B-series for Stochastic Differential Equations.

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- Part 1: Introduction to B-series.
- Part 2: Stochastic B-series
- Part 3: B-series and preservation of quadratic invariants

Part I

Introduction to B-series

Why B-series?

Taylor expansions in terms of rooted trees

Formal derivation of B-series for ODEs

Order conditions and rooted trees

Why B-series?

Idea:

Whenever a method for solving a time dependent problem is proposed, a *local error analysis* is needed.

This usually means doing a Taylor-expansion of the exact and the numerical solution, and compare equal powers of the stepsize h.

B-series is nothing but an efficient way of expressing these series.

(De)motivating example

ODE:

$$y' = f(t, y)$$

One step of a 2-stage Runge-Kutta method:

$$k1 = f(t_0, y_0)$$
$$k_2 = f(t_0 + c_i h, y_0 + a_{21} h k_1)$$
$$y_1 = y_0 + h b_1 k_1 + b_2 k_2$$

(De)motivating example cont.

Power expansion of the exact solution:

$$\begin{aligned} y(t_0+h) &= y_0 + hy' + \frac{1}{2}h^2y'' + \frac{1}{6}h^3y''' + \cdots \\ &= y_0 + hf + \frac{1}{2}h^2(f_t + f_yf) + \frac{1}{6}h^3(f_{tt} + 2f_{t,y}f + f_{yy}ff + f_yf_t + f_yf_yf) + \ldots \end{aligned}$$

and of the numerical solution:

$$\begin{aligned} k_1 &= f \\ k_2 &= f + h(c_2f_t + a_{21}f_yf) + h^2\left(\frac{1}{2}c_2^2f_{tt} + c_2a_{21}f_{ty}f + \frac{1}{2}a_{21}^2f_{yy}ff\right) + \ldots \\ y_1 &= y_0 + h(b_1+b_2)f + h^2\left(b_2c_2f_t + b_2a_{21}f_yf\right) \\ &\quad + h^3\left(\frac{1}{2}b_2c_2^2f_{tt} + b_2c_2a_{21}f_{ty}f + \frac{1}{2}b_2a_{21}^2f_{yy}ff\right) + \ldots \end{aligned}$$

(De)motivating example cont.

Power expansion of the exact solution:

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and of the numerical solution:

$$\begin{aligned} k_1 &= f \\ k_2 &= f + h(c_2 f_t + a_{21} f_y f) + h^2\left(\frac{1}{2}c_2^2 f_{tt} + c_2 a_{21} f_{ty} f + \frac{1}{2}a_{21}^2 f_{yy} ff\right) + \dots \\ y_1 &= y_0 + h(b_1 + b_2)f + h^2\left(b_2 c_2 f_t + b_2 a_{21} f_y f\right) \\ &\quad + h^3\left(\frac{1}{2}b_2 c_2^2 f_{tt} + b_2 c_2 a_{21} f_{ty} f + \frac{1}{2}b_2 a_{21}^2 f_{yy} ff\right) + \dots \end{aligned}$$

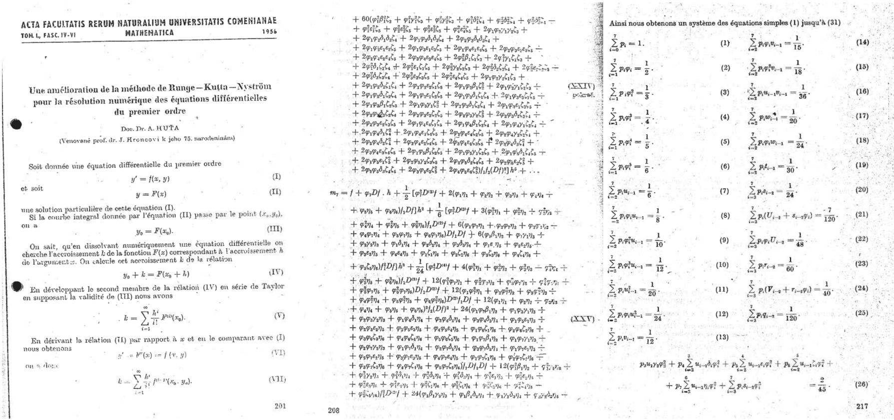
By comparing equal terms, we find that the method is of order 2 (local order 3) if

$$b_1 + b_2 = 1,\, b_2 c_2 = \frac{1}{2},\, b_2 a_{21} = \frac{1}{2}$$

But it can not be of order 3.

The paper of Hut'a

In 1956, Anton Hut'a published a paper in which a the order conditions for an 8-stage explicit Runge-Kutta method of order 6 was derived, using the procedure of the previous slide.


ACTA FACULTATIS RERUM NATURALIUM UNIVERSITATIS COMENIANAE

TOM. I., FASC. IV-VI MATHEMATICA 1956

Une amélioration de la méthode de Runge—Kutta—Nyström pour la résolution numérique des équations différentielles du premier ordre

Doc. Dr. A. HUŤA

(Venované prof. dr. J. Hroncovi k jeho 75. narodeninám)

Soit donnée une équation différentielle du premier ordre

$$y' = f(x, y) \quad (I)$$

et soit

$$y = F(x) \quad (II)$$

une solution particulière de cette équation (I). Si la courbe integral donnée par l'équation (II) passe par le point (x_0, y_0), on a

$$y_0 = F(x_0). \quad (III)$$

On sait, qu'en dissolvant numériquement une équation différentielle on cherche l'accroissement k de la fonction $F(x)$ correspondant à l'accroissement h de l'argument x. On calcule cet accroissement k de la rélation

$$y_0 + k = F(x_0 + h) \quad (IV)$$

En développant le second membre de la rélation (IV) en série de Taylor en supposant la validité de (III) nous avons

$$k = \sum_{i=1}^{\infty} \frac{h^i}{i!} F^{(i)}(x_0). \quad (V)$$

En dérivant la rélation (II) par rapport à x et en le comparant avec (I) nous obtenons

$$y' = F'(x) = f(x, y) \quad (VI)$$

on a donc

$$k = \sum_{i=1}^{\infty} \frac{h^i}{i!} f^{(i-1)}(x_0, y_0). \quad (VII)$$

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Ainsi nous obtenons un système des équations simples (1) jusqu'à (31)

$$\sum_{i=0}^{7} p_i = 1. \quad (1) \qquad \sum_{i=2}^{7} p_i\varphi_i v_{i-1} = \frac{1}{15}. \quad (14)$$
$$\sum_{i=1}^{7} p_i\varphi_i = \frac{1}{2}. \quad (2) \qquad \sum_{i=2}^{7} p_i\varphi_i^2 v_{i-1} = \frac{1}{18}. \quad (15)$$
$$\sum_{i=1}^{7} p_i\varphi_i^2 = \frac{1}{3}. \quad (3) \qquad \sum_{i=2}^{7} p_i u_{i-1} v_{i-1} = \frac{1}{36}. \quad (16)$$
$$\sum_{i=1}^{7} p_i\varphi_i^3 = \frac{1}{4}. \quad (4) \qquad \sum_{i=2}^{7} p_i w_{i-1} = \frac{1}{20}. \quad (17)$$
$$\sum_{i=1}^{7} p_i\varphi_i^4 = \frac{1}{5}. \quad (5) \qquad \sum_{i=2}^{7} p_i\varphi_i w_{i-1} = \frac{1}{24}. \quad (18)$$
$$\sum_{i=1}^{7} p_i\varphi_i^5 = \frac{1}{6}. \quad (6) \qquad \sum_{i=2}^{7} p_i t_{i-1} = \frac{1}{30}. \quad (19)$$
$$\sum_{i=2}^{7} p_i u_{i-1} = \frac{1}{6}. \quad (7) \qquad \sum_{i=3}^{7} p_i s_{i-2} = \frac{1}{24}. \quad (20)$$
$$\sum_{i=2}^{7} p_i\varphi_i u_{i-1} = \frac{1}{8}. \quad (8) \qquad \sum_{i=3}^{7} p_i(U_{i-2} + s_{i-2}\varphi_i) = \frac{7}{120}. \quad (21)$$
$$\sum_{i=2}^{7} p_i\varphi_i^2 u_{i-1} = \frac{1}{10}. \quad (9) \qquad \sum_{i=3}^{7} p_i\varphi_i U_{i-2} = \frac{1}{48}. \quad (22)$$
$$\sum_{i=2}^{7} p_i\varphi_i^3 u_{i-1} = \frac{1}{12}. \quad (10) \qquad \sum_{i=3}^{7} p_i r_{i-2} = \frac{1}{60}. \quad (23)$$
$$\sum_{i=2}^{7} p_i u_{i-1}^2 = \frac{1}{20}. \quad (11) \qquad \sum_{i=3}^{7} p_i(V_{i-2} + r_{i-2}\varphi_i) = \frac{1}{40}. \quad (24)$$
$$\sum_{i=2}^{7} p_i\varphi_i u_{i-1}^2 = \frac{1}{24}. \quad (12) \qquad \sum_{i=3}^{7} p_i q_{i-2} = \frac{1}{120}. \quad (25)$$
$$\sum_{i=2}^{7} p_i v_{i-1} = \frac{1}{12}. \quad (13)$$

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Two simplifications

- Autonomous systems: $y' = f(y)$ (S. Giles 1951)
- The use of rooted trees:
  (R.H. Merson 1957, J.C. Butcher 1963 and E. Hairer, G.Wanner 1974).

Rooted trees and elementary differentials

ODE:

$$y' = f(y)$$

Taylor expansion of the exact solution:

$$y(t+h) = y(t) + hy'(t) + \frac{1}{2}h^2 y''(t) + \frac{1}{6}h^3 y'''(t) + \frac{1}{24}h^4 y^{(4)}(t) + \cdots$$

Repeated use of the chain rules gives

$$\begin{aligned} y' &= f \\ y'' &= f'f \\ y''' &= f''ff + f'f'f \\ y^{(4)} &= f'''fff + 3f''f'ff + f'f''ff + f'f'f'f \end{aligned}$$

Each of these terms, *elementary differentials*, can be identified by a rooted tree.

Rooted trees and elementary differentials (cont.)

- Each node • is associated with the function f.

• $\quad f$

Rooted trees and elementary differentials (cont.)

- Each node ● is associated with the function f.
- Each branch from the node is associated with the derivative of f with respect to y.

f'

Rooted trees and elementary differentials (cont.)

- Each node ● is associated with the function f.
- Each branch from the node is associated with the derivative of f with respect to y.
- And since the chain rule apply, all branches will be concluded with a node ●.

$f' f$

Rooted trees and elementary differentials (cont.)

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- And since the chain rule apply, all branches will be concluded with a node ●.

$f^{'} f$

The *order of a tree* $\rho(\tau)$ is the number of nodes.

Frechet derivatives

The κth Frechet derivative $f^{(\kappa)}(y)$ of $f \in C^{\infty}(\mathbb{R}^d, \mathbb{R}^d)$:

$$f^{(\kappa)}(y)\Big(v_1, v_2, \cdots, v_\kappa\Big)$$

or

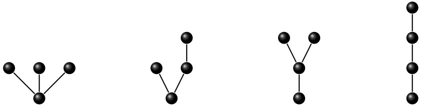
$$\Big[f^{(\kappa)}(y)(v_1, v_2, \cdots, v_\kappa)\Big]_i = \sum_{j_1=1}^{d}\sum_{j_2=1}^{d}\cdots\sum_{j_\kappa=1}^{d} \frac{\partial^\kappa f_i(y)}{\partial y_{j_1}\partial y_{j_2}\cdots\partial y_{j_\kappa}} v_{1,j_1} v_{2,j_2}\cdots v_{\kappa,j_\kappa}, \quad i = 1\ldots, d$$

Properties:

- $f^{(\kappa)}(y) : \overbrace{\mathbb{R}^d \times \mathbb{R}^d \times \cdots \times \mathbb{R}^d}^{\kappa \text{ times}} \to \mathbb{R}^d$
- Linear in each of its operands
- Symmetric in each of its operands

Trees up to order 4

f $\quad f'f$ $\quad f''(f,f)$ $\quad f'f'f$



$f'''(f,f,f)$ $\quad f''(f,f'f)$ $\quad f'f''(f,f)$ $\quad f'f'f'f$

The exact solution of $y' = f(y)$ can now be expressed as a series in terms of trees:

$$y(t_0 + h) = y_0 + \sum_{\tau \in \bar{T}} \xi(\tau) \cdot \frac{h^{\rho(\tau)}}{\rho(\tau)!} \cdot F(\tau)(y_0)$$

and we want to express the numerical solution in a similar series:

$$y_1 = y_0 + \sum_{\tau \in \bar{T}} \xi(\tau) \cdot \psi(\tau) \cdot \frac{h^{\rho(\tau)}}{\rho(\tau)!} \cdot F(\tau)(y_0)$$

Thus the method is of order p if

$$\psi(\tau) = 1, \qquad \text{for all } \tau \in T, \qquad \rho(\tau) \leq p$$

Definition of B-series

In the following, B-series is defined as a formal series by:

$$B(\varphi, h; x_0) = x_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \varphi(\tau)(h) \cdot F(\tau)(x_0)$$

in which the following elements are involved:

- *The set of trees* T, $\bar{T} = T \backslash \{\emptyset\}$.
- *The elementary differentials:* $F(\tau)(x_0)$, $F(\emptyset)(x_0) = x_0$.
- *The elementary weight functions:* $\varphi(\tau)(h)$, with $\varphi(\emptyset)(h) = 1$.
- *A combinatorial term* $\alpha(\tau)$, with $\alpha(\emptyset) = 1$.

The series is consistent if $B(\varphi, 0; x_0) = x_0$ and $\varphi(\tau)(0) = 0$ for all $\tau \neq \emptyset$.

