NIDS Session 6

$\boxed{1}$ Given a RK method with coefficients satisfying

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \quad (*)$$

Let's show that under condition (*) it preserves invariants of the form

$$I(y(t)) = y(t)^T C y(t) + d^T y(t) + e$$

$$C \in \mathbb{R}^{m \times m}, \quad d \in \mathbb{R}^m, \quad e \in \mathbb{R}$$

$$I(y) = I_2(y) + I_1(y) + I_0(y)$$

$$I_2(y(t)) = y(t)^T C y(t) \quad (\text{quadratic})$$

$$I_1(y(t)) = d^T y(t) \quad (\text{linear})$$

$$I_0(y(t)) = e \quad (\text{constant})$$

A RK method preserves constant (obviously) invariants, linear ones (see course), and quadratic ones under condition (*)

$$I(y_1) = I_2(y_1) + I_1(y_1) + I_0(y_1)$$
$$= I_2(y_0) + I_1(y_0) + I_0(y_0) = I(y_0)$$

2 Consider the partitioned system

$$\left.\begin{aligned} \dot y(t) &= f(y(t), z(t)) \\ \dot z(t) &= g(y(t), z(t)) \end{aligned}\right\} \quad (2)$$

Symplectic Euler $\qquad Q(y,z) = y^T D z$ is invariant

$$y_1 = y_0 + h k_1 \quad \text{where} \quad k_1 = f(y_0 + h k_1, z_0) \qquad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} + \begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

$$z_1 = z_0 + h l_1 \quad \text{where} \quad l_1 = g(y_0 + h k_1, z_0)$$

Q is a first integral $\Rightarrow Q'(y,z)\begin{pmatrix} f \\ g \end{pmatrix} = 0$

$$\Leftrightarrow \underbrace{f(y,z)^T D z + y^T D g(y,z)} = 0$$

$$Q(y_1, z_1) = (y_0 + h k_1)^T D (z_0 + h l_1)$$

$$= y_0^T D z_0 + h\Big(\underbrace{k_1^T D z_0 + (\overbrace{y_0 + h k_1}^{=y_1})^T D l_1}_{f(y_1,z_0)^T D z_0 + y_1^T D g(y_1,z_0) = 0}\Big) \qquad k_1 = f(y_1, z_0), \quad l_1 = g(y_1, z_0)$$

$$= Q(y_0, z_0)$$

3 Back to the partitioned system (2) with the same invariant $Q(y(t), z(t)) = y(t)^T D z(t)$

$$\frac{d}{dt} Q(y(t), z(t)) = f(y(t), z(t))^T D z(t) + y(t)^T D g(y(t), z(t)) = 0$$

Let's consider a general partitioned RK method:

$$k_i = f(g_i, \hat{g}_i)$$

$$\hat{k}_i = g(g_i, \hat{g}_i)$$

where
$$g_i = y_0 + h \sum_{j=1}^{s} a_{ij} k_j$$
$$\hat{g}_i = p_0 + h \sum_{j=1}^{s} \hat{a}_{ij} \hat{k}_j$$

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i$$
$$p_1 = p_0 + h \sum_{i=1}^{s} \hat{b}_i \hat{k}_i$$

We compute

$$Q(y_1, p_1) - Q(y_0, p_0)$$
$$= \left(y_0 + h \sum_{i=1}^{s} b_i k_i\right)^T D \left(p_0 + h \sum_{i=1}^{s} \hat{b}_i \hat{k}_i\right) - y_0^T D p_0$$
$$= h\left(\sum_{i=1}^{s} \hat{b}_i \, y_0^T D \hat{k}_i + b_i k_i^T D p_0\right) + h^2 \sum_{i,j=1}^{s} b_i \hat{b}_j k_i^T D \hat{k}_j \quad (3)$$

Write $y_0 = g_i - h \sum_{j=1}^{s} a_{ij} k_j$ and substitute
$p_0 = \hat{g}_i - h \sum_{j=1}^{s} \hat{a}_{ij} \hat{k}_j$ in (3)

and we eventually obtain

$$h \sum_{i=1}^{s} \left(\hat{b}_i g_i^T D \hat{k}_i + b_i k_i^T D \hat{g}_i \right)$$

$$+ h^2 \sum_{i,j=1}^{s} \left(b_i \hat{b}_j - \hat{b}_j a_{ji} - b_i \hat{a}_{ij} \right) k_i^T D \hat{k}_j$$

