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BUTCHER SERIES FOR EVOLUTIONS ON CLIFFORD ALGEBRAS

Alžběta Haková *

Abstract

Numerical solution methods for dynamical systems are known to be organized by the algebra of rooted trees which also allows to manipulate them due to its Hopf algebra structure. The particular case of evolution on Clifford algebras is discussed.

1 Introduction

The aim of this paper is to discuss the solution of the differential equation $dx(s)/ds = F[x(s)]$ which is known as a flow of a vector field. There is a special numerical method which solves this differential equation and it is known as the Runge-Kutta method. In 1972 John Butcher published an article where he analysed general Runge-Kutta methods on the basis of the algebra of rooted trees. He also defined sums over trees which form another type of algorithms solving our differential equation. These sums are now called B-series in honour of Butcher.

We assume that the function F in the equation is a commutator in generators of the Clifford algebra and we compare the solution that provides Runge-Kutta methods and B-series.

The paper is organized as follows. In Section 2 we introduce notations and necessary concepts concerning Clifford algebras, rooted trees and Butcher series. In Section 3 we show that B-series and Runge-Kutta methods coincide in the case of a second order commutator on the right hand side and in Section 4 we discuss the situation in the fourth order case.

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2 Definitions and known results

2.1 Clifford algebras

Let V be an arbitrary real vector space upon which $g : V \times V \to \mathbb{R}$ is a positive-definite inner product. By a *Clifford map* on V we shall mean a real-linear map $f : V \to B$ into a unital associative complex algebra B such that if $v \in V$ then $f(v)^2 = g(v,v)1$. We define a *complex Clifford algebra* over V to be a unital associative complex algebra A together with a Clifford map $\Phi : V \to A$ satisfying the following *universal mapping property*: if $f : V \to B$ is any Clifford map, then there exists a unique algebra map $F : A \to B$ such that $F \circ \Phi = f$. We denote $Cl(V,g)$ a complex Clifford algebra over V.

Theorem 2.1.1([6], Theorem 1.1.1) *The complex Clifford algebra $Cl(V,g)$ is generated by its real subspace V satisfying the Clifford relations*

$$x, y \in V \quad \Rightarrow \quad xy + yx = 2g(x,y)1. \tag{1}$$

2.2 Rooted trees

A *rooted tree* is a graph with a designated vertex called a root such that there is a unique path from the root to any other vertex in the tree (see [7]). In what follows, we will use several operations and functions on trees.

If $t_1, t_2, ..., t_k$ are trees, $t = B^+(t_1, t_2, ..., t_k)$ is defined as the tree obtained by creating a new vertex r and by joining the roots of $t_1, t_2, ..., t_k$ to r, which becomes the root of t. This operation is called *merging of trees.*

We denote by $|t|$ the *number of vertices* of a tree t.

The *tree factorial* $t!$ is defined recursively as

$$\begin{aligned} \circ\,! &= 1, && (2)\\ B^+(t_1, t_2, ..., t_k)! &= |B^+(t_1, t_2, ..., t_k)|t_1!t_2!...t_k!. && (3) \end{aligned}$$

$\alpha(t)$ is defined as the number of times tree t appears in $N^{|t|}(1)$.

Assume we want to solve the equation

$$\frac{dx(s)}{ds} = F[x(s)], \tag{4}$$

where $x(s_0) = x_0$, s is a real, x is in $\mathbb{R}^{\mathbb{N}}$ and F is a smooth function from $\mathbb{R}^{\mathbb{N}}$ to $\mathbb{R}^{\mathbb{N}}$ with components $f^i(x)$. This is the equation of flow of a vector field.

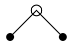
If we use the following notation

$$\begin{aligned} f^i &= f^i[x(s)] && (5)\\ f^i_{j_1 j_2 ... j_k} &= \frac{\partial^k f^i}{\partial x_{j_1} ... \partial x_{j_k}}[x(s)] && (6) \end{aligned}$$

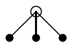
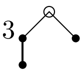
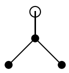
we can write the derivatives of the i-th component of $x(s)$ with respect to s:

$$\frac{dx^i(s)}{ds} = f^i = \circ \tag{7}$$

$$\frac{d^2x^i(s)}{ds^2} = f^i_j f^j = \tag{8}$$


$$\frac{d^3x^i(s)}{ds^3} = f^i_{jk} f^j f^k + f^i_j f^j_k f^k = \tag{9}$$
 $+$ 

$$\frac{d^4x^i(s)}{ds^4} = f^i_{jkl} f^j f^k f^l + 3 f^i_{jk} f^j_l f^k f^l + f^i_j f^j_{kl} f^k f^l + f^i_j f^j_k f^k_l f^l = \tag{10}$$

 $+\,3$  $+$  $+$  (11)

This one-to-one relation between a rooted tree with n vertices and a term $d^n x(s)/ds^n$ was established by Arthur Cayley in 1857 (see [4]).

