := \{\hat{h} \in \overline{\mathbb{C}} : |R(\hat{h})| \leq 1\}$$

is called the absolute stability domain of the method.

Some examples with RK methods

$$y' = \lambda y, \quad \Re\lambda < 0$$

- $y_{n+1} = y_n + hf(x_n + h/2, y_n + h/2 f(x_n, y_n))$

$$y_{n+1} = y_n + \lambda h (y_n + \frac{h}{2}\lambda y_n) = (1 + (\lambda h) + \frac{(\lambda h)^2}{2}) y_n$$

  and $\{y_n\}$ bounded iff $|1 + \hat{h} + \frac{\hat{h}^2}{2}| \leq 1$, with $\hat{h} := \lambda h$.

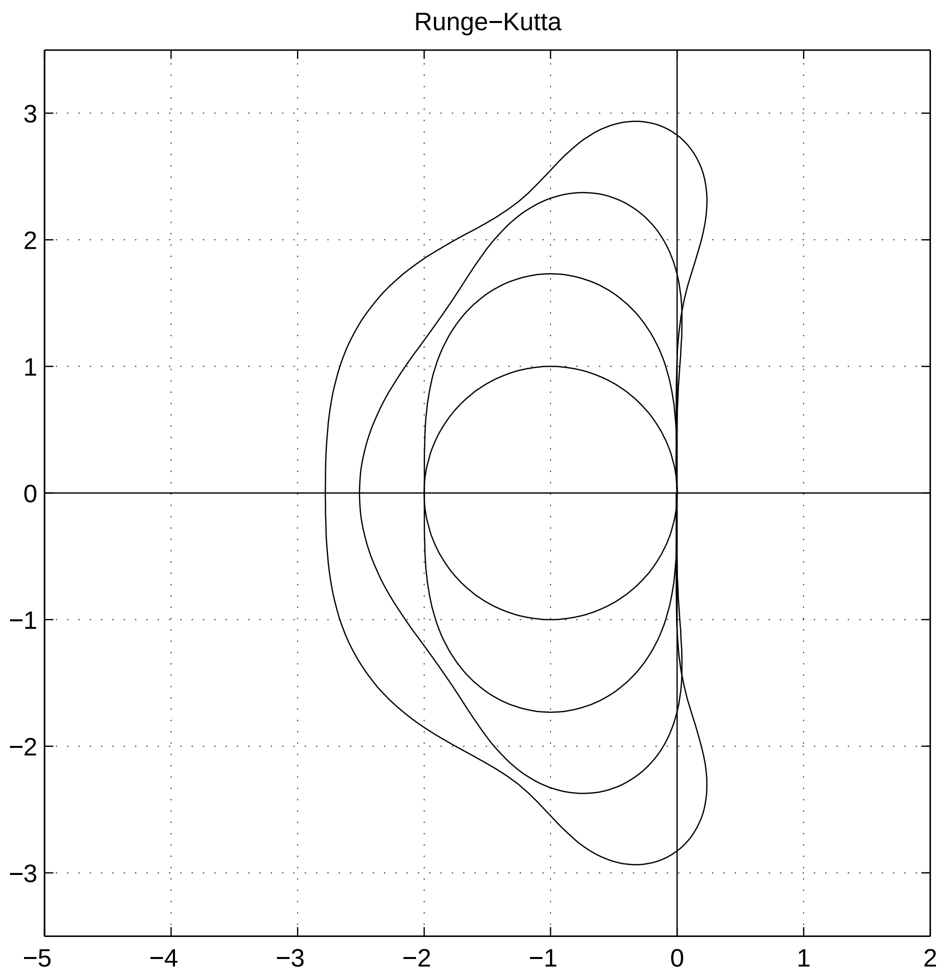
- $y_{n+1} = y_n + \frac{h}{2}(f(x_n, y_n) + f(x_n + h, y_{n+1})$

$$y_{n+1} = y_n + \frac{h}{2}(\lambda y_n + \lambda y_{n+1}), \quad \Longrightarrow y_{n+1} = \frac{1 + \frac{\lambda h}{2}}{1 - \frac{\lambda h}{2}} y_n$$

  and $\{y_n\}$ bounded iff

$$\left| \frac{1 + \frac{\hat{h}}{2}}{1 - \frac{\hat{h}}{2}} \right| \leq 1, \quad \hat{h} := \lambda h.$$

