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Efficient Simulation of Stiff Stochastic Differential Equations

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Motivation

- Stochasticity and stiffness in wide range of physical systems
- Large range of time-scales in the formulation of system governing equations
- Particular interest: time integration of stiff stochastic chemical systems
- Governing system: chemical Langevin equations with significant degree of stiffness
- Focus of this talk: time integration of stiff stochastic differential equations with fast diffusion processes

Background: Chemical Reaction Networks

A collection of chemical reactions that involves

- a set of N "species":

$$S_i, \quad i \in \{1, \ldots, N\}$$

- a set of M chemical reactions $\mathcal{R}_j, \quad j \in \{1, \ldots, M\}$:

$$\mathcal{R}_j : \quad \sum_{i=1}^{N} \alpha_{ij} S_i \rightarrow \sum_{i=1}^{N} \beta_{ij} S_i$$

For $i = 1, \ldots, N, \quad j = 1, \ldots, M$

- $\alpha_{ij}, \beta_{ij} \in \mathbb{Z}^+$ - stoichiometry coefficients
- $v_{ij} = \beta_{ij} - \alpha_{ij}$, $\mathbf{v}_j := (v_{1j}, \cdots, v_{Nj})$ - change in molecular population caused by one $\mathcal{R}_j$ reaction
- $V = (v_{ij})_{N \times M}$ - stoichiometry matrix.

Model Set-up

Assumption: the system is well-stirred:

- constant volume Ω
- in thermal equilibrium at some constant temperature
- positions and velocities of the individual molecules ignored

$X_i(t)$ - the number of the species S_i in the system at time t.

Goal estimate the state vector

$$\mathbf{X}(t) := (X_1(t), \cdots, X_N(t))$$

given that the system was in state $\mathbf{X}(t_0) = \mathbf{x}_0$ at initial time t_0.

Stochastic Models

- $X_i(t)$: number of species S_i at time t $(i = 1, \ldots, N)$.
- $\boldsymbol{X}(t) = (X_1(t), \ldots, X_N(t))^T$ - column-vector Markov stochastic process.
- $k = (k_1, \ldots, k_N)^T \in \mathbb{Z}_+^N$ - state of the process.
- $p_k(t) = \mathbb{P}[\boldsymbol{X}(t) = k$, given $X(t_0) = \mathbf{k}_0]$ - the probability that, at time t, there are k_1 units of species S_1, k_2 units of species S_2, ..., given $\boldsymbol{X}(t_0) = \mathbf{k}_0$.
- $\rho_j : \mathbb{Z}_+^N \to \mathbb{R}_+$ - propensity function for the respective reaction $\mathcal{R}_j$.
- $\rho_j(\mathbf{k})\mathrm{d}t$ - given $\boldsymbol{X}(t) = k$, the probability that reaction $\mathcal{R}_j$ takes place in the next infinitesimal time interval $[t, t + \mathrm{d}t)$.
- v_j - the jth column of stoichiometry matrix V.

Chemical Langevin equation (CLE)

Chemical Langevin Difference Equation

$$\boldsymbol{X}(t+\mathrm{d}t) = \boldsymbol{X}(t) + \sum_{j=1}^{M} \mathbf{v}_j \rho_j(k)\mathrm{d}t + \sum_{j=1}^{M} \mathbf{v}_j \sqrt{\rho_j(k)}\mathcal{N}_j(0,1)\sqrt{\mathrm{d}t}$$

By theory of continuous Markov processes
Chemical Langevin Differential Equation

$$d\boldsymbol{X}(t) = \sum_{j=1}^{M} \mathbf{v}_j \rho_j(\boldsymbol{X}(t))dt + \sum_{j=1}^{M} \mathbf{v}_j \sqrt{\rho_j(\boldsymbol{X}(t))}dW_j(t)$$

$W_j(t)$ - independent Gaussian white noise processes.

