New simplifying assumptions for RK methods

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Plan

Preliminaries

Consider the standard Butcher tableau

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

with the order conditions

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

for each rooted tree t, which form very large polynomial systems:

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

Extended matrix

For my purposes it is convenient to use an *extended* $(s+1)\times(s+1)$-matrix A of the RK-method that is defined as follows.

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ a_{21} & 0 & 0 & 0 & \dots & 0 \\ a_{31} & a_{32} & 0 & 0 & \dots & 0 \\ & \dots & & & & \\ a_{s1} & a_{s2} & \dots & a_{s,s-1} & 0 & 0 \\ b_1 & b_2 & \dots & b_{s-1} & b_s & 0 \end{pmatrix}$$

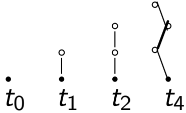
where as usual the first column can be expressed in terms of the others:

$$a_{k1} = c_k - a_{k2} - \dots - a_{k,k-1} \quad \forall k = 2 \dots s \ .$$

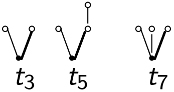
Trees

Following standard Butcher's approach, we use trees. We recall operations from graph theory.

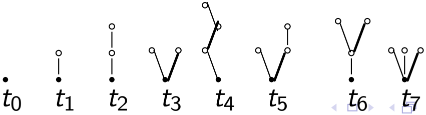
Here t_0 is a tree with only one vertex,
$t_1 = \alpha t_0$ – adding a vertex and an edge to the root,
$t_2 = \alpha^2 t_0$,
$t_4 = \alpha(t_2) = \alpha^3(t_0)$.



Multiplication of trees:
$t_3 = t_1 \cdot t_1$,
$t_5 = t_1 \cdot t_2$,
$t_7 = t_1 \cdot t_1 \cdot t_1$.



So we have the following 8 trees of weight ≤ 3.



Also we have almost standard vectors Φ (not completely standard as we use the extended matrix A here):

$$\begin{aligned} \Phi(t_0) &= e, & \Phi(t_4) &= A^3e, \\ \Phi(t_1) &= Ae, & \Phi(t_5) &= Ae * A^2e, \\ \Phi(t_2) &= A^2e, & \Phi(t_6) &= A(Ae * Ae), \\ \Phi(t_3) &= Ae * Ae, & \Phi(t_7) &= Ae * Ae * Ae, \end{aligned}$$

where $e = (1, \ldots, 1)^t$ and "$*$" – coordinate-wise multiplication in $\mathbb{R}^{s+1}$.

Subspaces L_k and M_k

Consider subspaces generated by $\Phi_t(A)$ with trees of weight k:

$$L_k = < \Phi_t(A) \mid w(t) = k > \subset \mathbb{R}^{s+1} .$$

For example,

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

Consider a filtration in $\mathbb{R}^{s+1}$: 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

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

Classical simplifying assumption $C(2)$

The famous simplifying assumption called $C(2)$ is equivalent to a condition on subspaces !!!!

$$M_{p-1} = \mathbb{R}^{s+1} \ .$$

Theorem Let A be the extended matrix of an s-stage RK-method of order p. The following statements are equivalent:

1. $C(2)$ applies;
2. subspace M_{p-1} coincide with total space $\mathbb{R}^{s+1}$;
3. $Td = T^2 d + Ae{*}Td$, where $T = A^t$ is the transposed matrix, and $d = (0, \ldots, 0, 1)^t$.

In this case the equations that correspond to trees of the form αt for an arbitrary tree t ("maimed" trees) will be consequences of the others.

Remark. The last (vector) equation allows us to express the elements of the penultimate row of the matrix A in terms of the other elements in the matrix.

Classical simplifying assumption $D(1)$

The famous simplifying assumption called $D(1)$ is also equivalent to a condition on subspaces:

$$M_{p-2} = \mathbb{R}^{s+1} \ .$$

Theorem. Let A be the extended matrix of an s-stage RK-method of order p. The following statements are equivalent:

1. $D(1)$ applies;
2. subspace M_{p-2} coincide with total space $\mathbb{R}^{s+1}$;
3. $(Ae{*}Ae - 2A^2e){*}Td = 0$, where $T = A^t$ is the transposed matrix, and $d = (0, \ldots, 0, 1)^t$.