Absolute Stability of ERK



Implicit RK methods (Gaussian)

- Implicit RK methods

$$
\begin{aligned}
\mathbf{y}_{n+1} &= \mathbf{y}_n + h\sum_{i=1}^{s} b_i \mathbf{f}(x_n + c_i h, \mathbf{Y}_i),\\
\mathbf{Y}_i &= \mathbf{y}_n + h\sum_{j=1}^{s} a_{ij} \mathbf{f}(x_n + c_i h, \mathbf{Y}_j), \quad i = 1, \ldots, s.
\end{aligned}
$$

with Butcher's array

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

- If $a_{ij} = 0, j > i$, the nonlinear system in the inner stages $\mathbf{Y}_i, i = 1, \ldots, s$ decouples in s different nonlinear systems, each one of order d. (**diagonally implicit RK method (DIRK)**). If $a_{ii} = \gamma, i = 1, \ldots, s$, (**single diagonally implicit (SDIRK)**).

An example of an implicit RK method

$$\begin{array}{c|cc} c_1 & a_{11} & a_{12} \\ c_2 & a_{21} & a_{22} \\ \hline & b_1 & b_2 \end{array}, \qquad \begin{aligned} & b_1 + b_2 = 1, \\ & b_1 c_1 + b_2 c_2 = 1/2 \\ & b_1 c_1^2 + b_2 c_2^2 = 1/3 \\ & b_1(a_{11}c_1 + a_{12}c_2) + b_2(a_{21}c_1 + a_{22}c_2) = 1/6. \end{aligned}$$

The quadrature rule $\int_0^1 g(t)dt \approx b_1 g(c_1) + b_2 g(c_2)$ is exact for polinomials up to the third degree.Hence $\int_0^1 (x - c_1)(x - c_2)dx = 0 \Longrightarrow c_2 = \dfrac{3c_1 - 2}{6c_1 - 3}$. Then

$$b_1 = \frac{c_2 - 1/2}{c_2 - c_1}, \quad b_2 = \frac{c_1 - 1/2}{c_1 - c_2}, a_{22} = \frac{1/6 - b_1 a_{12}(c_2 - c_1) - c_1/2}{b_2(c_2 - c_1)}.$$

($a_{12} = 0, a_{11} = a_{22} = \gamma, a_{21} = 1 - \gamma, b_1 = b_2 = 1/2, \gamma = (3 \pm \sqrt{3})/6$) . For order 4

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

Test of Stiffness

- System 1

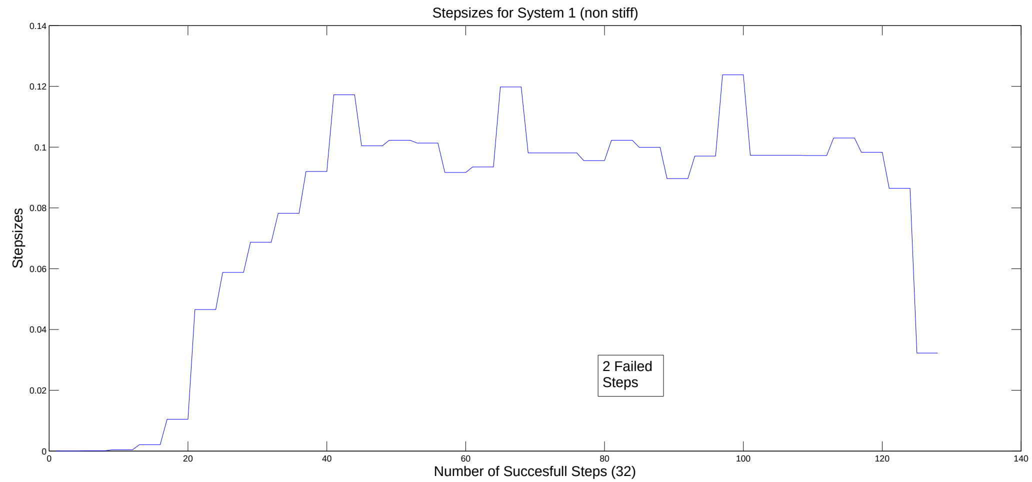
$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} -2 & 1 \\ 1 & -2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} + \begin{bmatrix} 2\sin x \\ 2(\cos x - \sin x) \end{bmatrix}$$