Previous works: time-integration strategies based on stochastic singular perturbation

SDE with fast diffusion

$$\mathrm{d}\boldsymbol{X}(t) = f(\boldsymbol{X}(t))\mathrm{d}t + \sum_{k=1}^{m} g_k(\boldsymbol{X}(t))\mathrm{d}W_k(t), \quad \boldsymbol{X}(0) = \boldsymbol{x}_0$$

Assumptions:

- The diffusion coefficients $\{g_k\}_{k=1,\cdots,m}$ exhibit a large range of magnitudes.
- There exists $M \in \{1, \cdots, m\}$ such that

$$|g_1|, \cdots, |g_M| \gg |g_{M+1}|, \cdots |g_m|.$$

- $|g_1|, \cdots, |g_M|$: fast processes
- $|g_{M+1}|, \cdots |g_m|$: slow processes

Euler-Maruyama (EM) and modified EM

- Simplest one-step EM

$$
\begin{aligned}
\boldsymbol{x}_{n+1} &= \boldsymbol{x}_n + f(\boldsymbol{x}_n)\Delta t + \sum_{k=1}^{m} g_k(\boldsymbol{x}_n)\Delta W_{k,n} \\
\Delta W_{k,n} &= W_k(t_{n+1}) - W_k(t_n)
\end{aligned}
$$

- Requires Δt to be extremely small for the above SDE with fast diffusions.
- Modified EM

$$
\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta t f(\boldsymbol{x}_n) + \sum_{k=M+1}^{m} g_k(\boldsymbol{x}_n)\Delta W_{k,n} + \eta_{n+1}
$$

Goal: develop models for η_{n+1} that approximates the fast diffusion processes more accurately than $\sum_{k=1}^{M} g_k(\boldsymbol{x}_n)\Delta W_{k,n}$.

Approximation of fast diffusion processes

Given any $\mathbb{R}^d$-valued stochastic process $\boldsymbol{X}(t)$, define

$$\mathscr{D}_n^{\boldsymbol{X}}(t) = \sum_{k=1}^{M} \int_{t_n}^{t} g_k(\boldsymbol{X}(s))\mathrm{d}W_k(s), \quad t \in [t_n, t_{n+1}).$$

Let $\hat{\boldsymbol{X}}(t)$ be the solution to the diffusion only SDE

$$\mathrm{d}\hat{\boldsymbol{X}}(t) = \sum_{k=1}^{M} g_k(\hat{\boldsymbol{X}}(t))\mathrm{d}W_k(t), \quad \hat{\boldsymbol{X}}(t_n) = \boldsymbol{x}_n, \quad t \in [t_n, t_{n+1})$$

- Idea: Approximating $\mathscr{D}_n^{\boldsymbol{X}}(t)$ where $\boldsymbol{X}$ is the solution to the original SDE, by $\mathscr{D}_n^{\hat{\boldsymbol{X}}}(t)$

Justification

Error of the approximation $|\mathscr{D}_n^{\boldsymbol{X}}(t) - \mathscr{D}_n^{\hat{\boldsymbol{X}}}(t)|$ is

- equal to zero if $g_k(\boldsymbol{X})_{k=1}^{M}$ are decoupled from $g_k(\boldsymbol{X})_{k=M+1}^{m}$ and $f(\boldsymbol{X})$.
- relatively small compared to the error of the EM scheme applied to the slow diffusion processes (in the context of chemical reaction systems when the magnitudes of $g_1, \ldots, g_M$ are much larger than $g_{M+1}, \ldots g_m$ which indicates the evolution of $\hat{\boldsymbol{X}}(t)$ is only weakly coupled with $\boldsymbol{X}(t)$)

First step: approximating

$$\mathscr{D}_n^{\hat{\boldsymbol{X}}}(t) = \sum_{k=1}^{M} \int_{t_n}^{t} g_k(\hat{\boldsymbol{X}}(s)) \mathrm{d}W_k(s), \quad t \in [t_n, t_{n+1}),$$

where $\hat{\boldsymbol{X}}$ is the solution to the fast diffusion only SDE.

I. Linear approximation at pathwise initial state

- Set $\boldsymbol{Y}_n(t) = \hat{\boldsymbol{X}}(t) - \boldsymbol{x}_n$ for $t \in [t_n, t_{n+1})$.
- Notice $\boldsymbol{Y}_n(t_{n+1}) = \mathscr{D}_n^{\hat{\boldsymbol{X}}}(t_{n+1})$.
- Use $\boldsymbol{Y}_n(t_{n+1})$ to approximate $\mathscr{D}_n^{\boldsymbol{X}}(t_{n+1})$.
- Model the random variable η_{n+1} by $\boldsymbol{Y}_n(t_{n+1})$.

