Challenges in S(P)DEs and Bayesian inference

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Brown report

Applied mathematics at the US Department of Energy:

> *Develop new approaches for efficient modeling of large stochastic systems.*
>
> *... particularly spatially dependent systems.*
>
> *Invest in analysis and algorithms for stochastic optimization.*
>
> *How do we modify models of the atmosphere and clouds to incorporate newly collected data of possibly of new types?*

Stochastic differential equations

$$\mathrm{d}y_t = \tilde{V}_0(y_t)\,\mathrm{d}t + V_1(y_t)\,\mathrm{d}W_t^1 + \cdots + V_d(y_t)\,\mathrm{d}W_t^d$$

Four approaches to approximation, solve:

- PDE (transition probability distribution)
- for a weak approximation (Monte–Carlo)
- for a strong approximation (Monte–Carlo)
- pathwise (rough paths)

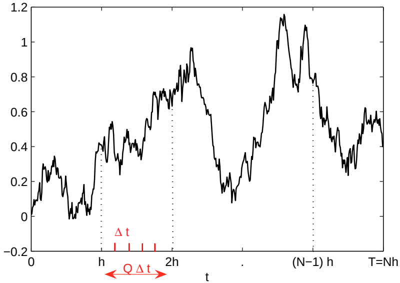
First three: expectation and higher moments of solution sought.

Basic setting

$$y_t = y_0 + \int_0^t \tilde{V}_0(y_\tau)\,\mathrm{d}\tau + \sum_{i=1}^{d} \int_0^t V_i(y_\tau)\,\mathrm{d}W_\tau^i$$

- Itô 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

Applications

- *Finance*: Heston model for pricing options. Stock price is a stochastic process u with stochastic volatility v:

$$
\begin{aligned}
\mathrm{d}u_t &= \mu u_t \,\mathrm{d}t + \sqrt{v_t}\, u_t \,\mathrm{d}W_t \\
\mathrm{d}v_t &= \kappa(\theta - v_t)\,\mathrm{d}t + \varepsilon\sqrt{v_t}\,\mathrm{d}Z_t
\end{aligned}
$$

- Molecular simulation: Langevin dynamics
- DNA damage dynamics (Chickarmane *et al.*)
- Neuronal dynamics (Coombes & Lord)
- Biochemical reactions (Burrage)
- Ocean/weather modelling: Bayesian inference (Stuart, Jones)
- Oil extraction: porous media
- Subspace tracking: inference on manifolds (Srivastava)

Itô's lemma

$$\mathrm{d}y = \tilde{V}_0 \circ y \,\mathrm{d}t + \sum_{i=1}^{d} V_i \circ y \,\mathrm{d}W^i$$

$$\Rightarrow \quad \mathrm{d}(f \circ y) = \tilde{V}_0 \cdot \partial_y (f \circ y) \,\mathrm{d}t \; + \sum_{i=1}^{d} V_i \cdot \partial_y (f \circ y) \,\mathrm{d}W^i$$

$$+ \tfrac{1}{2} \sum_{i=1}^{d} (V_i \otimes V_i) : \partial_{yy} (f \circ y) \text{ “}\mathrm{d}t\text{“}$$

$$\Rightarrow \quad \mathrm{d}(f \circ y) = \mathcal{L}(f \circ y) \,\mathrm{d}t + \sum_{i=1}^{d} V_i \cdot \partial_y (f \circ y) \,\mathrm{d}W_t^i$$

where

$$\mathcal{L} := \tilde{V}_0 \cdot \partial_y + \tfrac{1}{2} \sum_{i=1}^{d} (V_i \otimes V_i) : \partial_{yy}$$

Related PDE

- Consider Itô SDE for $f \circ y_t$ with initial data $y_0 \equiv y$:

$$\Rightarrow \quad f \circ y_t = f \circ y + \int_0^t \mathcal{L}\,(f \circ y_\tau)\,\mathrm{d}\tau + \sum_{i=1}^{d} \int_0^t V_i \cdot \partial_y (f \circ y_\tau)\,\mathrm{d}W_\tau^i$$

- Feynman–Kac $\Rightarrow$ solution of PDE

$$\partial_t u = \mathcal{L}\, u \qquad \text{with} \qquad u(0, y) = f(y)$$

is $u(t, y) = \mathbb{E}\big(f(y_t)\big)$

Black–Scholes–Merton PDE

- Recall:

$$\mathcal{L} := \tilde{V}_0 \cdot \partial_y + \tfrac{1}{2} \sum_{i=1}^{d} (V_i \otimes V_i) : \partial_{yy}$$