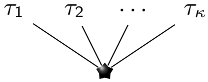
The bracket notation

If $\tau_1, \tau_2, \ldots, \tau_\kappa$ are trees, then

$$[\tau_1, \tau_2, \ldots, \tau_\kappa]_{\bigstar}$$

is the tree formed by joining the subtrees $\tau_1, \tau_2, \ldots, \tau_\kappa$ each by a single branch to a common root $\bigstar$:

$$\tau = [\tau_1, \tau_2, \ldots, \tau_\kappa]_{\bigstar} \qquad =$$



Key lemma: The series of functions of B-series

If $X(t) = B(\varphi, t; x_0)$ is some consistent B–series and $f \in C^\infty(\mathbb{R}^d, \mathbb{R}^{\hat{d}})$ then $f(X(t))$ can be written as a formal series of the form

$$f(X(t)) = f(x_0) + \sum_{u \in U_f \setminus [\emptyset]_f} \beta(u) \cdot \psi_\varphi(u)(t) \cdot G(u)(x_0)$$

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where U_f is a set of trees derived from T, by

a) $[\emptyset]_f \in U_f$, and if $\tau_1, \tau_2, \cdots, \tau_\kappa \in T$ then $u = [\tau_1, \tau_2, \cdots, \tau_\kappa]_f \in U_f$.

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c) $G([\emptyset]_f)(x_0) = f(x_0)$ and

$$G(u = [\tau_1, \cdots, \tau_\kappa]_f)(x_0) = f^{(\kappa)}(x_0)\Big(F(\tau_1)(x_0), \cdots, F(\tau_\kappa)(x_0)\Big).$$

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b) $\psi_\varphi([\emptyset]_f)(t) = 1$ and $\psi_\varphi(u = [\tau_1, \cdots, \tau_\kappa]_f)(t) = \prod_{j=1}^{\kappa} \varphi(\tau_j)(t)$.

sde

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$$G(u = [\tau_1, \cdots, \tau_\kappa]_f)(x_0) = f^{(\kappa)}(x_0)\Big(F(\tau_1)(x_0), \cdots, F(\tau_\kappa)(x_0)\Big).$$

b) $\psi_\varphi([\emptyset]_f)(t) = 1$ and $\psi_\varphi(u = [\tau_1, \cdots, \tau_\kappa]_f)(t) = \prod_{j=1}^{\kappa} \varphi(\tau_j)(t)$.

d) $\beta([\emptyset]_f) = 1$ and $\beta(u = [\tau_1, \cdots, \tau_\kappa]_f) = \dfrac{1}{r_1! r_2! \cdots r_q!} \prod_{j=1}^{\kappa} \alpha(\tau_j)$,

where $r_1, r_2, \cdots, r_q$ count equal trees among $\tau_1, \tau_2, \cdots, \tau_\kappa$.

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Key lemma: Sketch of the proof

- Use consistency:

$$X(t) = B(x_0, t; \varphi) = x_0 + \delta$$

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- Use Taylor's theorem

$$f(x_0 + \delta) = f(x_0) + \frac{1}{\kappa!} \sum_{\kappa=1}^{\infty} f^{(\kappa)}(x_0)(\overbrace{\delta, \cdots, \delta}^{\kappa \text{ times}})$$

Key lemma: Sketch of the proof

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- Use the linearity and symmetry of the Frechet derivative.

B-series for ODEs

- Write the ODE in integral form

$$y(t_0+h) = y_0 + \int_0^h f(y(t_0+s))\,\mathrm{d}s.$$

- Write the solution as a B-series:

$$y(t_0+h) = y_0 + \sum_{\tau\in\bar{T}} \alpha(\tau)\cdot\eta(\tau)(h)\cdot F(\tau)(y_0)$$

- Apply the key lemma on $f(y(t_0+s))$:

$$y(t_0+h) = y_0 + \sum_{u\in U_f} \beta(u)\cdot\int_0^h \psi_\eta(u)(s)\mathrm{d}s\cdot G(u)(y_0)$$

- Compare term by term:

B-series for the ODEs

$$y(t_0 + h) = y_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \eta(\tau)(h) \cdot F(\tau)(y_0)$$
$$= y_0 + \sum_{u \in U_f} \beta(u) \cdot \int_0^h \psi_\eta(u)(s)\mathrm{d}s \cdot G(u)(y_0)$$

From the Key Lemma:

$$[\emptyset]_f \in U_f, \text{ and if } \tau_1, \tau_2, \cdots, \tau_\kappa \in T \text{ then } u = [\tau_1, \tau_2, \cdots, \tau_\kappa]_f \in U_f$$

Corresponding trees in T:

$$\bullet \in T, \text{ and if } \tau_1, \tau_2, \cdots, \tau_\kappa \in T \text{ then } \tau = [\tau_1, \tau_2, \cdots, \tau_\kappa]_\bullet \in T$$

When only one kind of nodes are involved, the $\bullet$ is usually omitted.

B-series for the ODEs

$$y(t_0+h) = y_0 + \sum_{\tau\in\bar{T}} \alpha(\tau)\cdot\eta(\tau)(h)\cdot F(\tau)(y_0)$$

$$= y_0 + \sum_{u\in U_f} \beta(u)\cdot\int_0^h \psi_\eta(u)(s)\mathrm{d}s\cdot G(u)(y_0)$$

From the Key Lemma:

$$G([\emptyset]_f)(y_0) = f(y_0), \qquad G(u)(y_0) = f^{(\kappa)}(y_0)\big(F(\tau_1)(y_0),\cdots,F(\tau_\kappa)(y_0)\big)$$

correspond to

$$F(\bullet)(y_0) = f(y_0), \qquad F(\tau)(y_0) = f^{\kappa}(y_0)\big(F(\tau_1)(y_0),\cdots,F(\tau_\kappa)(y_0)\big)$$

B-series for the ODEs

$$y(t_0+h) = y_0 + \sum_{\tau\in\bar{T}} \alpha(\tau)\cdot\eta(\tau)(h)\cdot F(\tau)(y_0)$$
$$= y_0 + \sum_{u\in U_f} \beta(u)\cdot\int_0^h \psi_\eta(u)(s)\mathrm{d}s\cdot G(u)(y_0)$$

From the Key Lemma:

$$\beta([\emptyset]_f) = 1, \qquad \beta(u) = \frac{1}{r_1!r_2!\cdots r_q!}\prod_{j=1}^{\kappa}\alpha(\tau_j)$$

correspond to

$$\alpha(\bullet) = 1, \qquad \alpha(\tau) = \frac{1}{r_1!r_2!\cdots r_q!}\prod_{j=1}^{\kappa}\alpha(\tau_j)$$

where $r_1, r_2, \cdots, r_q$ count equal trees among $\tau_1, \tau_2, \cdots, \tau_\kappa$.

B-series for the ODEs

$$y(t_0+h) = y_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \eta(\tau)(h) \cdot F(\tau)(y_0)$$

$$= y_0 + \sum_{u \in U_f} \beta(u) \cdot \int_0^h \psi_\eta(u)(s) \mathrm{d}s \cdot G(u)(y_0)$$

From the Key Lemma:

$$\psi_\eta([\emptyset]_f)(t) = 1, \qquad \psi_\eta(u)(t) = \prod_{j=1}^{\kappa} \eta(\tau_j)(t)$$

correspond to

$$\eta(\bullet)(h) = h, \qquad \eta(\tau)(h) = \int_0^h \prod_{j=1}^{\kappa} \eta(\tau_j)(s)\, \mathrm{d}s$$

Different formulations

The exact solution of an $y' = f(y)$ can be written as a formal series:

$$y(t_0 + h) = y_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \eta(\tau)(h) \cdot F(\tau)(y_0) \quad \textit{in the remaining}$$

$$= y_0 + \sum_{\tau \in \bar{T}} \xi(\tau) \cdot \frac{h^{\rho(\tau)}}{\rho(\tau)!} \cdot F(\tau)(y_0) \quad \textit{introduction}$$

$$= y_0 + \sum_{\tau \in \bar{T}} \frac{1}{\sigma(\tau)} \cdot \frac{h^{\rho(\tau)}}{\gamma(\tau)} \cdot F(\tau)(y_0) \quad \textit{Butcher, Hairer and Wanner}.$$

with the relations:

$$\eta(\tau)(h) = \frac{h^{\rho(\tau)}}{\gamma(\tau)}, \qquad \alpha(\tau) = \frac{1}{\sigma(\tau)}, \qquad \xi(\tau) = \frac{\rho(\tau)!}{\gamma(\tau)\sigma(\tau)}$$

What next?

Given the B-series for the exact solution,

$$y(t_0 + h) = B(\eta, h; y_0) = y_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \eta(\tau)(h) \cdot F(\tau)(y_0)$$

the next step is to find the corresponding B-series for the numerical solution:

$$y_1 = B(\phi, h; y_0) = y_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \phi(\tau)(h) \cdot F(\tau)(y_0)$$

Runge–Kutta methods

Given an s-stage Runge–Kutta (RK) method:

$$Y_i = y_n + h \sum_{j=1}^{s} a_{ij} f(Y_j) \qquad i = 1, 2, \ldots, s$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i f(Y_i)$$

where the method coefficients are given in the Butcher tableau

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \qquad \text{or in short} \qquad \begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

with

$$c_i = \sum_{j=1}^{s} a_{ij}, \quad i = 1, \cdots, s \qquad \text{or in short} \qquad c = A\mathbb{1}_s.$$

B-series for RK-solutions

- Write the stage values Y_i as B-series of ODEs:

$$Y_i = B(\Phi_i, h; y_0) = y_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \Phi_i(\tau)(h) \cdot F(\tau)(y_0)$$

- Insert this in the right hand side

$$Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} f(B(\Phi_j, h; y_0))$$

- Apply the key lemma and compare equal terms:

$$\Phi_i(\emptyset)(h) = 1, \qquad \Phi_i(\bullet) = hc_i, \qquad \Phi_i(\tau)(h) = h \sum_{j=1}^{s} a_{ij} \prod_{k=1}^{\kappa} \Phi_j(\tau_k)(h)$$

- Similar for $y_1 = B(\phi, h; y_0)$, with

$$\phi(\emptyset)(h) = 1, \qquad \Phi_i(\bullet) = h \sum_{i=1}^{s} b_i, \qquad \phi(\tau)(h) = h \sum_{i=1}^{s} b_i \prod_{k=1}^{\kappa} \Phi(\tau_k)(h)$$

Order conditions for Runge-Kutta methods applied to ODEs

A method is of order p if $\phi(\tau)(h) = \eta(\tau)(h)$ for all $\tau \in T$, $\rho(\tau) \le p$.

f

$\sum b_i = 1$

$f'f$

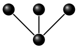
$\sum b_i c_i = 1/2$

$f''(f,f)$

$\sum b_i c_i^2 = 1/3$

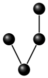
$f'f'f$

$\sum b_i a_{ij} c_j = 1/6$



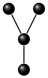
$f'''(f,f,f)$

$\sum b_i c_i^3 = 1/4$



$f''(f,f'f)$

$\sum b_i c_i a_{ij} c_j = 1/8$



$f'f''(f,f)$

$\sum b_i a_{ij} c_j^2 = 1/12$

$f'f'f'f$

$\sum_i a_{ij} a_{jk} c_k = 1/24$

Part 1: Summary

To find B-series for a given problem:

- Write the equation in integral form if possible.
- Write the solution in $t_0 + h$ as an (unknown) B-series.
  Check for consistency.
- Insert this into the equation, and apply the Key lemma on functions of B-series.
- Compare equal terms.
- For the numerical solution, repeat the process. It should result in similar series, but with different weight functions $\varphi(\tau)$.

Biodiversity

- There are all kind of trees:
  - The nodes can have different shapes and colors
  - Not all trees has to be represented
  - They can be non-symmetric

$\vdots$

- There are similar lemmas as the Key Lemma for:
  - $f'(B(\varphi, h; y_0))$
  - $B(\varphi_1, h; B(\varphi_2, h, y_0))$ (Splitting and composition methods)

$\vdots$

Part II

Stochastic B-series

joint with Kristian Debrabant, SDU, Denmark

Introduction

The stochastic differential equation of our interest is of the form: SDE:

$$X(t) = x_0 + \sum_{m=0}^{M} \int_0^t g_m(X(s)) * dW_m(s)$$

with

- m independent Wiener processes, $W_m(s)$, $m = 1, \ldots, M$.
- smooth functions g_m, $\mathbb{R}^d \to \mathbb{R}^d$.
- Itô or Stratonovich integrals.
- For convenience, $W_0(t) = t$.

Stochastical integrals (notation)

- Stochastical integrals:

$$I^*_{(m_1,\dots,m_r)}(t) = \int_0^t \int_0^{s_r} \cdots \int_0^{s_2} W_{m_1}(s_1) * \cdots * \mathrm{d}W_{m_r}(s_r)$$

- For the numerical solutions, realizations of the integrals

$$I^*_\alpha = I^*_\alpha(h), \qquad \text{with} \quad \alpha = (m_1, \dots, m_r)$$

  are generated for each step.
- As usual, I_α, J_α refer to Itô respectively Stratonovich integrals
- $\Delta W_m = I^*_{(m)}$

Numerical solutions of SDEs

- The Euler-Maruyama scheme:

$$Y_{n+1} = Y_n + \sum_{m=1}^{M} g_m(Y_n)\Delta W_m$$

- Milstein scheme:

$$Y_{n+1} = Y_n + \sum_{m=1}^{M} g_m(Y_n)\Delta W_m + \sum_{m_1,m_2=1}^{M} g'_{m_1} g_{m_2}(Y_n)\ I^*_{(m_1,m_2)}$$

Stochastic Runge-Kutta methods:

$$H_i = Y_n + \sum_{m=0}^{M} \sum_{j=1}^{s} Z_{ij}^{(m)} g_m(H_j), \qquad i = 1, \dots, s$$

$$Y_{n+1} = Y_n + \sum_{m=0}^{M} \sum_{i=1}^{s} z_i^{(m)} g_m(H_i)$$

- The coefficients $Z_{ij}^{(m)}$ and $z_i^{(m)}$ are depends on random variables, often constructed from stochastic integrals.
- Given a RK method for ODEs, an SRK can be constructed by

$$Z_{ij}^{(m)} = a_{ij}\Delta W_m \qquad \text{and} \qquad z_i^{(m)} = b_i \Delta W_m$$

Such methods has in general at most strong order 1 if $M = 1$, otherwise strong order $1/2$.

