

# On the construction of explicit exponential-based schemes for stiff SDEs

Hugo de la Cruz

**Escola de Matemática Aplicada (FGV-EMAp)**  
**Rio de Janeiro**

*(NUMDIFF 2015. Halle. Germany)*

$$dx(t) = f(t, x(t))dt + \sum_{j=1}^m g_j(t, x(t))dw_t^j$$

$$x \in \mathbb{R}^d$$

$w_t = (w_t^1, \dots, w_t^m)$   $m$ -dimensional Brownian Motion,

$$f : [0, T] \times \mathbb{R}^d \longrightarrow \mathbb{R}^d$$

$$g_j : [0, T] \times \mathbb{R}^d \longrightarrow \mathbb{R}^d$$

## semi-linear SDE

$$dx(t) = (Ax(t) + f(x(t))) dt + \sum_{j=1}^m g_j(x(t)) dw_t^j$$



Y. Komori, K. Burrage, A stochastic **Exponential Euler scheme** for simulation of stiff biochemical reaction system, BIT, 10.1007/s10543-014-0485-1 (2014)



C. Shi, Y. Xiao, C. Zhang, The convergence and MS stability of **Exponential Euler method** for semilinear SDEs, Abstract and Applied Analysis, 10.1155/2012/350407 (2012)

By Ito formula to  $f, L^0 f, L^j f$ :

$$f(t, x(t)) = f(t_n, x(t_n)) + \int_{t_n}^{t_{n+1}} L^0 f(s, x(s)) ds + \sum_{j=1}^m \int_{t_n}^{t_{n+1}} L^j f(s, x(s)) dw_t^j$$

By Ito formula to  $f, L^0 f, L^j f$ :

$$\begin{aligned} f(t, x(t)) &= f(t_n, x(t_n)) + \int_{t_n}^{t_{n+1}} L^0 f(s, x(s)) ds + \sum_{j=1}^m \int_{t_n}^{t_{n+1}} L^j f(s, x(s)) dw_t^j \\ &= f(t_n, x(t_n)) + L^0 f(t_n, x(t_n)) \int_{t_n}^{t_{n+1}} ds + \sum_{j=1}^m L^j f(t_n, x(t_n)) \int_{t_n}^{t_{n+1}} dw_t^j + R \end{aligned}$$

By Ito formula to  $f, L^0 f, L^j f$ :

$$\begin{aligned} f(t, x(t)) &= f(t_n, x(t_n)) + \int_{t_n}^{t_{n+1}} L^0 f(s, x(s)) ds + \sum_{j=1}^m \int_{t_n}^{t_{n+1}} L^j f(s, x(s)) dw_t^j \\ &= f(t_n, x(t_n)) + L^0 f(t_n, x(t_n)) \int_{t_n}^{t_{n+1}} ds + \sum_{j=1}^m L^j f(t_n, x(t_n)) \int_{t_n}^{t_{n+1}} dw_t^j + R \end{aligned}$$

where

$$L^0 f = \frac{\partial f}{\partial t} + J_f f + \frac{1}{2} \sum_{j=1}^m (\mathbf{I} \otimes g_j^\top) f_{xx} g_j$$

$$L^j f = J_f g_j,$$

Then:

$$\begin{aligned}
 f(t, x(t)) &= f(t_n, x(t_n)) + \left[ \frac{\partial f}{\partial t} + J_f f + \frac{1}{2} \sum_{j=1}^m (\mathbf{I} \otimes \mathbf{g}_j^T) f_{xx} \mathbf{g}_j \right]_{(t_n, x(t_n))} (t - t_n) \\
 &\quad + \sum_{j=1}^m [J_f \mathbf{g}_j]_{(t_n, x(t_n))} (w_t^j - w_{t_n}^j) + R_1
 \end{aligned}$$

Then:

$$\begin{aligned} f(t, x(t)) &= f(t_n, x(t_n)) + \left[ \frac{\partial f}{\partial t} + J_f f + \frac{1}{2} \sum_{j=1}^m (\mathbf{I} \otimes g_j^T) f_{xx} g_j \right]_{(t_n, x(t_n))} (t - t_n) \\ &\quad + \sum_{j=1}^m [J_f g_j]_{(t_n, x(t_n))} (w_t^j - w_{t_n}^j) + R_1 \end{aligned}$$