And now we use our conditions:

$$\begin{cases} b_i = \hat{b}_i & (1)' \\ b_i a_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j & (2)' \end{cases}$$

From (2)', the second term vanishes and thanks to (1)',

$$Q(y_1, p_1) - Q(y_0, p_0)$$

$$= h \sum_{i=1}^{s} b_i \underbrace{\left(g_i^T D \hat{k}_i + k_i^T D \hat{g}_i \right)}_{g_i^T D\, g(g_i, \hat{g}_i) + f(g_i, \hat{g}_i)^T D \hat{g}_i \,=\, 0}$$

$\Rightarrow \quad Q(q_1, p_1) = Q(q_0, p_0)$

$\boxed{4}$ Consider the RK methods defined by

$\{(b_i, a_{ij})\}$ and $\{(\hat{b}_i, \hat{a}_{ij})\}$

An irreducible RK method is such that

$$k_i \neq k_j \qquad i \neq j$$

for h small enough ($\exists\, h_0 > 0$ such that this is satisfied for all $h < h_0$)

Recall that if the RK method is irreducible, then the Cooper conditions are satisfied.

Since both methods are assumed irreducible, then

$$\begin{cases} b_i a_{ij} + b_j a_{ji} = b_i b_j & i, j = 1 \dots s \\ \hat{b}_i \hat{a}_{ij} + \hat{b}_j \hat{a}_{ji} = \hat{b}_i \hat{b}_j & i, j = 1 \dots s \end{cases}$$

are satisfied. Consequently, from the lecture both methods preserve quadratic first integrals i.e. $Q_C(q) = q^T C q$ and $Q_E(\beta) = \beta^T E \beta$

$(C \in \mathbb{R}^{n \times n}, \ E \in \mathbb{R}^{m \times m})$

$Q_C(q) = Q(q, 0) = Q(y_0, 0) = Q_C(q_0)$

(similarly for $Q_E(\beta)$)

(ii) Recall that a partitioned RK is reducible if

$$k_i = k_j \quad i \neq j \quad \text{and} \quad \hat{k}_i = \hat{k}_j \quad i \neq j$$

By assumption our RK methods are irreducible, meaning

$$k_i \neq k_j \quad i \neq j \quad \text{and} \quad \hat{k}_i \neq \hat{k}_j \quad i \neq j$$

Consequently, the partitioned RK method is irreducible and thus the Cooper condition for the partitioned RK method is satisfied.

(iii)

Combine
$$\begin{cases} b_i a_{ij} + b_j a_{ji} = b_i b_j & (1) \\ b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j & (2) \end{cases}$$

Since $b_i = \hat{b}_i$, $(1) - (2) \Rightarrow b_i a_{ij} = b_i \hat{a}_{ij}$

iv) Let's define

$$\beta = \{ i : b_i = 0 \}$$ and its complement

$$\beta^c = \{ i : b_i \neq 0 \}$$

$$g_1 = g_0 + h\sum_{i=1}^{s} b_i k_i$$

$$\hat{g}_1 = g_0 + h\sum_{i=1}^{s} \hat{b}_i \hat{k}_i$$

$$g_1 - \hat{g}_1 = h\sum_{i\in\beta^c} b_i (k_i - \hat{k}_i)$$

$$k_i = f\Big(g_0 + h\sum_{j=1}^{s} a_{ij} k_j\Big) \quad (1) \qquad i \in \beta^c$$

$$\hat{k}_i = f\Big(g_0 + h\sum_{j=1}^{s} \hat{a}_{ij} \hat{k}_j\Big) \quad (2) \qquad i \in \beta^c$$

From iii) $\quad b_i a_{ij} = b_i \hat{a}_{ij}$

For $i \in \beta^c$ $(b_i \neq 0)$

$$\Rightarrow \quad a_{ij} = \hat{a}_{ij} \qquad j = 1, \ldots, s$$

Substituting this in (2)

$$k_i = f\left(q_0 + h \sum_{j=1}^{n} a_{ij} k_j\right) \quad (3)$$

$$\hat{k}_i = f\left(q_0 + h \sum_{j=1}^{n} \hat{a}_{ij} \hat{k}_j\right) \quad (4)$$

take $i \in B^c$ and $j \in B$, then

$$\underbrace{b_i}_{\neq 0} a_{ij} + \underbrace{b_j}_{=0} a_{ji} = \underbrace{b_i b_j}_{=0}$$

$$\Rightarrow \quad b_i a_{ij} = 0 \quad \Rightarrow \quad a_{ij} = 0 \quad (\text{because } b_i \neq 0)$$