Given $\hat{\boldsymbol{X}}(t_n) = \boldsymbol{x}_n$, approximate $g_k(\hat{\boldsymbol{X}})$ by

$$g_k(\hat{X}(t)) \approx \boldsymbol{b}_{k,n} + J_{k,n}(\hat{X}(t) - \boldsymbol{x}_n), \quad t \in [t_n, t_{n+1}),$$

where $J_{k,n}$ is the Jacobian of g_k evaluated at $\boldsymbol{x}_n$ and $\boldsymbol{b}_{k,n} = g_k(\boldsymbol{x}_n)$. Then $\boldsymbol{Y}_n$ satisfies

$$\mathrm{d}\boldsymbol{Y}_n(t) = \sum_{k=1}^{M} \big(\boldsymbol{b}_{k,n} + J_{k,n} Y_n(t)\big)\mathrm{d}W_k(t), \quad \boldsymbol{Y}_n(t_n) = 0,\ t \in [t_n, t_{n+1})$$

Exact solution $Y_n(t)$

$$
\begin{aligned}
Y_n(t) &= \Phi_n(t)\left(-\int_{t_n}^{t}\Phi_n^{-1}(s)\sum_{k=1}^{M}J_{k,n}\boldsymbol{b}_{k,n}\mathrm{d}s\right.\\
&\quad \left.+\int_{t_n}^{t}\Phi_n^{-1}(s)\sum_{k=1}^{M}\boldsymbol{b}_{k,n}\mathrm{d}W_k(s)\right)\\
\mathrm{d}\Phi_n(t) &= \sum_{k=1}^{M}J_{k,n}\Phi_n(t)\mathrm{d}W_k(t), \quad t\in[t_n,t_{n+1}), \quad \Phi_n(t_n)=I_d\\
\eta_{n+1} &= Y_n(t_{n+1})\\
\Phi_n(t) &\approx I_d+\sum_{k=1}^{M}J_{k,n}(W_k(t)-W_k(t_n)).
\end{aligned}
$$

II. Linear approximation at the mean initial state

- The previous method evaluate $J_{k,n}$ for each sample path.
- Reduce computational cost by approximating of $g_k(\boldsymbol{X}(t))$ at the path independent mean state $\bar{\boldsymbol{x}}_n := \mathbb{E}[\boldsymbol{x}_n(\omega)]$:

$$g_k(\boldsymbol{X}(t)) \approx \bar{\boldsymbol{b}}_{k,n} + \bar{J}_{k,n}(\boldsymbol{X}(t) - \bar{\boldsymbol{x}}_n), \quad t \in [t_n, t_{n+1}),$$

$\bar{J}_{k,n}$ is the Jacobian of g_k evaluated at $\bar{\boldsymbol{x}}_n$ and $\bar{\boldsymbol{b}}_{k,n} = g_k(\bar{x}_n)$.

- $Y_n(t)$ satisfies the approximating SDE

$$\mathrm{d}\boldsymbol{Y}_n(t) = \sum_{k=1}^{M} \left(\bar{J}_{k,n}\boldsymbol{Y}_n(t) + \boldsymbol{c}_{k,n}\right)\mathrm{d}W_k(t), \quad t \in [t_n, t_{n+1}),$$

where $\boldsymbol{c}_{k,n} = \bar{\boldsymbol{b}}_{k,n} + \bar{J}_{k,n}(\boldsymbol{x}_n - \bar{\boldsymbol{x}}_n)$.

