Order conditions for RK methods

Question: How to choose c_i, a_{ij}, b_i in order to achieve a given accuracy?

First simplification: Transform $y' = f(t, y(t))$ (see $(*)$) in autonomous form $(y' = f(y))$:

Introduce $Y = \begin{pmatrix} t \\ y \end{pmatrix}$, $Y' = \begin{pmatrix} 1 \\ f(t,y) \end{pmatrix} = F(Y)$ $\qquad (**)$

Lemma: Assume a RK method has order p for $(**)$ and that $\sum_{i=1}^{s} b_i = 1$ (for consistency) and $c_i = \sum_{j=1}^{s} a_{ij}$, then the RK method has order p for $(*)$.

Proof: See exercises.

Rem.:

Σ

$$\begin{array}{c|ccc}
c_1 & a_{11} & \cdots & a_{1s} \\
\vdots & & & \\
c_s & a_{s1} & \cdots & a_{ss} \\
\hline
 & b_1 & \cdots & b_s
\end{array}$$

$\hookrightarrow \Sigma = 1$

AB

NIDS

Recall: $f: \mathbb{R}^d \to \mathbb{R}^d$, $f(y) = \begin{pmatrix} f_1(y_1, \dots, y_d) \\ \vdots \\ f_d(y_1, \dots, y_d) \end{pmatrix}$

- $f'(y): \mathbb{R}^d \to \mathbb{R}^d$ (Jacobian matrix)

  $u \mapsto f'(y)(u)$

  $(f'(y)u)_i = \sum_{j=1}^{d} \frac{\partial f_i(y)}{\partial y_j} u_j$ (linear form)

- $f''(y): \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$

  $(u,v) \mapsto f''(y)(u,v)$

  $(f''(y)(u,v))_i = \sum_{j,k=1}^{d} \frac{\partial^2 f_i(y)}{\partial y_j \partial y_k} u_j v_k$ (bilinear form)

  $= u^T \underbrace{D^2 f_i(y)}_{\text{Hessian of ith component}} v$

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Strategy: Taylor expansion of the exact and the RK solutions and then compare the terms.

Exact: $y(t_0+h) = y_0 + \sum_{k=1}^{p} \frac{h^k}{k!} y^{(k)}(t_0) + O(h^{p+1})$

Numerical: $y_1(h) = y_0 + \sum_{k=1}^{p} \frac{h^k}{k!} y_1^{(k)}(0) + O(h^{p+1})$

By defn of RK order p iff $y^{(k)}(t_0) = y_1^{(k)}(0)$, $\forall k \leq p$.

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<u>Exact solution:</u> We have

$$y'(t) = f(y(t))$$
$$y''(t) = f'(y(t))\, y'(t) = f'(y(t))\, f(y(t))$$
$$y'''(t) = f''(y(t))\,(y'(t), f(y(t))) + f'(y(t))\, f'(y(t))\, y'(t)$$
$$= f''(y(t))\,(f(y(t)), f(y(t))) + f'(y(t))\, f'(y(t))\, f(y(t))$$

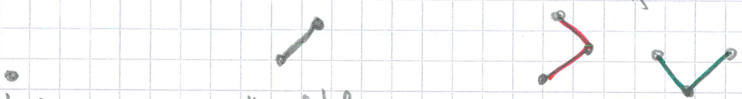
We call $f^{(k)} = f^{(k)}(y(t_0))$, so that

$y'(t_0) = f$ $\qquad$ $y'''(t_0) = f''(f,f) + f'f'f$

$y''(t_0) = f'f$ $\qquad$ $y^{IV}(t_0) = ?$

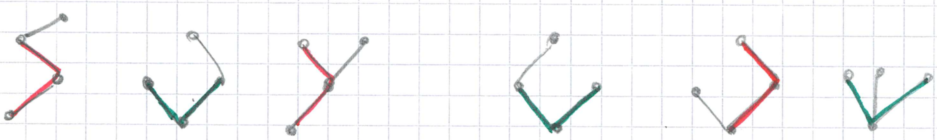
<u>Idea:</u> Use rooted trees: $f \leftrightarrow \circ$ (vertex)

$f^{(k)} \leftrightarrow$ (k branches)



