Symplectic Runge-Kutta methods satisfying effective order conditions

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11–15 July, 2011

International Conference on Scientific Computation and Differential equations (SciCADE 2011)

University of Toronto, Canada

Introduction

1. The idea of effective order was first introduced by Butcher in 1969 for explicit Runge–Kutta methods as a mean of overcoming the 5^{th} order 5 stage barrier.
2. This was extended to Singly Implicit Runge–Kutta methods by Butcher and Chartier in 1997.
3. The idea was later used for Diagonally Extended Singly Implicit Runge–Kutta methods by Butcher and Diamantakis in 1998 and by Butcher and Chen in 2000 .
4. The accuracy of symplectic integrators for Hamiltonian systems was enhanced using effective order by M A Lopéz-Marcos, J M Sanz-Serna and R D Skeel in 1996.

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The purpose of this presentation is to develop some special symplectic effective order methods with low implementation costs.

Differential Equations with Invariants

Consider an initial value problem

$$y'(x) = f(y(x)), \qquad y(x_0) = y_0. \tag{1}$$

Suppose $Q(y) = y^T M y$ is a quadratic invariant , that is

$$Q'(y)f(y) = 0,$$

or

$$y^T M f(y) = 0.$$

Methods which conserve quadratic invariants are said to be "Canonical" or "Symplectic".

Outline

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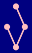
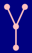
Algebraic interpretation

1. We introduce an algebraic system which represents indvidual Runge–Kutta methods and also composition of methods.
2. This centres on the meaning of order for Runge–Kutta methods and leads to the possible generalisation to the "effective order".
3. We introduce a group G whose elements are mapping from T (rooted –trees) to real numbers and where the group operation is defined according to the algebraic theory of Runge–Kutta methods or to the theory of B–series.
4. Members of G represents Runge–Kutta methods with E representing the exact solution. That is, $E : T \to \mathbb{R}$ is defined by

$$E(t) = \frac{1}{\gamma(t)}, \quad \forall t$$

Table: Group Operation

t	$r(t)$	$\alpha(t)$	$\beta(t)$	$(\alpha\beta)(t)$	$E(t)$
	1	α_1	β_1	$\alpha_1\beta_0 + \beta_1$	1
	2	α_2	β_2	$\alpha_2\beta_0 + \beta_2 + \alpha_1\beta_1$	$\frac{1}{2}$
	3	α_3	β_3	$\alpha_3\beta_0 + \beta_3 + \alpha_1^2\beta_1 + 2\alpha_1\beta_2$	$\frac{1}{3}$
	3	α_4	β_4	$\alpha_4\beta_0 + \beta_4 + \alpha_1\beta_2 + \alpha_2\beta_1$	$\frac{1}{6}$
	4	α_5	β_5	$\alpha_5\beta_0 + \beta_5 + 3\alpha_1\beta_3 + \alpha_1^2\beta_1 + \alpha_1^3\beta_1$	$\frac{1}{4}$
	4	α_6	β_6	$\alpha_6\beta_0 + \beta_6 + \alpha_1\beta_4 + \alpha_1\beta_3 +$ $\alpha_1^2\beta_2 + \alpha_2\beta_2 + \alpha_1\alpha_2\beta_1$	$\frac{1}{8}$
	4	α_7	β_7	$\alpha_7\beta_0 + \beta_7 + 2\alpha_1\beta_4 + \alpha_3\beta_1 + \alpha_1^2\beta_2$	$\frac{1}{12}$
	4	α_8	β_8	$\alpha_8\beta_0 + \beta_8 + \alpha_2\beta_2 + \alpha_1\beta_4 + \alpha_4\beta_1$	$\frac{1}{24}$

We introduce N_p as a normal subgroup, which is defined by

$$N_p = \{\alpha \in \mathbb{G} : \alpha(t) = 0, \text{whenever} \quad r(t) \leq p\}$$

A Runge- Kutta method with group element α is of order p, if it is in the same coset as EN_p , that is