We call *elementary differentials* (see [3])the δ_t defined recursively for each rooted tree t by

$$\delta^i_\circ = f^i \tag{12}$$

$$\delta^i_t = f^i_{j_1 j_2 \ldots j_k} \delta^{j_1}_{t_1} \delta^{j_2}_{t_2} \ldots \delta^{j_k}_{t_k} \quad \text{where} \quad t = B^+(t_1, t_2, \ldots, t_k). \tag{13}$$

2.3 Butcher series

To solve a flow equation $dx(s)/ds = F[x(s)]$, some efficient numerical algorithms are known as Runge-Kutta methods. They are determined by an $m \times m$ matrix a and an m-dimensional vector b. At each step a vector x_n is defined as a function of the previous value x_{n-1} by:

$$X_i = x_{n-1} + h \sum_{j=1}^{m} a_{ij} F(X_j), \tag{14}$$

$$x_n = x_{n-1} + h \sum_{j=1}^{m} b_j F(X_j), \tag{15}$$

where i ranges from 1 to m.

In [2] Butcher proved that the solution of the corresponding equations

$$X_i(s) = x_0 + (s - s_0) \sum_{j=1}^{m} a_{ij} F(X_j(s)), \tag{16}$$

$$x(s) = x_0 + (s - s_0) \sum_{j=1}^{m} b_j F(X_j(s)) \tag{17}$$

is given by

$$X_i(s) = x_0 + \sum_t \frac{(s-s_0)^{|t|}}{|t|!}\alpha(t)\sum_{j=1}^m a_{ij}\phi_j(t)\delta_t(s_0), \tag{18}$$

$$x(s) = x_0 + \sum_t \frac{(s-s_0)^{|t|}}{|t|!}\alpha(t)t!\phi(t)\delta_t(s_0). \tag{19}$$

These series over trees are called B-series in honour of John Butcher (see [5]). The homomorphism ϕ is defined recursively as a function of a and b, for $i = 1, ..., m$:

$$\phi_i(\circ) = 1, \tag{20}$$

$$\phi_i(B^+(t_1, ..., t_k)) = \sum_{j_1,\dots,j_k} a_{ij_1}...a_{ij_k}\phi_{j_1}(t_1)...\phi_{j_k}(t_k), \tag{21}$$

$$\phi(t) = \sum_{i=1}^m b_i\phi_i(t). \tag{22}$$

For more see [1].

3 An example in the second order case

In this section, we assume that the right hand side of (4) is a commutator in generators of the Clifford algebra and show that in this case Runge-Kutta methods and B-series coincide.

Let V be a vector space, y^1, y^2, y^3, y^4 its orthonormal basis. By $Cl(V, g)$ we denote a Clifford algebra over V, $g(y^i, y^j) = \delta^i_j$. We want to solve the following equation:

$$\frac{dy^i}{ds} = [y^1y^2 - y^2y^1, y^i] \tag{23}$$

$$= 4y^1g(y^2, y^i) - 4y^2g(y^1, y^i). \tag{24}$$

Therefore

$$\frac{dy^1}{ds} = -4y^2, \quad \frac{dy^2}{ds} = 4y^1 \quad \text{and} \quad \frac{dy^3}{ds} = \frac{dy^4}{ds} = 0. \tag{25}$$

The classical 4-th order Runge-Kutta method is given by

$$k_1 = f(x_n, y_n), \tag{26}$$

$$k_2 = f\left(x_n + \frac{h_n}{2}, y_n + \frac{h_n}{2}k_1\right), \tag{27}$$

$$
\begin{aligned}
k_3 &= f\left(x_n + \frac{h_n}{2}, y_n + \frac{h_n}{2}k_2\right), && (28)\\
k_4 &= f(x_{n+1}, y_n + h_n k_3), && (29)\\
y_{n+1} &= y_n + h_n\frac{k_1 + 2k_2 + 2k_3 + k_4}{6} && (30)
\end{aligned}
$$

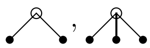
Using this algorithm we receive the solution

$$
y(s) = y^1(\cos(4s)) - y^2(\sin(4s)). \tag{31}
$$

Now, we want to know what trees may appear in sums for B-series:

