Butcher Algebras

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September 12, 2012

Preliminaries

Butcher tableau is the standard method method of description of Runge-Kutta method:

$$\begin{array}{c|cccccc} c_2 & a_{21} \\ c_3 & a_{31} & a_{32} \\ c_4 & a_{41} & a_{42} & a_{43} \\ c_5 & a_{51} & a_{52} & a_{53} & a_{54} \\ c_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} \\ \hline & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 \end{array}$$

The coefficients of this table should satisfy order conditions:

$$(b, \Phi_t(A)) = 1/\gamma(t)$$

for each rooted tree t.

Number of eqs, N stages

This polynomial system of equation is large and difficult to solve:

order	1	2	3	4	5	6	7	8	9	10
numb. of eqs	1	2	4	8	17	37	85	200	486	1205
min. stages :				4	6	7	9	11	13	≤ 17

Simplifying assumptions

"Simplifying assumptions" are often used to simplify the system:
1st simplifying assumptions ($C(2)$, with $c_n = 1$).
2nd simplifying assumptions ($D(1)$, with $b_2 = 0$).

order/stages	4/4	5/6	6/7	7/9	8/11	9/13
none : *eqs/vars*	8/10	17/21	37/28	85/45	200/66	486/91
1 : *eqs/vars*	4/6	9/15	20/21	48/36	115/55	286/78
2 : *eqs/vars*		6/11	13/16	32/29	79/46	202/67

Result: algebraic classification of Runge-Kutta methods

- Introduced using Abstract Algebra.
- New simplifying assumptions that
  - are as good as simplifying assumptions 1 and 2 (no solution loss), and
  - used jointly with assumptions 1 and 2 simplifies the system drastically.
- Using new assumptions we were able to obtain new RK methods of order 9.

Vectors

Consider a vector space $\mathbb{R}^n$, where vectors are considered as columns and

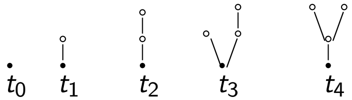
$$e = \begin{pmatrix} 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix}, \; d = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}.$$

Let $*$ be the coordinate-wise multiplication in $\mathbb{R}^n$:

$$(x_1, \ldots, x_n)^t * (y_1, \ldots, y_n)^t = (x_1 y_1, \ldots, x_n y_n)^t.$$

Trees multiplication, operators α, Φ

Let t_0 – tree with only one vertex, $t_1 = \alpha t_0$ – two vertex and one edge, $t_2 = \alpha^2 t_0$, $t_3 = t_1 \cdot t_2$, $t_4 = \alpha(t_1 \cdot t_1)$. So



Weight $w(t)$ – number of edges. For arbitrary square matrix A and $e = (1, \ldots, 1)^t$ we have the weights and operator $\Phi_t(A)$ as follows:

$$
\begin{aligned}
w(t_0) &= 0, & \Phi_{t_0}(A) &= e, \\
w(t_1) &= 1, & \Phi_{t_1}(A) &= Ae, \\
w(t_2) &= 2, & \Phi_{t_2}(A) &= A^2 e, \\
w(t_3) &= 3, & \Phi_{t_3}(A) &= Ae * A^2 e, \\
w(t_4) &= 3, & \Phi_{t_4}(A) &= A(Ae * Ae)
\end{aligned}
$$

Subspaces L_k

For arbitrary square matrix A of size $n \times n$ consider subspaces generated by $\Phi_t(A)$ with trees of weight k:

$$L_k = < \Phi_t(A) | w(t) = k > \subset \mathbb{R}^n .$$

For example,

$$\begin{aligned} L_0 &= < e > , \\ L_1 &= < Ae > , \\ L_2 &= < A^2 e, \ Ae * Ae > , \\ L_3 &= < A^3 e, \ A(Ae * Ae), \ A^2 e * Ae, \ Ae * Ae * Ae > , \\ \ldots \end{aligned}$$

Subspaces M_k

For given matrix A consider a filtration in $\mathbb{R}^n$: chain of subspaces $0 \subset M_0 \subset M_1 \subset M_2 \ldots$:

$$\begin{aligned} M_0 &= L_0 \ , \\ M_1 &= L_0 + L_1 \ , \\ M_2 &= L_0 + L_1 + L_2 \ , \\ M_3 &= L_0 + L_1 + L_2 + L_3 \ , \\ \ldots \end{aligned}$$

Theorem This filtration corresponds to the multiplication, that is

$$M_i * M_j \subset M_{i+j}, \quad A(M_i) \subset M_{i+1} \ .$$

Remark. 1st simplifying assumption holds iff $M_p = \mathbb{R}^{s+1}$.
2nd simplifying assumption holds iff $M_{p-1} = \mathbb{R}^{s+1}$.

Algebra B

Definition. We say that the adjoint algebra corresponding to the filtration $0 \subset M_0 \subset M_1 \subset M_2 \ldots$:

$$B(A) = \bigoplus_{k=0}^{n} \underbrace{M_k / M_{k-1}}_{B_k(A)}$$

is an upper Butcher algebra of matrix A.

