Series 6

Exercise 1. Show that if the coefficients of a Runge–Kutta method satisfy $b_i a_{ij} + b_j a_{ji} = b_i b_j$ for $i, j = 1, \ldots, s$, then the method conserves all invariants of the form $I(y) = y^\top C y + d^\top y + e$, where $C \in \mathbb{R}^{n \times n}$, $d \in \mathbb{R}^n$ and $e \in \mathbb{R}$.

Exercise 2. Consider the partitioned system

$$\dot{y} = f(y, z), \qquad \dot{z} = g(y, z), \tag{1}$$

where $y(t) \in \mathbb{R}^n$ and $z(t) \in \mathbb{R}^m$. Without using the Cooper theorem proved in Exercise 3, show that the symplectic Euler method conserves all quadratic invariants of the form $Q(y, z) = y^\top D z$, where $D \in \mathbb{R}^{n \times m}$.

Exercise 3. (Cooper theorem for partitioned RK methods) Consider the partitioned system (1). Show that if the coefficients of a partitioned Runge–Kutta method satisfy

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

then the method conserves all quadratic invariants of the form $Q(y, z) = y^\top D z$, where $D \in \mathbb{R}^{n \times m}$.

Exercise 4. Consider the partitioned system (1) and let $\left\{ \{b_i, a_{ij}\}, \{\hat{b}_i, \hat{a}_{ij}\} \right\}$ be a partitioned method which conserves all quadratic invariants of the form

$$Q(y, z) = y^\top C y + 2 y^\top D z + z^\top E z,$$

where $C \in \mathbb{R}^{n \times n}$, $D \in \mathbb{R}^{n \times m}$, $E \in \mathbb{R}^{m \times m}$. Moreover, let both methods $\{b_i, a_{ij}\}$ and $\{\hat{b}_i, \hat{a}_{ij}\}$ be irreducible.

i) Prove that $\{b_i, a_{ij}\}$ conserves quadratic invariants of the form $Q_C(y) = y^\top C y$ and $\{\hat{b}_i, \hat{a}_{ij}\}$ conserves quadratic invariants of the form $Q_E(z) = z^\top E z$ and deduce that

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

ii) Prove that the partitioned method $\left\{ \{b_i, a_{ij}\}, \{\hat{b}_i, \hat{a}_{ij}\} \right\}$ is irreducible and deduce that

$$\begin{aligned} b_i \hat{a}_{ij} + \hat{b}_j a_{ji} &= b_i b_j, \quad i, j = 1, \ldots, s, \\ b_i &= \hat{b}_i, \qquad i = 1, \ldots, s. \end{aligned}$$

iii) Combining points *i)* and *ii)*, show that

$$b_i a_{ij} = b_i \hat{a}_{ij}, \quad i, j = 1, \ldots, s.$$

iv) Using point *iii)*, prove that the Runge–Kutta methods $\{b_i, a_{ij}\}$ and $\{\hat{b}_i, \hat{a}_{ij}\}$ define the same numerical scheme, i.e., that $y_1 = \hat{y}_1$.
Hint: split the indices $i = 1, \ldots, s$ in two sets depending on whether $b_i = 0$ or $b_i \neq 0$.

Exercise 5. (Isospectral flows and isospectral methods) Consider the matrix differential equation

$$L' = [B(L), L], \qquad L(0) = L_0, \tag{2}$$

where $L \in \mathbb{R}^{d\times d}$, $L_0 \in \mathbb{R}^{d\times d}$ is symmetric, $B(L) \in \mathbb{R}^{d\times d}$ is skew-symmetric for all L and $[B, L] = BL - LB$ is the commutator between B and L.

i) Define the problem

$$U' = B(L)U, \qquad U(0) = I_d,$$

where $U \in \mathbb{R}^{d\times d}$ and deduce that $U(t)$ is orthogonal for all $t \geq 0$.

ii) Which Runge–Kutta method would you use to approximate $U_1 \approx U(h)$ in order to conserve the orthogonality?

iii) Show that $L(t) = U(t)L_0U(t)^\top$ and deduce that $L(t)$ is symmetric for all $t \geq 0$.

iv) Prove that the characteristic polynomial $\det(L(t) - \lambda I)$ is constant in time and deduce that the eigenvalues of $L(t)$ are constant in time as well.

It follows that the characteristic polynomial $\det(L(t)-\lambda I) = \sum_{k=0}^{d} \alpha_k(t)\lambda^k$ is invariant, hence its coefficients $\alpha_k(t)$ are independent of t. The coefficients are polynomial invariants as $\alpha_0 = \det L$, $\alpha_{d-1} = (-1)^{d-1}\mathrm{trace}\, L$, etc. For $d \geq 3$, this is a higher-order invariant and there is no hope for a Runge–Kutta method to automatically conserve it, hence the eigenvalues neither. In the remaining of this exercise we derive isospectral methods, which conserve the eigenvalues of $L(t)$ (Calvo, Iserles & Zanna, 1999). Assume that L_n, an approximation of $L(t_n)$, is known. Solve numerically the problem

$$U' = B(UL_nU^T)U, \qquad U(0) = I, \tag{3}$$

from $t = 0$ to $t = h$ and denote its solution by U_1^n. Then set $L_{n+1} = U_1^n L_n (U_1^n)^T$ for obtaining an approximation of $L(t_{n+1})$.

v) Explain why, choosing the right numerical method to solve (3), the spectra of L_n and L_{n+1} are equivalent.

We consider now a particular case of (2), the Toda lattice, which represents a system of particles on a line interacting pairwise with exponential forces. The system is Hamiltonian and after a change of variables it can be written as (2) where

$$L_0 = \begin{pmatrix} a_1 & b_1 & & & & b_d \\ b_1 & a_2 & b_2 & & & \\ & b_2 & a_3 & b_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & b_{d-2} & a_{d-1} & b_{d-1} \\ b_d & & & & b_{d-1} & a_d \end{pmatrix}$$

with zeros everywhere else and $B(L) = L_+ - L_-$, where L_+ denotes the part of L strictly above the diagonal and L_- the part of L strictly below the diagonal.

vi) Fix the dimension $d = 10$, the values $a_i = b_i = i/d$ for $i = 1, \dots, d$, the step size $h = 1$ and the final time $T = 100$. Solve numerically equation (2) using the implicit midpoint rule and verify that the eigenvalues of L are not conserved. Then, apply the isospectral method using the implicit midpoint rule to solve (3) and verify that the eigenvalues of L are now conserved up to machine precision, i.e., $\sim 10^{-16}$.