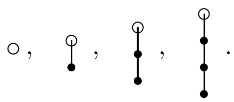
$$
\begin{aligned}
\circ :\quad f^1 &= \frac{dy^1}{ds} = -4y^2\\
f^2 &= \frac{dy^2}{ds} = 4y^1\\
f^3 &= f^4 = 0
\end{aligned}
$$

$$
\begin{aligned}
:\quad f_1^1 &= f_2^2 = 0\\
f_1^2 &= -f_2^1 = 4
\end{aligned}
$$



$$
:\quad f_{jk}^i = f_{jkl}^i = 0 \quad \text{for all } i, j, k \in \{1, 2, 3, 4\}.
$$

It turns out that in B-series will be only following trees



The B-series for initial conditions $y^1(0) = y^1$, $y^2(0) = y^2$ and a_{ij}, b_j representing the classical 4-th order Runge-Kutta method are

$$
\begin{aligned}
y(s) &= y^1\left(1 - \frac{(4s)^2}{2!} + \frac{(4s)^4}{4!}\right) + y^2\left(-4s + \frac{(4s)^3}{3!}\right), && (32)\\
y(s) &= y^1\left(4s - \frac{(4s)^3}{3!}\right) + y^2\left(1 - \frac{(4s)^2}{2!} + \frac{(4s)^4}{4!}\right). && (33)
\end{aligned}
$$

Therefore

$$
\begin{aligned}
y(s) &= y^1(\cos(4s)) - y^2(\sin(4s)), && (34)\\
y(s) &= y^1(\sin(4s)) + y^2(\cos(4s)). && (35)
\end{aligned}
$$

We see that B-series and Runge-Kutta methods coincide.

4 The 4-th order case

In this section we discuss the solution of our differential equation in the case that function F is a 4-th order commutator in generators of the Clifford algebra.

Let $y^1, y^2, ..., y^n$ be an orthonormal basis of V, $g(y^i, y^j) = \delta^i_j$. We want to solve the equation

$$\frac{dy^i}{ds} = [y^1y^2y^3y^4, y^i]. \tag{36}$$

Then

$$\frac{dy^1}{ds} = -2y^2y^3y^4, \qquad \frac{dy^2}{ds} = 2y^1y^3y^4, \tag{37}$$

$$\frac{dy^3}{ds} = -2y^1y^2y^4, \qquad \frac{dy^4}{ds} = 2y^1y^2y^3, \tag{38}$$

$$\frac{dy^i}{ds} = 0 \qquad \text{for all} \quad i > 4. \tag{39}$$

Trees available in B-series are

$$\circ : \quad f^i = \frac{dy^i}{ds}, \tag{40}$$

 :

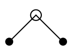
$$f^1_2 = -2y^3y^4, \qquad f^2_1 = 2y^3y^4, \qquad f^2_3 = -2y^1y^4 \tag{41}$$

$$f^3_1 = -2y^2y^4, \qquad f^1_3 = 2y^2y^4, \qquad f^3_2 = 2y^1y^4, \tag{42}$$

$$f^1_4 = -2y^2y^3, \qquad f^4_1 = 2y^2y^3, \qquad f^3_4 = -2y^1y^2, \tag{43}$$

$$f^4_2 = -2y^1y^3, \qquad f^2_4 = 2y^1y^3, \qquad f^4_3 = 2y^1y^2, \tag{44}$$

$$\Rightarrow \qquad f^i_j = -f^j_i \qquad \text{for} \quad i, j \in \{1, 2, ..., n\}. \tag{45}$$

 :

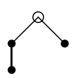
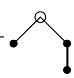
$$f^1_{23} = 2y^4, \qquad f^1_{32} = -2y^4, \tag{46}$$

$$f^1_{34} = 2y^2, \qquad f^1_{43} = -2y^2, \tag{47}$$

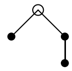
$$f^2_{31} = 2y^4, \qquad f^2_{13} = -2y^4, \text{etc.} \tag{48}$$

$$\Rightarrow \quad f^i_{jk} = -f^i_{jk} \quad \text{for} \quad i, j \in \{1, 2, ..., n\}. \tag{49}$$

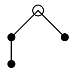
We conclude that these trees have the following surprising proposition

 $= -$  (50)

because



$$= f^i_{jk} f^k_l f^j f^l, \tag{51}$$



$$= f^i_{jk} f^j_l f^k f^l = f^i_{kj} f^k_l f^j f^l. \tag{52}$$

$$\tag{53}$$

Now, we want to compute the Runge-Kutta method so first of all it is necessary to look for a Taylor expansion of a function on generators of a Clifford algebra

$$y = \sum_{\substack{k=0 \\ i_1 < i_2 < \ldots < i_k}}^{n} a_{i_1 i_2 \ldots i_k} y^{i_1} y^{i_2} \ldots y^{i_k} \tag{54}$$

