On B-series and their structure-preserving properties.

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Hairer60, June 18th 2009
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Outline

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   - B-series
   - Structure preserving B-series

2. Modified vector fields
   - Energy-preserving and Hamiltonian modified vector fields
   - Linear subspaces of Hamiltonian and energy-preserving B-series

3. Dimensions and annihilators

4. Conjugate B-series

5. Energy preserving conjugate-Hamiltonian B-series (EPCH)
\[ \dot{y} = f(y), \]

where \( y \) lies in a vector space, we consider numerical integrators \( y \mapsto \Phi_h(y) \) that have B-series

\[
\Phi_h(y) = \left[ \text{id} + hf + h^2 a(\bullet) f'(f) + h^3 \left( \frac{1}{2} a(\triangledown) f''(f, f) + a(\bullet) f'(f(f)) \right) + \ldots \right](y)
\]

\[
= \sum_{\tau \in T \cup \emptyset} h^{\vert \tau \vert} \frac{a(\tau)}{\sigma(\tau)} F(\tau)(y)
\]

\[ T := \{ \bullet, \triangledown, \bar{\bullet}, \bar{\triangledown}, \cdot, \ldots \} \quad \text{set of rooted trees}, \]

\[ T^n \quad \text{trees of order } n, \]

\[ |\tau| \quad \text{number of nodes of } \tau, \]

\[ \sigma(\tau) \quad \text{the symmetry of } \tau, \]

\[ F(\tau) \quad \text{elementary differential of } \tau: \]

\[ F(\bullet) = f, \quad F(\bar{\bullet}) = f' f, \quad F(\triangledown) = f''(f, f), \quad F(\bar{\triangledown}) = f' f' f, \quad \ldots \]

\[ T = \bigoplus_{n=1}^{\infty} T^n \]
Find a differential equation whose solution at \( t = t_n \) is the numerical approximation \( y_n \).

\[
\begin{align*}
\text{numerical} & \quad \dot{y} = f(y) & \text{exact} \\
y_n = \phi_h(y_{n-1}) & \quad y(t_n) = \varphi_{t_n}(y_0) \\
\dot{\tilde{y}} = f_h(\tilde{y}) & \quad \tilde{y}(0) = y_0 \\
s.t. \tilde{y}(t_n) = y_n
\end{align*}
\]

**Modified vector field (MVF)**

\[
f_h(\tilde{y}) = f(\tilde{y}) + hf_2(\tilde{y}) + h^2f_3(\tilde{y}) + \cdots = \sum_{\tau \in T \cup \emptyset} h^{\left|\tau\right|} \frac{a(\tau)}{\sigma(\tau)} F(\tau)(y).
\]

\( \phi_h(y), \varphi_{t_n}(y_0), f_h(\tilde{y}) \) and \( f(y) \) have a B-series.
Consider
\[ \dot{y} = f(y) = \Omega^{-1} \nabla H(y), \quad \Omega^T = -\Omega, \quad \det(\Omega) \neq 0, \quad \Omega \text{ constant}. \]

Energy is preserved along solutions: \[ \frac{dH(y(t))}{dt} = \nabla H^T \Omega^{-1} \nabla H = 0. \]

Symplecticity of the flow: for \( \psi(t) := \frac{\partial \varphi_t(y_0)}{\partial y_0} \) one has \( \psi^T \Omega^{-1} \psi = \Omega^{-1} \).
Consider
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### Definitions

The energy-preserving subspace (of order \( n \)) is defined by
\[ T^n_H := \{ t \in T^n : F(t) \text{ has first integral } H \text{ when } f = \Omega^{-1} \nabla H \} \]

The Hamiltonian subspace (of order \( n \)) is defined by
\[ T^n_\Omega := \{ t \in T^n : F(t) \text{ is Hamiltonian w.r.t } \Omega^{-1} \text{ when } f = \Omega^{-1} \nabla H \} \]

\[ T_H = \bigoplus_{n=1}^{\infty} T^n_H \quad T_\Omega = \bigoplus_{n=1}^{\infty} T^n_\Omega \]

and \( F(T^n_{(H,\Omega)}) \) is the set of B-series of modified vector fields.
Butcher product and free trees

A recursive representation of trees is given as follows:

\[
t \in T = \begin{cases} 
    \bullet = [\emptyset] \\
    [t_1, \ldots, t_n]
\end{cases}
\]

\([t_1, \ldots, t_n]\) obtained by joining the roots of each tree \(t_i\) to a new common root, thus \(|t| = 1 + \sum_i |t_i|\).