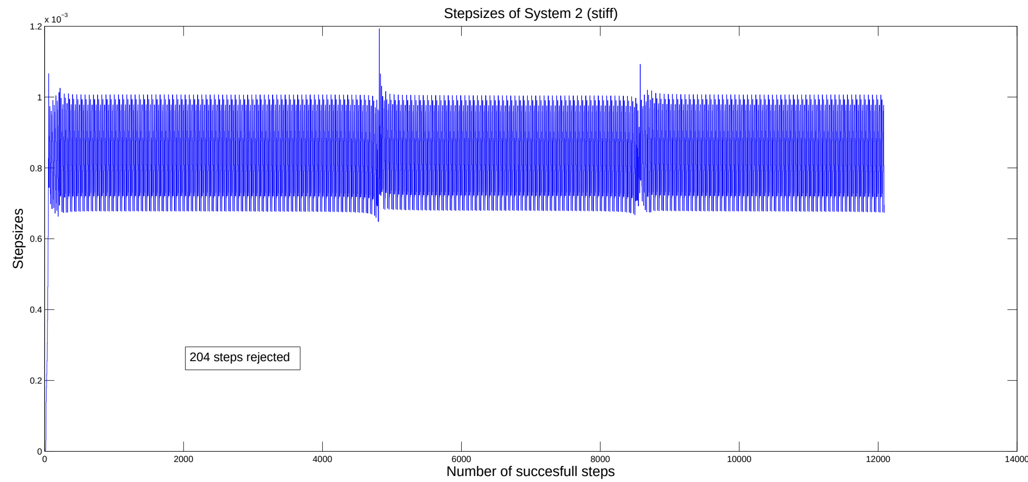
- System 2

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} -2 & 1 \\ 998 & -999 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} + \begin{bmatrix} 2\sin x \\ 999(\cos x - \sin x) \end{bmatrix}$$

- The solution $\mathbf{y} = [\sin(x), \cos(x)]^T$
- Both systems integrated with ODE45 (RK pair 5(4)).
  System 1 Stats: 32 Succesful steps, 2 rejected, 205 number of evaluations of $\mathbf{f}$.
  System 2 Stats: 3023 Succesful steps, 205 rejected, 19363 number of evaluations of $\mathbf{f}$.

Test problems





Predictor-Corrector Schemes

$$y' = f(x,y), \quad y(a) = A$$

- An example ($d=1$):

$$y_{n+1} - y_n = \frac{1}{12}h(5f(x_{n+1},y_{n+1}) + 8f_n - f_{n-1}), \quad f_j = f(x_j,y_j), \quad j = n, n-1$$

If we solve the nonlinear system at each step by fixed point iteration, ($\frac{5}{12}hL < 1$)

$$y_{n+1}^{(\nu+1)} = \frac{5}{12}hf(x_{n+1}, y_{n+1}^{(\nu)}) + g_n \quad g_n := y_n + \frac{h}{12}(8f_n - f_{n-1}).$$

The predictor provides a good initial approximation $y_{n+1}^{(0)}$. The procedure could be:

$$\begin{aligned} P: &\quad y_{n+1}^{(0)} = -4y_n + 5y_{n-1} + h(4f_n + f_{n-1}), \\ E: &\quad f_{n+1}^{(0)} = f(x_{n+1}, y_{n+1}^{(0)}), \\ C: &\quad y_{n+1}^{(1)} = y_n + \tfrac{5}{12}hf_{n+1}^{(0)} + g_n, \\ E: &\quad f_{n+1}^{(1)} = f(x_{n+1}, y_{n+1}^{(1)}) \end{aligned}$$

- Other modes: $PECECE$, $PE(CE)^k$, PEC (one uses $f_{n+1}^{(0)}$), and up to the convergence.

