We have for I_1:

$$2 g_i^T C k_i = 2 g_i^T C f(g_i) = Q'(g_i) f(g_i) = 0 \Rightarrow \underline{\underline{I_1 = 0}}$$

For I_2:

$$I_2 = -h^2 \sum_{i,j=1}^{s} b_i a_{ij} k_j^T C k_i - h^2 \sum_{i,j=1}^{s} b_j a_{ji} k_i^T C k_j \qquad (i \Leftrightarrow j)$$

Observe that $k_i^T C k_j = k_j^T C k_i$

$$\Rightarrow I_2 = -h^2 \sum_{i,j=1}^{s} (b_i a_{ij} + b_j a_{ji}) k_j^T C k_i$$

$$\Rightarrow I_2 + I_3 = h^2 \sum_{i,j=1}^{s} \underbrace{(b_i b_j - b_i a_{ij} - b_j a_{ji})}_{= 0 \text{ by hypothesis}} k_j^T C k_i = \underline{\underline{0}}$$

$$\Rightarrow Q(y_1) = Q(y_0). \qquad \#$$

<u>Defn.:</u> (equivalent RK)

The stages $i \neq j$ of a RK method are equivalent if for all suff. smooth functions there exists $h_0 > 0$, s.t. $\forall h < h_0$ it holds: $k_i = k_j$.

<u>Defn.:</u> (irreducible RK)

A RK method is irreducible if it has no equivalent stages, reducible otherwise.

<u>Remark:</u> Cooper's condition is necessary for irreducible RK methods.

(without proof, advanced RK theory, RK can be too large, so can break the "necessary" condition).

(to show not iff condition in Cooper's thm)

Example: let α, β be real:

$$\begin{array}{c|cc} 1/2 & \alpha & 1/2-\alpha \\ 1/2 & \beta & 1/2-\beta \\ \hline & 1/2 & 1/2 \end{array} \qquad (*)$$

(existence thm for implicit methods ↳ unique soln)

$\Rightarrow$ If h small enough so that RK method is well-posed, then

$$k_1 = k_2 = k = f(y_0 + \tfrac{1}{2}k)$$

$\Rightarrow$ Method equivalent to $\begin{array}{c|c} \frac{1}{2} & 1/2 \\ \hline & 1 \end{array}$ (implicit midpoint rule)

$\Rightarrow$ conserves quadratic first integrals (Gauss method)

But the tableau $(*)$ does not satisfy Cooper's condition.

Rem.: Gauss methods are the only collocation (and discontinuous collocation) methods conserving quadratic first integrals. (proof requires advanced knowledge).

Partitioned RK

Consider $y \in \mathbb{R}^{d_1}$, $z \in \mathbb{R}^{d_2}$ solution of

$$\begin{cases} y' = f(y,z) \\ z' = g(y,z) \end{cases} \qquad \begin{array}{l} f: \mathbb{R}^{d_1 \times d_2} \to \mathbb{R}^{d_1} \\ g: \mathbb{R}^{d_1 \times d_2} \to \mathbb{R}^{d_2} \end{array}$$

We study a quadratic invariant of the form:

$$Q(y,z) = y^T D z, \qquad D \in \mathbb{R}^{d_1 \times d_2} \text{ matrix}$$

We have

$$\begin{aligned} Q(y+h_1, z+h_2) &= (y+h_1)^T D (z+h_2) \\ &= \underbrace{y^T D z}_{=Q(y,z)} + \underbrace{h_1^T D z + y^T D h_2}_{=Q'(y,z)(h_1,h_2)} + \underbrace{h_1^T D h_2}_{\text{higher order term}} \end{aligned}$$

$$\Rightarrow \quad Q'(y,z)(v,w) = v^T D z + y^T D w$$

Conserved if

$$Q'(y,z)\big(f(y,z), g(y,z)\big) = 0 \quad \forall y \in \mathbb{R}^{d_1}, z \in \mathbb{R}^{d_2}.$$

Rem: $Q'(y,z)(v,w) = Q(v,z) + Q(y,w)$.

Theorem: (Sun 1993)

If the coefficients of a PRK satisfy:

$$(*) \begin{cases} b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j & , \; i,j = 1,2,\dots,s \\ b_i = \hat{b}_i & , \; i = 1,2,\dots,s \end{cases} \qquad (*)$$

then the PRK conserves quadratic first integrals of the form $Q(y,z) = y^T D z$.

Proof: Exercises (same as Cooper, just compute).

Rem: (i) Condition $(*)$ is also necessary for irreducible PRK methods.

(ii) Störmer-Verlet conserves quadratic first integrals of the form $y^T D z$.

