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John C. Butcher

B-Series

Algebraic Analysis of Numerical Methods

Springer

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Foreword

In Spring 1965 I took part in a scientific meeting in Vienna, where I gave a talk on Lie derivatives and Lie series, research done together with Hans Knapp under the supervision of Wolfgang Gröbner at the University of Innsbruck. Right after, in the same session, was a talk by Dietmar Sommer from Aachen on a sensation: Implicit Runge–Kutta methods of **any** order, together with impressive numerical results and trajectory plots. Back in Innsbruck, the paper in question was quickly found in volume 18 of *Mathematics of Computation* from 1964, but not at all quickly understood. Definition, Definition, so-called “trees” were expressions composed of brackets and τ’s, Lemma, Proof, Lemma, Proof, Theorem, Proof, etc.

Apparently, another paper of John Butcher’s was required to stand a chance to understand it, but that paper was in the Journal of the Australian Mathematical Society, a journal almost completely unknown in Austria, at a time long before the internet when even access to a Xerox copying machine required permission from the Rektorat. John told me later that this paper had previously been refused for publication in *Numerische Mathematik* for its lack of practical interest, no Algol code, no impressive numerical results with thousands of digits, and no rigorous error bounds.

These two papers of Butcher brought elegance and order into the theory of Runge–Kutta methods. Earlier, these methods were very popular for practical applications; one of the first computers, ENIAC (Electronic Numerical Integrator and Computer), containing only a few “registers”, had mainly been built for solving differential equations using a Runge–Kutta method. The very first program which G. Dahlquist wrote for the first Swedish computer was a Runge–Kutta code. But not much theoretical progress had been achieved in these methods after Kutta’s paper from 1901. For example, the question whether a fifth order method can be found with only five stages was open for half a century, until Butcher had proved that such methods were impossible.

The next sensation came when, “at the Dundee Conference in 1969, a paper by J. Butcher was read which contained a surprising result” [1]. The idea of combining

[1] H. J. Stetter 1971

different fourth order methods with five stages in such a way, that their **composition** leads to a fifth order numerical result, culminated in Butcher's **algebraic** theory of integration methods, first accessible as a preprint with beautiful Māori design, then published in an accessible journal, but which was "admirantur plures quam intelligant" [2].

Fortunately, in the academic year 1968/69 I had the chance to deliver a first year Analysis course in Innsbruck, where a couple of very brilliant students continued to participate in a subsequent seminar on Numerical Analysis, above all Ernst Hairer, in whose hand this Māori-design preprint eventually arrived. Many months later, Ernst suddenly came to me and said: "Iatz hab i's verstandn"[3].

But to push all these Runge–Kutta and generalized Runge–Kutta spaces into a brain that has worked for years on Lie series and Taylor series, was another adventure. The best procedure was finally to bring the algebraic structures directly into the series themselves. So we arrived at the composition of B-series.

Gerhard Wanner

[2] more admired than understood, (A. Taquet 1672)

[3] now I have understood it

Preface

The term “B-series”, also known as “Butcher series”, was introduced by Ernst Hairer and Gerhard Wanner [52] (1974).

In 1970, I was invited to visit the University of Innsbruck to give a series of lectures to a very talented audience, which included Ernst and Gerhard. At that time, my 1972 paper [14] had not been published, but a preprint was available. A few years later the important Hairer–Wanner paper [52] appeared .

“B-series” refers to a special type of Taylor series associated with initial-value problems

$$y'(x) = f\big(y(x)\big), \qquad y(x_0) = y_0,$$

and the need to approximate $y(x_0 + h)$, with h a specified “stepsize”, using Runge–Kutta and other numerical methods.

The formal Taylor series of the solution about the initial point x_0 is a sum of terms containing two factors:

(i) a factor related to a specific initial value problem; and
(ii) a coefficient factor which is the same for each initial value problem.

If, instead of the *exact solution* to an initial value problem, it is required to find the Taylor series for an *approximate solution*, calculated by a specific Runge–Kutta method, the terms in (i) are unchanged, but the coefficients in (ii) are replaced by a different sequence of coefficients, which are characteristic of particular Runge–Kutta methods.

This factorization effectively divides mathematical questions, about initial value problems and approximate solutions, into two components: questions about f analytical in nature, and essentially algebraic questions concerning coefficient sequences. An important point to note is that, in the various Taylor series, the terms in the sequences are best not thought of in terms of indices $0, 1, 2, 3, 4, \ldots$, but in terms of graph-theoretic indices: $\varnothing$, $\ldots$ The sequence of graphs which appears here consists of the empty tree, followed by the sequence of all rooted trees.

The significance of trees in mathematics was pointed out by Arthur Cayley [28] (1857), and the name “tree”, referring to these objects, is usually atributed to him.

The use of trees in the analysis of Runge–Kutta methods seems to have been due to S. Gill [45] (1951), and then by R. H. Merson [72] (1957). The present author has also developed these ideas [7, 14] (1963, 1972), leading to the use of group and other algebraic structures in the analysis of B-series coefficients. The Butcher group, referred to in this volume as the “B-group”, is central to this theory, and is related to algebraic structures with applications in Physics and Geometry – see [4], (Brouder, 2000).

Chapter 1 is a broad and elementary introduction to differential equation systems and numerical methods for their solution. It also contains an introduction to some of the topics included in later chapters. Chapter 2 is concerned with trees and related graphical structures.

B-series, with further properties, especially those associated with compositions of series, are introduced in Chapter 3

Properties of the B-group are explored in Chapter 4. This chapter is also concerned with “integration methods” in the sense of [14]. Integration methods were intended as a unifying theory that includes Runge–Kutta methods, with a finite number of stages, and continuous stage Runge–Kutta methods, such as in the kernel of the Picard–Lindelöf theorem – see for example [30] (Coddington and Levinson, 1957).

Chapter 5 deals with Runge–Kutta methods with an emphasis on the B-series analysis of these methods. Multivalue methods are the subject of Chapter 6. This includes linear multistep methods and so-called “general linear methods”. In these general linear methods, multistage and multivalue aspects of numerical methods fit together in a balanced way. In the final Chapter 7, the B-series approach is applied to limited aspects of the burgeoning subject of Geometric Integration.

In addition to exercises scattered throughout the book, especially in the early chapters, a number of substantial “projects” are added at the end of each chapter. Unlike the exercises, the projects are open-ended and of a more challenging nature and no answers are given to these.

Throughout the volume, a number of algorithms have been included. As far as I am aware, the first B-series algorithm was composed by Jim Verner and myself on 1 January 1970. A shared interest in related algorithms has been maintained between us to this day.

Amongst the many people who have taken an interest in this work, I would like to mention four people who have read all or part of the text and given me detailed advice. I express my gratitude for this valuable help to Adrian Hill, Yuto Miyatake, Helmut Podhaisky and Shun Sato. Special thanks to Tommaso Buvoli, Valentin Dallerit, Anita Kean and Helmut Podhaisky, who are kindly working with me on the support page.

Support page

A support page for this book is being developed at

`jcbutcher.com/B-series-book`

Amongst other information, the Algorithms in the book will be re-presented as procedures or functions in one or more standard languages. The support page will also contain some informal essays on some of the broad topics of the book.

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