Structure of B-series for some classes of geometric integrators

Elena Celledoni*, Robert I. McLachlan†, Brynjulf Owren* and GRW Quispel**

*Department of Mathematical Sciences, NTNU, N-7491 Trondheim, Norway
†Institute of Fundamental Sciences, Massey University, Palmerston North, New Zealand
**Mathematics Department, La Trobe University, VIC 3086 Australia

Abstract.
The characterizations of B-series of symplectic and energy preserving integrators are well-known. The graded Lie algebra of B-series of modified vector fields include the Hamiltonian and energy preserving classes as Lie subalgebras, these spaces are relatively well understood. However, two other important classes are the integrators which are conjugate to Hamiltonian and energy preserving methods respectively. The modified vector fields of such methods do not form linear subspaces and the notion of a grading must be reconsidered. We suggest to study these spaces as filtrations, and viewing each element of the filtraton as a trivial vector bundle whose typical fiber replaces the graded homogeneous components. In particular, we shall study properties of these fibers, a particular result is that, in the energy preserving case, the fiber of degree n is a direct sum of the nth graded component of the Hamiltonian and energy preserving space. We also give formulas for the dimension of each fiber, thereby providing insight into the range of integrators which are conjugate to symplectic or energy preserving.

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INTRODUCTION

In recent years the conservation of geometric properties in numerical integrators has attracted a lot of interest. Examples of such geometric properties are symplecticity, preservation first integrals, and volume preservation. For Runge-Kutta methods some early and important results were: They conserve all linear invariants and there exists a subclass of methods which conserves quadratic invariants and symplecticity. No Runge-Kutta method conserves volume for every divergence free vector field. More recently, much attention has been given to a more general class of integrators which include the Runge-Kutta methods as a subclass. These are in general the schemes which can be expanded in a *B*-series, see e.g. [6]. Several classes of integration methods belong to this class, usual denoted *B*-series methods, but one should keep in mind that not every *B*-series corresponds to a scheme of a known format. In particular, the exact solution of the ODE system can be expanded in a *B*-series. In the sequel we shall mostly consider properties of *B*-series without paying particular attention to whether each series correspond to a computable integration scheme. This approach was taken for instance in [3, 4, 5] where results similar to those mentioned above for Runge-Kutta methods were proved in more generality. An important result was that for canonical Hamiltonian problems there exists a large class of *B*-series schemes which preserve the Hamiltonian. Later, it was observed by Quispel and McLaren [7] that the Averaged Vector Field (AVF) method is energy preserving for Hamiltonian problems. This scheme is defined as

$$y^{n+1} = y^n + h\int_0^1 f((1-\xi)y^n + \xi y^{n+1})\,\mathrm{d}\xi$$

when applied to autonomous ODEs $y' = f(y)$. Note that the integral in the AVF method is calculated on the interval $[0,1]$ for a real variable ξ. For many known Hamiltonian problems, this integral can be computed exactly a priori.

Insisting on the preservation of geometric structure in numerical integrators may sometimes cause the resulting schemes to be somewhat computational expensive or may alternatively exclude integrators that we know from experience has good long term properties. It may therefore be advantageous to relax on the preservation principle by allowing for *conjugacy*. For an integrator represented as a map ϕ_h, one may take any consistent integrator χ_x and construct the conjugate scheme $\bar{\phi}_h = \chi_h \circ \phi_h \circ \chi_h^{-1}$. Applying this new scheme over N time steps results in the approximation $\bar{\phi}_h^n = \chi_h \circ \phi_h^n \circ \chi_h^{-1}$ showing that the long term behaviour of two conjugate methods do not depend on the number of time steps taken. It is of interest to understand the structure and richness of integrators which are conjugate to symplectic or energy preserving, and this will be discussed in what remains of this paper.