Theorem: The pair Lobatto IIIA + Lobatto IIIB conserves quadratic first integrals of the form

$$Q(y,z) = y^T D z .$$

Proof: Let $u(t), v(t)$ be the polynomials of Lobatto IIIA / B respectively.

$$Q(u(t_0+h), v(t_0+h)) - Q(u(t_0), v(t_0)) = \int_{t_0}^{t_0+h} \frac{d}{dt} Q(u(t), v(t))\, dt$$

$$= \int_{t_0}^{t_0+h} Q'(u(t), v(t))\,(u'(t), v'(t))\, dt$$

$$= h \int_0^1 Q'(u(t_0+rh), v(t_0+rh))\,(u'(t_0+rh), v'(t_0+rh))\, dr$$

$$= h \int_0^1 \underbrace{\underbrace{u'(t_0+rh)^T}_{\#s-1} D \underbrace{v(t_0+rh)}_{\#s-2} + \underbrace{u(t_0+rh)^T}_{\#s} D \underbrace{v'(t_0+rh)}_{\#s-3}}_{\#2s-3} dr$$

$$\overset{\text{QF order } 2s-2}{=} h \sum_{i=1}^{s} b_i\, Q'(u(t_0+c_i h), v(t_0+c_i h))\,(u'(t_0+c_i h), v'(t_0+c_i h))$$

for $i = 2, 3, \dots, s-1$
$$\begin{cases} u'(t_0+c_i h) = f(u(t_0+c_i h)) \\ v'(t_0+c_i h) = g(v(t_0+c_i h)) \end{cases}$$

$\Rightarrow$ elements $2, 3, \dots, s-1$ in the sum vanish $(=0)$.

$$\Rightarrow Q(u(t_0+h), v(t_0+h)) - Q(u(t_0), v(t_0))$$

$$= h b_1 Q'(u(t_0), v(t_0))\,(f(u(t_0), v(t_0)), v'(t_0))$$

$$+ h b_s Q'(u(t_0+h), v(t_0+h))\,(f(u(t_0+h), v(t_0+h)), v'(t_0+h))$$

Remarks:

(1) $Q'(y,z)(v,w) = v^T D z + y^T D w = Q(v,z) + Q(y,w)$

Since $Q'(y,z)(f(y,z), g(y,z)) = 0$

$\Rightarrow Q(f(y,z), z) = -Q(y, g(y,z))$

(2) $\forall\, \alpha, \beta \in \mathbb{R}$ (Q bilinear)

$Q(v, \alpha w + \beta z) = \alpha Q(v,w) + \beta Q(v,z)$

Applying (1) yields

$$Q(u(t_0+h), v(t_0+h)) - Q(u(t_0), v(t_0))$$

$$\overset{(1)}{=} h\, b_1\, Q(f(u(t_0), v(t_0)), v(t_0)) + h b_1\, Q(u(t_0), v'(t_0))$$

$$+ h\, b_s\, Q(f(u(t_0+h), v(t_0+h)), v(t_0+h)) + h b_s\, Q(u(t_0+h), v'(t_0+h))$$

$$\overset{(2)}{=} h\, b_1\, Q(u(t_0), \delta(t_0)) + h b_s\, Q(u(t_0+h), \delta(t_0+h))$$

with $\delta(t) = v'(t) - g(u(t), v(t))$.

<u>Remark:</u> $u(t_0) = y_0$ $\qquad v(t_0) = z_0 - h b_1 \delta(t_0)$

$u(t_0+h) = y_1$ $\qquad v(t_0+h) = z_1 + h b_s \delta(t_0+h)$

Hence, we can rewrite the LHS as:

$$Q(u(t_0+h), v(t_0+h)) - Q(u(t_0), v(t_0))$$

$$\overset{(2)}{=} Q(y_1, z_1) - Q(y_0, z_0) + h b_s\, Q(y_1, \delta(t_0+h)) + h b_1\, Q(y_0, \delta(t_0))$$

Thus, $\quad Q(y_1, z_1) - Q(y_0, z_0) = 0 \iff Q(y_1, z_1) = Q(y_0, z_0)$. #

Polynomial first integral of degree higher than two

<u>Theorem</u>: For $n \geq 3$, no consistent RK method can conserve all polynomial first integrals of degree n.

The proof of the theorem is split into four lemmas. The idea is finding a polynomial invariant that <u>cannot</u> be conserved by any RK method.

<u>Lemma 1</u>: (Abel – Liouville – Jacobi – Ostrogradaski identity)

Consider $\begin{cases} Y' = AY \\ Y(0) = Y_0 \end{cases}$, $A, Y \in \mathbb{R}^{n \times n}$ and $g(Y) = \det(Y)$

Then $g'(Y)(AY) = \operatorname{trace}(A) \cdot \det(Y)$.

<u>Proof</u>: Let $f: \mathbb{R} \to \mathbb{R}$

$\varepsilon \mapsto f(\varepsilon) = g(Y + \varepsilon AY)$.

Observe that
- $f(0) = g(Y) = \det(Y)$
- $f'(\varepsilon) = g'(Y + \varepsilon AY)(AY)$
- $f'(0) = g'(Y)(AY)$.

