AB

NIDS

Discontinuous collocation methods

Defn.: (discontinuous collocation method)

Let $0 < c_2 < \dots < c_{s-1} < 1$, $c_1 = 0$, $c_s = 1$, b_1, b_s be real numbers. Define a polynomial of degree $s-2$ satisfying

$$\begin{cases} u(t_0) = y_0 - h b_1 \overbrace{\left(u'(t_0) - f(t_0, u(t_0))\right)}^{\text{correction}} \\ u'(t_0 + c_i h) = f(t_0 + c_i h, u(t_0 + c_i h)), \quad i = 2, \dots, s-1 \end{cases}$$

A discontinuous collocation method is given by:

$$y_1 = u(t_0 + h) - h b_s \left(u'(t_0 + h) - f(t_0 + h, u(t_0 + h))\right).$$

Theorem 3: The discontinuous collocation method is equivalent to a s-stage RK method given by

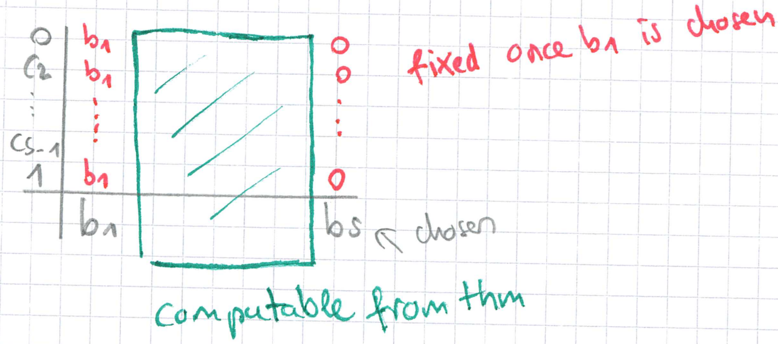
$$0 = c_1 < c_2 < \dots < c_s = 1, \quad a_{i1} = b_1, \quad a_{is} = 0 \quad \text{and}$$

$$a_{ij} = \int_0^{c_i} l_j(t)\,dt - b_1 l_j(0) \qquad \begin{array}{l} i = 1, 2, \dots, s \\ j = 2, \dots, s-1 \end{array}$$

$$b_i = \int_0^1 l_i(t)\,dt - b_1 l_i(0) - b_s l_i(1), \quad i = 2, \dots, s-1$$

with $l_j(t) = \prod_{\substack{k=2 \\ k \neq j}}^{s-1} \frac{(t - c_k)}{(c_j - c_k)}$. (Lagrange interpolation polynomials)

Proof: Similar to the proof for continuous collocation methods (see exercises).



Rem.: Fixing $b_1 = b_s = 0 \Rightarrow$ we obtain a $(s-2)$-stage collocation method.

Example: (Lobatto III B)