Exact solution $\boldsymbol{Y}_n(t)$

$$
\begin{aligned}
\boldsymbol{Y}_n(t) &= \bar{\Phi}_n(t)\left(-\int_{t_n}^{t}\bar{\Phi}_n^{-1}(s)\sum_{k=1}^{M}\bar{J}_{k,n}\boldsymbol{c}_{k,n}\mathrm{d}s\right.\\
&\quad\left.+\int_{t_n}^{t}\bar{\Phi}_n^{-1}(s)\sum_{k=1}^{M}\boldsymbol{c}_{k,n}\mathrm{d}W_k(s)\right),\\
\bar{\Phi}_n(t) &= \exp\left\{-\frac{1}{2}\sum_{k=1}^{M}\bar{J}_{k,n}^2(t-t_n)+\sum_{k=1}^{M}\bar{J}_{k,n}(W_k(t)-W_k(t_n))\right\}\\
\eta_{n+1} &= Y_n(t_{n+1})\\
\bar{\Phi}_n(t) &\approx I_d+\sum_{k=1}^{M}\bar{J}_{k,n}(W_k(t)-W_k(t_n))
\end{aligned}
$$

III. Moment approximations

- Model η_{n+1} in distribution by computing the moments for $\boldsymbol{Y}_n(t_{n+1})$.
- The mean $\mu_n(t) = \mathbb{E}[\boldsymbol{Y}_n(t)]$ and second moment $P_n(t) = \mathbb{E}[\boldsymbol{Y}_n(t)\boldsymbol{Y}_n^T(t)]$ of $\boldsymbol{Y}_n(t)$ satisfy

$$\begin{aligned} \frac{\mathrm{d}\mu_n(t)}{\mathrm{d}t} &= 0, \\ \frac{\mathrm{d}P_n(t)}{\mathrm{d}t} &= \sum_{k=1}^{M} \left(J_{k,n} P_n J_{k,n}^T + J_{k,n}\mu_n \boldsymbol{b}_{k,n}^T + \boldsymbol{b}_{k,n}\mu_n^T J_{k,n}^T + \boldsymbol{b}_{k,n}\boldsymbol{b}_{k,n}^T \right) \end{aligned}$$

Solutions to the moment system

- $\mu_n(t) \equiv 0$ on $[t_n, t_{n+1})$.
- Covariance matrix $C_n(t) = \mathbb{E}[\boldsymbol{Y}_n(t)\boldsymbol{Y}_n^T(t)]$ satisfies

$$\frac{\mathrm{d}C_n(t)}{\mathrm{d}t} = \sum_{k=1}^{M} J_{k,n} C_n(t) J_{k,n}^T + \sum_{k=1}^{M} \boldsymbol{b}_{k,n}\boldsymbol{b}_{k,n}^T, \quad t \in [t_n, t_{n+1}).$$

- Model η_{n+1} as the d-variate normal distribution $\eta_{n+1} \sim \mathcal{N}\left(0, C_n(t_{n+1})\right)$, with

$$C_n(t_{n+1}) \approx \Delta t \sum_{k=1}^{M} \boldsymbol{b}_{k,n}\boldsymbol{b}_{k,n}^T.$$

Numerical algorithms

For $n = 0, \cdots, N$:

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta t f(\boldsymbol{x}_n) + \sum_{k=M+1}^{m} g_k(\boldsymbol{x}_n)\Delta W_{k,n} + \eta_{n+1} \text{ with}$$

[FPM-LP] $$\eta_{n+1} = \left(I_d + \sum_{k=1}^{M} J_{k,n}\Delta W_{k,n}\right) \sum_{k=1}^{M} \left(-J_{k,n}\boldsymbol{b}_{k,n}\Delta t + \boldsymbol{b}_{k,n}\Delta W_{k,n}\right)$$

[FPM-LM] $$\eta_{n+1} = \left(I_d + \sum_{k=1}^{M} \bar{J}_{k,n}\Delta W_{k,n}\right) \sum_{k=1}^{M} \left(-\bar{J}_{k,n}\boldsymbol{c}_{k,n}\Delta t + \boldsymbol{c}_{k,n}\Delta W_{k,n}\right)$$

