B-series

Algebraic analysis of numerical methods

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Outline

What are B-series?

The problem defined by the trio (y_0, f, h) can be used to ask various questions such as

1. What is the formal Taylor series of $y(x_0 + h)$ to the solution to the initial value problem

$$\begin{aligned} y'(x) &= f(y(x)), \\ y(x_0) &= y_0? \end{aligned}$$

2. What is the formal Taylor series of the numerical approximation computed by a Runge–Kutta method (A, b, c)?

The solution to each of these problems, and many closely related problems, can be written in the form

$$a(\varnothing)y_0 + \sum_{t\in T} a(t)\frac{h^{|t|}}{\sigma(t)}F(t),$$

where $a : \{\varnothing\} \cup T \to \mathbb{R}$ is characteristic of the particular question being asked.

These are B-series

But why are we doing this?

Because operations in analysis such as compositions, mapping inverses, conjugates and linear operations, all have exact counterparts in B-series manipulations.

We obtain a group (the “B-group") which corresponds to everything related to compositions.

And linear combinations of mappings correspond to linear combinations of B-series.

These combine to give us an algebra which can be used to analyse properties of numerical methods by analysing their algebraic counterparts.

Book chapters

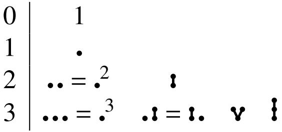
1. Differential equations, numerical methods and algebraic analysts
2. Trees and forests
3. B-series and algebraic analysis
4. Algebraic analysis and integration methods
5. B-series and Runge–Kutta methods
6. B-series and multivalue methods
7. B-series and geometric integration

Trees and forests: trees

Here are the first few trees along with their order, symmetry and factorial

$\lvert t\rvert$	t	$\sigma(t)$	$t!$
1		1	1
2		1	2
3		2	3
3		1	6
4		6	4
4		1	8
4		2	12
4		1	24

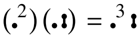
Here are some forests of increasing orders



alternative terminology

0	[0]
1	[1]
2	[2] [0, 1]
3	[3] [1, 1] [0, 0, 1] [0, 0, 0, 1]

examples of forest by forest multiplication



$$[2][0,0,1] = [2,0,1]$$

Composition and the B-group

Given two Runge–Kutta tableaux, R and R', we can consider three related constructs

RR', the product tableau

$\phi'_h \circ \phi_h$, the composition of the corresponding mappings

aa', the product of the corresponding B-series

Generalize to

$R\big(\sum_{i=1}^{n} c_i R_i\big)$,

$\big(\sum_{i=1}^{n} c_i \phi_{ih}\big) \circ \phi_h$,

$a\big(\sum_{i=1}^{n} c_i a_i\big)$

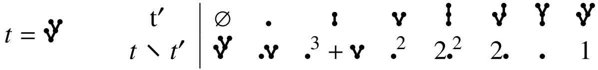
Composition and the B-group: Supertrees and subtrees

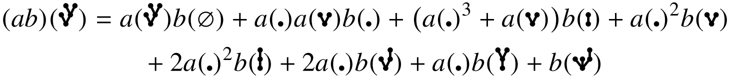
- We can prune elements from a tree to obtain a subtree.
- We can splice additional elements to a tree to obtain a supertree

Notation

- $t' \leq t$
- $t \setminus t'$

Example





left-distribution

$$a(C_1 b_1 + C_2 b_2) = C_1 a b_1 + C_2 a b_2$$

Composition and the B-group: Special members of B^*

- $\mathbf{i} \in \mathsf{B}$ corresponds to the identity map.
  Its value is

$$\begin{aligned} \mathbf{i}(\emptyset) &= 1, \\ \mathbf{i}(t) &= 0. \end{aligned}$$

- $\mathbf{E} \in \mathsf{B}$ corresponds to the flow of the solution through a step h.
  Its value is known to be

$$\mathbf{E}(t) = \frac{1}{t!}$$

- $\mathbf{D} \in \mathsf{B}^*$ corresponds to $y \mapsto hf(y)$.
  Its value is

$$\begin{aligned} \mathbf{D}(\emptyset) &= 0, \\ \mathbf{D}(\bullet) &= 1, \\ \mathbf{D}(t) &= 0, \qquad |t| > 1. \end{aligned}$$

Finally, introduce $\mathbf{O}_q \in \mathsf{B}^*$ corresponding to $O(h^q)$, so that $1 + \mathbf{O}_q$ is a normal subgroup of B.

Order conditions

For a Runge–Kutta method written in the form

$$
\begin{aligned}
Y_i &= y_0 + h \sum_{j=1}^{s} a_{ij} f Y_j), \qquad 1 \leq i s, \\
y(x_0 + h) &= y_0 + h \sum_{i=1}^{s} b_i f(Y_i) + O(h^{p+1}),
\end{aligned}
$$

we can use the corresponding B-series formulation

$$
\begin{aligned}
\eta &= \mathbf{i} + A\mathbf{D}\eta, \\
\mathbf{E} &= \mathbf{i} + b^{\mathsf{T}}\mathbf{D}\eta + \mathbf{O}_{p+1}.
\end{aligned}
$$

Analysis of a sixth order method: Structure of the method

The method G6245 [Butcher, Imran, Podhaisky (2017)], is G-symplectic with

- Order 6
- Stage order 2
- 4 values passed from step to step
- 5 stages

is characterized by 4 matrices $\begin{bmatrix} A & U \\ B & V \end{bmatrix}$ with A lower triangular with diagonal $[0, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, 0]$, and $\sigma(V) = \left\{ \pm 1, \pm\sqrt{-1} \right\}$.

The coefficients are chosen so that the parasitic growth factors are zero.

Simulations confirm that approximate symplectic behaviour is maintained for millions of time steps with deterioration at a rate comparable to the growth of rounding errors.

Analysis of a sixth order method: What is still needed

A difficult part of the implementation is the evaluation of starting methods

- Direct evaluation
- Low order direct evaluation with iterative refinement

The rather coarse evaluations in existing simulations still give remarkably effective results but more is needed.

We also need accurate multilength arithmetic to get the best out of the methods.

In future work along these lines, B-series will be needed.

This is one of many potential applications and I am confident that

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B-series are here to stay

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