Predictor-Corrector Schemes

$$y' = f(x,y), \quad y(a) = A$$

- We have two formulae: one explicit (the predictor) and the other one implicit (the corrector)

$$\sum_{j=0}^{k} \alpha_j^* \mathbf{y}_{n+j} = h \sum_{j=0}^{k-1} \beta_j^* \mathbf{f}_{n+j}, \quad |\alpha_0^*| + |\beta_0^*| \neq 0, \alpha_k^* \neq 0$$

$$\sum_{j=0}^{k} \alpha_j \mathbf{y}_{n+j} = h \sum_{j=0}^{k} \beta_j \mathbf{f}_{n+j}, \qquad \alpha_k \neq 0$$

-

$$P: \qquad \mathbf{y}_{n+k}^{[0]} + \sum_{j=1}^{k-1} \alpha_j^* \mathbf{y}_{n+j}^{[m]} = h \sum_{j=0}^{k-1} \beta_j^* \mathbf{f}_{n+j}^{[m-t]},$$

$$(EC)^m: \qquad \mathbf{f}_{n+k}^{[\nu]} = f(x_{n+k}, \mathbf{y}_{n+k}^{[\nu]})$$

$$\mathbf{y}_{n+k}^{[\nu+1]} + \sum_{j=0}^{k-1} \alpha_j \mathbf{y}_{n+j}^{[m]} = h\beta_k \mathbf{f}_{n+k}^{[\nu]} + h \sum_{j=0}^{k-1} \beta_j \mathbf{f}_{n+j}^{[m-t]}$$

$$\nu = 1, \ldots, m-1$$

$$E^{(1-t)}: \qquad \mathbf{f}_{n+k}^{[m]} = f(x_{n+k}, \mathbf{y}_{n+k}^{[m]}), \quad \text{si } t = 0.$$

Order of a Predictor-Corrector Schemes

- We assume that $(x_n, \mathbf{y}_n), (x_{n-1}, \mathbf{y}_{n-1})$ are in the same curve $\mathbf{u}(x)$ ("local solution").
- The local error for the predicted value is given by

$$u(x_{n+1}) - y_{n+1}^{(0)} = -\frac{1}{6}h^4 u^{(4)}(x_n) + O(h^5).$$

- The order of the corrector formula in the example is

$$u(x_n+h) - u(x_n) - \frac{1}{12}h(5u'(x_n+h) + 8u'(x_n) - u'(x_{n-1})) = \frac{1}{24}h^4 u^{(4)}(x_n) + O(h^5).$$

$$y_{n+1}^{(1)} - y_n - \frac{1}{12}h(5f(x_{n+1}, y_{n+1}^{(0)}) + 8f_n - f_{n-1}) = 0$$

and substracting the second equation from the first one

$$u(x_{n+1}) - y_{n+1}^{(1)} - \frac{5h}{12}\underbrace{[f(x_{n+1}, u(x_{n+1})) - f(x_{n+1}, y_{n+1}^{(0)})]}_{\frac{\partial f}{\partial y}(x_{n+1},\zeta)(u(x_{n+1}) - y_{n+1}^{(0)})} = \frac{1}{24}h^4 y^{(4)}(x_n) + O(h^5).$$

-

$$u(x_{n+1}) - y_{n+1}^{(\nu+1)} - \frac{5h}{12}[f(x_{n+1}, u(x_{n+1})) - f(x_{n+1}, y_{n+1}^{(\nu)})] = \frac{1}{24}h^4 y^{(4)}(x_n) + O(h^5).$$

Error estimation in Predictor Corrector Schemes

- With a predictor of order p and a corrector of order $p+1$.
- With a predictor and a corrector both of order p.