Theorem

"This algebra has nice properties":

- *it is graduated,*
- *operator A acts on it.*

Example: “rule 3/8“

Extended Butcher table $\widetilde{A}$ defining this method is

$$\widetilde{A} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 & 0 \\ -1/3 & 1 & 0 & 0 & 0 \\ 1 & -1 & 1 & 0 & 0 \\ 1/8 & 3/8 & 3/8 & 1/8 & 0 \end{pmatrix}.$$

Algebraic constructions above may be completely computed:

$$L_0 : \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \; L_1 : \begin{pmatrix} 0 \\ 1/3 \\ 2/3 \\ 1 \\ 1 \end{pmatrix}, \; L_2 : \begin{pmatrix} 0 & 0 \\ 0 & 1/9 \\ 1/3 & 4/9 \\ 1/3 & 1 \\ 1/2 & 1 \end{pmatrix},$$

Example: "rule 3/8"

$$M_0 : \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \; M_1 : \begin{pmatrix} 1 & 0 \\ 1 & 1/3 \\ 1 & 2/3 \\ 1 & 1 \\ 1 & 1 \end{pmatrix}, \; M_2 : \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1/3 & 0 & 1/9 \\ 1 & 2/3 & 1/3 & 4/9 \\ 1 & 1 & 1/3 & 1 \\ 1 & 1 & 1/2 & 1 \end{pmatrix},$$

$M_3 = \mathbb{R}^5$. So:

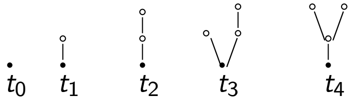
$$\begin{aligned} B_0 &= M_0, & \dim = 1, \quad & B_0 = < e > , \\ B_1 &= M_1/M_0, & \dim = 1, \quad & B_1 = < Ae > , \\ B_2 &= M_2/M_1, & \dim = 2, \quad & B_2 = < A^2e, Ae * Ae > , \\ B_3 &= M_3/M_2, & \dim = 1, \quad & B_3 = < R = Ae * Ae * Ae > , \end{aligned}$$

$$A^2e * Ae = 3/2R, \; A^3e = 15/4R, \; A(Ae * Ae) = 0.$$

δ: trees $\to \mathbb{N}$

I suggest to slightly change the standard γ function (call it δ here):

1. $\delta(t_0) = 1$,
2. $\delta(t_1 t_2) = \delta(t_1)\delta(t_2)$ for any $t_1, t_2 \in \mathcal{T}$,
3. $\delta(\alpha t) = \delta(t)(w(t) + 1)$ for any $t \in \mathcal{T}$.



t	t_0	t_1	t_2	t_3	t_4
$w(t)$	0	1	2	3	3
$\delta(t)$	1	1	2	2	3
$\gamma(t)$	1	2	6	8	12

Subspaces L'_k

Here we upgrade our construction a little bit (subspaces L'_k and everything denoted by primes).

Definition. For an arbitrary tree t denote by $\Phi'(t)(A)$ vector

$$\Phi'_t(A) = \delta(t)\Phi_t(A) - \underbrace{Ae * \cdots * Ae}_{d},$$

where $d = w(t)$ is the weight of the tree.

Definition. For a given matrix A consider subspaces L'_k, $k = 0, 1, \ldots$ generated by vectors $\Phi'_t(A)$ for all trees t of weight k.

$$L'_0 = L'_1 = 0, \;\; L'_2 =< 2A^2e - Ae{*}Ae >$$

$$L'_3 =< 6A^3e - Ae{*}Ae{*}Ae, \; 3A(Ae{*}Ae) - Ae{*}Ae{*}Ae,$$

$$2A^2e{*}Ae - Ae{*}Ae{*}Ae >$$

Subspaces M'_k

For given matrix A consider the filtration $0 \subset M'_2 \subset M'_3 \ldots$:

$$\begin{aligned} M'_2 &= L'_2 \ , \\ M'_3 &= L'_2 + L'_3 \ , \\ M'_4 &= L'_2 + L'_3 + L'_4 \ , \\ \ldots \end{aligned}$$

This filtration corresponds to the multiplication, that is

$$M'_i * M'_j \subset M'_{i+j}, \quad A(M'_i) \subset M'_{i+1} \ .$$

Algebra B'

Definition. We say that the adjoint algebra corresponding to the filtration $0 \subset M'_2 \subset M'_3 \subset \ldots$:

$$B'(A) = \bigoplus_{k=0}^{n} B'_k(A) = \bigoplus_{k=0}^{n} M'_k / M'_{k-1}$$

is an lower Butcher algebra of matrix A.

Remark. Note that all constructions above can be done for an arbitrary square matrix A.