Example of a Stochastic Runge-Kutta methods

Runge-Kutta method applied to an SDE ($M = 1$):

$$H_i = Y_n + \sum_{i=1}^{s} Z_{ij}^{(0)} g_0(H_j) + \sum_{l=1}^{s} Z_{ij}^{(1)} g_1(H_j), \quad i = 1, 2, \cdots, s$$

$$Y_{n+1} = Y_n + \sum_{i=1}^{s} z_i^{(0)} g_0(H_i) + \sum_{l=1}^{s} z_i^{(1)} g_1(H_i),$$

The coefficient matrices $Z^{(l)}$, $z^{(l)}$ depends on the stepsize h and random variables.

Example (RK method of order 1, Itô SDE)

$$H_1 = Y_n$$

$$H_2 = Y_n + \sqrt{h}\, g_1(Y_n)$$

$$Y_{n+1} = Y_n + h\, g_0(H_1) + \left(I_{(1)} - \frac{I_{(1,1)}}{\sqrt{h}}\right) g_1(H_1) + \frac{I_{(1,1)}}{\sqrt{h}}\, g_1(H_2)$$

Platen 1984

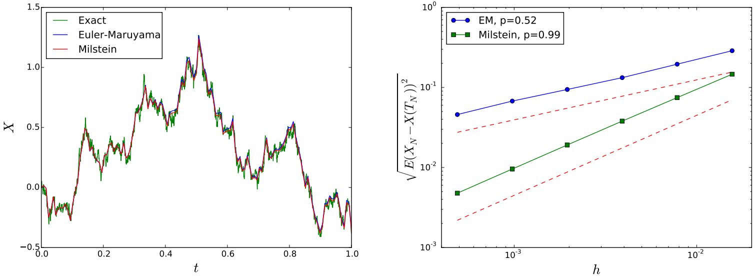
Strong Approximation

In this case, we are interested in each solution path $X(t,\omega)$.

Example

SDE: $$dX = (\frac{1}{2}X + \sqrt{X^2+1})\mathrm{d}t + \sqrt{X^2+1}\mathrm{d}W(t)$$

Solution: $$X(t) = \sinh(t + W(t)),$$



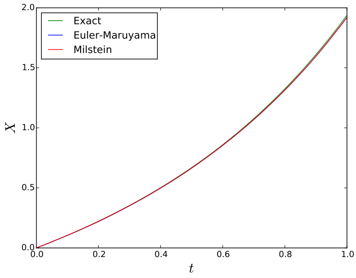
Weak Approximation

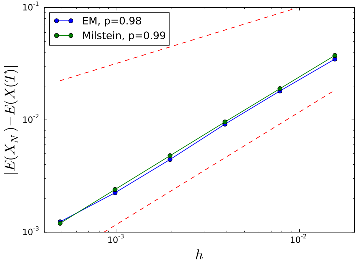
In this case, we are interested in the expectation value of some derived quantity $\Psi : \mathbb{R}^r \to \mathbb{R}$.

Example

SDE: $dX = (\frac{1}{2}X + \sqrt{X^2+1})\mathrm{d}t + \sqrt{X^2+1}\mathrm{d}W(t), \qquad \Psi(X) = X$

Solution: $X(t) = \sinh(t + W(t)), \qquad \mathbb{E}X(t) = \frac{1}{2}(\mathrm{e}^{\frac{3}{2}t} - \mathrm{e}^{\frac{1}{2}t})$





Error Analysis Cheat Sheet

Error Concepts

	Global error E	Local error δ
Strong	$\max_n \mathbb{E}\lvert X(t_n) - X_n\rvert$	$\mathbb{E}(X(t_{n+1}) - X_{n+1} \mid X(t_n) = X_n)$
Mean Square	$\max_n \sqrt{\mathbb{E}\lvert X(t_n) - X_n\rvert^2}$	$\sqrt{\mathbb{E}(X(t_{n+1}) - X_{n+1})^2 \mid X(t_n) = X_n)}$
Weak	$\max_n \lvert\mathbb{E}\Psi(X(t_n)) - \mathbb{E}\Psi(X_n)\rvert$	$\mathbb{E}(\Psi(X(t_{n+1}) - \Psi(X_{n+1})\lvert X(t_n) = X_n)$

$\Psi : \mathbb{R}^d \to \mathbb{R}$.

Theorem: Local $\to$ Global Error (Milstein -95)

- Strong Convergence:

$$\begin{array}{l} |\delta^s| \leq Kh^{p+1} \\ \delta^{ms} \leq Kh^{p+\frac{1}{2}} \end{array} \quad \Rightarrow \quad E^{ms} \leq Kh^p \quad \Rightarrow \quad E^s \leq Kh^p$$

- Weak Convergence

$$|\delta^w| \leq Kh^{p+1} \quad \Rightarrow \quad E^w \leq Kh^p$$

K is some generic constant

Previous work on B–series for SDEs

- Y. Komori, T. Mitsui, H. Sugiura (1997)
- P. M. Burrage (1999)
- P. M. Burrage, K. Burrage (2000)
- A. Rößler (2004, 2006)
- Y. Komori (2007)

B–series for SDEs

SDE:

$$X(t) = x_0 + \sum_{m=0}^{M} \int_0^t g_m(X(s)) * dW_m(s)$$

B–series:

$$B(\varphi, t; x_0) = x_0 + \sum_{\tau \in \bar{T}} \alpha(\tau) \cdot \varphi(\tau)(h) \cdot F(\tau)(x_0)$$

where

T	:	The set of trees
$\varphi(\tau)$	:	The weight functions
$F(\tau)$	:	The elementary differentials
$\alpha(\tau)$	:	A combinatorial term

Theorem: Convergence of the numerical solution

If the exact and numerical solutions both can be written as B–series,

$$X(h) = B(\eta, h; x_0), \qquad Y_1 = B(\phi, h; x_0)$$

then:

- The method is weak consistent of order p iff

$$\mathbb{E} \prod_{k=1}^{\kappa} \phi(\tau_k)(h) = \mathbb{E} \prod_{k=1}^{\kappa} \eta(\tau_i)(h) + \mathcal{O}(h^{p+1})$$

  for all $[\tau_1, \tau_2, \ldots, \tau_\kappa]$, $\tau_k \in T$, $\sum_{i=1}^{m} \rho(\tau_i) \leq p + \frac{1}{2}$.

- The method has mean square global order p if

$$\phi(\tau)(h) = \eta(\tau)(h) + \mathcal{O}(h^{p+\frac{1}{2}}), \qquad \rho(\tau) \leq p$$

$$E\phi(\tau)(h) = E\eta(\tau)(h) + \mathcal{O}(h^{p+1}), \qquad \rho(\tau) \leq p + \frac{1}{2}$$

B–series for SDEs

SDE:

$$X(t) = x_0 + \sum_{m=0}^{M} \int_0^t g_m(X(s)) * dW_m(s) = x_0 + \sum_{m=0}^{M} \int_0^t g_m(x_0) * dW_m(s) + \cdots$$

B–series:

$$X(t) = B(\eta, t; x_0) = \sum_{\tau \in T} \alpha(\tau) \cdot \eta(\tau)(t) \cdot F(\tau)(x_0),$$

Clearly:

$$\emptyset \in T, \quad \alpha(\emptyset) = 1, \quad \eta(\emptyset)(t) = 1, \quad F(\emptyset)(x_0) = x_0,$$

$$\bullet_m \in T, \quad \alpha(\bullet_m) = 1, \quad \eta(\bullet_m)(t) = \int_0^t dW_m(s) = W_m(t), \quad F(\bullet_m)(x_0) = g_m(x_0)$$

for $m = 0, 1, \ldots, M$.

We have

$$X(t) = x_0 + \sum_{m=0}^{M} \int_0^t g_m(X(s)) * dW_m(s)$$

B–series:

$$X(t) = B(\eta, t; x_0) = \sum_{\tau \in T} \alpha(\tau) \cdot \eta(\tau)(t) \cdot F(\tau)(x_0)$$

Apply the Key lemma for functions of B-series:

$$B(\eta, t; x_0) = x_0 + \sum_{m=0}^{M} \int_0^t \sum_{u \in U_{g_m}} \beta(u) \cdot \psi_\eta(u)(s) \cdot G(u)(x_0) * dW_m(s)$$

We have

$$X(t) = x_0 + \sum_{m=0}^{M} \int_0^t g_m(X(s)) * dW_m(s)$$

B–series:

$$X(t) = B(\eta, t; x_0) = \sum_{\tau \in T} \alpha(\tau) \cdot \eta(\tau)(t) \cdot F(\tau)(x_0)$$

Apply the Key lemma for functions of B-series:

$$B(\eta, t; x_0) = x_0 + \sum_{m=0}^{M} \int_0^t \sum_{u \in U_{g_m}} \beta(u) \cdot \psi_\eta(u)(s) \cdot G(u)(x_0) * dW_m(s)$$

Compare term by term: $\emptyset \in T$, $\bullet_m = [\emptyset]_m \in T_m$ and

a) $u = [\tau_1, \dots, \tau_\kappa]_{g_m} \in U_{g_m} \;\rightarrow\; \tau = [\tau_1, \dots, \tau_\kappa]_m \in T_m, \quad T = T_0 \cup \cdots \cup T_M \cup \emptyset$

b) $\eta(\tau)(t) = \int_0^t \psi_\eta(u) * dW_m(s) = \int_0^t \prod_{k=1}^{\kappa} \eta(\tau_k)(s) * dW_m(s)$

c) $F(\tau)(x_0) = G(u)(x_0) = g_m^{(\kappa)}(x_0)\Big(F(\tau_1)(x_0), \cdots, F(\tau_\kappa)(x_0)\Big)$

Debrabant & K, (2008)

B–series for SDEs

$$X(t) = \sum_{\tau \in T} \alpha(\tau) \cdot \eta(\tau)(t) \cdot F(\tau)(x_0)$$

with

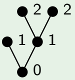
a) $\bullet_m = [\emptyset]_m \in T_m, \qquad \tau = [\tau_1, \dots, \tau_\kappa]_m \in T_m, \qquad T = T_0 \cup T_1 \cup \cdots \cup T_m \cup \emptyset$

b) $\eta(\bullet_m)(t) = W_m(t), \qquad \eta(\tau)(t) = \int_0^t \prod_{j=1}^{\kappa} \eta(\tau_j)(s) * dW_m(s)$

c) $F(\bullet_m)(x_0) = g_m(x_0), \quad F(\tau)(x_0) = g_m^{(\kappa)}(x_0)\Big(F(\tau_1)(x_0), \cdots, F(\tau_\kappa)(x_0)\Big)$

Example

$$\eta(\tau)(t) = \int_0^t W_1(s_1)\left(\int_0^{s_1} W_2(s_2)^2 * dW_1(s_2)\right) * ds_1$$

$\tau =$ 

$, \quad F(\tau)(x_0) = g_0''(g_1, g_1''(g_2, g_2))(x_0)$

$$\alpha(\tau) = \tfrac{1}{2}, \qquad \rho(\tau) = 3.$$

B-series for stochastic Runge-Kutta solutions

$$H_i = x_0 + \sum_{m=0}^{M} \sum_{j=1}^{s} Z_{ij}^{(m)} g_m(H_j), \qquad i = 1, \dots, s$$

$$Y_1 = x_0 + \sum_{m=0}^{M} \sum_{i=1}^{s} z_i^{(m)} g_m(H_i)$$

- Write H_i and Y_1 as B-series:

$$H_i = B(\Phi_i, h; x_0), \qquad Y_1 = B(\phi, h; x_0)$$

- Apply the key lemma and compare equal terms:

$$\Phi_i(\emptyset) = 1, \quad \Phi_i(\bullet_m) = \sum_{j=1}^{s} Z_{ij}^{(m)}, \quad \Phi_i(\tau) = \sum_{j=1}^{s} Z_{ij}^{(m)} \prod_{k=1}^{\kappa} \Phi_j(\tau_k) \quad \text{for } \tau \in T_m$$

$$\phi(\emptyset) = 1, \quad \Phi_i(\bullet_m) = \sum_{i=1}^{s} z_i^{(m)}, \quad \phi(\tau) = \sum_{j=1}^{s} z_i^{(m)} \prod_{k=1}^{\kappa} \phi(\tau_k) \quad \text{for } \tau \in T_m$$

Strong Order 1 Conditions for M=1

τ	$\rho(\tau)$	$\eta(\tau)$	$\mathbb{E}\,\eta(\tau)(h)$		$\phi(\tau)$
			I	S	
	$1/2$	$W(h)$	0	0	$z^{(1)}\mathbb{1}_s$
	1	h	h	h	$z^{(0)}\mathbb{1}_s$
	1	$\int_0^h W(s)\star dW(s)$	0	$h/2$	$z^{(1)}Z^{(1)}\mathbb{1}_s$
	$3/2$	$\int_0^h W(s)ds$	0	0	$\mathbb{E}\,z^{(0)}Z^{(1)}\mathbb{1}_s$
	$3/2$	$\int_0^h s\star dW(s)$	0	0	$\mathbb{E}\,z^{(1)}Z^{(0)}\mathbb{1}_s$
	$3/2$	$\int_0^h W(s)^2\star dW(s)$	0	0	$\mathbb{E}\,z^{(1)}\left(Z^{(1)}\mathbb{1}_s\right)^2$
	$3/2$	$\int_0^h\int_0^s W(s_1)\star dW(s_1)\star dW(s)$	0	0	$\mathbb{E}\,z^{(1)}Z^{(1)}Z^{(1)}\mathbb{1}_s$