In this case the equations that correspond to trees of the form $t \cdot t_2$, where t is an arbitrary tree, will be consequences of the others.

t_2

Classical simplifying assumptions

The following table shows how the number of variables and the number of equations change when one of the simplifying assumptions is applied.

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
$C(2)$: *eqs/vars*	4/6	9/15	20/21	48/36	115/55	286/78
$D(1)$: *eqs/vars*		6/11	13/16	32/29	79/46	202/67

Note that $C(2)$ is the consequence of $D(1)$.
There exist methods of order 5, for which $C(2)$ does not hold.
There exist methods of orders up to 7 inclusive, for which $D(1)$ does not hold.

Simplifying assumptions via subspaces

Thus,

1. $M_{p-1} = \mathbb{R}^{s+1}$ is the same as $C(2)$;
2. $M_{p-2} = \mathbb{R}^{s+1}$ is the same as $D(1)$;
3. $M_{p-3} = \mathbb{R}^{s+1}$???? (shall we name it $E(0)$???)

Theoretically, we can find further simplifying assumptions as $M_{p-3} = \mathbb{R}^{s+1}, \dots$. However, it turns out that they are not true for many interesting methods.

That is why we suggest further modification of our idea.

Subspaces L'_k

Thus, we change our construction a little (our new subspaces are denoted by primes).

Definition. For an arbitrary tree t, define the vector

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

where $d = w(t)$ is the weight of the tree, and $\delta(t)$ is some modification of the standard $\gamma(t)$.

Note that the order conditions imply that the last coordinate of this vector is zero for $d < p$.

Definition. For a given matrix A consider subspaces L'_k, $k = 0, 1, \dots$ 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 $0 \subset M'_2 \subset M'_3 \ldots$:

$$\begin{aligned} M'_0 &= 0 \,, \\ M'_1 &= 0 \,, \\ M'_2 &= L'_2 \,, \quad (\dim M'_2 = 1) \\ M'_3 &= L'_2 + L'_3 \,, \\ M'_4 &= L'_2 + L'_3 + L'_4 \,, \\ \ldots \end{aligned}$$

This filtration corresponds to the multiplication, that is

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

New simplifying assumptions

We calculate the dimensions of the introduced subspaces $B'_k = M'_k / M'_{k-1}$ for all known RK-methods:

Method, k:	0	1	2	3	4	5	6	7	8
RK(p=3,s= 3) :	0	0	1	1	–	–	–	–	–
RK(p=4,s= 4) :	0	0	1	1	1	–	–	–	–
RK(p=5,s= 6) :	0	0	1	2	1	1	–	–	–
RK(p=6,s= 7) :	0	0	1	1	2	1	1	–	–
RK(p=7,s= 9) :	0	0	1	1	2	2	1	1	–
RK(p=8,s=11) :	0	0	1	1	2	2	2	1	1

Note that the sum of the elements in each row is $s-1$.
We suggest the next new simplifying assumption: $\dim B'_3 = 1$. We see from the table that RK($p=5, s=6$) will not satisfy this condition. However, for all known higher order RK methods it holds.

Vectors w_k

Now more detailed computations.

Definition

For $k \geq 2$ denote by w_k vector

$$w_k = kA(\underbrace{Ae * \cdots * Ae}_{k-1}) - \underbrace{Ae * \cdots * Ae}_{k} \in L'_k.$$

That is

$$\begin{aligned} w_2 &= 2A^2e - Ae * Ae, \\ w_3 &= 3A(Ae * Ae) - Ae * Ae * Ae, \\ w_4 &= 4A(Ae * Ae * Ae) - Ae * Ae * Ae * Ae, \\ &\ldots, \end{aligned}$$

This vectors w_k allow us to define L'_k recursively (we shall omit the details here, and show only the consequences).

Simplifying assumptions of level $3, 4$

We propose to call

1. $C(2)$ level 1 simplification;
2. $D(1)$ level 2 simplification.

Simplifying assumptions of level 3: $\dim B'_3 = 1$, that is $\dim M'_3 = 2$.
In other words, the dimension of subspace in $\mathbb{R}^{s+1}$ generated by $w_2, w_3,\ Ae * w_2,\ Aw_2$ equals 2.