$\boxed{s=2}$

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

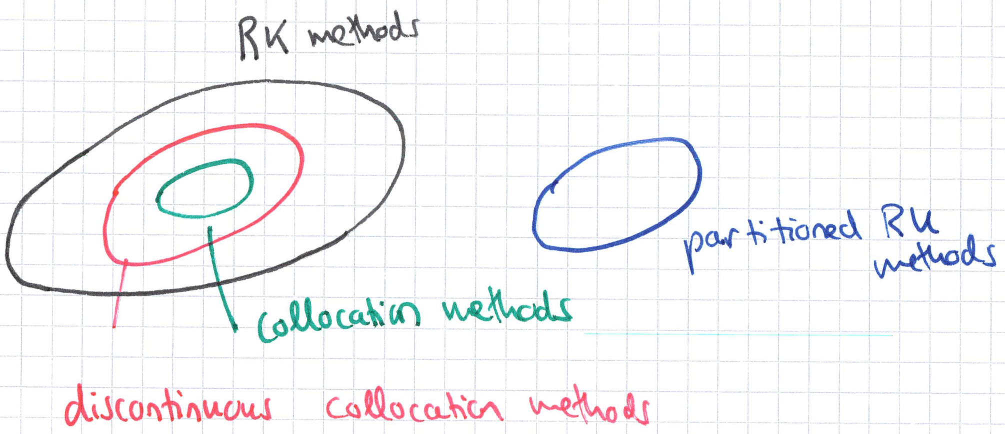
$\boxed{s=3}$

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

Theorem 4. Consider $\begin{cases} y' = f(t, y(t)) \\ y(t_0) = y_0 \end{cases}$ and a discontinuous collocation method. Assume f is Lipschitz (in its second argument) and smooth.
If $B(p)$ holds for some $p \geq s-2$,
then $\| y(t_0+h) - u(t_0+h) \| \leq C h^{p+1}$ for h small enough.

Proof: see Hairer et al. 2006, Chap. II.
(Similar to the Thm of Guillou & Soulé)

Rem: Lobatto III B methods have order $2s-2$.



4. Partitioned Runge-Kutta methods

Important methods that do not belong to the class of RK methods.

Consider
$$\begin{cases} y' = f(y,z), & y(t_0) = y_0 \\ z' = g(y,z), & z(t_0) = z_0 \end{cases} \qquad (*)$$

$f: \mathbb{R}^{d_1} \times \mathbb{R}^{d_2} \to \mathbb{R}^{d_1}$ $\quad g: \mathbb{R}^{d_1} \times \mathbb{R}^{d_2} \to \mathbb{R}^{d_2}$ (often $d_1 = d_2$) (we mainly use it for Hamiltonian systems)

Example: (Hamiltonian systems)
$$\begin{cases} p' = -\frac{\partial H}{\partial q}(p,q) \\ q' = \frac{\partial H}{\partial p}(p,q) \end{cases}$$

Defn: (Partitioned Runge-Kutta, PRK)

Take two RK methods (a_{ij}, b_i), $(\hat{a}_{ij}, \hat{b}_i)$, $i,j = 1,2,\dots,s$.
A partitioned RK method for $(*)$ is given by

$$\begin{cases} k_i = f\left(y_0 + h \sum_{j=1}^{s} a_{ij} k_j, \; z_0 + h \sum_{j=1}^{s} \hat{a}_{ij} l_j\right) \\ l_i = g\left(y_0 + h \sum_{j=1}^{s} a_{ij} k_j, \; z_0 + h \sum_{j=1}^{s} \hat{a}_{ij} l_j\right) \end{cases} \quad i = 1,2,\dots,s$$

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i$$

$$z_1 = z_0 + h \sum_{i=1}^{s} \hat{b}_i l_i .$$

Rem: WLOG autonomous, general case put $t' = 1$ (see proof of order conditions).

(Important for geometric integration)

Example: 1) Symplectic Euler

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \quad + \quad \begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \quad \Rightarrow \text{ symplectic Euler (PRK)}$$

implicit Euler   explicit Euler

2) Lobatto IIIA (collocation method) + Lobatto IIIB (discontinuous collocation method)

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

$s=2$
$$\begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array} \Rightarrow \text{Störmer-Verlet (PRK)}$$

Thm: The partitioned RK method composed of Lobatto IIIA and Lobatto IIIB has order $p = 2s-2$.

Order conditions for PRK

Two methods $\rightsquigarrow$ "bicolor" trees:

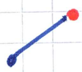
$p=1$

$\sum_{i=1}^{s} b_i = 1$

$\sum_{i=1}^{s} \hat{b}_i = 1$

$p=2$

$\sum_{i,j} b_i a_{ij} = \frac{1}{2}$



$\sum_{i,j} b_i \hat{a}_{ij} = \frac{1}{2}$

$\sum_{i,j} \hat{b}_i a_{ij} = \frac{1}{2}$

$\sum_{i,j} \hat{b}_i \hat{a}_{ij} = \frac{1}{2}$.

cross-product

$\Rightarrow$ a lot of conditions.