- Constant volatility v, stock/index value u_t evolves:

$$\mathrm{d}u_t = \mu u_t \, \mathrm{d}t + \sqrt{v} \, u_t \, \mathrm{d}W_t$$

- Current price of option at time t is $C(t) = f(t, u_t)$
- Itô formula and financial argument to duplicate C by a portfolio consisting of investment of u and a bond (risk-free with interest rate r) $\Rightarrow$

$$\partial_t f + ru \, \partial_u f + \tfrac{1}{2} v u^2 \, \partial_{uu} f - r \, f = 0$$

Weak approximation

- Replace Gaussian increments $\Delta W^i(t_n, t_{n+1})$ by simpler RVs $\Delta \hat{W}^i(t_n, t_{n+1})$ with appropriate moment properties, eg. by branching process:

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

- Expectation of approximation $\hat{y}_T$ across all paths at the final time T is close to the expectation of the true solution:

$$\|\mathbb{E}\,(y_T) - \mathbb{E}\,(\hat{y}_T)\| = \mathcal{O}(h^p)$$

- No pathwise comparison: paths not "close" to Wiener paths

Strong approximation

- Generate approximate Wiener process paths
- Pick independent increments from

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

- Since we have followed Wiener path approximations, we can compare y_T with $\hat{y}_T$, they're close in the sense:

$$\mathbb{E}\,\|y_T - \hat{y}_T\| = \mathcal{O}\big(h^{\frac{p}{2}}\big)$$

Rough paths (Lyons)

- Does solution depend continuously on driving path?
- Lévy area $A_{ij} \equiv \frac{1}{2}(J_{ij} - J_{ji})$
- V_i non-commuting $\Rightarrow$ y_t depends continuously on W_i, A_{ij}
- i.e. $(\hat{W}_i, \hat{A}_{ij}) \rightarrow (W_i, A_{ij}) \Rightarrow \hat{y} \rightarrow y$
- A_{ij} not included $\exists$ example: $W_i \rightarrow 0$ but $\hat{y} \not\rightarrow 0$
- Back to strong solutions:

$$\hat{W}^i \rightarrow W^i \qquad \Rightarrow \qquad \mathbb{E}\|\hat{y}_t - y_t\|^2_{L^2} \rightarrow 0$$

Stochastic chain rule (Stratonovich)

$$y_t = y_0 + \sum_i \int_0^t V_i \circ y_\tau \, \mathrm{d}W_\tau^i$$

Itô lemma (stochastic chain rule) $\Rightarrow$

$$f \circ y_t = f \circ y_0 + \sum_j \int_0^t V_j \circ f \circ y_\tau \, \mathrm{d}W_\tau^j$$

e.g. $$V_i \circ y_t = V_i \circ y_0 + \sum_j \int_0^t V_j \circ V_i \circ y_\tau \, \mathrm{d}W_\tau^j$$

$$y_t = y_0 + \sum_i \int_0^t \left(V_i \circ y_0 + \sum_j \int_0^{\tau_1} V_j \circ V_i \circ y_{\tau_2} \, \mathrm{d}W_{\tau_2}^j \right) \mathrm{d}W_{\tau_1}^i$$

Stochastic Taylor series

$$y_t = y_0 + \sum_i \int_0^t \mathrm{d}W^i_{\tau_1} V_i \circ y_0 + \sum_{i,j} \int_0^t \int_0^{\tau_1} V_j \circ V_i \circ y_{\tau_2} \, \mathrm{d}W^j_{\tau_2} \, \mathrm{d}W^i_{\tau_1}$$

Now choose $f = V_j \circ V_i \Rightarrow$

$$y_t = y_0 + \sum_i \underbrace{\int_0^t \mathrm{d}W^i_{\tau_1}}_{J_i(t)} V_i \circ y_0 + \sum_{i,j} \underbrace{\int_0^t \int_0^{\tau_1} \mathrm{d}W^j_{\tau_2} \, \mathrm{d}W^i_{\tau_1}}_{J_{ji}(t)} V_j \circ V_i \circ y_0 + \cdots$$

- Feynman–Dyson path ordered exponential, Neumann series, Peano–Baker series, Chen-Fleiss series, stochastic B-series,...
- Euler-Maruyama and Milstein methods
- Need approximations for iterated integrals

Flow map/exponential Lie series

$$y_t = \varphi_t \circ y_0$$

$$\varphi_t = \mathrm{id} + \sum_i J_i(t) V_i + \sum_{i,j} J_{ji}(t) V_j \circ V_i + \sum_{i,j,k} J_{kji}(t) V_k \circ V_j \circ V_i + \cdots$$

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

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

- *Magnus* 1954, *Chen* 1957, *Kunita* 1980, *Strichartz* 1987, *Ben Arous* 1989, *Castell* 1993, *Castell–Gaines* 1995, *Moan* 2004

Castell–Gaines (ODE) method

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

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

Approximate solution:

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

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 $u(1) \approx y_{t_{n+1}}$.