[FPM-MM] $$\eta_{n+1} \sim \mathcal{N}\left(0, \Delta t \sum_{k=1}^{M} \boldsymbol{b}_{k,n}\boldsymbol{b}_{k,n}^T\right)$$

where
$$\bar{\boldsymbol{x}}_n = \mathbb{E}[\boldsymbol{x}_n], \quad \boldsymbol{b}_{k,n} = g_k(\boldsymbol{x}_n), \quad \boldsymbol{c}_{k,n} = g_k(\bar{\boldsymbol{x}}_n) + \bar{J}_{k,n}(\boldsymbol{x}_n - \bar{\boldsymbol{x}}_n),$$
$$J_{k,n} = \left(\frac{\partial g_k}{\partial X_1}, \cdots, \frac{\partial g_k}{\partial X_d}\right)\Bigg|_{\boldsymbol{X}=\boldsymbol{x}_n}, \quad \bar{J}_{k,n} = \left(\frac{\partial g_k}{\partial X_1}, \cdots, \frac{\partial g_k}{\partial X_d}\right)\Bigg|_{\boldsymbol{X}=\bar{\boldsymbol{x}}_n}.$$

Convergence experiments

- Example system of stiff SDE in $\mathbb{R}^2$, with $m = 3$ Brownian motions, and order-p polynomial drift and diffusion terms

$$f(\boldsymbol{X}(t)) = (A\boldsymbol{X}(t))^{\circ p}\,; \qquad g_k(\boldsymbol{X}(t)) = (B_k\boldsymbol{X}(t))^{\circ p}\,, \quad k = 1, \cdots, m$$

where the operation $()^{\circ p}$ denotes the Hadamard power.

- Sample matrices

$$A = \alpha \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix}, \quad B_1 = \beta_1 \begin{bmatrix} -1 & 2 \\ 3 & -6 \end{bmatrix}, \quad B_2 = \beta_2 \begin{bmatrix} 3 & -2 \\ -3 & 8 \end{bmatrix}, \quad B_3 = \beta_3 \begin{bmatrix} 1 & 4 \\ 6 & -9 \end{bmatrix}$$

- Scaling coefficients $\alpha = 0.1$, $\beta = (0.05, 0.05, 5 \times 10^{-7})$ for the linear ($p = 1$) case, and $(0.04, 0.04, 5 \times 10^{-4})$ for the quadratic ($p = 2$) case.

Sample paths computed by FPM-LP

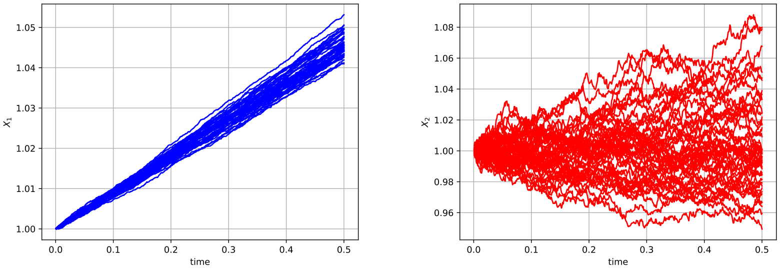


Figure: Illustrated sample paths computed with FPM-LP for X_1 (left) and X_2 (right), quadratic SDE.

Convergence of FPM-LP

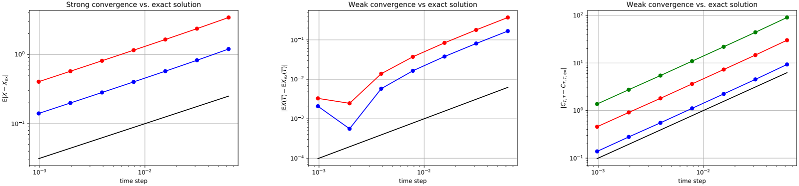


Figure: Convergence of FPM-LP vs the exact solution for the linear SDE system. Results highlight the expected 1/2-order strong convergence, and first order weak convergence.