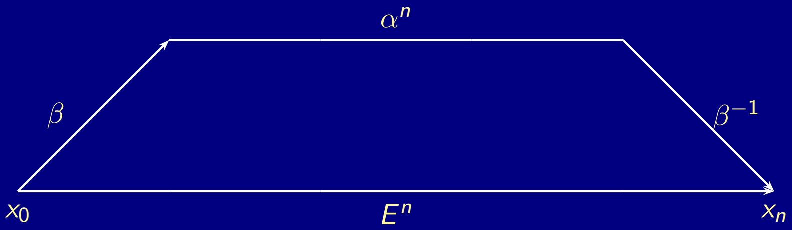
$$\alpha N_p = EN_p$$

A Runge- Kutta method has an "effective order" p if there exist another Runge - Kutta method with corresponding group element β, such that

$$\beta\alpha N_p = E\beta N_p$$

Computational interpretation

The conjugacy concept in group theory provides a computational interpretation of the effective order. This means that, “every input value for effective order method α is perturbed by a method β”.
Therefore the starting method β offers some freedom of the order conditions of the effective order method α.
Every output value could also be perturbed back to the origional trajectory using method β^{-1}.



Symplectic Runge– Kutta methods

A Runge–Kutta method is said to be canonical or symplectic if the numerical solution y_n also has the quadratic invariant $Q(y_n)$ i.e.

$$\langle y_n, y_n \rangle = \langle y_{n-1}, y_{n-1} \rangle$$

A method has this property if and only if,

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0$$

for all i, j.

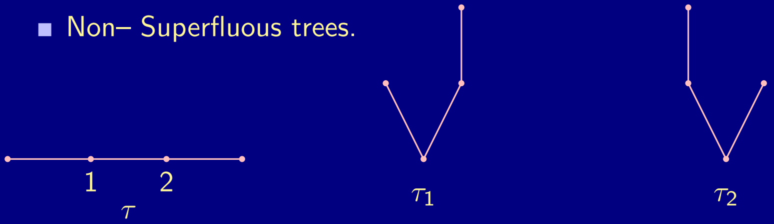
Superfluous and Non–superfluous trees

It is a consequence of the symplectic condition that if τ_1 and τ_2 are rooted trees corressponding to the same tree τ then

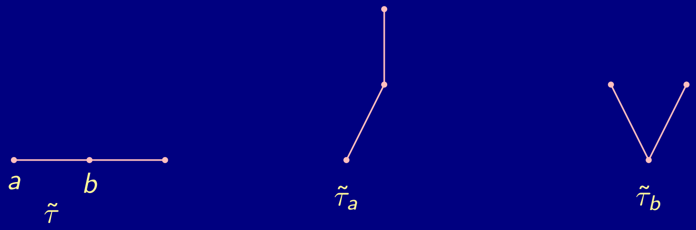
$$\phi(\tau_1) = \frac{1}{\gamma(\tau_1)}, \quad \phi(\tau_2) = \frac{1}{\gamma(\tau_2)}$$

For Symplectic Runge–Kutta methods, we distinguish trees in two ways.

- Superfluous trees,
- Non– Superfluous trees.



Order conditions corresponding to non–superfluous trees are transformed into one order condition.



Order Conditions for Symplectic Runge–Kutta methods

The number of order conditions for symplectic Runge–Kutta methods is less than the number of order conditions for a general Runge–Kutta method.

Case 1: Suppose the method is of order at least 1, $(\sum_i b_i = 1)$,

$$\sum_{i,j} b_i a_{ij} + \sum_{i,j} b_j a_{ji} - \sum_{i,j} b_i b_j = 0$$

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

Therefore for symplectic Runge–Kutta method the second order condition is automatically satisfied and hence not required.

Order Conditions for Symplectic Runge–Kutta methods

Case 2 : Suppose the method is of order at least 2, $(\sum_i b_i c_i = \frac{1}{2})$, Consider the symplectic condition,

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0$$

Multiply with c_j and take summation,

$$\sum_{i,j} b_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} - \sum_{i,j} b_i b_j c_j = 0$$

$$\Rightarrow (\sum_{i,j} b_i a_{ij} c_j - \tfrac{1}{6}) + (\sum_j b_j c_j^2 - \tfrac{1}{3}) = 0$$

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Order	General RK method	Symplectic RK method
1	1	1
2	2	1
3	4	2
4	8	3

Table: Order conditions for general and symplectic Runge–Kutta methods up to order 4.