Challenges?

- Combinatorial Hopf algebras
- Positivity preservation
- SPDEs and inference

Basic idea

$$\varphi_t = \mathrm{id} + \sum_i J_i(t) V_i + \sum_{i,j} J_{ji}(t) V_j \circ V_i + \sum_{i,j,k} J_{kji}(t) V_k \circ V_j \circ V_i + \cdots$$

$$\varphi = \sum_{w \in \mathbb{A}^*} J_w \, V_w$$

$$\begin{aligned} \psi &= \sum_{k=1}^{\infty} C_k \, (\varphi - \mathrm{id})^k \\ &= \sum_{w \in \mathbb{A}^*} K_w \, V_w \end{aligned}$$

$\mathbb{A}^* = \{\text{words over } \mathbb{A} = \{0, 1, \ldots, d\}\}$

Hopf algebra of words

Shuffle relations:

$$\begin{aligned} J_{a_1} J_{a_2} &= J_{a_1 a_2} + J_{a_2 a_1} \\ J_{a_1} J_{a_2 a_3} &= J_{a_1 a_2 a_3} + J_{a_2 a_1 a_3} + J_{a_2 a_3 a_1} \\ J_{a_1 a_2} J_{a_3 a_4} &= J_{a_1 a_2 a_3 a_4} + J_{a_1 a_3 a_2 a_4} + J_{a_1 a_3 a_4 a_2} \\ &\quad + J_{a_3 a_1 a_4 a_2} + J_{a_3 a_1 a_2 a_4} + J_{a_3 a_4 a_1 a_2} \end{aligned}$$

Shuffle product: $J_u J_v \longrightarrow u \sqcup\!\sqcup\, v$

Two *Hopf algebra* structures, set:

$$\mathcal{H} = \mathbb{R}\langle \mathbb{A} \rangle \otimes \mathbb{R}\langle \mathbb{A} \rangle$$

$$(u \otimes x)(v \otimes y) = (u \sqcup\!\sqcup\, v) \otimes (xy)$$

Pullback to Hopf algebra

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

$$\begin{aligned}
\Rightarrow \quad \psi &= \sum_{k \geq 1} C_k \big(\varphi - 1 \otimes 1\big)^k \\
&= \sum_{k \geq 1} C_k \left(\sum_{w \in \mathbb{A}^+} w \otimes w \right)^k \\
&= \sum_{k \geq 1} C_k \sum_{u_1, \ldots, u_k \in \mathbb{A}^+} (u_1 \sqcup\!\sqcup \ldots \sqcup\!\sqcup u_k) \otimes (u_1 \ldots u_k) \\
&= \sum_{w \in \mathbb{A}^*} \left(\sum_{k=1}^{|w|} C_k \sum_{\substack{u_1, \ldots, u_k \in \mathbb{A}^+ \\ w = u_1 \ldots u_k}} u_1 \sqcup\!\sqcup \ldots \sqcup\!\sqcup u_k \right) \otimes w
\end{aligned}$$

Sinh-log series?

- Diffusion vector fields commute: exponential Lie series has smaller mean-square error (orders 1/2, 1, 3/2)
- Do not commute: counter-example for order 1
- *Assume no drift*: $\Rightarrow$ sinh-log series:
  - $K_w \equiv \frac{1}{2}(J_w - J_{\alpha \circ w})$
  - Use concatenation-shuffle operator algebra
  - Remainder is smaller

Positivity preservation

Recall Heston model for pricing options:

$$\mathrm{d}u_t = \mu u_t \,\mathrm{d}t + \sqrt{v_t}\, u_t \,\mathrm{d}W_t$$
$$\mathrm{d}v_t = \kappa(\theta - v_t)\,\mathrm{d}t + \varepsilon\sqrt{v_t}\,\mathrm{d}Z_t$$

- Square-root diffusions prototypical Langevin dynamics
- Degrees of freedom $\nu := 4\kappa\theta/\varepsilon^2$
- Transition probability $\mathrm{P}(v_t < x \colon v_0)$ is:

$$F_{\chi^2_\nu(\lambda)}(z) = \frac{\mathrm{e}^{-\lambda/2}}{2^{\nu/2}} \sum_{j=0}^{\infty} \frac{(\lambda/2)^j}{j!2^j\Gamma(\nu/2+j)} \int_0^z \xi^{\nu/2+j-1}\mathrm{e}^{-\xi/2}\,\mathrm{d}\xi$$

where $z = x\,\hat{\eta}(t)$ and $\lambda = v_0\,\eta(t)$ (see e.g. Andersen)