Elementary differentials:
\[F(\bullet) = f, \ F(t)(y) = f^{(m)}(y)(F(t_1), \ldots, F(t_m)), \ t = [t_1, \ldots, t_n].\]

The Butcher product: let \(u = [u_1, \ldots, u_n]\) and \(v \in T\) is defined as

\[u \circ v = [u_1, \ldots, u_n, v], \quad u \circ v \neq v \circ u.\]

Consider the equivalence relation \(u \sim v\) iff \(u\) and \(v\) have the same graph, and differ only in the position of the root.\(^1\) Each equivalence class is called a free tree.

\(^1\) the smallest equivalence relation satisfying \(u \circ v \sim v \circ u\) for every \(u, v \in T\).
Free trees

Two equivalent trees have the same graph, and differ only in the position of the root.

Example

The trees with 4 nodes are $\frac{1}{6}$, $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$, there are two free trees (two equivalence classes):

$\{\begin{array}{c} Y, \quad \mathcal{Y} \end{array}\}$, and $\{\begin{array}{c} V, \quad \mathcal{Y} \end{array}\}$.

A free tree is called **superfluous** if one of the elements in the class can be factorized as $u \circ u$.

Example

$$v = \mathcal{1} \circ 1$$

the free tree $\{\begin{array}{c} v, \quad 1 \end{array}\}$ is superfluous.
Calvo and Sanz-Serna ’94 (Num. Math.) characterization of the canonical B-series (i.e. corresponding to symplectic transformations).

If $V \subset \mathcal{T}$ is a linear subspace of $\mathcal{T}$, denote $\text{Ann}(V) = \{ u^* \in \mathcal{T}^* \mid u^*(v) = 0, \forall v \in V \}$ annihilator of $V \subset \mathcal{T}$, and $u^*(v) = \delta_{u,v}$ for $u$ and $v$ in $\mathcal{T}$.

- $\text{Ann}(\mathcal{T}_\Omega^n) = \text{span}\{(u \circ v)^* + (v \circ u)^* : u, v \in \mathcal{T}, |u| + |v| = n\}$

order 4 trees

$$(\circ Y)^* + (Y \circ \bullet)^* = Y^* + Y^*, \ (\bullet \circ \bullet)^* + (\bullet \circ \bullet)^* = V^* + I^*, \ (\bigcirc \bigcirc)^* = V^*$$

the Hamiltonian tree of order 4 is $3Y - V$.

- $|\mathcal{T}_\Omega^n|$ is the number of nonsuperfluous free trees with $n$ nodes.

(See also GI book by Hairer, Lubich and Wanner).
Energy-preserving B-series $\mathcal{T}_H = \oplus \mathcal{T}_H^n$

Faou, Hairer and Pham 2004.

A basis for $\text{Ann}(\mathcal{T}_H^n)$ depends on the nonsuperfluous free trees with $n + 1$ nodes:

$$
\text{Ann}(\mathcal{T}_H^n) = \text{span}\left\{ \sum_{\tau \in \pi^{-1}(\phi) \atop \tau = [\bar{\tau}]} (-1)^{\kappa(\tau_0, \tau)} \frac{1}{\sigma(\tau)} \bar{\tau}^* : \phi \in FT^{n+1}, \ \phi \ \text{nonsuperfluous} \right\}
$$

where $\tau_0$ is a designated element of $\pi^{-1}(\phi)$. The sum is taken over all trees $\tau \in \pi^{-1}(\phi)$ having precisely one subtree.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\tau_0 \in T^{n+1}$</th>
<th>basis of $\text{Ann}(\mathcal{T}_H^n)$</th>
<th>EP trees</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$\bullet$</td>
<td>$\bullet^*$</td>
<td>$\cdot$</td>
</tr>
</tbody>
</table>

- $|\mathcal{T}_H^n| = |\mathcal{T}^n| - |\mathcal{T}_\Omega^{n+1}|$
- $\mathcal{T}_\Omega \cap \mathcal{T}_H = \cdot$

The only symplectic B-series that conserves the Hamiltonian for arbitrary $H$ is the scaled exact flow of the original differential equation. (Chartier, Faou, Murua 06). See also Ge and Marsden 1988.
Energy-preserving B-series

Quispel and McLaren 2008.

\[ t + (-1)^m \hat{t} \quad t \in T^n \]

and

\[ t = \ldots \quad \text{and} \quad \hat{t} = \ldots \]

For order 4

\[ \Psi + \Psi, \quad \Psi - \Psi = 0, \quad 1 - 1 = 0 \]

We proved that this is a system of generators of

\[ T^n_H = \text{span}\{ t + (-1)^m \hat{t} \mid t \in T^n \}. \]
Conjugate to symplectic and conjugate to energy-preserving B-series