Gauss method

For example, consider applying Gauss method to the harmonic oscillator problem given below:

$$q' = p, \qquad p' = -q.$$

The energy is given by,

$$H = \frac{p^2}{2} + \frac{q^2}{2}.$$

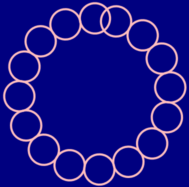
The exact solution is,

$$\begin{bmatrix} p(x) \\ q(x) \end{bmatrix} = \begin{bmatrix} \cos(x) & -\sin(x) \\ \sin(x) & \cos(x) \end{bmatrix} \begin{bmatrix} p(0) \\ q(0) \end{bmatrix}.$$

This problem describes the motion of a unit mass attached to a spring with momentum p and position co-ordinates q defines a Hamiltonian system.

we consider the two stage order four Gauss method,

$$\begin{array}{c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{2}$$



Gauss method approximately conserve the total energy of the himiltonian system .

Effective order with symplectic integrator

We show a way of analyzing methods of effective order 4 having symplectic condition with three stages.

$$
\begin{aligned}
(\beta\alpha)(\tau) &= \beta(\tau) + \alpha(\tau) \\
(\beta\alpha)([\tau,\tau]) &= \beta([\tau,\tau]) + 2\beta(\tau)\alpha([\tau]) + \beta^2(\tau)\alpha(\tau) + \alpha([\tau,\tau]) \\
(\beta\alpha)([\tau,\tau,\tau]) &= \alpha([\tau,\tau,\tau]) + 3\beta(\tau)\alpha([\tau,\tau]) + 3\beta^2(\tau)\alpha([\tau]) \\
&\quad + \beta^3(\tau)\alpha(\tau) + \beta([\tau,\tau,\tau])
\end{aligned}
$$

New Implicit methods

We present two examples of symplectic effective order methods:

- Method A - has real and distinct eigenvalues

$$\begin{array}{c|ccc} \frac{3}{8} & \frac{7}{15} & -\frac{163}{504} & \frac{73}{315} \\ \frac{5}{8} & -\frac{17}{40} & -\frac{1}{9} & \frac{209}{180} \\ 1 & \frac{12}{65} & \frac{157}{234} & \frac{13}{90} \\ \hline & \frac{14}{15} & -\frac{2}{9} & \frac{13}{45} \end{array}$$

- Method B - has complex eigenvalues

$$\begin{array}{c|ccc} \frac{1}{6} & \frac{3}{14} & -\frac{1}{21} & 0 \\ \frac{3}{4} & -\frac{5}{7} & -\frac{1}{28} & 0 \\ \frac{3}{4} & -\frac{3}{7} & \frac{1}{14} & \frac{1}{4} \\ \hline & \frac{3}{7} & \frac{1}{14} & \frac{1}{2} \end{array}$$

Cheap implementation

Since method A have real eigenvalues, it is therefore of interest.This is because we can obtain a cheaper implementation. Here we are considering only method A.
The general form of an s-stage implicit method is

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(x_n + hc_i, Y_i),$$

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f(x_n + hc_j, Y_j)$$

The stage equations can be written in the form

$$Y = e \otimes y_n + h(A \otimes I_m)F(Y)$$

We use modified Newton Raphson iteration scheme to solve the above equation. This can be defined as

$$M\Delta Y^{[k]} = G(Y^{[k]})$$
$$Y^{[k+1]} = Y^{[k]} + \Delta Y^{[k]}$$

where

$$M = I_s \otimes I_m - h(A \otimes J)$$
$$G(Y^{[k]}) = -Y^{[k]} + e \otimes y_n + h(A \otimes I_m)F(Y)$$

The total computational cost in this scheme include

- the evaluation of F and G,
- the evaluation of J,
- the evaluation of M,
- LU factorization of the iteration matrix, M,
- back substitution to get the Newton update vector, $\Delta Y^{[k]}$.

Transformation

To reduce computational cost of fully implicit RK method, we use transformation. The transformation matrix T for method A is given by

$$T = \begin{bmatrix} 0.262527404618574 & 0.949059020237884 & -0.235024483067430 \\ 0.812033424383500 & -0.068304645470165 & 0.765241433855123 \\ -0.521230351675958 & 0.307606000449118 & 0.599307133505220 \end{bmatrix}$$

The transformation matrix has the property,

$$T^{-1}AT = \begin{bmatrix} -0.993809382166128 & 0 & 0 \\ 0 & 0.565055763297954 & 0 \\ 0 & 0 & 0.928753618868175 \end{bmatrix}$$

where -0.993809382166128, 0.565055763297954, and 0.928753618868175 are three distinct real eigenvalues