Also

$$x(t) = x(t_n) + f(t_n, x(t_n))(t - t_n) + \sum_{j=1}^m g_j(t_n, x(t_n))(w_t^j - w_{t_n}^j) + R_2$$

thus,

$$J_f (x(t) - x(t_n)) = J_f f(t_n, x(t_n))(t - t_n) + \sum_{j=1}^m [J_f g_j]_{(t_n, x(t_n))} (w_t^j - w_{t_n}^j) + \bar{R}_2$$

Then:

$$f(t, x(t)) \approx f(t_n, x(t_n)) + J_f(x(t) - x(t_n)) + \left[ \frac{\partial f}{\partial t} + \frac{1}{2} \sum_{j=1}^m (\mathbf{l} \otimes \mathbf{g}_j^T) f_{xx} \mathbf{g}_j \right]_{(t_n, x(t_n))} (t - t_n)$$

$$\begin{aligned}
 dx(t) = & \left( J_f(x(t) - x_n) + \left[ \frac{\partial f}{\partial t} + \frac{1}{2} \sum_{j=1}^m (\mathbf{I} \otimes g_j^\top) f_{xx} g_j \right]_{(t_n, x_n)} (t - t_n) + f(t_n, x_n) \right) dt \\
 & + \sum_{j=1}^m g_j(t, x_n) dw_t^j
 \end{aligned}$$

$$\begin{aligned}
dx(t) &= \left( J_f(x(t) - x_n) + \left[ \frac{\partial f}{\partial t} + \frac{1}{2} \sum_{j=1}^m (\mathbf{I} \otimes g_j^\top) f_{xx} g_j \right]_{(t_n, x_n)} (t - t_n) + f(t_n, x_n) \right) dt \\
&\quad + \sum_{j=1}^m g_j(t, x_n) dW_t^j \\
&= (\mathbf{A}_n(x(t) - x_n) + \mathbf{b}_n(t - t_n) + f(t_n, x_n)) dt + G(t, x_n) dW_t
\end{aligned}$$

Let  $\mathbf{Z}(t) = (x(t) - x_n, t - t_n, f(t_n, x_n), 1)^\top \in \mathbb{R}^{2d+2}$  then

$$d\mathbf{Z}(t) = \mathbf{M} \mathbf{Z}(t)dt + \begin{pmatrix} G(t, x_n) \\ 0 \\ 0 \end{pmatrix} dW_t$$

$$\mathbf{Z}(t_n) = [\mathbf{0}_{1 \times d} \ 0 \ f(t_n, x_n) \ 1]^\top,$$

where

$$\mathbf{M} = \begin{pmatrix} \mathbf{A}_n & \mathbf{b}_n & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 0 \end{pmatrix}.$$

Solution:

$$\mathbf{Z}(t) = e^{\mathbf{M}(t-t_n)} \mathbf{Z}(t_n) + \int_{t_n}^t e^{\mathbf{M}(t-s)} \begin{pmatrix} G(t, x_n) \\ 0 \\ 0 \end{pmatrix} dW_s$$

Solution:

$$\mathbf{Z}(t) = e^{\mathbf{M}(t-t_n)} \mathbf{Z}(t_n) + \int_{t_n}^t e^{\mathbf{M}(t-s)} \begin{pmatrix} G(t, x_n) \\ 0 \\ 0 \end{pmatrix} dW_s$$

-Looking at the first component of  $\mathbf{Z}(t)$ , it follows that  $x(t)$ , can be computed by

$$\begin{aligned} x(t) &= x_n + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} e^{\mathbf{M}(t-t_n)} [\mathbf{0}_{d \times d} \ 0 \ f(t_n, x_n) \ 1]^\top \\ &\quad + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} \int_{t_n}^t e^{\mathbf{M}(t-s)} \begin{pmatrix} G(t, x_n) \\ 0 \\ 0 \end{pmatrix} dW_s \\ &= x_n + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} e^{\mathbf{M}(t-t_n)} [\mathbf{0}_{d \times d} \ 0 \ f(t_n, x_n) \ 1]^\top + \int_{t_n}^t e^{\mathbf{A}_n(t-s)} G(t, x_n) dW_s \end{aligned}$$