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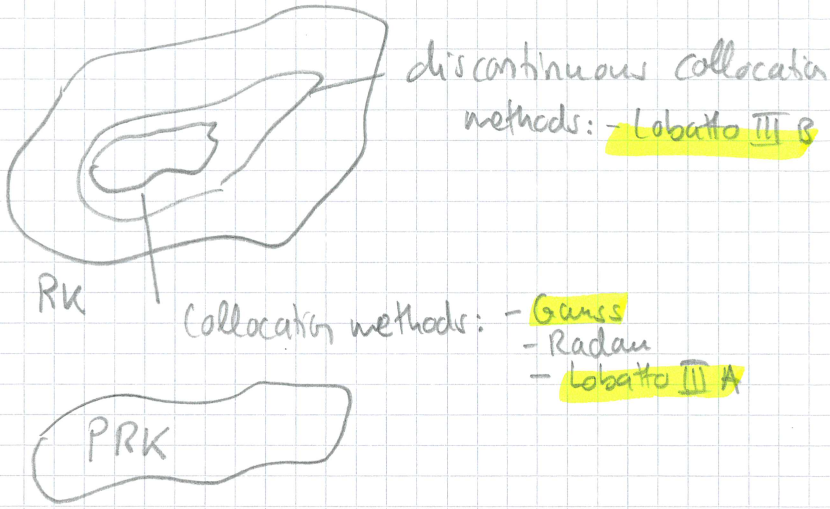
Summary:

$y' = f(t, y)$

For geometric integration



$$\begin{cases} y' = f(y, z) \\ z' = g(y, z) \end{cases}$$

- Lobatto III A + Lobatto III B
- Symplectic Euler method (implicit + explicit Euler)

II Geometric numerical integration of dynamical systems

1. Numerical conservation of invariants

Recall: Given $\begin{cases} y' = f(y) \\ y(t_0) = y_0 \end{cases}$ and $I: \mathbb{R}^d \to \mathbb{R}$ non-constant.

Then I is invariant or a first integral (FI) if

$$I'(y) f(y) = 0 \quad \forall y \in \mathbb{R}^d$$

$$\Leftrightarrow \frac{d}{dt} I(y(t)) = 0$$

In this case $I(y(t)) = I(y_0) = \text{constant}.$

Example:
- The Hamiltonian fct $H(p,q)$ in a Hamiltonian system
- $L(p,q) = q_1 p_2 - p_1 q_2$ (angular momentum for Kepler problem)
- Volterra-Lotka problem: u: predator, v: prey

$$u' = u(v-2), \quad u(t_0) = u_0$$
$$v' = v(1-u), \quad v(t_0) = v_0$$

$I(u,v) = u + v - \ln(u) - 2\ln(v)$ is a first integral of the system.

$$I'(u,v)\begin{pmatrix} u(v-2) \\ v(1-u) \end{pmatrix} = \begin{pmatrix} 1-\frac{1}{u} & 1-\frac{2}{v} \end{pmatrix}\begin{pmatrix} u(v-2) \\ v(1-u) \end{pmatrix}$$
$$= u(v-2) - (v-2) + v(1-u) - 2(1-u)$$
$$= (u-1)(v-2) - (u-1)(v-2) = \underline{\underline{0}}$$

Goal: Study polynomial invariants

Linear first integral

Example: chemical reaction

species 1, rate, species 2

$$\begin{cases} S_1 \xrightarrow{\alpha_1} S_2 \\ S_2 + S_2 \xrightarrow{\alpha_2} S_2 + S_3 \\ S_2 + S_3 \xrightarrow{\alpha_3} S_1 + S_3 \end{cases}$$

(ODE solvers often used in chemistry → chemical reactions)

$$y(t) = \begin{pmatrix} y_1(t) \\ y_2(t) \\ y_3(t) \end{pmatrix}$$ with $y_i(t)$ = concentration of molecules of S_i at time t.