<u>Idea</u>: find another way to derivate $f(\varepsilon)$

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We have

$$f(\varepsilon) = g(Y + \varepsilon AY) = \det(Y + \varepsilon AY) = \det((I + \varepsilon A)Y)$$
$$= \det(I + \varepsilon A)\det(Y)$$
$$= (1 + \varepsilon\, \mathrm{trace}(A) + O(\varepsilon^2))\overbrace{\det(Y)}^{= f(0)}$$

$$\Rightarrow f'(0) = \lim_{\varepsilon \to 0} \frac{f(\varepsilon) - f(0)}{\varepsilon} = \mathrm{trace}(A) f(0)$$
$$= \mathrm{trace}(A)\det(Y).$$

#

Lemma 2: Consider $Y' = AY$ with $\mathrm{trace}(A) = 0$.
Then $\det(Y)$ is a first integral of the system.

Proof: By lemma 1 calling $g(Y) = \det(Y)$:
$$g'(Y)(AY) = \mathrm{trace}(A)\det(Y) = 0.$$

#

Lemma 3: (Feng Kang and Shang Zai-jin 1995)

let $R(z)$ be analytic (fct) in a complex neighbourhood of zero.
Assume that $R(0) = R'(0) = 1$.
Then for $n \geq 3$, we have

$$\det(R(A)) = 1 \quad \forall\, A \in \mathbb{R}^{n\times n} \text{ s.t. } \mathrm{trace}(A) = 0$$

$$\Leftrightarrow \quad R(z) = e^z.$$

Proof: $\Leftarrow$:
① let $R(z) = e^z$.
Consider $\begin{cases} Y' = AY \\ Y(0) = I \end{cases}$ with $\mathrm{trace}(A) = 0$.

Then, by lemma 2, $\det(Y(t)) = \det(I) = 1 \quad \forall t \geq 0$.
Moreover, we know that
$$Y(t) = e^{tA} = R(tA).$$
Hence, in $t = 1$, $1 = \det(Y(1)) = \det(R(A))$.

② $\Rightarrow$: let R be an analytic fct with $R(0) = R'(0) = 1$ and s.t. $\det(R(A)) = 1 \quad \forall\, A \in \mathbb{R}^{n\times n}$, $\mathrm{trace}(A) = 0$.
$\overset{?}{\Rightarrow} \quad R(z) = e^z$.

let $\mu, \nu \in \mathbb{R}$ in a neighbourhood of zero.
Consider
$$A = \begin{pmatrix} \mu & & & & \\ & \nu & & & \\ & & -(\mu+\nu) & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix} \in \mathbb{R}^{n\times n}, \quad \mathrm{trace}(A) = 0.$$

$$R(A) \underset{\substack{\uparrow \\ A \text{ diagonal}}}{=} \begin{pmatrix} R(\mu) & & & & \\ & R(\nu) & & & \\ & & R(-(\mu+\nu)) & & \\ & & & R(0) & \\ & & & & \ddots \\ & & & & & R(0) \end{pmatrix} \quad \text{with } R(0) = 1.$$

$\Rightarrow \det(R(A)) = R(\mu)\cdot R(\nu)\cdot R(-(\mu+\nu)) = 1$ by hypothesis.

Fix $\nu = 0$

$$1 = R(\mu) \cdot \overbrace{R(0)}^{=1} \cdot R(-\mu) \Rightarrow R(\mu)^{-1} = R(-\mu).$$

Therefore,

$$1 = R(\mu) \cdot R(\nu) \cdot R(\mu+\nu)^{-1} \Rightarrow R(\mu) \cdot R(\nu) = R(\mu+\nu)$$

Derivate wrt ν

$$\Rightarrow R'(\nu)\, R(\mu) = R'(\mu+\nu)$$

Evaluate at $\nu = 0$

$$\Rightarrow \underbrace{R'(0)}_{=1} R(\mu) = R'(\mu)$$

$$\Rightarrow \begin{cases} R'(\mu) = R(\mu) \\ R(0) = 1 \end{cases} \text{ODE} \Rightarrow R(\mu) = e^{\mu}$$

#

<u>Lemma 4</u>: Consider a s-stage consistent RK method applied to $y' = Ay$.

Then $y_1 \overset{\text{(after one step)}}{=} R(hA)\, y_0$, where $R(z) = \dfrac{P(z)}{Q(z)}$ with P, Q polyn. of degree $\leq s$ and s.t. $R(0) = R'(0) = 1$.

<u>Proof</u>: See later (Chapter III).

<u>Examples</u>: Explicit Euler: $y_1 = y_0 + hAy_0 \Rightarrow R(z) = 1 + z$

Proof of the theorem: (Ad absurdum)

Consider $\begin{cases} Y' = AY \\ Y_0 = I \end{cases}$, trace$(A) = 0$.

By lemma 2, $\det(Y(t)) = 1$.

From lemma 4, we have $Y_1 = R(hA)Y_0$ with R a rational fct s.t. $R(0) = R'(0) = 1$.

Assume that the RK method conserves $\det(Y)$:

$$\det(Y_1) = \det(R(hA)) = \det(Y_0) = 1.$$

Since $R(0) = R'(0) = 1$, then by lemma 3 it follows that

$R(z) = e^z$, which contradicts $R(z) = \frac{P(z)}{Q(z)}$. #