Solution:

$$\mathbf{Z}(t) = e^{\mathbf{M}(t-t_n)} \mathbf{Z}(t_n) + \int_{t_n}^t e^{\mathbf{M}(t-s)} \begin{pmatrix} G(t, x_n) \\ 0 \\ 0 \end{pmatrix} dW_s$$

-Looking at the first component of  $\mathbf{Z}(t)$ , it follows that  $x(t)$ , can be computed by

$$\begin{aligned} x(t) &= x_n + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} e^{\mathbf{M}(t-t_n)} [\mathbf{0}_{d \times d} \ 0 \ f(t_n, x_n) \ 1]^\top \\ &\quad + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} \int_{t_n}^t e^{\mathbf{M}(t-s)} \begin{pmatrix} G(t, x_n) \\ 0 \\ 0 \end{pmatrix} dW_s \\ &= x_n + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} e^{\mathbf{M}(t-t_n)} [\mathbf{0}_{d \times d} \ 0 \ f(t_n, x_n) \ 1]^\top + \int_{t_n}^t e^{\mathbf{A}_n(t-s)} G(t, x_n) dW_s \end{aligned}$$

Thus, in particular

$$x(t_{n+1}) = x_n + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} e^{\mathbf{M}h} [\mathbf{0}_{d \times d} \ 0 \ f(t_n, x_n) \ 1]^\top + \int_{t_n}^{t_{n+1}} e^{\mathbf{A}_n(t_{n+1}-s)} G(t, x_n) dW_s$$

Let

$$\int_{t_n}^t e^{\mathbf{A}_n(t-s)} G(s, x_n) dW_s = e^{\mathbf{A}_n t} \boldsymbol{\eta}(t)$$

where

$$\boldsymbol{\eta}(t) = \sum_{i=1}^m \int_{t_n}^t e^{-\mathbf{A}_n u} g_i(u, x_n) dw_u^i$$

is the solution of the SDE

$$\begin{aligned} d\boldsymbol{\eta}(t) &= \sum_{i=1}^m e^{-\mathbf{A}_n t} g_i(t, x_n) dw_t^i \\ \boldsymbol{\eta}(t_n) &= \mathbf{0} \end{aligned}$$

- We need to compute  $e^{\mathbf{A}_n t_{n+1}} \boldsymbol{\eta}(t_{n+1})$

- We need to compute  $e^{\mathbf{A}_n t_{n+1}} \boldsymbol{\eta}(t_{n+1})$
- The application of the Ito formula to  $\mathbf{U}(t, \boldsymbol{\eta}) = \boldsymbol{\rho}(t) = e^{\mathbf{A}_n t_{n+1}} \boldsymbol{\eta}(t)$  yields

$$d\boldsymbol{\rho}(t) = \sum_{i=1}^m e^{\mathbf{A}_n(t_{n+1}-t)} g_i(t, x_n) dw^i(t)$$
$$\boldsymbol{\rho}(t_n) = \mathbf{0}$$

- We need to compute  $e^{\mathbf{A}_n t_{n+1}} \boldsymbol{\eta}(t_{n+1})$
- The application of the Ito formula to  $\mathbf{U}(t, \boldsymbol{\eta}) = \boldsymbol{\rho}(t) = e^{\mathbf{A}_n t_{n+1}} \boldsymbol{\eta}(t)$  yields

$$d\boldsymbol{\rho}(t) = \sum_{i=1}^m e^{\mathbf{A}_n(t_{n+1}-t)} g_i(t, x_n) dw^i(t)$$

$$\boldsymbol{\rho}(t_n) = \mathbf{0}$$

- By the order-1.5 strong Taylor scheme we have the approximation

$$\boldsymbol{\rho}(t_{n+1}) = e^{\mathbf{A}_n h} \sum_{i=1}^m \left( g_i(t_n, x_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, x_n) \Delta z_n^i + \frac{dg_i(t_n, x_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right)$$

where  $\Delta w_n^i = w_{t_{n+1}}^i - w_{t_n}^i = \sqrt{h} u_1^i$  and  $\Delta z_n^i = \int_{t_n}^{t_{n+1}} \int_{t_n}^{s_2} dw_{s_1}^i ds_2 = \frac{1}{2} h^{\frac{2}{3}} (u_1^i + \frac{1}{\sqrt{3}} u_2^i)$

$$\begin{aligned}
 x_{n+1} &= x_n + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} e^{\mathbf{M}h} \begin{bmatrix} \mathbf{0}_{d \times d} & 0 & f(t_n, x_n) & 1 \end{bmatrix}^\top \\
 &\quad + e^{\mathbf{A}_n h} \sum_{i=1}^m \left( g_i(t_n, x_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, x_n) \Delta z_n^i + \frac{dg_i(t_n, x_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right),
 \end{aligned}$$