Convergence of FPM-LM

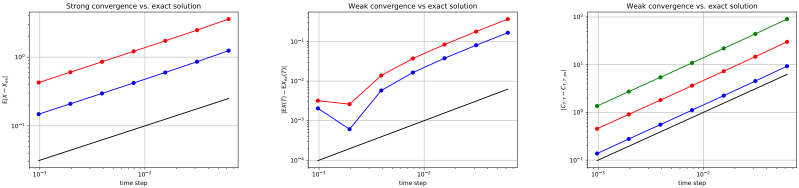


Figure: Convergence of FPM-LM vs the exact solution for the linear SDE

Convergence of FPM-MM

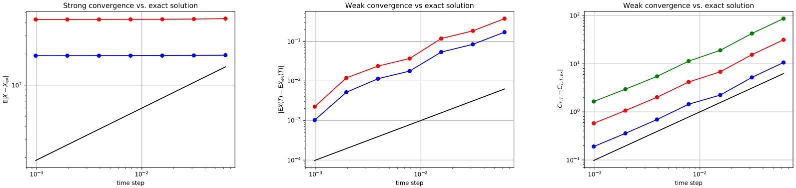
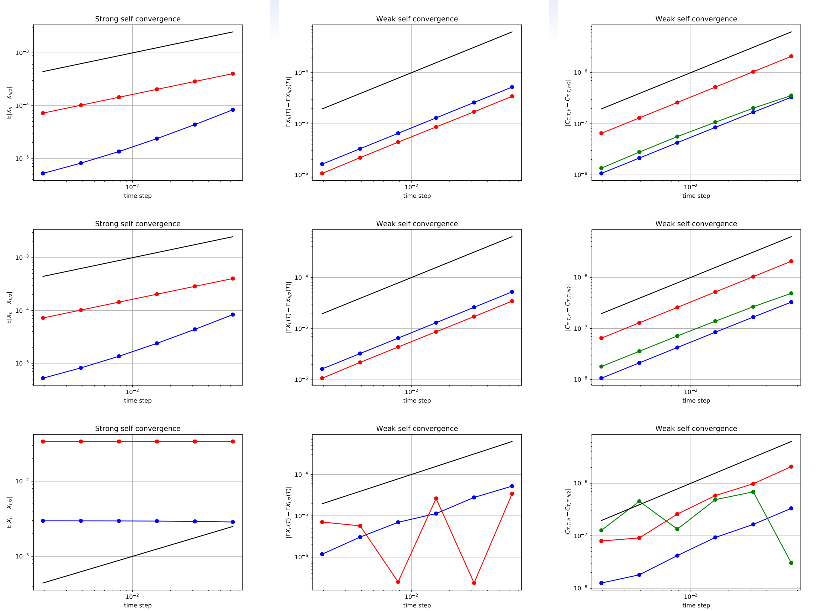
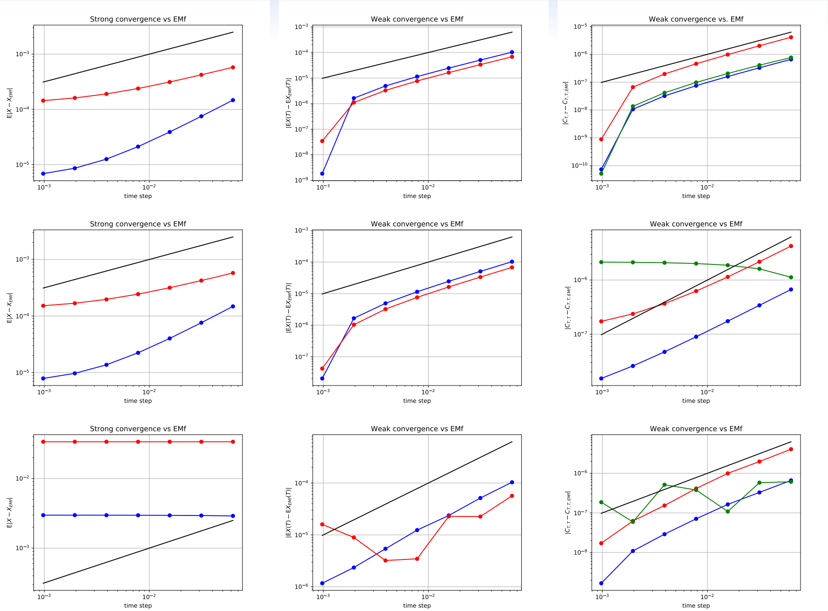


Figure: Convergence of FPM-MM vs the exact solution for the linear SDE system. Results show the expected absence of strong convergence, and the first order weak convergence.