  We can estimate the principal error terms of each formula (p.e. in PECE mode):

$$\begin{aligned} y_{n+1}^{(0)} - u(x_{n+1}) &= A_P h^{p+1} u^{(p+1)}(x_n) + O(h^{p+2}), \quad (h \to 0) \\ y_{n+1}^{(1)} - u(x_{n+1}) &= A_C h^{p+1} u^{(p+1)}(x_n) + O(h^{p+2}), \quad (h \to 0) \end{aligned}$$

This gives

$$y_{n+1}^{(0)} - y_{n+1}^{(1)} = (A_P - A_C) h^{p+1} u^{(p+1)}(x_n) + O(h^{p+2}), \quad (h \to 0).$$

from where

$$h^{p+1} u^{(p+1)}(x_n) = \frac{y_{n+1}^{(0)} - y_{n+1}^{(1)}}{A_P - A_C} + O(h^{p+2})$$

Usually the Predictor-Corrector pair is implemented in local extrapolation mode.

Interpolatory techniques

- If at $x = x_n$ the code do an steph length change from h to αh, k-steps linear multistep methods requiere the computation of new starter information if it is wanted to use the same formula at the grid points

$$x_n - \alpha h, x_n - 2\alpha - h, \ldots, x_n - (k-1)\alpha h.$$

- A practical approach is to interpolate the necessary information from the data.
1.- For a general k-step linear multistep method: consider the Hermite interpolating polynomial of the data $(x_{n-j}, \mathbf{y}_{n-j}, \mathbf{f}_{n-j}), j = 0, \ldots, k-1$. This is the only vector valued polynomial $P_{2k-1}(x)$, of degree less than or equal to $2k-1$, such that

$$P_{2k-1}(x_{n-j}) = \mathbf{y}_{n-j}, \quad P'_{2k-1}(x_{n-j}) = \mathbf{f}_{n-j}$$

2.- For a k steps Adams formula the stepping from $x = x_n$ to $x = x_{n+1}$ amounts to transform the data

$$(\mathbf{y}_n, \mathbf{y}'_n, \ldots, \mathbf{y}'_{n-k+1}) \rightarrow (\mathbf{y}_{n+1}, \mathbf{y}'_{n+1}, \ldots, \mathbf{y}'_{n-k+2}).$$

For doing that it is used the polynomial $I(x)$ of degree $\leq k$ that interpolate the data $(x_n, \mathbf{y}_n), (x_n, \mathbf{y}'_n), \ldots, (x_{n-k+1}, \mathbf{y}'_{n-k+1})$.

Adams formulas with variable coefficients

- Adams formulae extend easily to nonuniform grids of nodes.
- Adams-Bashforth formulae:

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} P^*_{k-1}(x)dx, \quad P^*_{k-1}(x_{n-j}) = f(x_{n-j}, y_{n-j}), \quad j = 0, \dots, k-1$$

We have

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1} \sum_{j=0}^{k-1} \alpha_j(n) \mathbf{f}[x_n, \dots, x_{n-j}], \tag{2}$$

where

$$\alpha_j(n) = \frac{1}{h_{n+1}} \int_{x_n}^{x_{n+1}} \prod_{i=0}^{j-1} (x - x_{n-i}) dt, \tag{3}$$

and $\mathbf{f}[x_n, \dots, x_{n-j}]$ denotes the j-th divided difference, which can be computed with the following recursive formulas

$$\mathbf{f}[x_n] = \mathbf{f}_n$$

$$\mathbf{f}[x_n, \dots, x_{n-j}] = \frac{\mathbf{f}[x_n, \dots, x_{n-j+1}] - \mathbf{f}[x_{n-1}, \dots, x_{n-j}]}{x_n - x_{n-j}}, \quad j = 1, \dots$$