# Implementation

The *Padé algorithm with scaling-squaring strategy* for computing  $e^{\mathbf{C}}$  [Golub-Van Loan]:

❶ Determine the minimum integer  $k$  such that  $\left\| \frac{\mathbf{C}}{2^k} \right\| < \frac{1}{2}$

❷ Compute

$$\begin{aligned}\mathbf{N}_q\left(\frac{\mathbf{C}}{2^k}\right) &= \sum_{j=0}^q \frac{(2q-j)!q!}{(2q)!j!(q-j)!} \mathbf{C}^j \\ \mathbf{D}_q\left(\frac{\mathbf{C}}{2^k}\right) &= \sum_{j=0}^q \frac{(2q-j)!q!}{(2q)!j!(q-j)!} (-\mathbf{C})^j.\end{aligned}$$

❸ Compute  $\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right) = [\mathbf{D}_q\left(\frac{\mathbf{C}}{2^k}\right)]^{-1} \mathbf{N}_q\left(\frac{\mathbf{C}}{2^k}\right)$ , (solving the system  $\mathbf{D}_q\left(\frac{\mathbf{C}}{2^k}\right) \mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right) = \mathbf{N}_q\left(\frac{\mathbf{C}}{2^k}\right)$ )

❹ Compute  $[\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)]^{2^k}$  by squaring  $\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)$   $k$  times

# The Adapted Padé algorithm for computing $\exp(\mathbf{M}h)$

$\mathbf{C} = \mathbf{M}h$ . Denote  $\mathbf{A} = \mathbf{A}_n h$  and  $\mathbf{b} = \mathbf{b}_n h$ , then

$$\left(\frac{\mathbf{C}}{2^k}\right) = \begin{pmatrix} \mathbf{A} & \mathbf{b} & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 0 \end{pmatrix} \frac{h}{2^k}$$

and, for any  $j \geq 2$

$$\left(\frac{\mathbf{C}}{2^k}\right)^j = \begin{pmatrix} \mathbf{A}^j & \mathbf{A}^{j-1}\mathbf{b} & \mathbf{A}^{j-1} & \mathbf{A}^{j-2}\mathbf{b} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 0 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 0 \end{pmatrix} \left(\frac{h}{2^k}\right)^j.$$

# The Adapted Padé algorithm for computing $\exp(\mathbf{M}h)$

$$\mathbf{N}_q\left(\frac{\mathbf{C}}{2^k}\right) = \begin{pmatrix} \mathbf{I} + \mathbf{A}(\alpha_1 \mathbf{I} + \mathbf{A}\mathbf{S}) & (\alpha_1 \mathbf{I} + \mathbf{A}\mathbf{S})\mathbf{b} & (\alpha_1 \mathbf{I} + \mathbf{A}\mathbf{S}) & \mathbf{S}\mathbf{b} \\ \mathbf{0}_{1 \times d} & 1 & \mathbf{0}_{1 \times d} & \alpha_1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \end{pmatrix},$$

and

$$\mathbf{D}_q\left(\frac{\mathbf{C}}{2^k}\right) = \begin{pmatrix} \mathbf{I} + \mathbf{A}(-\alpha_1 \mathbf{I} + \mathbf{A}\mathbf{S}) & (-\alpha_1 \mathbf{I} + \mathbf{A}\mathbf{S})\mathbf{b} & (-\alpha_1 \mathbf{I} + \mathbf{A}\mathbf{S}) & \mathbf{S}\mathbf{b} \\ \mathbf{0}_{1 \times d} & 1 & \mathbf{0}_{1 \times d} & -\alpha_1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \end{pmatrix},$$

where

$$\begin{aligned} \mathbf{S} &= (\alpha_2 \mathbf{I} + \alpha_3 \mathbf{A} + \dots + \alpha_q (\mathbf{A})^{q-2}), \\ \mathbf{S} &= (\alpha_2 \mathbf{I} - \alpha_3 \mathbf{A} + \dots + (-1)^{q-2} \alpha_q (\mathbf{A})^{q-2}), \end{aligned}$$

and  $\alpha_j = c_j \left(\frac{h}{2^k}\right)^j$ ,  $(c_j = \frac{(2q-j)!q!}{(2q)j!(q-j)!})$