$y' = f$ $\qquad$ $y'' = f'f$ $\qquad$ $y''' = f'f'f + f''(f,f)$

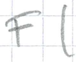
One observes that from $y^{(a)}$ to $y^{(a+1)}$ one has just to let the trees grow:



$f'f'f'f$ $\quad$ $f''(f'f,f)$ $\quad$ $f'f''(f,f)$ $\quad$ $f''(f'f,f)$ $\quad$ $f''(f'f,f)$ $\quad$ $f'''(f,f,f)$

$$\Rightarrow y^{IV}(t_0) = f'f'f'f + 3\, f''(f'f,f) + f'f''(f,f) + f'''(f,f,f)$$

Let τ denote a generic tree, let $|\tau|$ denote its order (i.e. number of nodes). Moreover, denote by $F(\tau)$ the differential associated to τ.

(e.g. $F($  $) = f'f'f$).

<u>Theorem:</u> $y^{(k)}(t_0) = \sum_{\tau : |\tau| = k} \alpha(\tau) F(\tau)$ for numbers $\alpha(\tau) \in \mathbb{N}$

<u>Example:</u> $\alpha(\cdot) = 1$, $\alpha($  $) = 3$ 3 ways (α: number of ways a tree can be built from the previous level)

previous level: 

<u>Rem:</u> The numbers $\alpha(\tau)$ are not relevant here, it will become clearer later on.

<u>Numerical solution:</u> We have

$$y_1(h) = y_0 + h \sum_{i=1}^{s} b_i K_i(h)$$
$$K_i(h) = f\left(y_0 + \sum_{j=1}^{s} a_{ij} h K_j(h)\right)$$

Notice that:

1) $K_i(0) = f(y_0) = f$

2) $(h K_i(h))^{(j)}\big|_{h=0} = j \, K_i^{(j-1)}(0)$ by Leibniz product rule (LPR)

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Hence $y_1'(0) = \sum_{i=1}^{s} b_i (h K_i(h))'\big|_{h=0} = \sum_{i=1}^{s} b_i K_i(0) = \left(\sum_{i=1}^{s} b_i\right) f$

For the second derivative:

$$k_i'(h) = f'\Big(y_0 + \sum_{j=1}^{s} a_{ij} h\, k_j(h)\Big) \cdot \sum_{j=1}^{s} a_{ij} \big(h k_j(h)\big)'$$

$$\Rightarrow k_i'(0) = f'(y_0) \sum_{j=1}^{s} a_{ij} \big(h k_j(h)\big)'\Big|_{h=0} = f'(y_0) \sum_{j=1}^{s} a_{ij} f(y_0)$$

$$= \Big(\sum_{j=1}^{s} a_{ij}\Big) f' f$$

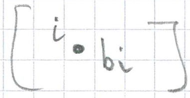
$$\Rightarrow y_1''(0) = \sum_{i=1}^{s} b_i \big(h k_i(h)\big)''\Big|_{h=0} \overset{LPR}{=} 2 \sum_{i=1}^{s} b_i k_i'(0)$$

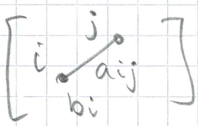
$$\overset{\text{above}}{=} 2 \Big(\sum_{i,j=1}^{s} b_i a_{ij}\Big) f' f \, .$$

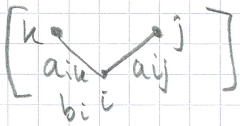
For higher order, we use a tree structure

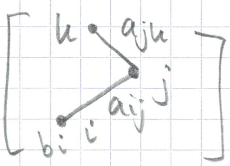
<u>Defn:</u> (fct ϕ)

Let τ be a tree representing a differential $F(\tau)$ and a_{ij}, b_i, $i,j = 1,2,\dots,s$ the coefficients of a RK method. We define a fct $\phi : \tau \mapsto \phi(\tau)$ recursively as:

$\phi(\cdot) = \sum_{i=1}^{s} b_i$ 

$\phi($$) = \sum_{i,j=1}^{s} b_i a_{ij}$ 

$\phi($$) = \sum_{i,j,k=1}^{s} b_i a_{ij} a_{ik}$ 

$\phi($$) = \sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk}$ 

etc.

Defn: (fct γ)

let $\gamma(\cdot) = 1$. Then $\gamma(\tau) = \underset{\substack{\uparrow \\ \text{number of nodes}}}{|\tau|} \prod_{n=1}^{N} \gamma(\tau_n)$,

where $\tau_1, \tau_2, \dots, \tau_N$ are the trees obtained by cutting the root of τ.

