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Using neural networks for the derivation of Runge–Kutta–Nyström pairs for integration of orbits

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ABSTRACT

In this paper we present Runge–Kutta–Nyström (RKN) pairs of orders 4(3) and 6(4). We choose a test orbit from the Kepler problem to integrate for a specific tolerance. Then we train the free parameters of the above RKN4(3) and RKN6(4) families to perform optimally. For that we form a neural network approach and minimize its objective function using a differential evolution optimization technique. Finally we observe that the produced pairs outperform standard pairs from the literature for Pleiades orbits and Kepler problem over a wide range of eccentricities and tolerances.

1. Introduction

Explicit Runge–Kutta–Nyström pairs are widely used for the numerical solution of the initial value problem

$$y'' = f(x, y), \quad y(x_0) = y_0 \in \mathbb{R}^m, \quad y'(x_0) = y'_0 \in \mathbb{R}^m, \quad x \in [x_0, x_e]$$

where $f : \mathbb{R} \times \mathbb{R}^m \mapsto \mathbb{R}^m$. We usually use the extended Butcher tableau Butcher, 1987 of the method's coefficients:

$$\begin{array}{c|c} c & A \\ \hline & b, b' \\ & \hat{b}, \hat{b}' \end{array}$$

to present the RKN pair. In such a tableau b^T, $\hat{b}^T$, b'^T, $\hat{b}'^T$, $c \in \mathbb{R}^s$ and $A \in \mathbb{R}^{s\times s}$ is strictly lower triangular.

Such a method implementing the following formulae:

$$y_{n+1} = y_n + h_n y'_n + h_n^2 \sum_{i=1}^{s} b_i f_{ni}$$

and

$$\hat{y}_{n+1} = y_n + h_n y'_n + h_n^2 \sum_{i=1}^{s} \hat{b}_i f_{ni}$$

advances the solution from x_n to $x_{n+1} = x_n + h_n$ computing at each step approximations y_{n+1}, $\hat{y}_{n+1}$ to $y(x_{n+1})$ of orders p and $p-1$ respectively.

It also produces two approximations y'_{n+1}, $\hat{y}'_{n+1}$ to $y'(x_{n+1})$ of orders p and $p-1$, given by

$$y'_{n+1} = y'_n + h_n \sum_{i=1}^{s} b'_i f_{ni}$$

and

$$\hat{y}'_{n+1} = y'_n + h_n \sum_{i=1}^{s} \hat{b}'_i f_{ni}.$$

Here

$$f_{ni} = f\left(x_n + c_i h_n, y_n + h_n \sum_{j=1}^{i-1} a_{ij} f_{nj}\right) \in \mathbb{R}^m$$

for $i = 1, 2, \ldots, s \geqslant p$. These embedded form methods (called RKN$p(p-1)$) are implemented with variable step-sizes as we can obtain an estimate

$$u_{n+1} = \max\left(\|y_{n+1} - \hat{y}_{n+1}\|_\infty, \|y'_{n+1} - \hat{y}'_{n+1}\|_\infty\right)$$

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of the local truncation error of the $p-1$ order formula. If this error estimation is grater than a requested tolerance TOL it is common to apply the step-size control algorithm

$$h_{n+1} = 0.9h_n \cdot \left(\frac{\mathrm{TOL}}{u_{n+1}}\right)^{1/p}$$

to compute the next step-size. If it is not, we use the same formula to recompute the current step. See Tsitouras and Papakostas, 1999 for more details on the implementation of these type of step size policies.

2. Derivation of the RKN pairs

The derivation of better RKN pairs is of continued interest the last $30-40$ years, see Tsitouras and Famelis, 2009 and references therein. The main framework for the construction of RKN pairs is matching Taylor series expansions of $y(x+h)-y_{n+1}$ and $y'(x+h)-y'_{n+1}$ after we have expanded the various f_{ni}'s.

2.1. RKN4(3) pairs

A pair of orders four and three as the one that interests us has to satisfy the following equations of condition:

$$b'e = 1, \quad b'c = \frac{1}{2}, \quad b'c^2 = \frac{1}{3}, \quad b'c^3 = \frac{1}{4} \quad \text{and} \quad b'Ac = \frac{1}{24} \tag{1}$$

when we set

$$Ae = \frac{c^2}{2} \tag{2}$$

and

$$b = b'(e-c) \tag{3}$$

with $e = [1,\ 1 \cdots 1]^T \in \mathbb{R}^s$.

Here we consider the family of Dormand et al. (1987) that needs four stages per step ($s = 4$). This family uses FSAL (First Stage As Last) device so it effectively needs only three stages per step. FSAL demands $c_4 = 1$ and $a_{4i} = b_i$, $i = 1,2,3$. Thus the parameters available for fulfilling the above mentioned five equations of condition are: $c_2,\ c_3,\ b'_1,\ b_2,\ b'_3,\ b'_4$ and a_{32}. Two of them are free to choose, namely c_2, and c_3. The simplifying assumptions define all the other coefficients..

