Stochastic expansions and Hopf algebras

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Brown report

Applied mathematics at the US Department of Energy 2008:

> *Develop new approaches for efficient modeling of large stochastic systems.*

> *Invest in analysis and algorithms for stochastic optimization.*

Langevin equation

Brownian motion: imagine pollen particle on water surface.

Equation of motion for its velocity y_t perhaps

$$\frac{\mathrm{d}y_t}{\mathrm{d}t} = -a\, y_t + \sqrt{b}\,\frac{\mathrm{d}W_t}{\mathrm{d}t}$$

where a and b are constants.

- Deterministic force: $-a\, y_t$,
- White noise force: $\sqrt{b}\,\mathrm{d}W_t/\mathrm{d}t$,
- Represents random buffeting by water molecules.

Stochastic differential equations

$$\mathrm{d}y_t = V_0(y_t)\,\mathrm{d}t + V_1(y_t)\,\mathrm{d}W_t^1 + \cdots + V_d(y_t)\,\mathrm{d}W_t^d$$

What information do we want to retrieve?

For $t \in [0, T]$, want to compute from paths $W(\omega)$

$$\mathrm{E}\, f(y_t) := \int f\big(y_t(\omega)\big)\,\mathrm{d}\mathrm{P}(\omega),$$

Or $f(t, y_s, s \leqslant t)$.

$$\|y_t\|_{L^p}^p := \int \|y_t(\omega)\|_p^p\,\mathrm{d}\mathrm{P}(\omega).$$

How do we retrieve it?

Simulation (PDE)

Solve a PDE for transition probability distribution:

Theorem (Feynman–Kac formula)

Consider the parabolic partial differential equation for $t \in [0, T]$:

$$\partial_t u = \mathcal{L} u,$$

with $u(0, y) = f(y)$. Here $\mathcal{L} := V_0 + \frac{1}{2}(V_1^2 + \cdots + V_d^2)$ is of order $2N$. Let y_t denote the solution to the SDE for $t \in [0, T]$:

$$\mathrm{d}y_t = V_0(y_t)\,\mathrm{d}t + \sum_{i=1}^{d} V_i(y_t)\,\mathrm{d}W_t^i.$$

Then, when $y_0 = y$ we have: $u(t, y) = \mathrm{E}\, f(y_t)$.

Simulation (Monte–Carlo)

Generate a set of suitable multi-d sample paths on $[0, T]$:

$$\hat{W}(\omega) := \Big(\hat{W}^1(\omega), \ldots, \hat{W}^d(\omega)\Big)$$

For each $\hat{W}(\omega)$, generate a sample path solution $\hat{y}_t(\omega)$.

Compute

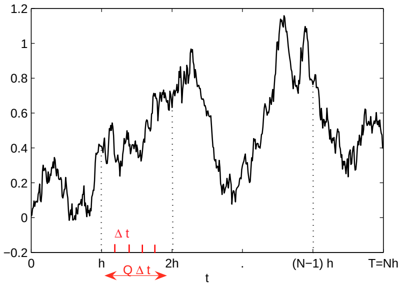
$$\int f\Big(y_t(\omega)\Big)\,\mathrm{dP}(\omega) \approx \tfrac{1}{P}\sum_{i=1}^{P} f\Big(y_t(\omega_i)\Big).$$

Basic setting

$$y_t = y_0 + \int_0^t V_0(y_\tau)\,\mathrm{d}\tau + \sum_{i=1}^{d} \int_0^t V_i(y_\tau)\,\mathrm{d}W_\tau^i$$