PRELIMINARIES

Through backward error analysis, we here represent every scheme by its modified equation, thus our focus is the set of *B*-series of the form

$$\sum_{t\in T}\frac{h^{|t|}}{\sigma(t)}b(t)F(t) \tag{1}$$

where T is the set of rooted trees, $|t|$ is the number of vertices in t, $\sigma(t)$ is the symmetry coefficient and $F(t)$ is the vector field represented by the elementary differential corresponding to the tree t. For details, see e.g. [1, 6] . The Lie bracket between two vector fields $F(u)$ and $F(v)$ yields another vector field which is a linear combination of vector fields $F(t)$ where $|t| = |u| + |v|$, and this naturally induces a graded Lie algebra on the $\mathbb{R}$-linear space having T as basis, henceforth denoted $\mathscr{T}$. For $u, v \in T$, one defines $[\![u,v]\!] \in \mathscr{T}$ by adding together all trees obtained by grafting u on each vertex of v and then subtracting all trees obtained by grafting v on each vertex of u. $\mathscr{T}$ is decomposed into homogeneous components $\mathscr{T}^n$ by the grading: $\mathscr{T}^n = \mathrm{span}\{t \in T : |t| = n\}$. Thus $\mathscr{T} = \mathscr{T}^1 \oplus \mathscr{T}^2 \oplus \cdots$. The *B*-series corresponding to symplectic methods are those whose modified equation is Hamiltonian, this is a linear subspace of $\mathscr{T}$, in fact even a graded Lie subalgebra, we denote it by $\mathscr{T}_\Omega$ and its graded components $\mathscr{T}_\Omega^n \subseteq \mathscr{T}^n$. Similarly, we may consider methods ϕ_h which preserve the Hamiltonian, i.e. $H(y) = H(\phi_h(y))$ for all y in phase space. Assuming that ϕ_h has a modified vector field, we shall say that this belongs to the space $\mathscr{T}_H$. This space is also a graded linear subspace of $\mathscr{T}$, with graded components $\mathscr{T}_H^n \subset \mathscr{T}^n$.

CONJUGATE SPACES

We now consider B-series that are conjugate (by a B-series) to an energy-preserving or a Hamiltonian B-series. Such B-series do not form linear spaces, but some of their properties—e.g., their dimension—can be described using two new linear spaces that we shall call $\mathscr{T}_{\widetilde{H}}^n$ and $\mathscr{T}_{\widetilde{\Omega}}^n$.

Let in general U and V be graded subspaces of $\mathscr{T}$ such that

$$U = \bigoplus_{n>0} U^n, \qquad V = \bigoplus_{n>0} V^n, \qquad U^n = \mathscr{T}^n \cap U, \quad V^n = \mathscr{T}^n \cap V$$

We study elements of $\mathscr{T}$ which are conjugations of elements of V by elements in U, following [2] we must then consider the set

$$\mathscr{M} = \{w = \exp(-\mathrm{ad}_u)\,v,\ u \in U, v \in V\}$$

where

$$w = \exp(-\mathrm{ad}_u)\,v = v - [\![u,v]\!] + \frac{1}{2}\,[\![u,[\![u,v]\!]]\!] + \cdots \tag{2}$$

$\mathscr{M}$ is not a graded linear subspace of $\mathscr{T}$ so we can not work with graded components as before. Instead we define a filtration through the quotient

$$G^n = \mathscr{T} / \bigoplus_{k>n} \mathscr{T}^k$$

We let $\mathscr{P}_n : \mathscr{T} \to G^n$ be the canonical projection and we consider the manifolds $\mathscr{M}^n = \mathscr{P}_n\mathscr{M}$ and their dimensions. We introduce the spaces $\mathscr{B}^n \subseteq G^n$ through

$$\mathscr{B}^n = \left\{ w = \mathscr{P}_n \exp(-\mathrm{ad}_u)v,\ u \in \bigoplus_{k\le n-2} U^k,\ v \in \bigoplus_{k\le n-1} V^k \right\}$$

In fact, due to the grading on $\mathscr{T}$, we could have written $\mathscr{M}^n$ in a similar way, just replacing the lower index bound in each direct sum by $n-1$ and n respectively. From this point, we assume $\bullet \in V$, and we consider only series $v = \sum v^k$,