I: Itô, S: Stratonovich

A 4-stage Drift-implicit SRK method of order 1.5

$$z^0 = h\alpha, \qquad z^1 = J_{(1)}\gamma^{(1)} + \frac{J_{(1,0)}}{h}\gamma^{(2)}$$

$$Z^{(0)} = hA, \qquad Z^{(1)} = J_{(1)}B^{(1)} + \frac{J_{(1,0)}}{h}B^{(2)} + \sqrt{h}B^{(3)},$$

$$\alpha^\top = (0.169775, 0.297820, 0.042159, 0.490244),$$

$$\gamma^{(1)\top} = (-1.008751, 0.285118, 0.760818, 0.962814),$$

$$\gamma^{(2)\top} = (1.507774, 1.085932, -1.458091, -1.135616),$$

$$A = \begin{pmatrix} 0.240968725 & 0 & 0 & 0 \\ 0.167810317 & 0.160243373 & 0 & 0 \\ -0.002766912 & 0.473332751 & 0.178081733 & 0 \\ 0.415057712 & 0.115126049 & 0.020652745 & 0.130541130 \end{pmatrix},$$

$$B_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -0.476890860 & 0 & 0 & 0 \\ 0.514160282 & 0.012424879 & 0 & 0 \\ -0.879966702 & 0.412866280 & 0.711524058 & 0 \end{pmatrix},$$

$$B_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1.287951512 & 0 & 0 & 0 \\ 0.665416412 & -0.686930244 & 0 & 0 \\ 0.703868780 & 0.876627859 & -0.321270197 & 0 \end{pmatrix},$$

$$B_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0.568300129 & -0.568300129 & 0 & 0 \\ 1.614193125 & -0.618659748 & -0.995533377 & 0 \\ 0.660721631 & -0.714401673 & -0.896487337 & 0.950167380 \end{pmatrix}$$

A surprising result

Given the rigid body model:

$$dX = A(X)Xdt + \sigma\, g_1(X) \circ dW(t)$$

with some constant σ, and

$$A(X) = \begin{pmatrix} 0 & x_3/I_3 & -x_2/I_2 \\ -x_3/I_3 & 0 & x_1/I_1 \\ x_2/I_2 & -x_1/I_1 & 0 \end{pmatrix}$$

with two different diffusion terms:

$$P1: \quad g_1(X) = A(X)X$$

$$P2: \quad g_1(X) = \begin{pmatrix} X_2 \\ -X_1 \\ 0 \end{pmatrix}$$

The problem were solved by the following order 1 methods:

- Platen's method
- Gauss' method, $s = 1$.
- Gauss' method, $s = 2$.

A surprising result

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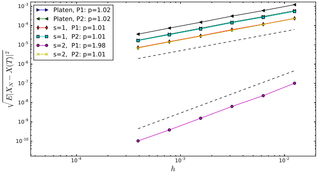
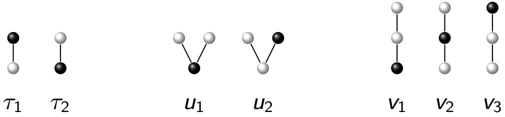


So why is the Gauss ($s = 2$) method of order 2 when applied to P1

The Gauss $s = 2$ method do not satisfy the order conditions for the following trees:



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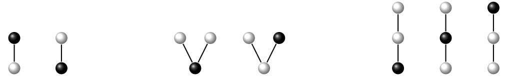

τ_1 τ_2 u_1 u_2 v_1 v_2 v_3

Problem P1 is of the form:

$$dX = g(X)dt + \sigma g(X) \circ dW(t)$$

Then $F(\tau_1) = F(\tau_2)$, $F(u_1) = F(u_2)$ and $F(v_1) = F(v_2) = F(v_3)$.

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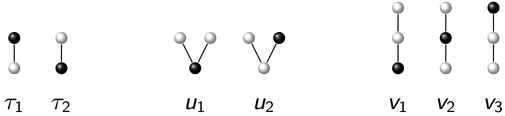

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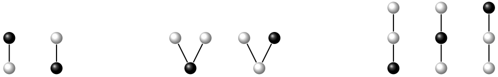
$$dX = g(X)dt + \sigma g(X) \circ dW(t)$$

Then $F(\tau_1) = F(\tau_2)$, $F(u_1) = F(u_2)$ and $F(v_1) = F(v_2) = F(v_3)$.
We can show:

$$\begin{aligned} \eta(\tau_1) + \eta(\tau_2) &= J_{10} + J_{01} & \qquad \phi(\tau_1) + \phi(\tau_2) &= h\Delta W_n \\ \frac{1}{2}\eta(u_1) + \eta(u_2) &= J_{110} + J_{011} + J_{101} & \qquad \frac{1}{2}\phi(u_1) + \phi(u_2) &= \frac{1}{2}h\Delta W_n^2 \\ \eta(v_1) + \eta(v_2) + \eta(v_3) &= J_{110} + J_{101} + J_{011} & \qquad \phi(v_1) + \phi(v_2) + \phi(v_3) &= \frac{1}{2}h\Delta W_n^2 \end{aligned}$$

So why is the Gauss ($s = 2$) method of order 2 when applied to P1

The Gauss $s = 2$ method do not satisfy the order conditions for the following trees:



τ_1 τ_2 u_1 u_2 v_1 v_2 v_3

Problem P1 is of the form:

$$dX = g(X)dt + \sigma g(X) \circ dW(t)$$

Then $F(\tau_1) = F(\tau_2)$, $F(u_1) = F(u_2)$ and $F(v_1) = F(v_2) = F(v_3)$.
We can show:

$$\eta(\tau_1) + \eta(\tau_2) = J_{10} + J_{01} = \phi(\tau_1) + \phi(\tau_2) = h\Delta W_n$$

$$\frac{1}{2}\eta(u_1) + \eta(u_2) = J_{110} + J_{011} + J_{101} = \frac{1}{2}\phi(u_1) + \phi(u_2) = \frac{1}{2}h\Delta W_n^2$$

$$\eta(v_1) + \eta(v_2) + \eta(v_3) = J_{110} + J_{101} + J_{011} = \phi(v_1) + \phi(v_2) + \phi(v_3) = \frac{1}{2}h\Delta W_n^2$$

Single integrand SDEs

These are Stratonovich SDEs of the form

$$X(t) = x_0 + \int_0^t g(X(s))ds + \sigma \int_0^t g(X(s)) \circ dW(s) = x_0 + \int_0^t g(X(s)) \circ d\mu(s)$$

where $\mu(t) = t + \sigma W(t)$.

Let $\mu_t(s) = \mu(t+s) - \mu(s)$ and let $\Delta\mu_n = \mu_{t_n}(h) = h + \sigma\Delta W_n$. Now we can write the exact solution $X(t+h)$ as a B-series around $X(t)$ in which the weight functions are Stratonovich integrals with respect to $\mu_t(s)$.

These integrals satisfy

$$\int_0^h \mu_t(s)^k \circ d\mu_t(s) = \frac{1}{k+1}\mu_t(h)^{k+1}$$

and

$$\mathbb{E}\mu_t(h)^k = \begin{cases} \mathcal{O}(h^{\frac{k}{2}}) & \text{if } k \text{ is even} \\ \mathcal{O}(h^{\frac{1}{k+1}}) & \text{if } k \text{ is odd} \end{cases}$$

Order results for single integrands SDEs

Given an ODE Runge–Kutta method (A, b) of order p. Solve the SDE

$$dX = g(X) \circ d\mu, \qquad X(0) = x0$$

by the stochastic version of the method:

$$H_i = Y_n + \Delta\mu_n \sum_{j=1}^{s} a_{ij} g(H_j),$$

$$Y_{n+1} = Y_n + \Delta\mu_n \sum_{i=1}^{s} b_i g(H_i).$$

where $\Delta\mu_n = h + \sigma\Delta W_n$.

Theorem

The proposed method is of mean square as well as of weak order $\lfloor p/2 \rfloor$.

Debrabant, K. (2017)

Stochastic Taylor expansions (Wagner–Platen series)

SDE:

$$X(t) = x_0 + \sum_{l=0}^{m} \int_0^t g_l(X(s)) * dW_l(s)$$

Wagner-Platen series is derived by repeated use of the Itô formula:

$$f(X(t)) = f(x_0) + \sum_{l=0}^{m} \int_0^t L^l f(X(s)) * dW_l(s),$$

in which

$$L^0 f = f' g_0 + \gamma^* \sum_{l=1}^{m} f''(g_l, g_l), \qquad L^l f = f' g_l, \quad l = 1, 2, \ldots, m$$

and $\gamma^* = 1/2$ in the Itô case and 0 in the Stratonovich case.

Wagner–Platen series

If $X(t)$ is a solution of the SDE, then $f(X(t))$ can be written as a formal series of the form

$$f(X(t)) = \sum_{\alpha \in \mathcal{M}} I^*_\alpha(t) f_\alpha(x_0).$$

Here, the *set of multi-indices* $\mathcal{M}$ is

$$\mathcal{M} = \Big\{ \alpha = (j_1, \dots, j_r) \,:\, j_i \in \{0, \dots, m\},\ i \in \{1, 2, \dots, r\} \text{ for } r = 1, 2, \dots \Big\}.$$

The *coefficient functions* f_α and the *multiple stochastic integrals* I^*_α are

$$f_\emptyset(x_0) = f(x_0), \qquad f_\alpha(x_0) = \Big(L^{j_1} L^{j_2} \cdots L^{j_r} f\Big)(x_0),$$

$$I^*_\emptyset(t) = 1, \qquad I^*_\alpha(t) = \int_0^t \int_0^{s_r} \cdots \int_0^{s_2} dW_{j_1}(s_1) * \cdots * dW_{j_r}(s_r).$$

For strong solutions: $f(x) = x$.

Notice! $I^*_\alpha(t) = \psi_\varphi(u)(t)$ for $u = [\,[\dots[\bullet_{j_1}]_{j_2} \cdots]_{j_r}\,]_f$.

Wagner and Platen (1982)

Wagner–Platen series vs. B–series

$$f(X(t)) = \sum_{\alpha\in\mathcal{M}} I^*_\alpha(t)\cdot f_\alpha(x_0) = \sum_{u\in U_f} \beta(u)\cdot\psi_\eta(u)(t)\cdot G(u)(x_0)$$

Trees and multi-indices are related by:

a) $$f_\alpha(x_0) = \sum_{u\in V(\alpha)} \mu^\alpha_u \cdot G(u)(x_0), \qquad V(\alpha)\subset U_f$$

b) $$\beta(u)\cdot\psi_\eta(t) = \sum_{\alpha\in\mathcal{A}(u)} \mu^\alpha_u \cdot I^*_\alpha(t), \qquad \mathcal{A}(u)\subset\mathcal{M}$$

Wagner–Platen series vs. B–series

$$f(X(t)) = \sum_{\alpha \in \mathcal{M}} I_\alpha^*(t) \cdot f_\alpha(x_0) = \sum_{u \in U_f} \beta(u) \cdot \psi_\eta(u)(t) \cdot G(u)(x_0)$$

Trees and multi-indices are related by:

$$\text{a)} \qquad f_\alpha(x_0) = \sum_{u \in V(\alpha)} \mu_u^\alpha \cdot G(u)(x_0), \qquad V(\alpha) \subset U_f$$

$$\text{b)} \qquad \beta(u) \cdot \psi_\eta(t) = \sum_{\alpha \in \mathcal{A}(u)} \mu_u^\alpha \cdot I_\alpha^*(t), \qquad \mathcal{A}(u) \subset \mathcal{M}$$

a) Expand $f_\alpha(x_0) = \left(L^{j_1} L^{j_2} \cdots L^{j_r} f\right)(x_0)$ and collect the elementary differentials that appear.
Used by Komori et.al, Burrage & Burrage, Rößler to derive B–series for SDEs.

Wagner–Platen series vs. B–series

$$f(X(t)) = \sum_{\alpha\in\mathcal{M}} I_\alpha^*(t)\cdot f_\alpha(x_0) = \sum_{u\in U_f} \beta(u)\cdot\psi_\eta(u)(t)\cdot G(u)(x_0)$$

Trees and multi-indices are related by:

$$\text{a)}\qquad f_\alpha(x_0) = \sum_{u\in V(\alpha)} \mu_u^\alpha \cdot G(u)(x_0), \qquad V(\alpha)\subset U_f$$

$$\text{b)}\qquad \beta(u)\cdot\psi_\eta(t) = \sum_{\alpha\in\mathcal{A}(u)} \mu_u^\alpha\cdot I_\alpha^*(t), \qquad \mathcal{A}(u)\subset\mathcal{M}$$

a) Expand $f_\alpha(x_0) = \left(L^{j_1}L^{j_2}\cdots L^{j_r}f\right)(x_0)$ and collect the elementary differentials that appear.
   Used by Komori et.al, Burrage & Burrage, Rößler to derive B–series for SDEs.

b) After the expansion a), collect all contributions to $G(u)(x_0)$.
   Can be used to derive relations between different representations of the stochastic integrals.