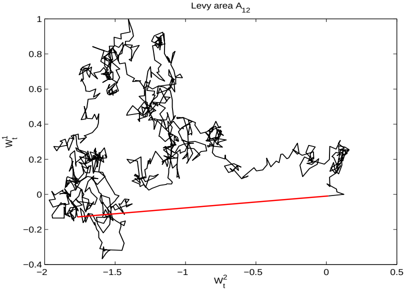
- Stratonovich form
- Non-commuting vector fields: $V_i = \sum_{j=1}^N V_i^j(y)\partial_{y_j}$
- d-dimensional driving signal: $(W^1, \ldots, W^d)$
- Convention: $W_t^0 \equiv t$
- Solution process: $y\colon \mathbb{R}_+ \to \mathbb{R}^N$

Wiener process



- $W_t - W_s \sim \mathrm{N}(0, \sqrt{t-s})$
- Independent increments
- Continuous, nowhere differentiable

Example two-dimensional Brownian path



Stokes' theorem $\implies$ the chordal area is

$$A_{12}(t) = \tfrac{1}{2}\left(\int_0^t W_\tau^1 \,\mathrm{d}W_\tau^2 - \int_0^t W_\tau^2 \,\mathrm{d}W_\tau^1\right).$$

Stochastic Taylor expansion

Flow-map $y_t = \varphi_t \circ y_0$ satisfies

$$\varphi_t = \mathrm{id} + \sum_{i=0}^{d} \int_0^t V_i \circ \varphi_\tau \, \mathrm{d}W_\tau^i .$$

$$\Longrightarrow \quad \varphi_t = \mathrm{id} + \sum_{i=0}^{d} \big(W_t^i\big) \, V_i + \sum_{i,j=0}^{d} \left(\int_0^t \int_0^{\tau_1} \mathrm{d}W_{\tau_2}^i \, \mathrm{d}W_{\tau_1}^j \right) V_{ij} + \cdots .$$

Here $V_{ij} \equiv V_i \circ V_j$. Thus have the *stochastic Taylor expansion*

$$y_t = y_0 + \sum_{i=0}^{d} \big(W_t^i\big) \, V_i(y_0) + \sum_{i,j=0}^{d} \left(\int_0^t \int_0^{\tau_1} \mathrm{d}W_{\tau_2}^i \, \mathrm{d}W_{\tau_1}^j \right) V_{ij}(y_0) + \cdots .$$

Stochastic Taylor approximations

Stochastic Taylor expansion:

$$y_t = y_0 + \sum_{i=0}^{d} J_i(t)\, V_i(y_0) + \sum_{i,j=0}^{d} J_{ij}(t)\, V_{ij}(y_0) + \cdots .$$

- Euler-Maruyama and Milstein methods
- Stochastic Runge–Kutta methods
- Need approximations for iterated integrals

Monte–Carlo: weak approximation

- Construct paths by generating increments $\Delta W^i(t_n, t_{n+1})$ by binomial branching process:

$$\mathrm{P}\Big(\Delta W^i(t_n, t_{n+1}) = \pm\sqrt{h}\Big) = \tfrac{1}{2}$$

- Expectation of approximation $\hat{y}_t$ across all paths is close to the expectation of the true solution:

$$\|\mathbb{E}\, f(y_t) - \mathbb{E}\, f(\hat{y}_t)\| = \mathcal{O}(h^p)$$

- No pathwise comparison: underlying paths not “close” to Wiener paths.

Monte–Carlo: strong approximation

- Generate each multi-d path $\hat{W}(\omega)$ by choosing increments

$$\Delta W^i(t_n, t_{n+1}) \sim \sqrt{h} \cdot \mathrm{N}(0, 1).$$

- More expensive, but can now compare $\hat{y}_t(\omega)$ and $y_t(\omega)$ directly in the sense:

$$\|y_t - \hat{y}_t\|^2_{L^2} = \mathrm{E}\,\|y_t - \hat{y}_t\|^2_2 = \mathcal{O}\big(h^p\big).$$

Exponential Lie series

$$y_t = \varphi_t \circ y_0$$

$$\varphi_t = \mathrm{id} + \sum_i J_i(t) V_i + \sum_{i,j} J_{ij}(t) V_{ij} + \sum_{i,j,k} J_{ijk}(t) V_{ijk} + \cdots$$