$v^k \in V^k$, such that $v^1 = \bullet$. Define the projection $\pi : \mathscr{M}^n \to \mathscr{B}^n$ obtained simply by removing the $n-1$-component of u and the n-component of v. Precisely, if

$$w = \mathscr{P}_n \exp(-\mathrm{ad}_u)v, \quad u = \sum_{k=1}^{n-1} u^k, \quad v = \bullet + \sum_{k=2}^{n} v^k,$$

then

$$\pi w = \mathscr{P}_n \exp(-\mathrm{ad}_{\bar{u}})\bar{v}, \quad \bar{u} = \sum_{k=1}^{n-2} u^k, \quad \bar{v} = \bullet + \sum_{k=2}^{n-1} v^k.$$

The triple $(\mathscr{M}^n, \mathscr{B}^n, \pi)$ forms a vector bundle with total space $\mathscr{M}^n$, base space $\mathscr{B}^n$ and projection π. The typical fiber is $F^n = \pi^{-1}(x)$, and by construction this space is obtained simply by considering all terms of (2) which depend only on the $n-1$-component of u and the n-component of v,

$$F^n = V^n + [\![U^{n-1}, \bullet]\!].$$

Using the natural identification of G^n with $\mathscr{T}^1 \oplus \cdots \oplus T^n$ it is easy to see that $\dim \mathscr{B}^n = \dim \mathscr{M}^{n-1}$, thus,

$$\dim \mathscr{M}^n = \dim \mathscr{B}^n + \dim F^n = \dim \mathscr{M}^{n-1} + \dim F^n$$

so that the dimension of $\mathscr{M}^n$ is obtained by summing up the dimensions of each F^k for $k = 1, \ldots, n$.

One may say that the fibers F^k play a similar role for the conjugate spaces as do the graded components $\mathscr{T}^n_\Omega$ and $\mathscr{T}^n_H$ for the Hamiltonian and energy preserving vector fields respectively. In our application we choose V to be either of $\mathscr{T}_\Omega$ or $\mathscr{T}_H$. The spaces we use conjugate with can in principle be $\mathscr{T}$ in both cases, but we find it reasonable to choose U to be a complement of $\mathscr{T}_\Omega$ in the Hamiltonian case and a complement of $\mathscr{T}_H$ in the energy preserving case. We denote such complements $\mathscr{T}'_\Omega$, $\mathscr{T}'_H$ respectively. The corresponding manifold $\mathscr{M}$ is characterized in terms of the bundles $(\mathscr{M}^n, \mathscr{B}^n, \pi)$ and the fibers F^n are denoted $\mathscr{T}^n_{\tilde{\Omega}}$, $\mathscr{T}^n_{\tilde{H}}$ respectively.

MAIN RESULTS

The results presented here are mostly taken from [2] and are presented without proofs. The reader may keep in mind that there are three important properties of the map $\mathrm{ad}_\bullet : t \mapsto [\![\bullet, t]\!]$ underlying many of the results used to characterize the conjugate fibers $\mathscr{T}^n_{\tilde{\Omega}}$ and $\mathscr{T}^n_{\tilde{H}}$. The first is that $\mathrm{ad}_\bullet$ is injective on $\mathscr{T}^n$, $n > 1$. The second is that $\mathrm{ad}_\bullet^{-1}(\mathscr{T}^{n+1}_\Omega) \subseteq \mathscr{T}^n_\Omega$ (and similarly with $\mathscr{T}_\Omega$ replaced by $\mathscr{T}_H$). The third an explicitly given decomposition of $\mathrm{ad}_\bullet(\tau)$ into the sum of two elements of $\mathscr{T}_\Omega$ and $\mathscr{T}_H$.

Theorem 1 *The dimension of* $\mathscr{T}^n_{\tilde{H}}$ *is*

$$\dim \mathscr{T}^n_{\tilde{H}} = \dim \mathscr{T}^n_H + \dim \mathscr{T}^{n-1} - \dim \mathscr{T}^{n-1}_H.$$

Theorem 2 *For* $n > 2$,

$$\mathscr{T}^n_{\tilde{H}} = \mathscr{T}^n_\Omega \oplus \mathscr{T}^n_H$$

Theorem 3 $\mathscr{T}_{\tilde{\Omega}} \subset \mathscr{T}_{\tilde{H}}$.