Example:

$$\gamma(/) = 2\,\gamma(\cdot) = 2$$

$$\gamma(\vee) = 3\,\gamma(\cdot)\cdot\gamma(\cdot) = 3\cdot 1\cdot 1 = 3.$$

$$\gamma(>) = 3\,\gamma(/) = 3\cdot 2 = 6$$

$$\gamma(Y) = 4\,\gamma(\vee) = 4\cdot 3 = 12$$

Recall:

$$y_1'(0) = \left(\sum_{i=1}^{s} b_i\right) f = \underbrace{\alpha(\cdot)}_{=1}\underbrace{\gamma(\cdot)}_{=1}\underbrace{\phi(\cdot)}_{\sum_{i=1}^{s} b_i}\underbrace{F(\cdot)}_{=f}$$

$$y_1''(0) = 2\left(\sum_{i,j=1}^{s} b_i a_{ij}\right) f'f$$

$$= \underbrace{\alpha(/)}_{=1}\underbrace{\gamma(/)}_{=2}\underbrace{\phi(/)}_{=\sum_{i,j=1}^{s} b_i a_{ij}}\underbrace{F(/)}_{=f'f}$$

In general, it holds:

Theorem: $$y_1^{(k)}(0) = \sum_{\tau:|\tau|=k} \alpha(\tau)\gamma(\tau)\phi(\tau)F(\tau)$$

Example: $\tau : |\tau| = 3 = \{\vee, >\}$

$$y_1'''(0) = \alpha(\vee)\gamma(\vee)\phi(\vee)F(\vee) + \alpha(>)\gamma(>)\phi(>)F(>)$$

$$= 1\cdot 3\cdot \sum_{i,j,k=1}^{s} b_i a_{ij} a_{ik} f''(f,f) + 1\cdot 6\cdot \sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} f'f'f$$

Rem:

$$y^{(k)}(t_0) = \sum_{\tau : |\tau| = k} \alpha(\tau) F(\tau)$$

$$y_1^{(k)}(0) = \sum_{\tau : |\tau| = k} \alpha(\tau)\, \phi(\tau)\, \gamma(\tau)\, F(\tau)$$

Theorem: A RK method has order p iff

$$\gamma(\tau)\phi(\tau) = 1 \qquad \forall\ \tau : |\tau| \leq p.$$

Examples:

$$\gamma(\bullet)\phi(\bullet) = 1 \iff \sum_{i=1}^{s} b_i = 1 \quad \Big]\ p=1$$

$$\gamma([\bullet])\phi([\bullet]) = 1 \iff \sum_{i,j=1}^{s} b_i a_{ij} = \frac{1}{2} \quad \Big]\ p=2$$

$$\gamma([\bullet,\bullet])\phi([\bullet,\bullet]) = 1 \iff \sum_{i,j,k=1}^{s} b_i a_{ij} a_{ik} = \frac{1}{3}$$

$$\gamma([[\bullet]])\phi([[\bullet]]) = 1 \iff \sum_{i,j,k=1}^{s} b_i\, a_{ij}\, a_{jk} = \frac{1}{6} \quad \Big]\ p=3$$

Rem: The cardinality of $\{\tau : |\tau| = k\}$ grows fast wrt k

order	1	2	3	4	5	6	7	8	9	10
number of conditions	1	2	4	8	17	35	85	200	486	1'205

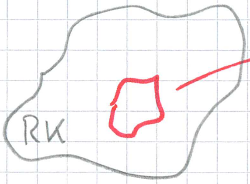
Consequences:

(i) We need another way to build higher-order methods.

(ii) Difficult to analyse the properties of a RK method without further "insight".

3. Collocation methods

Collocation methods are an important class of Runge-Kutta methods.