Set $\varphi_t = \exp \psi_t$ then $\Rightarrow$

$$\psi_t = (\varphi_t - \mathrm{id}) - \tfrac{1}{2}(\varphi_t - \mathrm{id})^2 + \tfrac{1}{3}(\varphi_t - \mathrm{id})^3 + \cdots$$
$$= \sum_{i=0}^{d} J_i V_i + \sum_{i>j} \tfrac{1}{2}(J_{ij} - J_{ji})[V_i, V_j] + \cdots$$

- *Magnus* 1954, *Chen* 1957, *Strichartz* 1987

Castell–Gaines (ODE) method

Truncated exponential Lie series across $[t_n, t_{n+1}]$:

$$\hat{\psi}_{t_n,t_{n+1}} = \hat{J}_1 V_1 + \hat{J}_2 V_2 + \hat{J}_0 V_0 + \tfrac{1}{2}(\hat{J}_{12} - \hat{J}_{21})[V_1, V_2]$$

$$\Rightarrow \quad y_{t_{n+1}} \approx \exp(\hat{\psi}_{t_n,t_{n+1}}) \circ y_{t_n}$$

Castell–Gaines: solve ODE

$$u'(\tau) = \hat{\psi}_{t_n,t_{n+1}} \circ u(\tau)$$

across $\tau \in [0, 1]$ with $u(0) = y_{t_n}$ gives $u(1) \approx y_{t_{n+1}}$.
Asymptotic efficiency.

Signature

Stochastic Taylor expansion:

$$\varphi_t = \mathrm{id} + \sum_i J_i(t)V_i + \sum_{i,j} J_{ij}(t)V_{ij} + \sum_{i,j,k} J_{ijk}(t)V_{ijk} + \cdots$$

Strip away unnecessary labels:

$$\sum_{w\in\mathbb{A}^*} J_w\, V_w \longrightarrow \sum_{w\in\mathbb{A}^*} w \otimes w$$

$\mathbb{A}^*$ is free monoid of words over $\mathbb{A} = \{0, 1, \dots, d\}$.

Hopf algebra of words

$$J_{a_1a_2}J_{a_3a_4} = J_{a_1a_2a_3a_4} + J_{a_1a_3a_2a_4} + J_{a_1a_3a_4a_2} + J_{a_3a_1a_4a_2} + J_{a_3a_1a_2a_4} + J_{a_3a_4a_1a_2}$$

Shuffle product: $J_uJ_v \longrightarrow u \sqcup\!\sqcup\, v$

Concatenation product: $V_uV_v \longrightarrow uv$

Two *Hopf algebra* structures:

$$(\mathbb{K}\langle\mathbb{A}\rangle, \mathrm{conc}, \Delta, u, c, S) \qquad \text{and} \qquad (\mathbb{K}\langle\mathbb{A}\rangle, \mathrm{sh}, \Delta', u, c, S).$$

Set

$$\mathcal{A} = \mathbb{R}\langle\mathbb{A}\rangle \otimes \mathbb{R}\langle\mathbb{A}\rangle \qquad \text{with} \qquad (u \otimes x)(v \otimes y) = (u \sqcup\!\sqcup\, v) \otimes (xy).$$

Recoding the signature

$$\varphi = \sum_{w \in \mathbb{A}^*} w \otimes w$$

$$\Rightarrow \quad \psi = \sum_{k \geq 1} c_k \Big(\varphi - 1 \otimes 1\Big)^k$$

$$= \sum_{k \geq 1} c_k \Bigg(\sum_{w \in \mathbb{A}^+} w \otimes w \Bigg)^k$$

$$= \sum_{k \geq 1} c_k \sum_{u_1, \ldots, u_k \in \mathbb{A}^+} (u_1 ⧢ \ldots ⧢ u_k) \otimes (u_1 \ldots u_k)$$