Extended matrix

Define the extended matrix, for example for 6-staged methods. For given RK-method

$$\begin{array}{c|cccccc} c_2 & a_{21} & & & & & \\ c_3 & a_{31} & a_{32} & & & & \\ c_4 & a_{41} & a_{42} & a_{43} & & & \\ c_5 & a_{51} & a_{52} & a_{53} & a_{54} & & \\ c_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & \\ \hline & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 \end{array}$$

extended RK matrix is

$$\widetilde{A} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{31} & a_{32} & 0 & 0 & 0 & 0 & 0 \\ a_{41} & a_{42} & a_{43} & 0 & 0 & 0 & 0 \\ a_{51} & a_{52} & a_{53} & a_{54} & 0 & 0 & 0 \\ a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & 0 & 0 \\ b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & 0 \end{pmatrix}.$$

Order equations in terms of L_k, L'_k

Theorem (Order equations in terms of L_k). An extended matrix $\widetilde{A}$ defines a RK method of order p if and only if

$$(d, \widetilde{A}v) = \frac{(d, v)}{k+1} \qquad (1)$$

holds for all k, $0 \leq k < p$ and for all $v \in L_k(\widetilde{A})$.

Theorem(Order equations in terms of L'_k). An extended matrix $\widetilde{A}$ defines a RK method of order p if and only if

$$\begin{array}{lllll} 1) & (d, \widetilde{A}^k e) = 1/k!, & \text{for} & k & = 0, \dots, p\ , \\ 2) & \forall v \in L'_k : (d, v) = 0, & \text{for} & k & < p\ . \end{array} \qquad (2)$$

Simplifying assumptions

Experimental Fact: For all known RK methods of orders 5 and higher the dimensions of B'_i spaces for small i are the same:

i :	0	1	2	3	4	...
$dim(B'_i)$:	0	0	1	1	2	...

As $B'_i = M'_i/M'_{i-1}$, so

i :	0	1	2	3	4	...
$dim(M'_i)$:	0	0	1	2	4	...
# of generators :	0	0	1	4	11	...

Remark: We see that the generators are obviously linearly dependent for known methods.

New simplifying assumptions: We assume that this tendency continues to unknown methods too.

Use new simplifying assumptions

Recall our notation:

$$\widetilde{A} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{31} & a_{32} & 0 & 0 & 0 & 0 & 0 \\ a_{41} & a_{42} & a_{43} & 0 & 0 & 0 & 0 \\ a_{51} & a_{52} & a_{53} & a_{54} & 0 & 0 & 0 \\ a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & 0 & 0 \\ & & \dots & & & & \end{pmatrix}, \quad \begin{aligned} c_2 &= a_{21} \\ c_3 &= a_{31} + a_{32} \\ c_4 &= a_{41} + a_{42} + a_{43} \\ \dots \end{aligned}$$

Denote two generating vectors:

$$\begin{aligned} w_2 &= 2\widetilde{A}^2 e \quad - \widetilde{A}e * \widetilde{A}e, \\ w_3 &= 6\widetilde{A}^3 e \quad - \widetilde{A}e * \widetilde{A}e * \widetilde{A}e. \end{aligned}$$

Use one of the new simplifying assumptions: $\dim M_3' = 2$.
This is the simplest simplifying assumption among our new.

So between four vectors $w_2, w_3, \ \widetilde{A}e * w_2, \ \widetilde{A}w_2$ there should be two relations. The exact coefficients in this relations can be obtained:

Theorem

The relations are:

$$\begin{aligned} K \cdot \widetilde{A}e * w_2 &= (2a_{32}c_2c_3) \cdot w_2 + (c_2 - c_3)(2a_{32}c_2 - c_3^2) \cdot w_3 \,, \\ K \cdot \widetilde{A}w_2 &= (a_{32}c_2^3) \cdot w_2 + (a_{32}c_2^2) \cdot w_3 \,. \end{aligned}$$

where $K = 2a_{32}c_2^2 - c_3^2(c_2 - c_3)$.

Second simplifying assumption together with one new

If matrix $\widetilde{A}$ satisfies second (classical) simplifying assumption, then the first relation is trivial and the second can be rewritten as

$$Aw_2 = -\frac{c_2^2}{2c_3} w_2 + \frac{c_2}{2c_3} w_3 \ .$$

Meaning of simplifying assumptions for matrices

- From the definition of c_k we have

$$a_{k1} = c_k - \sum_{i=2}^{k-1} a_{ki} \ .$$

- From the second simplifying assumption we have

$$a_{k2} = \left(c_k^2/2 - \sum_{i=3}^{k-1} a_{ki} c_i \right) / c_2 \ .$$

- From our new simplest simplifying assumption $\dim M_3' = 2$:

$$a_{k3} = \left(c_k^2 (c_k - c_3) - \sum_{i=4}^{k-1} a_{ki} c_i (3c_i - 2c_3) \right) / c_3^2 \ .$$

Conclusion

- We suggest an elegant abstract Algebra method for solution of systems appeared in connection with RK methods.
  - Upper and Lower Butcher Algebras are introduced.
  - New **"natural"** simplifying assumptions are suggested based on this structure.