An integration method $\Phi_h$ is conjugate-symplectic if it $\exists \Psi$ s.t. $\Psi \Phi_h \Psi^{-1}$ is symplectic (it preserves the symplectic form $(\Psi^{-1})^* \Omega$). Assume $c$ is a B-series and $\Psi = e^c$ is the corresponding flow. Assume $\hat{f}$ is an Hamiltonian B-series and $\tilde{f}$ a conjugate-Hamiltonian B-series such that

$$e^c e^{\tilde{f}} e^{-c} = e^{\hat{f}},$$

we are interested in the case $c$ is non-Hamiltonian. Characterization of conjugate-Hamiltonian B-series

$$\{ \tilde{f} \mid e^{\tilde{f}} = e^{-c} e^{\hat{f}} e^c \},$$

$$\tilde{f} = e^{-\text{ad}_c}(\hat{f}) = \hat{f} - [c, \hat{f}] + \frac{1}{2} [[c, [c, \hat{f}]]] - \ldots, c \in T, \hat{f} \in T\Omega,$$

and $[\cdot, \cdot]$ is the Lie bracket of vector fields. It induces a bracket on $T$ via the elementary differentials

$$[[F(u), F(v)] = F([u, v])$$

and $[u, v] = (\text{attach } u \text{ to all nodes of } v) - (\text{attach } v \text{ to all the nodes of } u)$.
\[ \mathcal{M} = \{ e^{-\text{ad}_c(\hat{f})}, \ c \in U, \ \hat{f} \in V \}, \quad U = \bigoplus_{n \geq 0} U^n, \quad V = \bigoplus_{n \geq 0} V^n, \ U, V \subset \mathcal{T}. \]

\[ G^n = \mathcal{T} / \bigoplus_{k > n} \mathcal{T}^k, \quad \mathcal{P}^n : \mathcal{T} \mapsto G^n, \quad \mathcal{M}^n := \mathcal{P}^n \mathcal{M}, \]

\[ \mathcal{M}^n = \{ w = \mathcal{P}^n \exp(-\text{ad}_c)(\hat{f}), \ c \in \bigoplus_{k \leq n-1} U^k, \ \hat{f} \in \bigoplus_{k \leq n} V^k \}. \]
Conjugate B-series CH and CEP

\[ \mathcal{M} = \{ e^{-\text{ad}_c}(\hat{f}), \ c \in U, \ \hat{f} \in V \}, \quad U = \bigoplus_{n \geq 0} U^n \quad V = \bigoplus_{n \geq 0} V^n, \ U, V \subset \mathcal{T}. \]

\[ G^n = \mathcal{T} / \bigoplus_{k > n} \mathcal{T}^k, \quad \mathcal{P}^n : \mathcal{T} \mapsto G^n, \quad \mathcal{M}^n := \mathcal{P}^n \mathcal{M}, \]

\[ \mathcal{M}^n = \{ w = \mathcal{P}^n \exp(-\text{ad}_c)(\hat{f}), \ c \in \bigoplus_{k \leq n-1} U^k, \ \hat{f} \in \bigoplus_{k \leq n} V^k \}. \]

**Structure of vector bundle on \( \mathcal{M}^n \):**

\[ \mathcal{B}^n := \{ w = \mathcal{P}^n \exp(-\text{ad}_c)(\hat{f}), \ c \in \bigoplus_{k \leq n-2} U^k, \ \hat{f} \in \bigoplus_{k \leq n-1} V^k \}, \]

\[ \mathcal{M}^{n-1} = \mathcal{P}^{n-1} \mathcal{B}^n \text{ and } \pi : \mathcal{M}^n \mapsto \mathcal{B}^n \text{ the projection. Then } (\mathcal{M}^n, \mathcal{B}^n, \pi) \text{ is a vector bundle, } b \in \mathcal{B}^n \]

\[ \pi^{-1}(b) = F^n = V^n + [U^{n-1}, \bullet], \]

\[ |\mathcal{M}^n| = |\mathcal{B}^n| + |F^n| = |\mathcal{M}^{n-1}| + |F^n| \]
We look at the linear spaces

\[ V^n + [U^{n-1}, \cdot], \quad \left\{ \begin{array}{ll}
V^n = T^n_\Omega, & U^{n-1} = T^{n-1} \quad \text{CH} \\
V^n = T^n_H, & U^{n-1} = T^{n-1} \quad \text{CEP.}
\end{array} \right. \]

Preliminaries.

**Lemma** \( \text{ad}_\cdot = [\cdot, \cdot] : T^n \hookrightarrow T^{n+1} \) is injective for \( n > 1 \).

Assume

\[ X : T^{n-1} \hookrightarrow T^n_\Omega, \]

\( X(t) \) is the Hamiltonian combination of trees associated to \([t]\) and

\[ \text{EP} : T^{n-1} \hookrightarrow T^n_H, \quad \text{EP}(\tau) = [\tau, \cdot] - X(\tau). \]

**Lemma** \( \text{ad}_\cdot(T^{n-1}) = X(T^{n-1}) \oplus \text{EP}(T^{n-1}). \)
A symplectic B-series is formally conjugate to a B-series which preserves the Hamiltonian exactly.