# The Adapted Padé algorithm for computing $\exp(\mathbf{M}h)$

## Padé Approximation

$$\mathbf{D}_q\left(\frac{\mathbf{C}}{2^k}\right)\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right) = \mathbf{N}_q\left(\frac{\mathbf{C}}{2^k}\right)$$

$\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)$  has the form:

$$\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right) = \begin{pmatrix} \mathbf{U1} & \mathbf{U2} & \mathbf{U3} & \mathbf{U4} \\ \mathbf{0}_{1 \times d} & 1 & \mathbf{0}_{1 \times d} & \alpha_1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \end{pmatrix}$$

# The Adapted Padé algorithm for computing $\exp(\mathbf{M}h)$

## Padé Approximation

$$\mathbf{D}_q\left(\frac{\mathbf{C}}{2^k}\right)\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right) = \mathbf{N}_q\left(\frac{\mathbf{C}}{2^k}\right)$$

$\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)$  has the form:

$$\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right) = \begin{pmatrix} \mathbf{U1} & \mathbf{U2} & \mathbf{U3} & \mathbf{U4} \\ \mathbf{0}_{1 \times d} & 1 & \mathbf{0}_{1 \times d} & \alpha_1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \end{pmatrix}$$

and  $\mathbf{U1}$ ,  $\mathbf{U2}$ ,  $\mathbf{U3}$ ,  $\mathbf{U4}$  satisfy:

$$\left[ \mathbf{I} + \mathbf{A} \left( -\alpha_1 \mathbf{I} + \mathbf{A}\hat{\mathbf{S}} \right) \right] \mathbf{U1} = \left[ \mathbf{I} + \mathbf{A} \left( \alpha_1 \mathbf{I} + \mathbf{A}\hat{\mathbf{S}} \right) \right]$$

$$\left[ \mathbf{I} + \mathbf{A} \left( -\alpha_1 \mathbf{I} + \mathbf{A}\hat{\mathbf{S}} \right) \right] \mathbf{U3} = \left( \alpha_1 \mathbf{I} + \mathbf{A}\hat{\mathbf{S}} \right) - \left( -\alpha_1 \mathbf{I} + \mathbf{A}\hat{\mathbf{S}} \right)$$

$$\left[ \mathbf{I} + \mathbf{A} \left( -\alpha_1 \mathbf{I} + \mathbf{A}\hat{\mathbf{S}} \right) \right] \mathbf{U4} = \left[ \mathbf{S} - 2\alpha_1 \left( -\alpha_1 \mathbf{I} + \mathbf{A}\hat{\mathbf{S}} \right) - \hat{\mathbf{S}} \right] \mathbf{b}$$

$$\mathbf{U2} = (\mathbf{U3})\mathbf{b}$$

# Squaring the scaled Padé Approx.

Once we have **U1**, **U2**, **U3**, **U4**, we can compute  $\left(\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)\right)^{2^k}$ :

$$\left(\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)\right)^{2^k} = \begin{pmatrix} (\mathbf{U1})^{2^k} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U2} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U3} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U4} + \alpha_1 \left(\sum_{i=0}^{2^k-2} (m-1-i) (\mathbf{U1})^i\right) \mathbf{U2} \\ \mathbf{0}_{1 \times d} & 1 & \mathbf{0}_{1 \times d} & 2^k \alpha_1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \end{pmatrix}$$