$$= \sum_{w \in \mathbb{A}^+} \Bigg(\sum_{k=1}^{|w|} c_k \sum_{w = u_1 \ldots u_k} u_1 ⧢ \ldots ⧢ u_k \Bigg) \otimes w$$

$$= \sum_{w \in \mathbb{A}^+} K(w) \otimes w$$

Representing endomorphisms

Strip away even more $\longrightarrow$ endomorphisms

The embedding $\mathrm{End}(\mathbb{K}\langle\mathbb{A}\rangle) \to \mathcal{A}$ (with shuffle as product)

$$K \mapsto \sum_{w \in \mathbb{A}^*} K(w) \otimes w$$

is an algebra homomorphism for the convolution product

$$K_1 \star K_2 = \mathrm{sh} \circ (K_1 \otimes K_2) \circ \Delta'$$

Idempotents

Define $J \in \mathrm{End}(\mathbb{K}\langle\mathbb{A}\rangle)$ by

$$J := \mathrm{id} - u \circ c.$$

Note J sends the empty word 1 to 0.

The *Eulerian idempotent* $e \in \mathrm{End}(\mathbb{K}\langle\mathbb{A}\rangle)$ is

$$e := \log^{\star}(\mathrm{id}) = \log^{\star}(u \circ c + J) = J - \tfrac{1}{2}J^{\star 2} + \cdots + \frac{(-1)^{n-1}}{n}J^{\star n} + \cdots,$$

where $J^{\star n} = J \star J \star \cdots \star J$ (n times); and $e \circ e = e$.

Sinh-log idempotent

General *integration by parts formula*:

$$S \star \mathrm{id} = \mathrm{id} \star S = u \circ c$$

$$S = (u \circ c + J)^{\star(-1)} = u \circ c - J + J^{\star 2} - J^{\star 3} + \cdots + (-1)^n J^{\star n} + \cdots .$$

The *sinh-log endomorphism* on $\mathbb{K}\langle\mathbb{A}\rangle$ is

$$\begin{aligned} P &:= \sinh\log^{\star}(\mathrm{id}) = \tfrac{1}{2}\Big(\mathrm{id} - \mathrm{id}^{\star(-1)}\Big) = \tfrac{1}{2}\Big(\mathrm{id} - S\Big) \\ &= J - \tfrac{1}{2}J^{\star 2} + \tfrac{1}{2}J^{\star 3} - \tfrac{1}{2}J^{\star 4} + \cdots \end{aligned}$$

and $P \circ P = P$ since

$$\tfrac{1}{2}(\mathrm{id}-S)\circ\tfrac{1}{2}(\mathrm{id}-S) = \tfrac{1}{4}(\mathrm{id}\circ\mathrm{id}-\mathrm{id}\circ S-S\circ\mathrm{id}+S\circ S) = \tfrac{1}{2}(\mathrm{id}-S).$$

Expectation

Set $\mathbb{D} = \{0, 11, 22, \ldots, dd\}$: then $\mathbb{D}^* \subset \mathbb{A}^*$

The linear map $\mathbb{E}\colon \mathbb{K}\langle\mathbb{A}\rangle \to \mathbb{K}$ given by

$$\mathbb{E}\, w = \begin{cases} \left(\frac{1}{2}\right)^{\mathrm{d}(w)} \frac{t^{\mathrm{n}(w)}}{\mathrm{n}(w)!}, & w \in \mathbb{D}^*; \\ 0, & w \in \mathbb{A}^* \backslash \mathbb{D}^*, \end{cases}$$

is the *expectation*. Here

- $\mathrm{d}(w) =$ number of non-zero consecutive pairs from $\mathbb{D}$ in w,
- $\mathrm{n}(w) = \mathrm{z}(w) + \mathrm{d}(w)$,
- $\mathrm{z}(w) =$ number of zeros in w.
- extends to $\mathbb{K}\langle\mathbb{A}\rangle$ by linearity.