Simplifying assumptions of level 4: $\dim B'_4 = 2$, that is $\dim M'_4 = 4$.
In other words, the dimension of subspace in $\mathbb{R}^{s+1}$ generated by $w_2, w_3,\ Ae * w_2,\ Aw_2,\ w_4,\ Ae{*}w_3,\ Aw_3, w_2 * w_2$ equals 4.

Simplification of level 3

Now more detils on simplification of level 3.
The condition of the linear dependency of the generating vectors implies that everything can be expressed in terms of w_2 and w_3:

$$\begin{aligned} d \cdot Aw_2 &= a_{32} c_2^2 (c_2 \cdot w_2 - w_3)\,, \\ d \cdot Ae * w_2 &= (3c_2 - 2c_3) c_2^2 a_{32} \cdot w_2 - (c_2 - c_3)(2a_{32} c_2 - c_3^2) \cdot w_3\,, \end{aligned}$$

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

If in addition, the simplifying assumption of level 2 holds and among all the b_i-s, only $b_2 = 0$, then we can simplify further:

$$\begin{aligned} Ae * w_2 &= c_2 w_2\,, \\ Aw_2 &= \frac{c_2}{2c_3}(-c_2 w_2 + w_3)\,. \end{aligned}$$

Meaning of simplifying assumptions for matrices

Now we show the result of these simplifications on matrix coefficients.

- 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 (we suggest to name them Level 2):

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

- From our new simplifying assumption $\dim M_3' = 2$ (we named them Level 3):

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

Simplification of level 4

M'_4 generated by M'_3 and 3 vectors: Aw_3, Aw_3 and $w_2{*}w_2$.
Subspace M'_3 is generated by (w_2, w_3),
subspace M'_4 is generated by $(w_2, w_3, w_4, Ae{*}w_3)$.
This is true under the small restriction $3c_2 \neq 2c_3$. If $3c_2 = 2c_3$ we have to take some other generators.

Since $w_2 = (0, -c_2^2, 0, \ldots, 0)^t$, then $w_2 * w_2 = -c_2^2/2w_2$, and, therefore, we have only one relation:

$$Aw_3 = x_2 w_2 + x_3 w_3 + x_4 w_4 + x_{4a} w_{42} \ ,$$

the coefficients of which can be found explicitly:

Simplification of level 4

$$
\begin{aligned}
x_2 &= 3a_{54}c_4(c_4-1)(c_4-c_5)(2c_4-3)/d,\\
x_3 &= 2x_2(c_4-2)/(2c_4-3),\\
x_4 &= (a_{54}c_4(1-c_4)(2c_4^2-c_4-c_5)+d_0)/d,\\
x_{4a} &= -x_2-x_3-x_4.
\end{aligned}
$$

where

$$
\begin{aligned}
d_0 &= c_5^2(c_5-1)(c_4-c_5),\\
d &= 2a_{54}c_4(c_4-1)(4c_4^2-3c_4c_5-5c_4+3c_5)-d_0.
\end{aligned}
$$

Simplification of level 4

Red coefficients can be expressed in terms of the others:

$$
\begin{array}{llllll}
c_2 & & & & & \\
c_3 & \color{red}{a_{32}} & & & & \\
c_4 & \color{red}{a_{42}} & \color{red}{a_{43}} & & & \\
c_5 & \color{red}{a_{52}} & \color{red}{a_{53}} & a_{54} & & \\
c_6 & \color{red}{a_{62}} & \color{red}{a_{63}} & \color{red}{a_{64}} & a_{65} & \\
c_7 & \color{red}{a_{72}} & \color{red}{a_{73}} & \color{red}{a_{74}} & a_{75} & \dots \\
c_8 & \color{red}{a_{82}} & \color{red}{a_{83}} & \color{red}{a_{84}} & a_{85} & \dots \\
 & & & \dots & &
\end{array}
$$

That is the number of the variables is reduced.
The number of equations (order conditions) is reduced too.
Indeed, only non-“maimed“ trees that is those that do not contain subtrees t_2 and t_6 are left.

Conclusion

1. The nature of the simplifying assumptions $C(2)$ and $D(1)$ is understood in a new way; they become a part of new systematic approach;
2. extending the approach to higher levels brings new simplifying assumptions. They reduce the number of variables and the number of equations.

Thank you!!!!