Zero boundary attracting, attainable?

i.e. solution of PDE $u_t = \mathcal{L}u$ is:

$$F_{\chi^2_\nu(\lambda)}(z) = \frac{\mathrm{e}^{-\lambda/2}}{2^{\nu/2}} \sum_{j=0}^{\infty} \frac{(\lambda/2)^j}{j! 2^j \Gamma(\nu/2+j)} \int_0^z \xi^{\nu/2+j-1} \mathrm{e}^{-\xi/2} \, \mathrm{d}\xi$$

Zero boundary, for:

- $\nu > 1$: non-attracting $\Rightarrow$ implicit numerical methods*
- $\nu \leq 1$: attracting and attainable $\Rightarrow$ transition prob

*with extreme caution depending on vector fields

Extension to SPDEs modelling biochemical reactions?

SPDEs

Gyöngy, Lord, Shardlow, Davie, Gaines, Stuart, Kloeden,. . .

- Brown report ⇒ major important challenge
- Stuart *et. al.* ⇒ path sampling, e.g. of bridge process
- Lots of physical/ocean/weather and defence applications

More challenges

- Numerical stability (Buckwar, . . .)
- Symplectic methods (Tretyakov, Bou–Rabee, . . .)
- Driving fractional Brownian motions (Baudoin, . . .)
- Driving processes with jumps, eg. Lévy processes
- Backward stochastic differential equations (Protter, . . .)

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

Îto or Stratonovich?

- Itô:

$$\int_0^T W_\tau^i \,\mathrm{d}W_\tau^i = \tfrac{1}{2}\left(W_T^i\right)^2 - \tfrac{1}{2}T$$

- Stratonovich:

$$\int_0^T W_\tau^i \circ \mathrm{d}W_\tau^i = \tfrac{1}{2}\left(W_T^i\right)^2$$

- Itô to Stratonovich:

$$V_0 = \tilde{V}_0 - \tfrac{1}{2}\sum_{i=1}^{d} V_i^2$$

- Stratonovich calculus familiar, easier, swapping to/back to Itô form trivial

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

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

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 $\xi = J_{12}(h)$ given $J_1(h)$, $J_2(h)$:

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

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

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

- 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

Stochastic integral properties

Stratonovich-to-Itô relations:

$$\begin{aligned} w = a_1 a_2: \ & J_w = I_w + \tfrac{1}{2} I_0\, \delta_{a_1=a_2\neq 0} \\ w = a_1 a_2 a_3: \ & J_w = I_w + \tfrac{1}{2}\big(I_{0a_3}\, \delta_{a_1=a_2\neq 0} + I_{a_1 0}\, \delta_{a_2=a_3\neq 0}\big) \\ w = a_1 a_2 a_3 a_4: \ & J_w = I_w + \tfrac{1}{4} I_{00}\, \delta_{a_1=a_2\neq 0}\delta_{a_3=a_4\neq 0} \\ & \quad + \tfrac{1}{2}\big(I_{0a_3a_4}\, \delta_{a_1=a_2\neq 0} + I_{a_1 0 a_4}\, \delta_{a_2=a_3\neq 0} + I_{a_1 a_2 0}\, \delta_{a_3=a_4\neq 0}\big) \end{aligned}$$

Expectations of Îto integrals: $\mathbb{E}(I_{\bullet j \bullet}) = 0$ for $j \neq 0 \Rightarrow$

$$\begin{aligned} \mathbb{E}(J_i) &= 0 \\ \mathbb{E}(J_{ij}) &= \tfrac{1}{2} h\, \delta_{i=j\neq 0} \\ \mathbb{E}(J_{ijk}) &= 0 \\ \mathbb{E}(J_{ijkl}) &= \tfrac{1}{8} h^2\, \delta_{i=j\neq 0}\delta_{k=l\neq 0} \end{aligned}$$

Basic idea

- Construct the new series $\psi_t = F(\varphi_t)$
- Truncate and use $\hat{J}_i$, $\hat{J}_{ij}$ to produce $\hat{\psi}_t$
- Approximate flow-map is $\hat{\varphi}_t = F^{-1}(\hat{\psi}_t)$
- "Flow error" is the flow remainder $R_t = \varphi_t - \hat{\varphi}_t$
- Approximate solution is $\hat{y}_t = \varphi_t \circ y_0$
- Error/remainder is $R_t \circ y_0$
- Mean-square error measure is

$$\|R_t \circ y_0\|_{L^2}^2 \equiv \mathbb{E}(R_t \circ y_0)^{\mathrm{T}}(R_t \circ y_0)$$