Wagner-Platen series:

$$\begin{aligned} f(X(t)) &= f + I^*_{(1)}L^1 f + I^*_{(0)}L^0 f + I^*_{(11)}L^1L^1 f + I^*_{(01)}L^0L^1 f + I^*_{(10)}L^1L^0 f + I^*_{(111)}L^1L^1L^1 f + \cdots \\ &= f + I^*_{(1)} f' g_1 + I^*_{(0)} \left(f'g_0 + \gamma^* f''(g_1,g_1)\right) + I^*_{(11)} \left(f''(g_1,g_1) + f' g_1' g_1 \right) \\ &+ I^*_{(01)} \left(f''(g_1,g_0) + f'g_1'g_0 + \gamma^* \left(f'''(g_1,g_1,g_1) + 2f''(g_1'g_1,g_1) + f'g_1''(g_1,g_1)\right)\right) \\ &+ I^*_{(10)} \left(f''(g_0,g_1) + f'g_0'g_1 + \gamma^* \left(f'''(g_1,g_1,g_1) + 2f''(g_1'g_1,g_1)\right)\right) \\ &+ I^*_{(111)} (f'''(g_1,g_1,g_1) + 3f''(g_1'g_1,g_1) + f'g_1''(g_1,g_1) + f'g_1'g_1'g_1) + \cdots \end{aligned}$$

B–series:

$$\begin{aligned} f(X(t)) &= f + I^*_{(1)} f'g_1 + I^*_{(0)} f'g_0 + I^*_{(11)} f'g_1'g_1 + \frac{1}{2}(I^*_{(1)})^2 f''(g_1,g_1) + I^*_{(0)} I^*_{(1)} f''(g_0,g_1) \\ &+ I^*_{(10)} f'g_0'g_1 + I^*_{(01)} f'g_1'g_0 + \frac{1}{6}(I^*_{(1)})^3 f'''(g_1,g_1,g_1) + I^*_{(1)} I^*_{(11)} f''(g_1'g_1,g_1) \\ &+ \frac{1}{2}\Psi f'g_1''(g_1,g_1) + I^*_{(111)} f'g_1'g_1'g_1 + \cdots \end{aligned}$$

Wagner-Platen series:

$$f(X(t)) = f + I^*_{(1)}L^1f + I^*_{(0)}L^0f + I^*_{(11)}L^1L^1f + I^*_{(01)}L^0L^1f + I^*_{(10)}L^1L^0f + I^*_{(111)}L^1L^1L^1f + \cdots$$
$$= f + I^*_{(1)}f'g_1 + I^*_{(0)}\left(f'g_0 + \gamma^* f''(g_1,g_1)\right) + I^*_{(11)}\left(f''(g_1,g_1) + f'g_1'g_1\right)$$
$$+ I^*_{(01)}\left(f''(g_1,g_0) + f'g_1'g_0 + \gamma^*\left(f'''(g_1,g_1,g_1) + 2f''(g_1'g_1,g_1) + f'g_1''(g_1,g_1)\right)\right)$$
$$+ I^*_{(10)}\left(f''(g_0,g_1) + f'g_0'g_1 + \gamma^*\left(f'''(g_1,g_1,g_1) + 2f''(g_1'g_1,g_1)\right)\right)$$
$$+ I^*_{(111)}(f'''(g_1,g_1,g_1) + 3f''(g_1'g_1,g_1) + f'g_1''(g_1,g_1) + f'g_1'g_1'g_1) + \cdots$$

B–series:

$$f(X(t)) = f + I^*_{(1)}f'g_1 + I^*_{(0)}f'g_0 + I^*_{(11)}f'g_1'g_1 + \frac{1}{2}(I^*_{(1)})^2 f''(g_1,g_1) + I^*_{(0)}I^*_{(1)}f''(g_0,g_1)$$
$$+ I^*_{(10)}f'g_0'g_1 + I^*_{(01)}f'g_1'g_0 + \frac{1}{6}(I^*_{(1)})^3 f'''(g_1,g_1,g_1) + I^*_{(1)}I^*_{(11)}f''(g_1'g_1,g_1)$$
$$+ \frac{1}{2}\Psi f'g_1''(g_1,g_1) + I^*_{(111)}f'g_1'g_1'g_1 + \cdots$$

Compare terms:

$$\gamma^* I^*_{(0)} + I^*_{(11)} = \frac{1}{2}(I^*_{(1)})^2$$

Wagner-Platen series:

$$\begin{aligned} f(X(t)) &= f + I^*_{(1)}L^1f + I^*_{(0)}L^0f + I^*_{(11)}L^1L^1f + I^*_{(01)}L^0L^1f + I^*_{(10)}L^1L^0f + I^*_{(111)}L^1L^1L^1f + \cdots \\ &= f + I^*_{(1)}f'g_1 + I^*_{(0)}\left(f'g_0 + \gamma^* f''(g_1,g_1)\right) + I^*_{(11)}\left(f''(g_1,g_1) + f'g_1'g_1\right) \\ &\quad + I^*_{(01)}\left(f''(g_1,g_0) + f'g_1'g_0 + \gamma^*\left(f'''(g_1,g_1,g_1) + 2f''(g_1'g_1,g_1) + f'g_1''(g_1,g_1)\right)\right) \\ &\quad + I^*_{(10)}\left(f''(g_0,g_1) + f'g_0'g_1 + \gamma^*\left(f'''(g_1,g_1,g_1) + 2f''(g_1'g_1,g_1)\right)\right) \\ &\quad + I^*_{(111)}(f'''(g_1,g_1,g_1) + 3f''(g_1'g_1,g_1) + f'g_1''(g_1,g_1) + f'g_1'g_1'g_1) + \cdots \end{aligned}$$

B–series:

$$\begin{aligned} f(X(t)) &= f + I^*_{(1)}f'g_1 + I^*_{(0)}f'g_0 + I^*_{(11)}f'g_1'g_1 + \frac{1}{2}(I^*_{(1)})^2 f''(g_1,g_1) + I^*_{(0)}I^*_{(1)}f''(g_0,g_1) \\ &+ I^*_{(10)}f'g_0'g_1 + I^*_{(01)}f'g_1'g_0 + \frac{1}{6}(I^*_{(1)})^3 f'''(g_1,g_1,g_1) + I^*_{(1)}I^*_{(11)}f''(g_1'g_1,g_1) \\ &+ \frac{1}{2}\Psi f'g_1''(g_1,g_1) + I^*_{(111)}f'g_1'g_1'g_1 + \cdots \end{aligned}$$

Compare terms:

$$\gamma^* I^*_{(0)} + I^*_{(11)} = \frac{1}{2}(I^*_{(1)})^2$$

$$2\gamma^*(I^*_{(01)} + I^*_{(10)}) + 3I^*_{(111)} = I^*_{(1)}I^*_{(11)}$$

Relations between integrals

$$\beta(u) \cdot \psi_\eta(u)(t) = \sum_{\alpha \in \mathcal{A}(u)} \mu_u^\alpha \cdot I_\alpha^*(t), \qquad \mathcal{A}(u) \subset \mathcal{M}$$

Find the set $\omega(u)$ of all monotonic labellings of the tree u. Then for each $\hat{u} \in \omega(u)$ do

1. $\alpha = (j_{r(u)}, j_{r(u)-1}, \ldots, j_1) \in L\mathcal{A}(\hat{u})$ and $\mu_{\hat{u}}^\alpha = 1$.
2. If $j_s = j_{s-1} \neq 0$ and vertex s is not above vertex $s-1$ on the same branch, then $(j_{r(u)}, j_{r(u)-1}, \ldots, j_{s+1}, 0, j_{s-2}, \ldots, j_1) \in L\mathcal{A}(\hat{u})$ and $\mu_{\hat{u}}^\alpha = \gamma^*$.
3. If there are k such pairs of indices, then each pair is replaced by 0, and the resulting multi-index is an element of $L\mathcal{A}(\hat{u})$. In this case $\mu_{\hat{u}}^\alpha = (\gamma^*)^k$.

Finally,

$$\mathcal{A}(u) = \bigcup_{\hat{u} \in \omega(u)} L\mathcal{A}(\hat{u}), \qquad \mu_u^\alpha = \sum_{\hat{u} \in \omega(u)} \mu_{\hat{u}}^\alpha.$$

Debrabant & K, Stochastic Analysis and Applications, (2010)

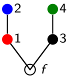
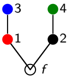
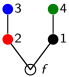
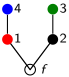
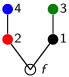
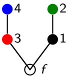
Relations between integrals

$$\beta(u) \cdot \psi(u)(t) = \sum_{\alpha \in \mathcal{A}(u)} \mu_u^\alpha \cdot I_\alpha^*(t), \qquad \mathcal{A}(u) \subset \mathcal{M}$$

For $u = [[\bullet]_\bullet, [\bullet]_\bullet]_f$ using the colors:

$$W_1(t),\ W_2(t),\ W_3(t),\ W_4(t)$$

we get:

$\hat{u}$						
$L\mathcal{A}(\hat{u})$	$\{4,3,2,1\}$	$\{4,2,3,1\}$	$\{4,2,1,3\}$	$\{2,4,3,1\}$	$\{2,4,1,3\}$	$\{2,1,4,3\}$

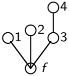
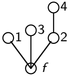
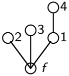
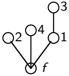
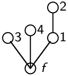
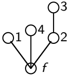
finally giving

$$\psi(u)(t) = I_{(21)}^* I_{(43)}^* = I_{(4321)}^* + I_{(4231)}^* + I_{(4213)}^* + I_{(2431)}^* + I_{(2413)}^* + I_{(2143)}^*$$

Relations between integrals

$$\beta(u) \cdot \psi(u)(t) = \sum_{\alpha \in \mathcal{A}(u)} \mu_u^{\alpha} \cdot I_{\alpha}^{*}(t), \qquad \mathcal{A}(u) \subset \mathcal{M}$$

For $u = [\circ, \circ, [\circ]]_f$ we get

					
$\{(1,1,1,1),$ $(1,1,0),$ $(1,0,1)\}$	$\{(1,1,1,1),$ $(1,1,0),$ $(1,0,1),$ $(0,1,1),$ $(0,0)\}$	$\{(1,1,1,1),$ $(1,1,0),$ $(1,0,1),$ $(0,1,1),$ $(0,0)\}$	$\{(1,1,1,1),$ $(1,1,0),$ $(1,0,1),$ $(0,1,1),$ $(0,0)\}$	$\{(1,1,1,1),$ $(1,0,1),$ $(0,1,1)\}$	$\{(1,1,1,1),$ $(1,1,0),$ $(0,1,1),$ $(0,0)\}$.

Taking into account $\beta(u) = \frac{1}{2}$ we obtain finally

$$\frac{1}{2}\psi(u)(t) = \frac{1}{2} I_{(1)}^{*} I_{(1)}^{*} I_{(11)}^{*} = 6 I_{(1111)}^{*} + \gamma^{*}(5 I_{(110)}^{*} + 5 I_{(101)}^{*} + 5 I_{(011)}^{*}) + 4(\gamma^{*})^{2} I_{(00)}^{*}.$$

Summary

Statement of the problem

Stochastic B-series

Order conditions for SRK

A surprising result (with explanation)

B-series vs. Wagner-Platen series

Part III

B-series and conservation of quadratic invariants

with

Sverre Anmarkrud, NMBU, Norway and Kristian Debrabant, SDU, Denmark

Background

- Sanz-Serna and Abia (1991) have proved that for Runge-Kutta methods preserving quadratic invariants only order conditions related to rootless trees have to be satisfied. The same authors proved a similar result for partitioned Runge-Kutta methods (1993).
- Is this true for stochastic methods as well?

Background

- Sanz-Serna and Abia (1991) have proved that for Runge-Kutta methods preserving quadratic invariants only order conditions related to rootless trees have to be satisfied. The same authors proved a similar result for partitioned Runge-Kutta methods (1993).
- Is this true for stochastic methods as well?
- The answer is yes
  (otherwise this talk would not be given).

This work was inspired by *J. Hong, D. Xu, P. Wang (2015)*.

Stochastic differential equations and invariants

Consider the Stratonovich SDEs

$$dX(t) = g_0(X(t))dt + \sum_{l=1}^{m} g_l(X(t)) \circ dW_l(t)$$

where $W_l(t)$ are independent Wiener processes, and the coefficient functions $g_l : \mathbb{R}^d \to \mathbb{R}^d$ are sufficiently smooth.
A function $\mathcal{I} : \mathbb{R}^d \to \mathbb{R}$ is an invariant, or a first integral of the SDE if

$$\mathcal{I}(X(t)) = \mathcal{I}(X(t_0))$$

for all possible solutions of the SDE, which is the case if and only if The function $\mathcal{I}$ is an invariant of the SDE if and only if

$$\nabla\mathcal{I}(x) \cdot g_l(x) = 0, \qquad l = 0, 1, \cdots, m, \qquad \forall x \in \mathbb{R}^n.$$

In this talk, we will only discuss quadratic invariants $\mathcal{I}(x) = x^T Cx$ for some constant matrix C.

Runge-Kutta method:

$$H_i = Y_n + \sum_{i=1}^{s} \sum_{l=0}^{m} Z_{ij}^{(l)} g_l(H_j), \quad i = 1, 2, \cdots, s$$

$$Y_{n+1} = Y_n + \sum_{i=1}^{s} \sum_{l=0}^{m} \gamma_i^{(l)} g_l(H_i).$$

Theorem

- *All SRKs preserves linear invariants.*
- *A SRK preserves all quadratic invariants if and only if*

$$\gamma_i^{(l)} Z_{ij}^{(k)} + \gamma_j^{(k)} Z_{ji}^{(l)} = \gamma_i^{(l)} \gamma_j^{(k)}, \qquad \forall i, j = 1, \ldots, s, \quad l, k = 0, \ldots, m.$$

- *No SRK preserves all polynomial invariants of degree 3.*

Milstein et.al. (2003), J.Hong et.al. (2015)

Numerical experiments:

Gauss method:

$$s = 1: \quad Z^{(l)} = \tfrac{1}{2}\Delta W_{l,n}, \qquad \gamma^{(l)} = \Delta W_{l,n}$$

$$s = 2: \quad Z^{(l)} = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \end{pmatrix} \Delta W_{l,n}, \quad \gamma^{(l)} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} \Delta W_{l,n}, \qquad l = 0, 1.$$

where $\Delta W_{0,n} = h$ and $\Delta W_{l,n} = W_l(t_n + h) - \Delta W_l(t_n)$ for $l > 0$ are the standard Wiener increments.

Both methods conserve quadratic invariants, they are of deterministic order 2 and 4 respectively, but of stochastic strong order 1.

For comparision we have applied Platen's method. The method is of stochastic strong order 1, but do not conserve quadratic invariants.