Self convergence for the quadratic SDE system



Convergence for the quadratic system vs EMf



Convergence analysis

Estimating

1. strong error $\mathfrak{E}^s := \max_{n=1,\cdots,N} \mathbb{E}[|X(t_n) - x_n|]$
2. weak error $\mathfrak{E}^w := \left|\mathbb{E}[\psi(x_N)] - \mathbb{E}[\psi(X(T))]\right|$

- x_n is computed using FPM-LP
- the piecewise continuous interpolation process of FPM-LP for $t \in [t_n, t_{n+1})$

$$x(t) = x_n + (t - t_n)f(x_n) + \sum_{k=M+1}^{m} g_k(x_n)(W_k(t) - W_k(t_n)) + \eta(t),$$

where

$$\eta(t) = \phi_n(t) \sum_{k=1}^{M} \Big(b_{k,n} \left(-a_{k,n}(t - t_n) + (W_k(t) - W_k(t_n))\right)\Big).$$

Strong convergence

Recall

1. $\eta(t)$ is an approximation for $Y_n(t)$ on $t \in [t_n, t_{n+1})$
2. $Y_n(t)$ satisfies the linear diffusion only SDE
3. define

$$y(t) = x_0 + \int_0^t f(\tilde{x}(s)) \mathrm{d}s + \sum_{k=M+1}^{m} \int_0^t g_k(\tilde{x}(s)) \mathrm{d}W_k(s) + Y(t).$$

4. piecewise constant process $\tilde{x}(t) \equiv x_n \quad \text{for} \quad t \in [t_n, t_{n+1})$
5. $x(t) = y(t) + \eta(t) - Y(t)$

$$\begin{aligned}
\mathfrak{E}^s &\leq \sup_{0 \leq t \leq T} \mathbb{E}\left[|X(t) - x(t)|\right] \\
&\leq \sup_{0 \leq t \leq T} \mathbb{E}\left[|X(t) - y(t)|\right] + \sup_{0 \leq t \leq T} \mathbb{E}\left[|\eta(t) - Y(t)|\right].
\end{aligned}$$

Strong convergence

Theorem. The FPM-LP scheme has a strong convergence order of 1/2, i.e., there exists C_T independent of Δt such that

$$\mathfrak{E}^s = \max_{n=1,\cdots,N} \mathbb{E}\left[|X(t_n) - x_n|\right] \leq C_T \Delta t^{1/2},$$

where x_n is computed according to FPM-LP.

Techniques: The term $\mathbb{E}\left[|X(t) - x(t)|\right]$ is split into 3 parts

$$\left(\sup_{0\leq t\leq T} \mathbb{E}\left[|X(t) - y(t)|\right]\right)^2 \leq 3\left(\mathbb{E}\left[\sup_{0\leq t\leq T} \mathcal{E}_1^2(t)\right] + \mathbb{E}\left[\sup_{0\leq t\leq T} \mathcal{E}_2^2(t)\right] + \mathbb{E}\left[\sup_{0\leq t\leq T} \mathcal{E}_3^2(t)\right]\right)$$

$$\begin{aligned}
\mathcal{E}_1^2(t) &= \left|\int_0^t \left(f(X(s)) - f(\tilde{x}(s))\right) \mathrm{d}s\right|^2, \\
\mathcal{E}_2^2(t) &= \left|\sum_{k=M+1}^{m} \int_0^t \left(g_k(X(s) - g_k(\tilde{x}(s))\right) \mathrm{d}W_k(s)\right|^2, \\
\mathcal{E}_3^2(t) &= \left|\sum_{k=1}^{M} \int_0^t \Big(g_k(X(s)) - g_k(\tilde{x}(s)) - g_k'(\tilde{x}(s))(\hat{X}(s) - \tilde{x}(s))\Big) \mathrm{d}W_k(s)\right|^2.
\end{aligned}$$

Weak Convergence

Theorem. The FPM-LP scheme has a weak convergence order of 1, i.e., there exists C_T independent of Δt such that

$$\mathfrak{E}^w \leq C_T \Delta t.$$

Techniques: the Feynman-Kac formula. The weak discretization error is split into 4 parts.

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Thanks for your attention!