Mass-action law: the rate at which a chemical is produced (or destroyed) is proportional to the product of the reactants:

destroyed

$$\Rightarrow \begin{cases} y_1'(t) = -\alpha_1 y_1(t) + \alpha_3 y_2(t) y_3(t) \\ y_2'(t) = \alpha_1 y_1(t) - \alpha_2 y_2^2(t) - \alpha_3 y_2(t) y_3(t) \\ y_3'(t) = \alpha_2 y_2^2(t) + 0\, \alpha_3 y_2(t) y_3(t) \end{cases}$$

created; $(-2+1)$

$(1-1)$ concentration of S_3 doesn't change (on both sides)

$$\Rightarrow y_1'(t) + y_2'(t) + y_3'(t) = 0$$

$$f(y) = \begin{pmatrix} -\alpha_1 y_1 + \alpha_3 y_2 y_1 \\ \vdots \end{pmatrix}$$

$$\Rightarrow \underbrace{\begin{pmatrix} 1 & 1 & 1 \end{pmatrix}}_{= I'(y)^T} \begin{pmatrix} f_1(y) \\ f_2(y) \\ f_3(y) \end{pmatrix} = 0$$

$$\Rightarrow \boxed{I(y) = y_1 + y_2 + y_3}$$ (total mass) is a first integral of the system.

Theorem: All RK methods conserve linear first integrals of the form $I(y) = v^T y$, $v \in \mathbb{R}^d$.
PRK methods conserve linear first integrals if $b_i = \hat{b}_i$, $i = 1, 2, \ldots, s$ or if the linear first integral I depends only on y (or z).

Proof: We need to show that $I(y_1) = I(y_0)$ (along trajectory conserved)
Remark: $I'(y)\, w = v^T w$

① Consider $y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i$, $k_i = f(y_0 + h \sum_{j=1}^{s} a_{ij} k_j)$
$i = 1, 2, \ldots, s$

$$I(y_1) = v^T y_1 = \overbrace{v^T y_0}^{= I(y_0)} + h \sum_{i=1}^{s} b_i v^T k_i$$

but $v^T k_i = \underbrace{I'(y_0 + h \sum_{j=1}^{s} a_{ij} k_j)\, f(y_0 + h \sum_{j=1}^{s} a_{ij} k_j)}_{= 0}$

↑ since I first integral

Hence $I(y_1) = I(y_0)$.

② For PRK: $\begin{cases} y' = f(y,z) \\ z' = g(y,z) \end{cases}$ $I(y,z) = (v_1^T \;\; v_2^T) \begin{pmatrix} y \\ z \end{pmatrix}$

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i, \quad z_1 = z_0 + h \sum_{i=1}^{s} \hat{b}_i l_i$$

$$I(y_1, z_1) = v_1^T y_1 + v_2^T z_1 = \overbrace{v_1^T y_0 + v_2^T z_0}^{= I(y_0, z_0)} + h \sum_{i=1}^{s} b_i v_1^T k_i + h \sum_{i=1}^{s} \hat{b}_i v_2^T l_i$$

$$\overset{b_i = \hat{b}_i}{=} I(y_0, z_0) + h \sum_{i=1}^{s} b_i \underbrace{(v_1^T \;\; v_2^T) \begin{pmatrix} k_i \\ l_i \end{pmatrix}}_{= 0 \text{ as above}} = I(y_0, z_0)$$

Hence $I(y_1, z_1) = I(y_0, z_0)$. #

(The case $I(y,z) = v_1^T y$ or $I(y,z) = v_2^T z$ is similar to the proof for non-partitioned RK methods).

Quadratic first integral

Consider $Q(y) = Q(y_1, y_2, \dots, y_d) = \sum_{ij=1}^{d} c_{ij} y_i y_j = y^T C y$
(quadratic form)

with $C \in \mathbb{R}^{d\times d}$ symmetric matrix.