The rigid body example

$$dX = A(X)Xdt + \sigma\, g_1(X) \circ dW(t)$$

with some constant σ and

$$A(X) = \begin{pmatrix} 0 & x_3/I_3 & -x_2/I_2 \\ -x_3/I_3 & 0 & x_1/I_1 \\ x_2/I_2 & -x_1/I_1 & 0 \end{pmatrix} \qquad \text{with} \qquad \begin{aligned} I_1 &= 2 \\ I_2 &= 1 \\ I_3 &= 2/3 \end{aligned}$$

Problem P1:

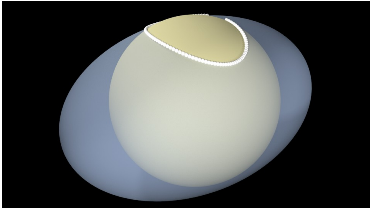
$$g_1(X) = A(X)X, \qquad \begin{cases} \mathcal{I}(X) = X_1^2 + X_2^2 + X_3^2 \\ \mathcal{H}(X) = \frac{1}{2}\left(X_1^2/I_1 + X_2^2/I_2 + X_3^2/I_3\right) \end{cases}$$

Problem P2:

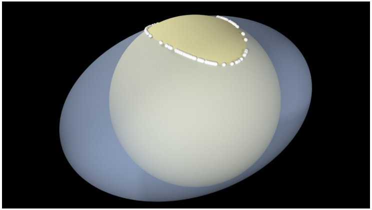
$$g_1(X) = \begin{pmatrix} X_2 \\ -X_1 \\ 0 \end{pmatrix}, \qquad \mathcal{I}(X) = (X_1^2 + X_2^2 + X_3^2)$$

The rigid body example

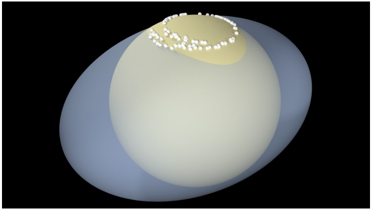
Deterministic



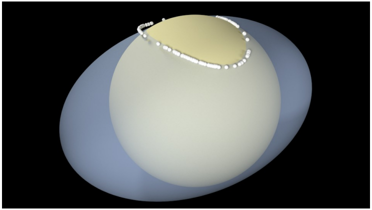
P1: Two invariants



P2: One invariant



P2: Two invariants, Platen's method



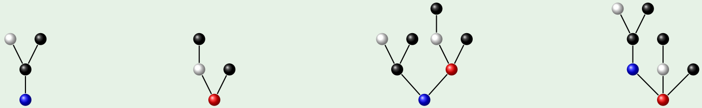
The first three are solved by a Gauss, $s = 2$ method.

The Butcher product

Given two trees $u = [u_1, \ldots, u_{\kappa_1}]_{l_1}$, $v = [v_1, \ldots, v_{\kappa_2}]_{l_2}$. Then the Butcher product of the two trees is defined by

$$u \circ v = [u_1, \cdots, u_{\kappa_1}, v]_{l_1}$$

Example



$u = [u_1]_{\bullet}$	$v = [v_1, v_2]_{\bullet}$	$u \circ v$	$v \circ u$
$\eta(u)$	$\eta(v)$	$\eta(u \circ v)$	$\eta(v \circ u)$
$\shortparallel$	$\shortparallel$	$\shortparallel$	$\shortparallel$
$\int_0^h \eta(u_1) \circ dW$	$\int_0^h \eta(v_1)\eta(v_2) \circ dW$	$\int_0^h \eta(u_1)\eta(v) \circ dW$	$\int_0^h \eta(u)\eta(v_1)\eta(v_2) \circ dW$

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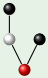
$$u \circ v = [u_1, \cdots, u_{\kappa_1}, v]_{l_1}$$

Example

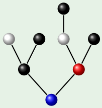
$u = [u_1]_{\color{blue}\bullet}$

$$\eta(u) = \int_0^h \eta(u_1) \circ dW$$



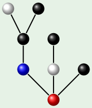
$v = [v_1, v_2]_{\color{red}\bullet}$

$$\eta(v) = \int_0^h \eta(v_1)\eta(v_2) \circ dW$$



$u \circ v$

$$\eta(u \circ v) = \int_0^h \eta(u_1)\eta(v) \circ dW$$



$v \circ u$

$$\eta(v \circ u) = \int_0^h \eta(u)\eta(v_1)\eta(v_2) \circ dW$$

By the chain rule for Stratonovich integrals and the definition of the elementary weight functions e, we get

$$\eta(u)\eta(v) = \eta(u \circ v) + \eta(v \circ u)$$

Let us put things together

SDE:

$$dX(t) = \sum_{l=0}^{m} g_l(Y(t)) \circ dW_l(t)$$

SRK:

$$H_i = Y_n + \sum_{l=0}^{m} \sum_{j=1}^{s} Z_{ij}^{(l)} g_l(H_j)$$

$$Y_{n+1} = Y_n + \sum_{l=0}^{m} \sum_{i=1}^{s} \gamma_i^{(l)} g_l(H_j)$$

Set of trees:

$$\tau = [\tau_1, \ldots, \tau_{\kappa_1}]_l \in T : \quad X(t),\ H_i,\ Y_1$$

Quadratic invariant condition:

$$\gamma_i^{(l)} Z_{ij}^{(k)} + \gamma_j^{(k)} Z_{ji}^{(l)} = \gamma_i^{(l)} \gamma_j^{(k)}$$

Cont.

Let

$$u = [u_1, \cdots, u_{\kappa_1}]_l \qquad v = [v_1, \cdots, v_{\kappa_2}]_k$$

$$u \circ v = [u_1, \cdots, u_{\kappa_1}, v]_l, \qquad v \circ u = [u, v_1, \cdots, v_{\kappa_2}]_k$$

Quadratic invariants:

$$(*) \quad \gamma_i^{(l)}\gamma_j^{(k)} = \gamma_i^{(l)} Z_{ij}^{(k)} + \gamma_j Z_{ji}^{(l)}$$

Weight functions of SRK:

Let $\mathcal{R}_i(u) = \prod_k \Phi_i(u_r)$, $\mathcal{R}_j(v) = \prod_k \Phi_j(v_r)$. Then

$$\phi(u) = \sum_i \gamma_i^{(l)} \mathcal{R}_i(u), \qquad \phi(v) = \sum_j \gamma_j^{(k)} \mathcal{R}_j(v)$$

Cont.

Let

$$u = [u_1, \cdots, u_{\kappa_1}]_l \qquad v = [v_1, \cdots, v_{\kappa_2}]_k$$
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Multiply $(*)$ by $\mathcal{R}_i(u) \cdot \mathcal{R}_j(v)$ and sum over all $i, j = 1, \ldots, s$:

$$\sum_i \gamma_i^{(l)} \mathcal{R}_i(u) \sum_j \gamma_j^{(k)} \mathcal{R}_j(v) = \sum_i \gamma_i^{(l)} \mathcal{R}_i(u) \Big(\sum_j Z_{ij}^{(k)} \mathcal{R}_j(v) \Big) + \sum_j \gamma_j^{(k)} \Big(\sum_i Z_{ji}^{(l)} \mathcal{R}_i(u) \Big) \mathcal{R}_j(v)$$

Cont.

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Multiply $(*)$ by $\mathcal{R}_i(u) \cdot \mathcal{R}_j(v)$ and sum over all $i, j = 1, \ldots, s$:

$$\overbrace{\sum_i \gamma_i^{(l)} \mathcal{R}_i(u)}^{\phi(u)} \overbrace{\sum_j \gamma_j^{(k)} \mathcal{R}_j(v)}^{\phi(v)} = \overbrace{\sum_i \gamma_i^{(l)} \mathcal{R}_i(u) \Big(\sum_j Z_{ij}^{(k)} \mathcal{R}_j(v) \Big)}^{\phi(u \circ v)} + \overbrace{\sum_j \gamma_j^{(k)} \Big(\sum_i Z_{ji}^{(l)} \mathcal{R}_i(u) \Big) \mathcal{R}_j(v)}^{\phi(v \circ u)}$$

Cont.

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Multiply $(*)$ by $\mathcal{R}_i(u) \cdot \mathcal{R}_j(v)$ and sum over all $i, j = 1, \ldots, s$:

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$$\phi(u)\phi(v) = \phi(u \circ v) + \phi(v \circ u)$$

Butcher product cont.

We have proved the following result:

Lemma

For all $u, v \in T$ *we have*

$$\eta(u)(h) \cdot \eta(v)(h) = \eta(u \circ v)(h) + \eta(v \circ u)(h).$$

If the SRK preserves quadratic invariants then

$$\phi(u)(h) \cdot \phi(v)(h) = \phi(u \circ v)(h) + \phi(v \circ u)(h).$$

Redundant order conditions

$$\text{Exact:} \qquad \eta(u)\eta(v) = \eta(u \circ v) + \eta(v \circ u)$$

$$\text{Numerical:} \qquad \phi(u)\phi(v) = \phi(u \circ v) + \phi(v \circ u)$$

Redundant order conditions

$$\begin{array}{lccccc} \text{Exact:} & \eta(u)\eta(v) & = & \eta(u \circ v) & + & \eta(v \circ u) \\ & \shortparallel \quad \shortparallel & & \shortparallel & & \\ \text{Numerical:} & \phi(u)\phi(v) & = & \phi(u \circ v) & + & \phi(v \circ u) \end{array}$$

Redundant order conditions

$$
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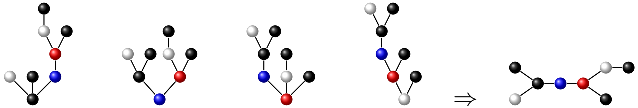

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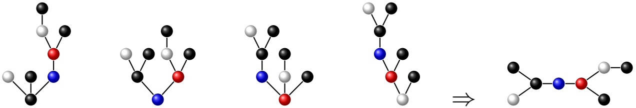

Consequence:

Assume that the order conditions $\phi(\tau) = \eta(\tau)$ for all trees with $\#$ nodes less than q. Then, to satisfy the order conditions for trees with q nodes, *we only have to consider one condition for each rootless tree.*

The number of trees to consider is significantly reduced.

Partitioned SDEs

SDE:

$$dX(t) = f_0(X(t), Y(t))dt + \sum_{l=1}^{m} f_l(X(t), Y(t)) \circ dW_l(t)$$

$$dY(t) = g_0(X(t), Y(t))dt + \sum_{l=1}^{m} g_l(X(t), Y(t)) \circ dW_l(t)$$

where

- $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \to \mathbb{R}^{n_x}$ and $g : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \to \mathbb{R}^{n_y}$
- $W_l(t)$ are standard Wiener processes.
  $W_0(t) = t$.
- Only Stratonovich integrals are considered

We consider quadratic invariants of the form

$$I(X, Y) = X(t)^T D\, Y(t), \qquad D \in \mathbb{R}^{n_x \times n_y}$$

Example: N-body system

Hamiltonian (total energy):

$$\mathcal{H}(\mathbf{p},\mathbf{q}) = T(\mathbf{p}) + V(\mathbf{q})$$

with

$$T(\mathbf{p}) = \sum_{i=1}^{N} \frac{|p_i|^2}{2m_i}, \qquad V(\mathbf{q}) = \sum_{i>j} V_{ij}(r_{ij}), \qquad r_{ij} = |q_i - q_j|.$$

Canonical equations:

$$dq_i = p_i\,(dt + \circ\alpha dW), \qquad dp_i = -\sum_{j=1}^{N} \frac{V'_{ij}}{r_{ij}}(q_i - q_j)\,(dt + \circ\alpha dW), \qquad i = 1, 2, \cdots, N$$

Preserved quantities:

- The total energy $\mathcal{H}(\mathbf{p},\mathbf{q})$ (nonlinear)
- The total momentum: $P = \sum_{i=1}^{N} p_i$ (linear)
- The angular momentum: $L = \sum_{i=1}^{N} q_i \times p_i$ (quadratic)

Why SPRK methods?

Consider the deterministic case

$$x' = f(x, y), \qquad y' = g(x, y)$$

The following method is known to preserve quadratic invariants:

$$\begin{aligned}
X_1 &= x_n, & Y_1 &= y_n + \frac{h}{2} g(X_1, Y_1), \\
X_2 &= x_n + \frac{h}{2}(f(X_1, Y_1) + f(X_2, Y_2)), & Y_2 &= y_n + \frac{h}{2} g(X_1, Y_1), \\
x_{n+1} &= x_n + \frac{h}{2}(f(X_1, Y_1) + f(X_2, Y_2)), & y_{n+1} &= y_n + \frac{h}{2}(g(X_1, Y_1) + g(X_2, Y_2)).
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\end{aligned}$$

But, if the system is *separable*, that is $f = f(y)$ and $g = g(x)$ this becomes

$$Y_1 = y_n + \frac{h}{2} g(x_n), \qquad x_{n+1} = x_n + hf(Y_1), \qquad y_{n+1} = y_n + \frac{h}{2}(g(x_n) + g(x_{n+1}))$$

Stochastic partitioned Runge-Kutta methods (SPRK)

SDE:

$$dX(t) = \sum_{l=0}^{m} f_l(X(t), Y(t)) \circ dW_l(t)$$

$$dY(t) = \sum_{l=0}^{m} g_l(X(t), Y(t)) \circ dW_l(t)$$

SPRK:

$$H_i = X_n + \sum_{l=0}^{m} \sum_{j=1}^{s} Z_{ij}^{(l)} f_l(H_j, K_j)$$

$$K_i = Y_n + \sum_{l=0}^{m} \sum_{j=1}^{s} \hat{Z}_{ij}^{(l)} g_l(H_j, K_j)$$

$$X_{n+1} = X_n + \sum_{l=0}^{m} \sum_{i=1}^{s} \gamma_i^{(l)} f_l(H_j, K_j)$$

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Example: Lobatto III A–B (Störmer-Verlet):

$$Z^{(1,l)} = \begin{pmatrix} 0 & 0 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} J_l, \qquad Z^{(2,l)} = \begin{pmatrix} \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \end{pmatrix} J_l$$

$$\gamma^{(1,l)} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} J_l, \qquad \gamma^{(2,l)} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} J_l.$$

for $l = 0, \dots, m$. Here $J_0 = h$, $J_l = \Delta W_l$.