# Squaring the scaled Padé Approx.

Once we have **U1**, **U2**, **U3**, **U4**, we can compute  $\left(\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)\right)^{2^k}$ :

$$\left(\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)\right)^{2^k} = \begin{pmatrix} (\mathbf{U1})^{2^k} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U2} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U3} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U4} + \alpha_1 \left(\sum_{i=0}^{2^k-2} (m-1-i) (\mathbf{U1})^i\right) \mathbf{U2} \\ \mathbf{0}_{1 \times d} & 1 & \mathbf{0}_{1 \times d} & 2^k \alpha_1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \end{pmatrix}$$

Thus,

$$\begin{aligned} x_{n+1} &= x_n + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} \left(\mathbf{P}_q\left(\frac{\mathbf{M}h}{2^k}\right)\right)^{2^k} \begin{bmatrix} \mathbf{0}_{d \times d} & 0 & f(t_n, x_n) & 1 \end{bmatrix}^\top \\ &+ \left(\mathbf{P}_q\left(\frac{\mathbf{A}_n h}{2^k}\right)\right)^{2^k} \sum_{i=1}^m \left( g_i(t_n, x_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, x_n) \Delta z_n^i + \frac{dg_i(t_n, x_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right) \end{aligned}$$

# Squaring the scaled Padé Approx.

Once we have **U1**, **U2**, **U3**, **U4**, we can compute  $\left(\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)\right)^{2^k}$ :

$$\left(\mathbf{P}_q\left(\frac{\mathbf{C}}{2^k}\right)\right)^{2^k} = \begin{pmatrix} (\mathbf{U1})^{2^k} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U2} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U3} & \left(\sum_{i=0}^{2^k-1} (\mathbf{U1})^i\right) \mathbf{U4} + \alpha_1 \left(\sum_{i=0}^{2^k-2} (m-1-i) (\mathbf{U1})^i\right) \mathbf{U2} \\ \mathbf{0}_{1 \times d} & 1 & \mathbf{0}_{1 \times d} & 2^k \alpha_1 \\ \mathbf{0}_{d \times d} & \mathbf{0}_{d \times 1} & \mathbf{I}_{d \times d} & \mathbf{0}_{d \times 1} \\ \mathbf{0}_{1 \times d} & 0 & \mathbf{0}_{1 \times d} & 1 \end{pmatrix}$$

Thus,

$$\begin{aligned} x_{n+1} &= x_n + \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} \left(\mathbf{P}_q\left(\frac{\mathbf{M}h}{2^k}\right)\right)^{2^k} \begin{bmatrix} \mathbf{0}_{d \times d} & 0 & f(t_n, x_n) & 1 \end{bmatrix}^\top \\ &\quad + \left(\mathbf{P}_q\left(\frac{\mathbf{A}_n h}{2^k}\right)\right)^{2^k} \sum_{i=1}^m \left( g_i(t_n, x_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, x_n) \Delta z_n^i + \frac{dg_i(t_n, x_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right) \\ &= x_n + \mathbf{L}f(t_n, x_n) + \mathbf{Q} \\ &\quad + \mathbf{R} \sum_{i=1}^m \left( g_i(t_n, x_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, x_n) \Delta z_n^i + \frac{dg_i(t_n, x_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right) \end{aligned}$$

# The Proposed Integrator

$$\begin{aligned}x_{n+1} &= x_n + \mathbf{L}f(t_n, x_n) + \mathbf{Q} \\ &\quad + \mathbf{R} \sum_{i=1}^m \left( g_i(t_n, x_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, x_n) \Delta z_n^i + \frac{dg_i(t_n, x_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right)\end{aligned}$$

where

$$\mathbf{L} = \left( \sum_{i=0}^{2^k-1} (\mathbf{U1})^i \right) \mathbf{U3},$$

$$\mathbf{Q} = \left( \sum_{i=0}^{2^k-1} (\mathbf{U1})^i \right) \mathbf{U4} + \alpha_1 \left( \sum_{i=0}^{2^k-2} (m-1-i) (\mathbf{U1})^i \right) (\mathbf{U3}) \mathbf{b}$$

$$\mathbf{R} = (\mathbf{U1})^{2^k}$$

## Convergence and Stability

Let

$$x_{n+1} = x_n + \phi(t_n, x_n; h) + \xi(t_n, x_n; h)$$

the order- $\gamma$  method, and

$$\tilde{x}_{n+1} = \tilde{x}_n + \tilde{\phi}(t_n, \tilde{x}_n; h) + \tilde{\xi}(t_n, \tilde{x}_n; h)$$