Theorem 4

(i) *From the four naturally-defined subspaces of B-series, namely* $\mathscr{T}^n_\Omega$, $\mathscr{T}^n_H$, $\mathscr{T}^n_{\tilde{\Omega}}$, *and* $\mathscr{T}^n_{\tilde{H}}$, *precisely one new subspace can be constructed using the natural subspace operations of intersection and sum. This is* $\mathscr{T}^n_{\tilde{\Omega}} \cap \mathscr{T}^n_H$, *the* energy-preserving conjugate-to-Hamiltonian *B-series.*

(ii) $\mathscr{T}^n_{\tilde{\Omega}} \cap \mathscr{T}^n_H$ *is isomorphic to* $\mathscr{T}^{n-1\prime}_\Omega$, *and an isomorphism is given by the map*

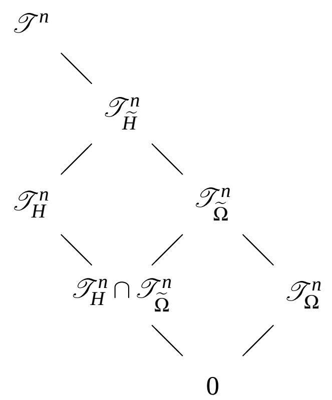
$$\mathscr{T}^{n-1\prime}_\Omega \to \mathscr{T}^n_{\tilde{\Omega}} \cap \mathscr{T}^n_H, \qquad t \mapsto [\![t, \bullet]\!] - X_{[t]} \tag{3}$$

(iii) *Its dimension is*

$$\dim \mathscr{T}^n_{\tilde{\Omega}} \cap \mathscr{T}^n_H = \dim \mathscr{T}^{n-1} - \dim \mathscr{T}^{n-1}_\Omega$$

(iv) There are B-series that are energy-preserving and conjugate-to-Hamiltonian, but are not the (reparameterized) flow of the original differential equation.

Theorem 5 *The (Hasse) order diagram under inclusion for the linear spaces $\mathscr{T}^n$, $\mathscr{T}^n_H$, $\mathscr{T}^n_\Omega$, $\mathscr{T}^n_{\tilde{H}}$, and $\mathscr{T}^n_{\tilde{\Omega}} \cap \mathscr{T}^n_H$ for $n > 2$ is*



and their dimensions up to order 10 are as given in Table 1. For $n = 1$ all these spaces are equal to $\mathrm{span}(\bullet)$*, while for $n = 2$ we have $\mathscr{T}^2 = \mathrm{span}([\bullet])$ and $\mathscr{T}^2_H = \mathscr{T}^2_\Omega = \mathscr{T}^2_{\tilde{H}} = \mathscr{T}^2_{\tilde{\Omega}} = \mathscr{T}^2_{\tilde{\Omega}} \cap \mathscr{T}^2_{\tilde{H}} = 0$.*

TABLE 1. Dimensions of the linear spaces spanned by the rooted trees and their 5 natural subspaces.

order	1	2	3	4	5	6	7	8	9	10
$\dim \mathscr{T}^n$	1	1	2	4	9	20	48	115	286	719
$\dim \mathscr{T}^n_\Omega$	1	0	1	1	3	4	11	19	47	97
$\dim \mathscr{T}^n_H$	1	0	1	1	5	9	29	68	189	484
$\dim \mathscr{T}^n_{\tilde{\Omega}}$	1	0	2	2	6	10	27	56	143	336
$\dim \mathscr{T}^n_{\tilde{H}}$	1	0	2	2	8	13	40	87	236	581
$\dim(\mathscr{T}^n_{\tilde{\Omega}} \cap \mathscr{T}^n_H)$	1	0	1	1	3	6	16	37	96	239

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