Thus we take $Q : \mathbb{R}^d \to \mathbb{R}$
$y \mapsto y^T C y$

Ex: Angular momentum (Kepler problem)

Recall: Q is a first integral of $\begin{cases} y' = f(y) \\ y(t_0) = y_0 \end{cases}$, $y \in \mathbb{R}^d$

$\Leftrightarrow Q'(y) f(y) = 0$.

Derivative of Q:

$$Q(y + \overset{\downarrow \text{perturbation}}{h}) = (y+h)^T C (y+h) = y^T C y + \underbrace{\overset{=(h^T C y)^T}{2 y^T C h}}_{\text{linear part}} + \underbrace{h^T C h}_{\text{quadratic part}}$$

$$= Q(y) + Q'(y) h + \mathcal{O}(h \cdot h)$$

$\Rightarrow$ Q first integral $\Leftrightarrow$ $\underbrace{2 y^T C}_{=Q'(y)} f(y) = 0 \ \forall y \in \mathbb{R}^d$.
(Q conserved)

Theorem: The Gauss methods (RK collocation methods) conserve quadratic first integrals.

Ex: Midpoint rule for angular momentum (see Exercises)

Proof: $Q(y_1) - Q(y_0) = Q(u(t_0+h)) - Q(u(t_0))$, $u(t)$ collocation polynomial of degree s (Gauss)

$$= \int_{t_0}^{t_0+h} \frac{dQ}{dt}(u(t))\, dt \leftarrow \text{(dense output)} = \int_{t_0}^{t_0+h} Q'(u(t)) u'(t)\, dt$$

$$= \int_{t_0}^{t_0+h} 2 u(t)^T C u'(t)\, dt$$

$$= h \int_0^1 \underbrace{\underbrace{2u(t_0 + rh)^T}_{\text{polyn. } \# s} C \underbrace{u'(t_0 + rh)}_{\text{polyn. } \# s-1}}_{\text{polyn. } \# 2s-1} dr$$

Gauss points / weights (a_i, b_i) give a QF of order $2s$

$$\Rightarrow \quad Q(y_1) - Q(y_0) \overset{\text{Gauss can approximate exactly}}{=} h \sum_{i=1}^{s} b_i \, 2u(t_0+c_i h)^T C u'(t_0+c_i h)$$

$$= h \sum_{i=1}^{s} b_i \underbrace{2u(t_0+c_i h)^T C f(u(t_0+c_i h))}_{=0}$$

$$= \underline{\underline{0}} \qquad \#$$

Next we show a condition on the coefficients a_{ij}, b_i of a RK method in order to conserve quadratic first integrals.

Theorem: (Cooper 1987)
If
$$b_i a_{ij} + b_j a_{ji} = b_i b_j \quad , \quad i,j = 1,2,\dots,s$$
then the RK method based on (b_i, a_{ij}) conserves quadratic first integrals.

Proof: Call $g_i = y_0 + h \sum_{j=1}^{s} a_{ij} k_j$

$\Rightarrow k_i = f(g_i)$

Remark: $y_0 = g_i - h \sum_{j=1}^{s} a_{ij} k_j \quad , \quad i = 1,2,\dots,s.$

$$Q(y_1) = y_1^T C y_1 = \Big(y_0 + h \sum_{i=1}^{s} b_i k_i\Big)^T C \Big(y_0 + h \sum_{j=1}^{s} b_j k_j\Big)$$

$$= \underbrace{y_0^T C y_0}_{=Q(y_0)} + \overbrace{2h \sum_{i=1}^{s} b_i y_0^T C k_i}^{=I_1} + h^2 \sum_{i,j=1}^{s} b_i b_j k_j^T C k_i$$

$$\Rightarrow Q(y_1) - Q(y_0) = 2h \sum_{i=1}^{s} b_i g_i^T C k_i \overbrace{- 2h^2 \sum_{i,j=1}^{s} b_i a_{ij} k_j^T C k_i}^{=I_2}$$

$$\underbrace{+ h^2 \sum_{i,j=1}^{s} b_i b_j k_j^T C k_i}_{=I_3}$$