It's easy to prove that

$$\frac{dy^i}{ds} y^j = -y^i \frac{dy^j}{ds} \tag{55}$$

Using (55) and (36)-(38) we conclude that

$$\frac{dy}{ds} = 2(-y^1 + y^2 - y^3 + y^4 - y^2 y^3 y^4 + y^1 y^3 y^4 - y^1 y^2 y^4 + y^1 y^2 y^3) R, \tag{56}$$

$$\frac{d^2 y}{ds^2} = 4(y^1 + y^2 + y^3 + y^4 + y^2 y^3 y^4 + y^1 y^3 y^4 + y^1 y^2 y^4 + y^1 y^2 y^3) R, \tag{57}$$

$$\frac{d^3 y}{ds^3} = 8(-y^1 + y^2 - y^3 + y^4 - y^2 y^3 y^4 + y^1 y^3 y^4 - y^1 y^2 y^4 + y^1 y^2 y^3) R, \tag{58}$$

$$\frac{d^4 y}{ds^4} = 16(y^1 + y^2 + y^3 + y^4 + y^2 y^3 y^4 + y^1 y^3 y^4 + y^1 y^2 y^4 + y^1 y^2 y^3) R, \tag{59}$$

where

$$R = \sum_{\substack{k=0 \\ 4 < i_1 < i_2 < \ldots < i_k}}^{n-4} a_{i_1 i_2 \ldots i_k} y^{i_1} y^{i_2} \ldots y^{i_k}. \tag{60}$$

A 4-th order Runge-Kutta method is given by

$$y(s+h) = y(s) + b_1 k_1 + b_2 k_2 + b_3 k_3 + b_4 k_4, \tag{61}$$

$$\text{where} \quad k_1 = h f(y), \tag{62}$$

$$k_2 = h f(y + a_1 k_1), \tag{63}$$

$$k_3 = h f(y + a_2 k_1 + a_3 k_2), \tag{64}$$

$$k_4 = h f(y + a_4 k_1 + a_5 k_2 + a_6 k_3). \tag{65}$$

In our case is

$$f(y) \quad = \quad \frac{dy}{ds}. \tag{66}$$

Therefore

$$\begin{aligned}
y(s+h) \quad &= \quad y(s) + \frac{dy}{ds}(b_1 h + b_2 h + b_3 h + b_4 h) + & (67)\\
&\quad \frac{d^2y}{ds^2}\, h^2(a_1 b_2 + a_2 b_3 + a_3 b_3 + a_4 b_4 + a_5 b_4 + a_6 b_4) + & (68)\\
&\quad \frac{d^3y}{ds^3}\, h^3(b_3 a_1 a_3 + b_4 a_1 a_5 + b_4 a_2 a_6 + b_4 a_3 a_6) + & (69)\\
&\quad \frac{d^4y}{ds^4}\, h^4(b_4 a_1 a_3 a_6). & (70)
\end{aligned}$$

If we compare this with the Taylor expansion

$$y(s+h) \quad = \quad y(s) + h\frac{dy}{ds} + \frac{h^2}{2!}\frac{d^2y}{ds^2} + \frac{h^3}{3!}\frac{d^3y}{ds^3} + \frac{h^4}{4!}\frac{d^4y}{ds^4} \tag{71}$$

we conclude

$$\begin{aligned}
&1) \quad 1 = b_1 + b_2 + b_3 + b_4 & (72)\\
&2) \quad \frac{1}{2} = a_1 b_2 + a_2 b_3 + a_3 b_3 + a_4 b_4 + a_5 b_4 + a_6 b_4 & (73)\\
&3) \quad \frac{1}{6} = b_3 a_1 a_3 + b_4 a_1 a_5 + b_4 a_2 a_6 + b_4 a_3 a_6 & (74)\\
&4) \quad \frac{1}{24} = b_4 a_1 a_3 a_6 & (75)
\end{aligned}$$

This leads to a classical 4-th order Runge-Kutta method

$$b_1 = \frac{1}{6}, \quad b_2 = \frac{1}{3}, \quad b_3 = \frac{1}{3}, \quad b_4 = \frac{1}{6}, \tag{76}$$

$$a_1 = \frac{1}{2}, \quad a_3 = \frac{1}{2}, \quad a_6 = 1, \quad a_2 = a_4 = a_5 = 0. \tag{77}$$

Acknowledgements

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Alžběta Haková, Mathematical Institute, Silesian University, 74601 Opava, Na Rybníčku 1, Czech republic, *e-mail*: Alzbeta.Hakova@math.slu.cz