a **numerical implementation** of  $x_{n+1}$ , where  $\tilde{\phi}$  and  $\tilde{\xi}$  denote **numerical algorithms to compute**  $\phi$  and  $\xi$ . And suppose that

$$\begin{aligned} & \left| E \left( \phi(t_n, \tilde{x}_n; h) - \tilde{\phi}(t_n, \tilde{x}_n; h) \mid \mathcal{F}_{t_n} \right) \right| \leq K_1 (1 + |\tilde{x}_n|^2)^{1/2} h^{k_1} \\ & \left( E \left( |\phi(t_n, \tilde{x}_n; h) - \tilde{\phi}(t_n, \tilde{x}_n; h)|^2 \mid \mathcal{F}_{t_n} \right) \right)^{1/2} \leq K_1 (1 + |\tilde{x}_n|^2)^{1/2} h^{k_2+1/2} \\ & \left| E \left( \xi(t_n, \tilde{x}_n; h) - \tilde{\xi}(t_n, \tilde{x}_n; h) \mid \mathcal{F}_{t_n} \right) \right| \leq K_2 (1 + |\tilde{x}_n|^2)^{1/2} h^{p_1} \\ & \left( E \left( |\xi(t_n, \tilde{x}_n; h) - \tilde{\xi}(t_n, \tilde{x}_n; h)|^2 \mid \mathcal{F}_{t_n} \right) \right)^{1/2} \leq K_2 (1 + |\tilde{x}_n|^2)^{1/2} h^{p_2+1/2} \end{aligned}$$

for some positive numbers  $k_2, p_2 \geq 1/2$ ,  $k_1 \geq k_2 + 1$ ,  $p_1 \geq p_2 + 1$ , then

$$\left( E \left( |x(t_n) - \tilde{x}_n|^2 \mid \mathcal{F}_{t_0} \right) \right)^{\frac{1}{2}} = O(h^{\min\{\gamma, k_2, p_2\}})$$

Note that we have

$$\begin{aligned}\tilde{\boldsymbol{\phi}}(t_n, \tilde{\mathbf{x}}_n; h) &= \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} \left( \mathbf{P}_q \left( \frac{\mathbf{M}h}{2^k} \right) \right)^{2^k} [\mathbf{0}_{d \times d} \ 0 \ f(t_n, \mathbf{x}_n) \ 1]^\top \\ \tilde{\boldsymbol{\xi}}(t_n, \tilde{\mathbf{y}}_n; h) &= \left( \mathbf{P}_q \left( \frac{\mathbf{A}_n h}{2^k} \right) \right)^{2^k} \sum_{i=1}^m \left( g_i(t_n, \mathbf{x}_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, \mathbf{x}_n) \Delta z_n^i + \frac{dg_i(t_n, \mathbf{x}_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right)\end{aligned}$$

Note that we have

$$\begin{aligned}\tilde{\boldsymbol{\phi}}(t_n, \tilde{\mathbf{x}}_n; h) &= \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} \left( \mathbf{P}_q \left( \frac{\mathbf{M}h}{2^k} \right) \right)^{2^k} [\mathbf{0}_{d \times d} \ 0 \ f(t_n, \mathbf{x}_n) \ 1]^\top \\ \tilde{\boldsymbol{\xi}}(t_n, \tilde{\mathbf{y}}_n; h) &= \left( \mathbf{P}_q \left( \frac{\mathbf{A}_n h}{2^k} \right) \right)^{2^k} \sum_{i=1}^m \left( g_i(t_n, \mathbf{x}_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, \mathbf{x}_n) \Delta z_n^i + \frac{dg_i(t_n, \mathbf{x}_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right)\end{aligned}$$

and by using that

$$\left| e^{\mathbf{X}} - (\mathbf{P}_q(2^{-k}\mathbf{X}))^{2^k} \right| \leq c_q(k, |\mathbf{X}|) |\mathbf{X}|^{\rho+q+1},$$

where  $c_q(k, |\mathbf{X}|) = \alpha 2^{-k(2q)+3} e^{(1+\epsilon_{\rho,q})|\mathbf{X}|}$  and  $\alpha = \frac{(q!)^2}{(2q)!(2q+1)!}$ ,  $\epsilon_q = \alpha(\frac{1}{2})^{2q-3}$