Adams formulae with variable coefficients

We introduce

$$\mathbf{\Phi}_j(n) := \left(\prod_{i=1}^{j}(x_n - x_{n-i})\right)\mathbf{f}[x_n,\ldots,x_{n-j}], \quad j = 0,\ldots; \tag{4}$$

that can be also computed recursively by the formulas

$$\mathbf{\Phi}_0(n) = \mathbf{f}_n,$$
$$\mathbf{\Phi}_j(n) = \mathbf{\Phi}_{j-1}(n) - \beta_{j-1}(n)\mathbf{\Phi}_{j-1}(n-1),$$

where $\beta_0(n) = 1$ and

$$\beta_j(n) = \prod_{i=1}^{j}\frac{x_n - x_{n-i}}{x_{n-1} - x_{n-1-i}}, \quad j = 1, 2, \ldots. \tag{5}$$

Then

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\sum_{j=0}^{k-1} g_j(n)\beta_j(n+1)\mathbf{\Phi}_j(n), \quad g_j(n) = \frac{1}{h_{n+1}}\int_{x_n}^{x_{n+1}}\prod_{i=0}^{j-1}\frac{x - x_{n-i}}{x_{n+1} - x_{n-i}}dt, j \geq 3$$

Adams-Moulton with variable coefficients

If we add to the interpolating polynomial of the explicit method the term

$$\left(\prod_{i=0}^{k-1}(x - x_{n-i})\right)\mathbf{f}[x_{n+1}, \ldots, x_{n-k+1}]$$

we get the polynomial of degree k that interpolate the $k+1$ data

$$(x_{n-k+1}, \mathbf{f}_{n-k+1}), \ldots, (x_n, \mathbf{f}_n), (x_{n+1}, \mathbf{f}_{n+1}).$$

Therefore, the k step implicit Adams method is given by the formula

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_{n+1}\sum_{j=0}^{k-1} g_j(n)\beta_j(n+1)\mathbf{\Phi}_j(n) + h_{n+1}g_k(n)\mathbf{\Phi}_k(n+1).$$

The coefficients $g_j(n) := g_{j,1}$ are also computed recursively with the formulas:

$$g_{1,q} = \frac{1}{q}, \quad g_{2,q} = \frac{q}{q+1}, \quad g_{j,q} = g_{j-1,q} - \frac{h_{n+1}}{x_{n+1} - x_{n+1-j}} g_{j-1,q+1}$$

Implementation aspects

- Codes for non stiff problems use to implement a Predictor-Corrector code based in the Adams-Basforth-Moulton formulae (in mode PECE, p.e.). It is common to have Adams-Bashforth and Adams-Moulton formulae for orders from $p = 1$ to $p = 12$ and the codes change the order of the method for efficiency.
- The starting procedure has two components:
  1. A prediction of the initial step size h_0 (p.e. $e_1 \approx h^2 \|f(x_0, \mathbf{y}_0)\|$).
  2. Order is raised and the step length is doubled after each successful step. This phase is terminated when we obtain the first rejection of a step.
- A strategie for changing the order.
  1. At each step, the method always compute the estimates for the local error with several formula and choose the one with the smallest estimate, or the one that allows a maximal step size.

Software

- Codes from www.netlib.org (Fortran 77 o Fortran 90, some in C)
  1. VODE (Adams methods in Nordsieck form (interpolation)), by Brown, Byrne and Hindmarsh (1989). Before was EPISODE by Byrne and Hindmarsh, 1975.
  2. LSODE. (Adams methods in Nordsieck form (interpolation)). This is a successor of the codes DIFSUB (Gear, 1971) and GEAR (Hindmarsh, 1972).
  3. DEABM. A modification of the code DE/STEP/INTRP in the book by Shampine and Gordon (1975)
- The codes in MATLAB 6.1
  1. ode45 (DOPRI5, no stiff), ode23 (RK embedded pair 3(2), no stiff), ode113 (PECE mode for Adams formula of orders 1-12 with modified divided differences, no stiff), ode23t (trapezoidal rule, moderate stiff), ode15s (NDF formula by Shampine of orders 1-5), ode23s (modified Rosenbrock (2,3) pair, stiff), ode23tb (implicit RK, moderate stiff)