Starting method

Solution of these equations give the starting method

$$
\begin{aligned}
(\alpha)(\tau) &= 1 \\
(\alpha)([\tau^2]) &= 2\beta(\tau) + \tfrac{1}{3} \\
(\alpha)([\tau^3]) &= 3\beta([\tau^2]) + 3\beta([\tau]) + \tfrac{1}{4}
\end{aligned}
$$

which is given by

$$
\begin{array}{c|ccc}
2 & \frac{13}{4608} & \frac{4595}{2304} & \frac{13}{4608} \\
0 & \frac{4621}{4608} & -\frac{13}{2304} & -\frac{4595}{4608} \\
-2 & \frac{13}{4608} & -\frac{4621}{2304} & \frac{13}{4608} \\
\hline
 & \frac{13}{2304} & -\frac{13}{1152} & \frac{13}{2304}
\end{array}
$$

Numerical Experiments

1. The Kepler's problem

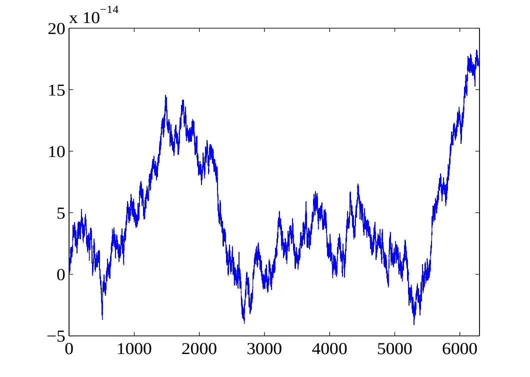
$$x_1' = y_1, \qquad x_2' = y_2,$$
$$y_1' = -\frac{x_1}{(x_1^2 + x_2^2)^{\frac{3}{2}}}, \qquad y_2' = -\frac{x_2}{(x_1^2 + x_2^2)^{\frac{3}{2}}}$$

where (x_1, x_2) are the position coordinates and (y_1, y_2) are the velocity components of the body.

$$(x_1, x_2, y_1, y_2) = (1 - e, 0, 0, \sqrt{(1 + e)/(1 - e)}),$$
$$H = \tfrac{1}{2}(y_1^2 + y_2^2) - \frac{1}{\sqrt{x_1^2 + x_2^2}}.$$

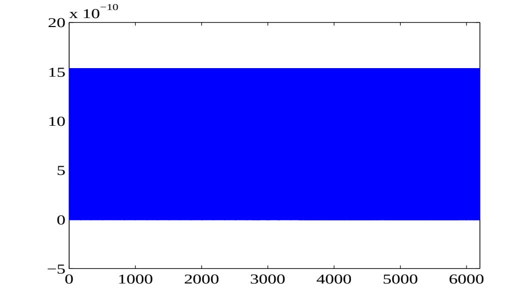
Kepler problem (e=0,h=0.01, $n = 10^6$)

Graph for Hamiltonian:
error VS time



Kepler problem (e=0.5,h=0.01, $n = 10^6$)

For Hamiltonian:
error VS time



1. The simple Pendulum

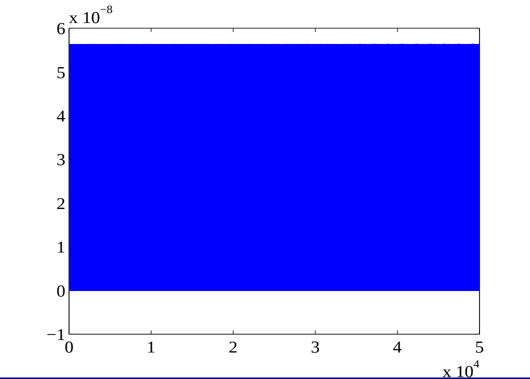
$$p' = -\sin(q), \qquad q' = p,$$

$$(p, q) = (0, 2.3).$$

$$H = \frac{p^2}{2} - \cos(q).$$

Simple Pendulum (h=0.05, $n = 10^6$)

For Hamiltonian:
error VS time



Conclusions

1. For problems that conserve some sort of invariant structure, it is a good idea to use numerical methods which mimic this behaviour.
2. Symplectic Runge–Kutta methods have this role for many important problems.
3. Because of greater flexibilty,effective order methods can provide greater efficiency as compared with methods with classical order.
4. It is possible to obtain cheap implementation cost if A has real eigenvalues.
5. These methods are suited for parallel computers which have very large number of processors.

Future work

1. Error estimates
2. Working on implicit methods with optimal choices of parameters.
3. Construct general linear methods with closely related properties.
4. Generalization of effective order on partioned Runge–Kutta methods for separable Hamiltonian.

THANK YOU