We look at the linear space of conjugate to energy preserving B-series (CEP)

\[
\mathcal{T}_H^n := \mathcal{T}_H^n + \mathcal{T}_H^{n-1}, \quad V^n = \mathcal{T}_H^n, \quad U^{n-1} = \mathcal{T}_H^{n-1}
\]

\(X : \mathcal{T}_H^{n-1} \mapsto \mathcal{T}_\Omega^n\), surjective and \(\text{ad}_X(\mathcal{T}_H^{n-1}) = X(\mathcal{T}_H^{n-1}) \oplus \text{EP}(\mathcal{T}_H^{n-1})\), then

**Theorem**

\[
\mathcal{T}_H^n = \mathcal{T}_H^n \oplus X(\mathcal{T}_H^{n-1}) = \mathcal{T}_H^n \oplus \mathcal{T}_\Omega^n, \quad n > 2,
\]

its dimension is \(|\mathcal{T}_H^n| = |\mathcal{T}_\Omega^n| + |\mathcal{T}_H^n|\).

\(\mathcal{T}_\Omega \subset \mathcal{T}_H\)
Existence of energy-preserving and conjugate to Hamiltonian B-series (EPCH)

For conjugate to energy-preserving

$$T^n_H = T^n_H \oplus T^n_\Omega, \ n > 2, \ \text{CEP.}$$

We look at the linear space of conjugate to Hamiltonian B-series

$$V^n + [U^{n-1}, \cdot] \quad V^n = T^n_\Omega, \quad U^{n-1} = T^{n-1},$$

$$T^n_\tilde{\Omega} := T^n_\Omega + [T^{n-1}, \cdot] \ \text{CH}$$

Theorem

1. $$T^n_\tilde{\Omega} = T^n_\Omega \oplus \text{EP}(T^{n-1})$$
   its dimension is $$|T^n_\tilde{\Omega}| = |T^n_\Omega| + |T^{n-1}| - |T^{n-1}_\Omega|.$$

2. $$T^n_\tilde{\Omega} \cap T^n_H = \text{EP}(T^{n-1}), \ \text{EPCH}$$
   its dimension is $$|T^n_\tilde{\Omega} \cap T^n_H| = |T^n_\Omega| - |T^n_\Omega| = |T^{n-1}| - |T^{n-1}_\Omega|.$$
Main result: EPCH has positive dimension for $n > 2$.

So

$$T^n_\tilde{\Omega} \cap T^n_H = \text{EP}(T^{n-1}),$$

and

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

This vector space has positive dimension for $n > 2$:
Main result: EPCH has positive dimension for $n > 2$. 

So

$$\mathcal{T}_\tilde{\Omega}^n \cap \mathcal{T}_H^n = \text{EP}(\mathcal{T}^{n-1}),$$

and

$$|\mathcal{T}_\tilde{\Omega}^n \cap \mathcal{T}_H^n| = |\mathcal{T}_\tilde{\Omega}^n| - |\mathcal{T}_\Omega^n| = |\mathcal{T}^{n-1}| - |\mathcal{T}_\Omega^{n-1}|.$$ 

This vector space has positive dimension for $n > 2$: there exist B-series which are conjugate-Hamiltonian and energy-preserving but are not the ( a reparametrization of) exact flow of the original differential equation.
### Table: Dimensions of the linear spaces spanned by the rooted trees and their 5 natural subspaces.

| order | $|T^n|$ | $|T^n_\Omega|$ | $|T^n_H|$ | $|T^n_{\Omega_\cap H}|$ |
|-------|-------|----------------|----------|-------------------|
| 1     | 1     | 1              | 1        | 1                |
| 2     | 1     | 0              | 1        | 0                |
| 3     | 2     | 1              | 1        | 2                |
| 4     | 4     | 1              | 1        | 4                |
| 5     | 9     | 3              | 5        | 9                |
| 6     | 20    | 4              | 9        | 20               |
| 7     | 48    | 11             | 29       | 48               |
| 8     | 115   | 19             | 68       | 115              |
| 9     | 286   | 47             | 189      | 286              |
| 10    | 719   | 97             | 484      | 719              |
| 11    | 115   | 336            |          |                  |
| 12    | 286   |                |          |                  |
| 13    | 719   |                |          |                  |

The table shows the dimensions of the linear spaces spanned by the rooted trees and their 5 natural subspaces for orders 1 to 10.


• P. Leone, PhD thesis (2002).


• J E Scully, A search for improved numerical integration methods using rooted trees and splitting, MSc Thesis, La Trobe University, 2002.

Thankyou for your attention.