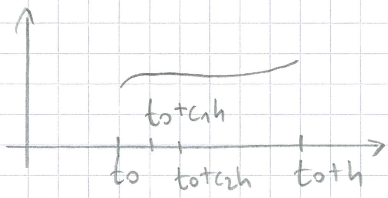


Collocation methods : Gauss method, Radau method, Lobatto method

Geometric integration

stiff problems

Consider $\begin{cases} y' = f(t,y) \\ y(t_0) = y_0 \end{cases}$



Defn: (Collocation method)

Let $0 \le c_1 < c_2 < \cdots < c_s \le 1$ be so-called collocation points. Define $u(t)$ a polynomial of degree s such that

$$\begin{cases} u(t_0) = y_0 \\ u'(t_0 + c_i h) = f(t_0 + c_i h, u(t_0 + c_i h)) \end{cases}, \quad i = 1, 2, \ldots, s.$$

The numerical approximation at $t_0 + h$ is defined by

$$y_1 = u(t_0 + h).$$

Example:

(i) $s = 1$, $c_1 = 0$, $u(t) = y_0 + \alpha(t - t_0)$

$$u'(t_0) = f(t_0, u(t_0)) = \alpha \Rightarrow \alpha = f(t_0, y_0)$$

$$\Rightarrow y_1 = u(t_0 + h) = y_0 + \overbrace{f(t_0, y_0)}^{=\alpha}(t_0 + h - t_0)$$

$$= \underline{y_0 + h f(t_0, y_0)} \quad \text{Explicit Euler method.}$$

(ii) $s = 1$, $c_1 = 1$ $\overset{\text{ex.}}{\Rightarrow}$ Implicit Euler method

(iii) $s = 2$, $c_1 = 0$, $c_2 = 1$ $\overset{\text{ex.}}{\Rightarrow}$ Implicit Midpoint rule

[redacted]

Rem: With collocation methods we do not only get a solution at t_0+h, but on the whole $[t_0, t_0+h]$ (dense output).

Theorem 1: (Guillou & Soulé 1969, Wright 1970)

A collocation method is equivalent to a s-stage RK method with coefficients:

$$a_{ij} = \int_0^{c_i} l_j(t)\,dt \,, \qquad b_i = \int_0^1 l_i(t)\,dt \qquad , i,j=1,2,\dots,s$$

where $l_i(t) = \prod_{\substack{j=1 \\ j\neq i}}^{s} \frac{t-c_j}{c_i-c_j}$. $\Leftarrow$ (polynomial of degree $s-1$) is $\equiv 1$ at collocation points $l_i(c_j) = \delta_{ij}$.

(Lagrange polynomial)

Rem: $l_i(t)$ is a polynomial of degree $s-1$ s.t. $l_i(c_i)=1$, $l_i(c_j)=0$ $(j\neq i)$.

Proof: Consider a collocation polynomial $u(t)$.

Define $K_i := f(t_0+c_ih, u(t_0+c_ih))$ for $i=1,2,\dots,s$ $(*)$.

① Observe that for $r\in[0,1]$:

$$\underbrace{u'(t_0+rh)}_{\text{polynomial of degree } s-1} = \underbrace{\sum_{j=1}^{s} l_j(r)K_j}_{\text{polynomial of degree } s-1} \qquad (**)$$

For all $i=1,2,\dots,s$

LHS: $u'(t_0+c_ih) \overset{\text{defn.}}{=} f(t_0+c_ih, u(t_0+c_ih))$

RHS: $\sum_{j=1}^{s} l_j(c_i)K_j = \sum_{j=1}^{s} \delta_{ij}K_j = K_i \overset{(*)}{=} f(t_0+c_ih, u(t_0+c_ih))$

So both (LHS and RHS) are polynomials of degree $s-1$ and they coincide on s points $\Rightarrow$ $(**)$ holds.

(2) Integrate

$$u(t_0+c_i h) \overset{\text{fundamental thm of Calculus}}{=} u(t_0) + \int_{t_0}^{t_0+c_i h} u'(s)\,ds$$

$$\overset{\text{change of variable}}{=} u(t_0) + h\int_0^{c_i} u'(t_0+rh)\,dr$$

$$\overset{(**)}{=} y_0 + h\int_0^{c_i} \sum_{j=1}^{s} \ell_j(r) K_j\,dr$$

Replace in $(*)$

$$K_i = f\left(t_0+c_i h,\ y_0 + h\sum_{j=1}^{s}\left(\int_0^{c_i}\ell_j(r)\,dr\right)K_j\right)$$

which is a RK system iff

$$\int_0^{c_i}\ell_j(r)\,dr = a_{ij} \qquad \forall\ i,j = 1,2,\dots,s.$$

(3) Similarly we obtain
(ex.)

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