Theorem (Hong et.al. 2015)

The SPRK preserves all linear invariants if $\gamma_i^{(l)} = \hat{\gamma}_i^{(l)}$ *and all quadratic invariants of the form* $I = X^T DY$ *if in addition*

$$\gamma_i^{(l)} \hat{Z}_{ij}^{(k)} + \hat{\gamma}_j^{(k)} Z_{ji}^{(l)} = \gamma_i^{(l)} \hat{\gamma}_j^{(k)}$$

for all $i, j = 1, \ldots, s$ *and* $l, k = 0, \ldots, m$.

For separable systems, the first condition is superfluous.

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For separable systems, the first condition is superfluous.

Tasks:

- Find the B-series for the exact and the numerical solution of the partitioned system.
- Prove that the if the theorem is satisfied, only rootless trees have to be considered.

Let us consider the system split into p partitions:
SDE:

$$dX_k(t) = \sum_{l=0}^{m} g_{k,l}(X_1(t),\dots,X_p(t)) \circ dW_l(t), \qquad k = 1,\cdots,p.$$

The B–series of the exact solution is a *formal* series of the form

$$X_k(h) = B_k(\eta,\mathbf{x_0};h) = \sum_{\tau\in T_k} \alpha(\tau)\cdot\eta(\tau)(h)\cdot F(\tau)(\mathbf{x}_0)$$

Each node $\bullet_{k,l}$ in a three $\tau \in T_k$ now has a *shape* k referring to the partition, and a color l referring to the Wiener process.

Here $\mathbf{x_0}$ refers to all the initial values.

B–series for the exact solution

$$\text{SDE:} \qquad dX_k(t) = \sum_{l=0}^{m} g_{k,l}(X_1(t), \ldots, X_p(t)) \circ dW_l(t), \qquad k = 1, \ldots, p$$

$$\text{B–series:} \quad X_k(h) = B_k(\eta, \mathbf{x}_0; h) = \sum_{\tau \in T_k} \alpha(\tau) \cdot \eta(\tau)(h) \cdot F(\tau)(\mathbf{x}_0)$$

- Trees:

$$\bullet_{k,l} = [\emptyset]_{k,l} \in T_{k,l}, \qquad \tau = [\tau_1, \ldots, \tau_\kappa]_{k,l} \in T_{k,l}, \qquad T_k = \cup_l T_{k,l}$$

- Elementary differentials:

$$F(\bullet_{k,l})(\mathbf{x}_0) = g_{k,l}(\mathbf{x}_0), \qquad F(\tau)(\mathbf{x}_0) = g_{k,l}^{(\kappa)}(\mathbf{x}_0)\Big(F(\tau_1)(\mathbf{x}_0), \cdots, F(\tau_\kappa)(\mathbf{x}_0)\Big)$$

- Elementary weight functions:

$$\eta(\bullet_{k,l})(h) = W_l(h), \qquad \eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$

- The order $\rho(\tau)$ of the three is the number or deterministic nodes + 1/2 times the number of stochastic nodes

Example

Let $m = 2, p = 3$:

	dt	W_1	W_2
$g_{1,l}$	●	●	●
$g_{2,l}$	■	■	■
$g_{3,l}$	★	★	★

$$\tau = [\tau_1, \ldots, \tau_\kappa]_{k,l} \in T_{k,l}, \qquad T_k = \cup_l T_{k,l}$$

$$F(\tau)(\mathbf{x}_0) = g_{k,l}^{(\kappa)}(\mathbf{x}_0)\Big(F(\tau_1)(\mathbf{x}_0), \cdots, F(\tau_\kappa)(\mathbf{x}_0)\Big)$$

$$\eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$

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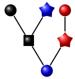
$$\tau = [\tau_1, \ldots, \tau_\kappa]_{k,l} \in T_{k,l}, \qquad T_k = \cup_l T_{k,l}$$

$$F(\tau)(\mathbf{x}_0) = g_{k,l}^{(\kappa)}(\mathbf{x}_0)\Big(F(\tau_1)(\mathbf{x}_0), \cdots, F(\tau_\kappa)(\mathbf{x}_0)\Big)$$

$$\eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$



Example

Let $m = 2, p = 3$:

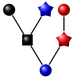
	dt	W_1	W_2
$g_{1,l}$	●	●	●
$g_{2,l}$	■	■	■
$g_{3,l}$	★	★	★

$$\tau = [\tau_1, \ldots, \tau_\kappa]_{k,l} \in T_{k,l}, \qquad T_k = \cup_l T_{k,l}$$

$$F(\tau)(\mathbf{x}_0) = g_{k,l}^{(\kappa)}(\mathbf{x}_0)\Big(F(\tau_1)(\mathbf{x}_0), \cdots, F(\tau_\kappa)(\mathbf{x}_0)\Big)$$

$$\eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$

- $\tau = \Big[\big[\bullet, \star\big]_{\blacksquare}, [\bullet]_{\star}\Big]_{\bullet}$



Example

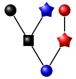
Let $m = 2, p = 3$:

	dt	W_1	W_2
$g_{1,l}$	● (black)	● (blue)	● (red)
$g_{2,l}$	■ (black)	■ (blue)	■ (red)
$g_{3,l}$	★ (black)	★ (blue)	★ (red)

$$\tau = [\tau_1, \ldots, \tau_\kappa]_{k,l} \in T_{k,l}, \qquad T_k = \cup_l T_{k,l}$$

$$F(\tau)(\mathbf{x}_0) = g_{k,l}^{(\kappa)}(\mathbf{x}_0)\Big(F(\tau_1)(\mathbf{x}_0), \cdots, F(\tau_\kappa)(\mathbf{x}_0)\Big)$$

$$\eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$



- $\tau = \Big[\big[●, ★\big]_{■}, [●]_{★}\Big]_{●}$
- $F(\tau) = \dfrac{\partial^2 g_{1,1}}{\partial X_2 \partial X_3}\left(\dfrac{\partial^2 g_{2,0}}{\partial X_1 \partial X_3}\big(g_{1,0}, g_{3,1}\big), \dfrac{\partial g_{3,2}}{\partial X_1} g_{1,2}\right)$

Example

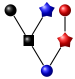
Let $m = 2, p = 3$:

	dt	W_1	W_2
$g_{1,l}$	●	●	●
$g_{2,l}$	■	■	■
$g_{3,l}$	★	★	★

$$\tau = [\tau_1, \dots, \tau_\kappa]_{k,l} \in T_{k,l}, \qquad T_k = \cup_l T_{k,l}$$

$$F(\tau)(\mathbf{x}_0) = g_{k,l}^{(\kappa)}(\mathbf{x}_0)\Big(F(\tau_1)(\mathbf{x}_0), \cdots, F(\tau_\kappa)(\mathbf{x}_0)\Big)$$

$$\eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$



- $\tau = \Big[\big[\bullet, \star\big]_{\blacksquare}, [\bullet]_{\star}\Big]_{\bullet}$
- $F(\tau) = \dfrac{\partial^2 g_{1,1}}{\partial X_2 \partial X_3}\left(\dfrac{\partial^2 g_{2,0}}{\partial X_1 \partial X_3}\big(g_{1,0}, g_{3,1}\big), \dfrac{\partial g_{3,2}}{\partial X_1} g_{1,2}\right)$
- $\eta(\tau)(h) = \displaystyle\int_0^h \left(\int_0^s s_1 W_1(s_1) ds_1\right)\left(\int_0^s W_3(s_2) \circ dW_3(s_2)\right) \circ dW_1(s)$

Example

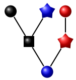
Let $m = 2, p = 3$:

	dt	W_1	W_2
$g_{1,l}$	$\bullet$	$\color{blue}\bullet$	$\color{red}\bullet$
$g_{2,l}$	$\blacksquare$	$\color{blue}\blacksquare$	$\color{red}\blacksquare$
$g_{3,l}$	$\bigstar$	$\color{blue}\bigstar$	$\color{red}\bigstar$

$$\tau = [\tau_1, \ldots, \tau_\kappa]_{k,l} \in T_{k,l}, \qquad T_k = \cup_l T_{k,l}$$

$$F(\tau)(\mathbf{x}_0) = g_{k,l}^{(\kappa)}(\mathbf{x}_0)\Big(F(\tau_1)(\mathbf{x}_0), \cdots, F(\tau_\kappa)(\mathbf{x}_0)\Big)$$

$$\eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$



- $\tau = \Big[\big[\bullet, {\color{blue}\bigstar}\big]_{\blacksquare}, [{\color{red}\bullet}]_{\color{red}\bigstar}\Big]_{\color{blue}\bullet}$
- $F(\tau) = \dfrac{\partial^2 g_{1,1}}{\partial X_2 \partial X_3}\left(\dfrac{\partial^2 g_{2,0}}{\partial X_1 \partial X_3}\big(g_{1,0}, g_{3,1}\big), \dfrac{\partial g_{3,2}}{\partial X_1} g_{1,2}\right)$
- $\eta(\tau)(h) = {\color{blue}\int_0^h}\left(\int_0^s s_1 {\color{blue}W_1(s_1)} ds_1\right){\color{red}\left(\int_0^s W_3(s_2) \circ dW_3(s_2)\right)} \circ {\color{blue}dW_1(s)}$
- The order of this tree is 4

B–series for SPRKs

SDE:

$$dX_k(t) = \sum_{l=0}^{m} g_{k,l}(X_1(t), \ldots, X_p(t)) \circ dW_l(t), \qquad k = 1, \ldots, p$$

SPRK with s stages:

$$H_{k,i} = x_0 + \sum_{l=0}^{m} \sum_{j=1}^{s} Z_{ij}^{(k,l)} g_{k,l}(H_{1,j}, \ldots, H_{p,j}), \qquad i = 1, \ldots, s$$

$$Y_{k,1} = x_0 + \sum_{l=0}^{m} \sum_{i=1}^{s} \gamma_i^{(k,l)} g_{k,l}(H_{1,j}, \ldots, H_{p,j})$$

SDE:

$$dX_k(t) = \sum_{l=0}^{m} g_{k,l}(X_1(t),\ldots,X_p(t)) \circ dW_l(t), \qquad k = 1,\ldots,p$$

SPRK with s stages:

$$H_{k,i} = x_0 + \sum_{l=0}^{m}\sum_{j=1}^{s} Z_{ij}^{(k,l)} g_{k,l}(H_{1,j},\ldots,H_{p,j}), \qquad i = 1,\ldots,s$$

$$Y_{k,1} = x_0 + \sum_{l=0}^{m}\sum_{i=1}^{s} \gamma_i^{(k,l)} g_{k,l}(H_{1,j},\ldots,H_{p,j})$$

Then $X_k(h) = B_k(\eta,\mathbf{x}_0;h)$, $H_{k,i} = B_k(\Phi_i,\mathbf{x}_0;h)$ and $Y_{k,1} = B_k(\phi,\mathbf{x}_0;h)$, with

$$X(h): \qquad \eta(\bullet_{k,l})(h) = W_l(h), \qquad \eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$

$$H_{k,i}: \qquad \Phi_i(\bullet_{k,l}) = \sum_j Z_{ij}^{(k,l)}, \quad \Phi_i(\tau) = \sum_j Z_{ij}^{(k,l)} \prod_{r=1}^{\kappa} \Phi_j(\tau_r)$$

$$Y_{k,1} \qquad \phi(\bullet_{k,l}) = \sum_j \gamma_i^{(k,l)}, \quad \phi(\tau) = \sum_j \gamma_i^{(k,l)} \prod_{r=1}^{\kappa} \Phi_i(\tau_r)$$

Theorem (Milstein -95)

The method has mean square global order q if

$$\phi(\tau)(h) = \eta(\tau)(h) + \mathcal{O}(h^{q+\frac{1}{2}}), \qquad \rho(\tau) \le q$$

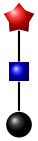
$$\mathbb{E}\phi(\tau)(h) = \mathbb{E}\eta(\tau)(h) + \mathcal{O}(h^{q+1}), \qquad \rho(\tau) \le q + \frac{1}{2}$$

Then $X_k(h) = B_k(\eta, \mathbf{x}_0; h)$, $H_{k,i} = B_k(\Phi_i, \mathbf{x}_0; h)$ and $Y_{k,1} = B_k(\phi, \mathbf{x}_0; h)$, with

$$X(h): \qquad \eta(\bullet_{k,l})(h) = W_l(h), \qquad \eta(\tau)(h) = \int_0^h \prod_{r=1}^{\kappa} \eta(\tau_r)(s) \circ dW_l(s)$$

$$H_{k,i}: \qquad \Phi_i(\bullet_{k,l}) = \sum_j Z_{ij}^{(k,l)}, \quad \Phi_i(\tau) = \sum_j Z_{ij}^{(k,l)} \prod_{r=1}^{\kappa} \Phi_j(\tau_r)$$

$$Y_{k,1} \qquad \phi(\bullet_{k,l}) = \sum_j \gamma_i^{(k,l)}, \qquad \phi(\tau) = \sum_j \gamma_i^{(k,l)} \prod_{r=1}^{\kappa} \Phi_i(\tau_r)$$

τ	η	ϕ
	$W_{l_1}(h)$	$\sum_i \gamma_i^{(k_1,l_1)}$
	$\int_0^h W_{l_2}(s_1) \circ dW_{l_1}(s)$	$\sum_{ij} \gamma_i^{(k_1,l_1} Z_{ij}^{(k_2,l_2)}$
	$\int_0^h W_{l_3}(s) W_{l_2}(s) \circ dW_{l_1}(s)$	$\sum_{ij} \gamma_i^{(k_1,l_1)} Z_{ij}^{(k_3,l_3)} Z_{ij}^{(k_2,l_2)}$
	$\int_0^h \int_0^{s_1} W_{l_3}(s_1) \circ dW_{l_2}(s_1) \circ dW_{l_1}(s)$	$\sum_{ijr} \gamma_i^{(k_1,l_1)} Z_{ij}^{(k_2,l_2)} Z_{jr}^{(k_3,l_3)}$