Similarly, for the coefficients of the lower order formulas after choosing a $\hat{b}'_4$ we solve

$$\hat{b}'e = 1, \quad \hat{b}'c = \frac{1}{2}, \quad \hat{b}'c^2 = \frac{1}{3}$$

for $\hat{b}'_1,\ \hat{b}'_2,\ \hat{b}'_3$.

Finally, we set $\hat{b}_3 = 0.15$ and $\hat{b}_4 = -1/20$ and solve

$$\hat{b} \cdot e = \frac{1}{2} \quad \text{and} \quad \hat{b} \cdot c = \frac{1}{6}$$

for $\hat{b}_i,\ i = 1,2$. The fixed coefficients for the lower order formulas affect mainly the step size. For example, smaller values may produce smaller estimations for the error and in consequence this is equivalent to using more lax tolerances. So for reasons of comparison we use the ones chosen in Dormand et al. (1987).

When we solve all the equations we conclude to the following expressions with respect to c_2 and c_3 (Tsitouras, 2008):

$$a_{21} = \frac{c_2^2}{2}, \quad a_{31} = \frac{\left(c_3\left(c_2^2(1-12c_3) + 6c_2^3c_3 - c_3^2 + 3c_2c_3(1+c_3)\right)\right)}{(6c_2(1-3c_2+2c_2^2))},$$

$$a_{32} = \frac{((c_2-c_3)c_3(-c_3+c_2(-1+3c_3)))}{(6c_2(1-3c_2+2c_2^2))},$$

$$a_{41} = \frac{(1-2c_2-2c_3+6c_2c_3)}{(12c_2c_3)},$$

$$a_{42} = \frac{(1-2c_3)}{(12c_2^2-12c_2c_3)},$$

$$a_{43} = \frac{(-1+2c_2)}{(12(c_2-c_3)c_3)},$$

$$b'_1 = \frac{(1-2c_2-2c_3+6c_2c_3)}{(12c_2c_3)},$$

$$b'_2 = \frac{(-1+2c_3)}{(12c_2(c_2^2+c_3-c_2(1+c_3)))},$$

$$b'_3 = \frac{(1-2c_2)}{(12(c_2-c_3)(-1+c_3)c_3)},$$

$$b'_4 = \frac{(3-4c_3+c_2(-4+6c_3))}{(12(-1+c_2)(-1+c_3))},$$

$$\hat{b}_1 = \frac{-13+24c_2+9c_3}{60c_2},$$

$$\hat{b}_2 = \frac{13-9c_3}{60c_2}, \quad \hat{b}'_1 = \frac{4-5c_2-5c_3+8c_2c_3}{6c_2c_3},$$

$$\hat{b}'_2 = \frac{4-5c_3}{6c_2^2-6c_2c_3}, \quad \hat{b}'_3 = -\frac{4-5c_2}{6c_2c_3-6c_3^2}.$$

2.2. RKN6(4) pairs

For the derivation of such type of pairs we need to solve more equations of condition along with those in Eq. (1). If assumptions (2 and 3) hold, to satisfy algebraic order five the additional conditions are:

$$b'c^4 = \frac{1}{5}, \quad b'Ac^2 = \frac{1}{60}, \quad b'cAc = \frac{1}{30}$$

and

$$b'c^5 = \frac{1}{6}, \quad b'Ac^3 = \frac{1}{120}, \quad b'A^2c = \frac{1}{720},$$

$$b'cAc^2 = \frac{1}{72}, \quad b'c^2Ac = \frac{1}{36}$$

to satisfy algebraic order six.

We consider again the family studied in Dormand et al. (1987, 1999) that needs six stages per step ($s = 6$). This family also uses FSAL device so it effectively needs only five stages per step. FSAL device enforces $c_6 = 1$ and $a_{6i} = b_i$, $i = 1,2,\ldots,5$. Among the parameters available for fulfilling the above mentioned equations of condition, we choose c_2, c_3, and c_4 freely. All the other coefficients are defined by the conditions and the simplifying assumptions. More details and the algorithm are given in Papakostas and Tsitouras (1999).

The lower order weights have to satisfy

$$\hat{b}'e = 1, \quad \hat{b}'c = \frac{1}{2}, \quad \hat{b}'c^2 = \frac{1}{3}, \quad \hat{b}'c^3 = \frac{1}{4} \quad \text{and} \quad \hat{b}'Ac = \frac{1}{24}.$$

These are five linear equations with six unknowns. We set $\hat{b}'_5 = -\frac{2}{5}$ (Dormand et al., 1987) and $\hat{b}'_6 = b'_6$ and solve four of the above equations for $\hat{b}'_1,\ \hat{b}'_2,\ \hat{b}'_3,\ \hat{b}'_4$ while we choose the remaining as in Dormand et al. (1987). We finally derive the coefficients of the vector $\hat{b}$ using the assumption $\hat{b} = \hat{b}'(e-c)$.

2.3. On the derivation of the pairs

The main question raising now is how to select the free parameters, i.e. c_2 and c_3 for the 4(3) pair and c_2,c_3, and c_4 for the 6(4) pair. For a p-order RKN method, the minimization of the $p+1$ order term in the truncation error expansion seems the best choice for the solution of a general problem. This technique does not consider the nature of each specific problem we want solved. Thus many