Inner product of endomorphisms

Accuracy with L^2-measure: $K \in \mathrm{End}(\mathbb{K}\langle\mathbb{A}\rangle)$ with image $\psi \in \mathcal{A}$:

$$\begin{aligned}\mathbb{E}\,|\psi(w)|^2 &= \mathbb{E}\,\psi(w)\cdot\psi(w)\\ &= \mathbb{E}\left(\sum_u K(u)\otimes u\right)\cdot\left(\sum_v K(v)\otimes v\right)\\ &= \sum_{u,v}\mathbb{E}\Big(K(u)\sqcup\!\sqcup K(v)\Big)\,u\cdot v,\end{aligned}$$

Definition (**Inner product**)

For $K_1, K_2 \in \mathrm{End}(\mathbb{K}\langle\mathbb{A}\rangle)$ define

$$\langle K_1, K_2\rangle := \frac{\sum_{u,v\in\mathbb{A}^+}\mathbb{E}\Big(K_1(u)\sqcup\!\sqcup K_2(v)\Big)}{\sum_{u,v\in\mathbb{A}^+}\mathbb{E}\,u\sqcup\!\sqcup v}.$$

Defined for some subset of $\mathbb{A}^*$ also.

Comparing the sinh-log and identity endomorphisms

Remainders of the stochastic Taylor and sinh-log expansions

$$R^{\mathrm{st}} = \sum_{\deg(w)=m+1} w \otimes w + \cdots$$

$$R^{\mathrm{sl}} = \sum_{\deg(w)=m+1} P(w) \otimes w + \cdots,$$

where $P := \frac{1}{2}(\mathrm{id} - S)$.

Lemma

If $\langle S, S \rangle = 1$ *then*

$$1 = \|\mathrm{id}\|^2 = \|P\|^2 + \left\|\tfrac{1}{2}(\mathrm{id} + S)\right\|^2.$$

Proof

$$
\begin{aligned}
\|\mathrm{id}\|^2 &= \langle \tfrac{1}{2}(\mathrm{id} - S) + \tfrac{1}{2}(\mathrm{id} + S), \tfrac{1}{2}(\mathrm{id} - S) + \tfrac{1}{2}(\mathrm{id} + S)\rangle \\
&= \|P\|^2 + \tfrac{3}{4}\langle \mathrm{id}, \mathrm{id}\rangle + \tfrac{1}{4}\Big(\langle \mathrm{id}, S\rangle + \langle S, \mathrm{id}\rangle\Big) - \tfrac{1}{4}\langle S, S\rangle \\
&= \|P\|^2 + \tfrac{1}{4}\langle \mathrm{id}, \mathrm{id}\rangle + \tfrac{1}{4}\Big(\langle \mathrm{id}, S\rangle + \langle S, \mathrm{id}\rangle\Big) + \tfrac{1}{4}\langle \mathrm{id}, \mathrm{id}\rangle \\
&\quad + \tfrac{1}{4}\Big(\langle \mathrm{id}, \mathrm{id}\rangle - \langle S, S\rangle\Big) \\
&= \|P\|^2 + \tfrac{1}{4}\Big(\langle \mathrm{id} + S, \mathrm{id} + S\rangle\Big),
\end{aligned}
$$

Lemma

On the subset generated by $\mathbb{A} = \{1, 2, \ldots, d\}$ or the subset from words of equal length, then $\langle S, S\rangle = 1$.

Final remark

We now intend to apply these ideas to investigate the underlying algebraic and combinatorial structure of SDEs driven by other processes and SPDEs.

Introductory references

- Theory:

  L.C. Evans: *An introduction to stochastic differential equations*

  `http://math.berkeley.edu/~evans`

- Numerics:

  D.J. Higham: *An algorithmic introduction to numerical simulation of stochastic differential equations*

  SIAM Review 43 (2001), pp. 525–546

Quadrature

How do we estimate $J_{12}(t_n, t_{n+1})$?