The Butcher product

Let

$$u = [u_1, \ldots, u_{\kappa_1}]_{l_1}, \qquad v = [v_1, \ldots, v_{\kappa_2}]_{l_2}$$

The Butcher product of the two trees are defined by

$$u \circ v = [u_1, \cdots, u_{\kappa_1}, v]_{l_1}$$

The Butcher product

Let

$$u = [u_1, \ldots, u_{\kappa_1}]_{l_1}, \qquad v = [v_1, \ldots, v_{\kappa_2}]_{l_2}$$

The Butcher product of the two trees are defined by

$$u \circ v = [u_1, \cdots, u_{\kappa_1}, v]_{l_1}$$

Example:

$u = [u_1]_{\bullet}$ $\quad v = [v_1]_{\bullet}$ $\quad u \circ v$ $\quad v \circ u$

The Butcher product

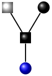
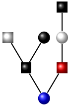
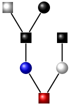
Let

$$u = [u_1, \ldots, u_{\kappa_1}]_{l_1}, \qquad v = [v_1, \ldots, v_{\kappa_2}]_{l_2}$$

The Butcher product of the two trees are defined by

$$u \circ v = [u_1, \cdots, u_{\kappa_1}, v]_{l_1}$$

Example:

			
$u = [u_1]_{\bullet}$	$v = [v_1]_{\bullet}$	$u \circ v$	$v \circ u$
$\eta(u)$	$\eta(v)$	$\eta(u \circ v)$	$\eta(v \circ u)$
=	=	=	=
$\int_0^h \eta(u_1) dW$	$\int_0^h \eta(v_1) dW$	$\int_0^h \eta(u_1)\eta(v) dW$	$\int_0^h \eta(u)\eta(v_1) dW$

Let

$$u = [u_1, \dots, u_{\kappa_1}]_{l_1}, \qquad v = [v_1, \dots, v_{\kappa_2}]_{l_2}$$

The Butcher product of the two trees are defined by

$$u \circ v = [u_1, \cdots, u_{\kappa_1}, v]_{l_1}$$

Example:

$u = [u_1]_{\bullet}$	$v = [v_1]_{\bullet}$	$u \circ v$	$v \circ u$
$\eta(u)$	$\eta(v)$	$\eta(u \circ v)$	$\eta(v \circ u)$
$=$	$=$	$=$	$=$
$\int_0^h \eta(u_1) dW$	$\int_0^h \eta(v_1) dW$	$\int_0^h \eta(u_1)\eta(v) dW$	$\int_0^h \eta(u)\eta(v_1) dW$

By the chain rule for Stratonovich integrals and the definition of the elementary weight functions e, we get

$$\eta(u)\eta(v) = \eta(u \circ v) + \eta(v \circ u)$$

Let us put things together

Separable partitioned SDE:

$$dX(t) = \sum_{l=0}^{m} f_l(Y(t)) \circ dW_l(t)$$

$$dY(t) = \sum_{l=0}^{m} g_l(X(t)) \circ dW_l(t)$$

Reduced set of trees:

$$\tau = [\hat{\tau}_1, \dots, \hat{\tau}_{\kappa_1}]_{\bullet} \in T : \quad X(t),\ H_i,\ X_1$$

$$\hat{\tau} = [\tau_1, \dots, \tau_{\kappa_2}]_{\blacksquare} \in \hat{T} : \quad Y(t),\ K_i,\ Y_1.$$

No child has the same shape as it's parent.

Quadratic invariant condition:

$$\gamma_i^{(l)} \hat{Z}_{ij}^{(k)} + \hat{\gamma}_j^{(k)} Z_{ji}^{(l)} = \gamma_i^{(l)} \hat{\gamma}_j^{(k)}$$

SPRK:

$$H_i = X_n + \sum_{l=0}^{m} \sum_{j=1}^{s} Z_{ij}^{(l)} f_l(K_j)$$

$$K_i = Y_n + \sum_{l=0}^{m} \sum_{j=1}^{s} \hat{Z}_{ij}^{(l)} g_l(H_j)$$

$$X_{n+1} = X_n + \sum_{l=0}^{m} \sum_{i=1}^{s} \gamma_i^{(l)} f_l(K_j)$$

$$Y_{n+1} = Y_n + \sum_{l=0}^{m} \sum_{i=1}^{s} \hat{\gamma}_i^{(l)} g_l(H_j)$$

Butcher product for SPRK methods on separable systems

Let

$$u = [\hat{u}_1, \cdots, \hat{u}_{\kappa_1}]_{\bullet} \in T \qquad \hat{v} = [v_1, \cdots, v_{\kappa_2}]_{\blacksquare} \in \hat{T}$$

$$u \circ \hat{v} = [\hat{u}_1, \cdots, \hat{u}_{\kappa_1}, \hat{v}]_{\bullet} \in T, \qquad \hat{v} \circ u = [u, v_1, \cdots, v_{\kappa_2}]_{\blacksquare} \in \hat{T}$$

Quadratic invariants:

$$(*) \quad \gamma_i^{(l)} \hat{\gamma}_j^{(k)} = \gamma_i^{(l)} \hat{Z}_{ij}^{(k)} + \hat{\gamma}_j Z_{ji}^{(l)}$$

Weight functions of SPRK:

Let $\mathcal{R}_i(u) = \prod_k \Phi_i(\hat{u}_r)$, $\mathcal{R}_j(\hat{v}) = \prod_k \Phi_j(v_r)$. Then

$$\phi(u) = \sum_i \gamma_i \mathcal{R}_i(u), \qquad \phi(\hat{v}) = \sum_j \hat{\gamma}_j \mathcal{R}_j(v)$$

Butcher product for SPRK methods on separable systems

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Weight functions of SPRK:

Let $\mathcal{R}_i(u) = \prod_k \Phi_i(\hat{u}_r)$, $\mathcal{R}_j(\hat{v}) = \prod_k \Phi_j(v_r)$. Then

$$\phi(u) = \sum_i \gamma_i \mathcal{R}_i(u), \qquad \phi(\hat{v}) = \sum_j \hat{\gamma}_j \mathcal{R}_j(v)$$

Multiply $(*)$ by $\mathcal{R}_i(u) \cdot \mathcal{R}_j(\hat{v})$ and sum over all $i, j = 1, \ldots, s$:

$$\sum_i \gamma_i^{(l)} \mathcal{R}_i(u) \sum_j \hat{\gamma}_j^{(k)} \mathcal{R}_j(\hat{v}) = \sum_i \gamma_i^{(l)} \mathcal{R}_i(u) \left(\sum_j \hat{Z}_{ij}^{(k)} \mathcal{R}_j(\hat{v}) \right) + \sum_j \hat{\gamma}_j^{(k)} \left(\sum_i Z_{ji}^{(l)} \mathcal{R}_i(u) \right) \mathcal{R}_j(\hat{v})$$

Butcher product for SPRK methods on separable systems

Let

$$u = [\hat{u}_1, \cdots, \hat{u}_{\kappa_1}]_{\bullet} \in T \qquad \hat{v} = [v_1, \cdots, v_{\kappa_2}]_{\blacksquare} \in \hat{T}$$

$$u \circ \hat{v} = [\hat{u}_1, \cdots, \hat{u}_{\kappa_1}, \hat{v}]_{\bullet} \in T, \qquad \hat{v} \circ u = [u, v_1, \cdots, v_{\kappa_2}]_{\blacksquare} \in \hat{T}$$

Quadratic invariants:

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$$\phi(u) = \sum_i \gamma_i \mathcal{R}_i(u), \qquad \phi(\hat{v}) = \sum_j \hat{\gamma}_j \mathcal{R}_j(v)$$

Multiply $(*)$ by $\mathcal{R}_i(u) \cdot \mathcal{R}_j(\hat{v})$ and sum over all $i, j = 1, \ldots, s$:

$$\overbrace{\sum_i \gamma_i^{(l)} \mathcal{R}_i(u)}^{\phi(u)} \overbrace{\sum_j \hat{\gamma}_j^{(k)} \mathcal{R}_j(\hat{v})}^{\phi(\hat{v})} = \overbrace{\sum_i \gamma_i^{(l)} \mathcal{R}_i(u) \Big(\sum_j \hat{Z}_{ij}^{(k)} \mathcal{R}_j(\hat{v}) \Big)}^{\phi(u \circ \hat{v})} + \overbrace{\sum_j \hat{\gamma}_j^{(k)} \Big(\sum_i Z_{ji}^{(l)} \mathcal{R}_i(u) \Big) \mathcal{R}_j(\hat{v})}^{\phi(\hat{v} \circ u)}$$

Butcher product for SPRK methods on separable systems

Let

$$u = [\hat{u}_1, \cdots, \hat{u}_{\kappa_1}]_{\bullet} \in T \qquad \hat{v} = [v_1, \cdots, v_{\kappa_2}]_{\blacksquare} \in \hat{T}$$

$$u \circ \hat{v} = [\hat{u}_1, \cdots, \hat{u}_{\kappa_1}, \hat{v}]_{\bullet} \in T, \qquad \hat{v} \circ u = [u, v_1, \cdots, v_{\kappa_2}]_{\blacksquare} \in \hat{T}$$

Quadratic invariants:

$$(*) \quad \gamma_i^{(l)} \hat{\gamma}_j^{(k)} = \gamma_i^{(l)} \hat{Z}_{ij}^{(k)} + \hat{\gamma}_j Z_{ji}^{(l)}$$

Weight functions of SPRK:

Let $\mathcal{R}_i(u) = \prod_k \Phi_i(\hat{u}_r)$, $\mathcal{R}_j(\hat{v}) = \prod_k \Phi_j(v_r)$. Then

$$\phi(u) = \sum_i \gamma_i \mathcal{R}_i(u), \qquad \phi(\hat{v}) = \sum_j \hat{\gamma}_j \mathcal{R}_j(v)$$

Multiply $(*)$ by $\mathcal{R}_i(u) \cdot \mathcal{R}_j(\hat{v})$ and sum over all $i, j = 1, \ldots, s$:

$$\overbrace{\sum_i \gamma_i^{(l)} \mathcal{R}_i(u)}^{\phi(u)} \overbrace{\sum_j \hat{\gamma}_j^{(k)} \mathcal{R}_j(\hat{v})}^{\phi(\hat{v})} = \overbrace{\sum_i \gamma_i^{(l)} \mathcal{R}_i(u) \left(\sum_j \hat{Z}_{ij}^{(k)} \mathcal{R}_j(\hat{v}) \right)}^{\phi(u \circ \hat{v})} + \overbrace{\sum_j \hat{\gamma}_j^{(k)} \left(\sum_i Z_{ji}^{(l)} \mathcal{R}_i(u) \right) \mathcal{R}_j(\hat{v})}^{\phi(\hat{v} \circ u)}$$

$$\phi(u)\phi(\hat{v}) = \phi(u \circ \hat{v}) + \phi(\hat{v} \circ u)$$

Redundant order conditions and rootless trees

SDE: $$\eta(u)\eta(\hat{v}) = \eta(u \circ \hat{v}) + \eta(\hat{v} \circ u)$$

SPRK: $$\phi(u)\phi(\hat{v}) = \phi(u \circ \hat{v}) + \phi(\hat{v} \circ u)$$

Redundant order conditions and rootless trees

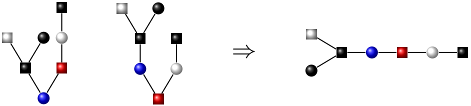
$$\begin{array}{lccccc} \text{SDE:} & \eta(u)\eta(\hat{v}) & = & \eta(u \circ \hat{v}) & + & \eta(\hat{v} \circ u) \\ & \shortparallel \quad \shortparallel & & \shortparallel & & \\ \text{SPRK:} & \phi(u)\phi(\hat{v}) & = & \phi(u \circ \hat{v}) & + & \phi(\hat{v} \circ u) \end{array}$$

Redundant order conditions and rootless trees

$$
\begin{array}{lccccc}
\text{SDE:} & \eta(u)\eta(\hat{v}) & = & \eta(u \circ \hat{v}) & + & \eta(\hat{v} \circ u) \\
 & \shortparallel \quad \shortparallel & & \shortparallel & & \shortparallel \\
\text{SPRK:} & \phi(u)\phi(\hat{v}) & = & \phi(u \circ \hat{v}) & + & \phi(\hat{v} \circ u)
\end{array}
$$

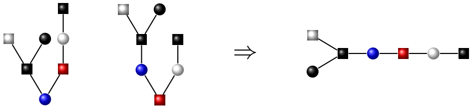
Redundant order conditions and rootless trees

$$
\begin{array}{lccccc}
\text{SDE:} & \eta(u)\eta(\hat{v}) & = & \eta(u \circ \hat{v}) & + & \eta(\hat{v} \circ u) \\
& \shortparallel \quad \shortparallel & & \shortparallel & & \shortparallel \\
\text{SPRK:} & \phi(u)\phi(\hat{v}) & = & \phi(u \circ \hat{v}) & + & \phi(\hat{v} \circ u)
\end{array}
$$



Redundant order conditions and rootless trees

SDE:	$\eta(u)\eta(\hat{v})$	$=$	$\eta(u \circ \hat{v})$	$+$	$\eta(\hat{v} \circ u)$
	$\shortparallel \quad \shortparallel$		$\shortparallel$		$\shortparallel$
SPRK:	$\phi(u)\phi(\hat{v})$	$=$	$\phi(u \circ \hat{v})$	$+$	$\phi(\hat{v} \circ u)$



Conclusion:

Assume that the order conditions $\phi(\tau) = \eta(\tau)$ for all trees with $\#$ nodes less than q. Then, to satisfy the order conditions for trees with q nodes, *we only have to consider one condition for each rootless tree.*

NB! Only for separable systems.

- Part 1: Introduction to B-series.
- Part 2: Stochastic B-series
- Part 3: B-series and preservation of quadratic invariants

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