(Similarly $\hat{a}_{ij} = 0 \quad i \in B^c, \; j \in B$)

Substituting in (3) and (4)

$$k_i = f\left(q_0 + h \sum_{j \in B^c} a_{ij} k_j\right) \quad (5)$$

$$\hat{k}_i = f\left(q_0 + h \sum_{j \in B^c} a_{ij} \hat{k}_j\right)$$

If h is small enough, the solution to (5) is unique $\Rightarrow \quad k_i = \hat{k}_i \quad i \in B^c$

Hence $y_1 - \hat{y}_1 = h \sum c_i (k_i - \hat{k}_i) = 0$

$$\Rightarrow \quad y_1 = \hat{y}_1$$

$\boxed{5}$ Let's consider the matrix differential equation

$$L'(t) = [B(L), L] \quad , \quad L(0) = L_0 \qquad (1)$$

where $[X, Y] = XY - YX$

- L_0 symmetric
- $L(t), \ B(L) \in \mathbb{R}^{d \times d}$
- $B(L)$ is skew symmetric

We define the auxiliary problem

$$\begin{cases} U'(t) = B(L)\, U(t) \\ U(0) = I_d \end{cases} \qquad (2)$$

i) From the last exercise set, since $B(L)$ is skew symmetric, then

$$I(U(t)) = U(t)^T U(t) \text{ is a first integral}$$

$$\Rightarrow \quad I(U(t)) = I(U(0)) = U(0)^T U(0) = I_d$$

$$\Rightarrow \quad U(t)^T U(t) = I_d \text{ and } U(t) \text{ is orthogonal}$$

ii) Again, we would use Gauss methods since in particular they preserve quadratic invariants and thus orthogonality

iii) Let's verify that $L(t) = U(t) L_0 U(t)^T$ is a solution of (7)

$$L'(t) = U'(t) L_0 U(t)^T + U(t) L_0 U(t)'^T$$

$$= B(L(t)) \underbrace{U(t) L_0 U(t)^T}_{L(t)} + U(t) L_0 U(t)^T B(L(t))^T$$

$$= B(L(t)) L(t) - L(t) B(L(t))$$

$$= [B(L(t)), L(t)]$$

$$L(0) = U(0) L_0 U(0)^T = L_0$$

So $L(t) = U(t) L_0 U(t)^T$ satisfies (7)

Moreover:

$$L(t)^T = U(t) L_0^T U(t)^T = U(t) L_0 U(t)^T$$
$$= L(t)$$

$L(t)$ is symmetric

iv/ $L(t) = U(t) L_0 U(t)^T$ is an orthogonal similarity transformation

Reminder: Two matrices $A, B \in M_n(K)$ (K is a field) are called similar $\exists\, P \in M_n(K)$ invertible such that $B = PAP^{-1}$

They are called orthogonaly similar if $P^{-1} = P^T$

Similar matrices have the same spectrum:

Indeed

$$
\begin{aligned}
p_B(\lambda) = \det(B - \lambda I) &= \det(PAP^{-1} - \lambda I) \\
&= \det(PAP^{-1} - \lambda PP^{-1}) \\
&= \det(P)\det(A - \lambda I)\det(P^{-1}) \\
&= \det(A - \lambda I) = p_A(\lambda)
\end{aligned}
$$

because $\det(P^{-1}) = \det(P)^{-1}$

Consequently $L(t)$ and L_0 have the same characteristic polynomial (and therefore the same spectrum)

Since L_0 does not depend on time, neither do its eigenvalues!

v) By definition $L_{n+1} = U_1^n L_n U_1^{n\,T}$

If U_1^n is orthogonal, L_{n+1} and L_n are (orthogonaly) similar and therefore share the same spectrum (see the reminder)

In particular, your methods preserve the orthogonality.