We can approximate it strongly using:

- Its conditional expection $\hat{J}_{12}(t_n, t_{n+1})$
- Karhunen–Loeve expansion (Fourier expansion)
- Wiktorsson's method (most promising) — looks at the joint probability distribution function for J_1, J_2 and J_{12}
- Stump and Hill's method (analogous)

Quadrature error I

With $\tau_q = t_n + q\Delta t$, $q = 0, \ldots, Q-1$, $Q\Delta t = h$

$$
\begin{aligned}
J_{12}(t_n, t_{n+1}) &= \int_{t_n}^{t_{n+1}} \int_{t_n}^{\tau} \mathrm{d}W^1_{\tau_1} \, \mathrm{d}W^2_{\tau} \\
&= \sum_{q=0}^{Q-1} \int_{\tau_q}^{\tau_{q+1}} W^1_{\tau} - W^1_{t_n} \, \mathrm{d}W^2_{\tau} \\
&= \sum_{q=0}^{Q-1} \int_{\tau_q}^{\tau_{q+1}} (W^1_{\tau} - W^1_{\tau_q}) + (W^1_{\tau_q} - W^1_{t_n}) \, \mathrm{d}W^2_{\tau} \\
&= \sum_{q=0}^{Q-1} J_{12}(\tau_q, \tau_{q+1}) + \sum_{q=0}^{Q-1} \left(W^1_{\tau_q} - W^1_{t_n} \right) \Delta W^2(\tau_q)
\end{aligned}
$$

Quadrature error II

With $\tau_q = t_n + q\Delta t$, $q = 0, \ldots, Q-1$, $Q\Delta t = h$

$$\begin{aligned}
\left\| J_{12}(t_n, t_{n+1}) - \hat{J}_{12}(t_n, t_{n+1}) \right\|_{L_2}^2 &= \sum_{q=0}^{Q-1} \left\| J_{12}(\tau_q, \tau_{q+1}) \right\|_{L^2}^2 \\
&= \sum_{q=0}^{Q-1} (\Delta t)^2 \\
&= Q(\Delta t)^2 \\
&= h^2/Q
\end{aligned}$$

$$\Rightarrow \quad \left\| J_{12}(t_n, t_{n+1}) - \hat{J}_{12}(t_n, t_{n+1}) \right\|_{L_2} = h/\sqrt{Q}$$

Wiktorsson: simulation of Lévy area I

- Conditional distribution of $\xi = A_{12}(h)$ given $J_1(h)$, $J_2(h)$:

$$\phi(\xi) = \frac{\frac{1}{2}h\xi}{\sinh(\frac{1}{2}h\xi)} \exp\Big(-a^2\big(\tfrac{1}{2}h\xi \coth(\tfrac{1}{2}h\xi) - 1\big)\Big)$$

  where $a^2 = \big(J_1^2(h) + J_2^2(h)\big)/(2h)$ and $b = J_1(h)J_2(h)/2h$
- Need to sample from this

Wiktorsson: simulation of Lévy area II

- Karhunen–Loeve $X_{ij}, Y_{ij} \sim \mathrm{N}(0,1)$:

$$A_{ij}(h) = \frac{h}{2\pi} \sum_{k=1}^{\infty} \frac{1}{k} \Big(X_{ik} \Big(Y_{jk} + \sqrt{\tfrac{2}{h}} J_j(h) \Big) - X_{jk} \Big(Y_{ik} + \sqrt{\tfrac{2}{h}} J_i(h) \Big) \Big)$$

- Truncate after Q terms, mean-square error $\mathcal{O}(h^2/Q)$
- Q large, tail sum $\sim$ multivariate Gaussian distribution
- Approximate with Gaussian RV: mean-square error $\mathcal{O}(h^2/Q^2)$
- SDELab: Gilsing & Shardlow