Note that we have

$$\begin{aligned}\tilde{\boldsymbol{\phi}}(t_n, \tilde{\mathbf{x}}_n; h) &= \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{0}_{d \times (d+2)} \end{bmatrix} \left( \mathbf{P}_q \left( \frac{\mathbf{M}h}{2^k} \right) \right)^{2^k} [\mathbf{0}_{d \times d} \ 0 \ f(t_n, \mathbf{x}_n) \ 1]^\top \\ \tilde{\boldsymbol{\xi}}(t_n, \tilde{\mathbf{y}}_n; h) &= \left( \mathbf{P}_q \left( \frac{\mathbf{A}_n h}{2^k} \right) \right)^{2^k} \sum_{i=1}^m \left( g_i(t_n, \mathbf{x}_n) \Delta w_n^i + (-\mathbf{A}_n g_i(t_n, \mathbf{x}_n) \Delta z_n^i + \frac{dg_i(t_n, \mathbf{x}_n)}{dt})(\Delta w_n^i h - \Delta z_n^i) \right)\end{aligned}$$

and by using that

$$\left| e^{\mathbf{X}} - (\mathbf{P}_q(2^{-k}\mathbf{X}))^{2^k} \right| \leq c_q(k, |\mathbf{X}|) |\mathbf{X}|^{\rho+q+1},$$

where  $c_q(k, |\mathbf{X}|) = \alpha 2^{-k(2q)+3} e^{(1+\epsilon_{p,q})|\mathbf{X}|}$  and  $\alpha = \frac{(q!)^2}{(2q)!(2q+1)!}$ ,  $\epsilon_q = \alpha(\frac{1}{2})^{2q-3}$

The scheme

$$\tilde{\mathbf{x}}_{n+1} = \tilde{\mathbf{x}}_n + \tilde{\boldsymbol{\phi}}(t_n, \tilde{\mathbf{x}}_n; h) + \tilde{\boldsymbol{\xi}}(t_n, \tilde{\mathbf{x}}_n; h)$$

satisfies

$$\left( E \left( |\mathbf{x}(t_n) - \tilde{\mathbf{x}}_n|^2 \mid \mathcal{F}_{t_0} \right) \right)^{\frac{1}{2}} = O(h^{\min\{\frac{1}{2}, q-1\}})$$

## Example

### Two connected oscillators

$$dx_1 = x_2$$

$$dx_2 = \left( \frac{1}{2}x_2(1 - x_1^2) - x_1 + 0.1x_3 \right)dt + 10^{-3}x_1dw^1$$

$$dx_3 = x_4$$

$$dx_4 = \left( 5x_4(1 - x_3^2) - x_3 + 0.1x_1 \right)dt + 10^{-3}x_3dw^2$$

$$(x_1^0, x_2^0, y_1^0, y_2^0) = (1, 1, 0, 0).$$

# phase space second V. der Pol oscillator

Click me!

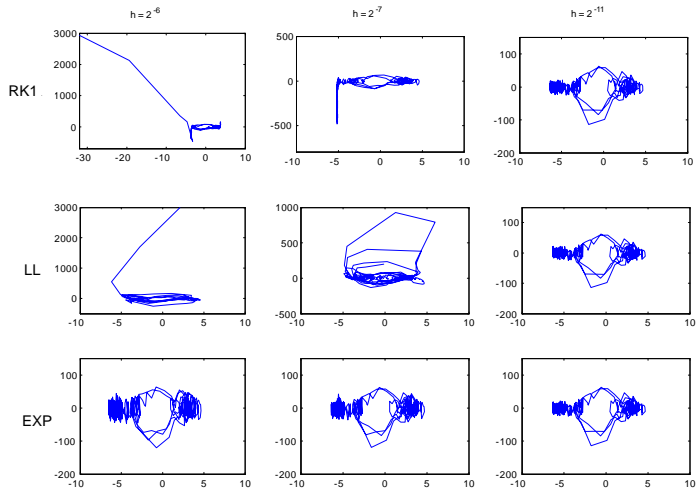
## Example

Stochastic Van der Pol equat.

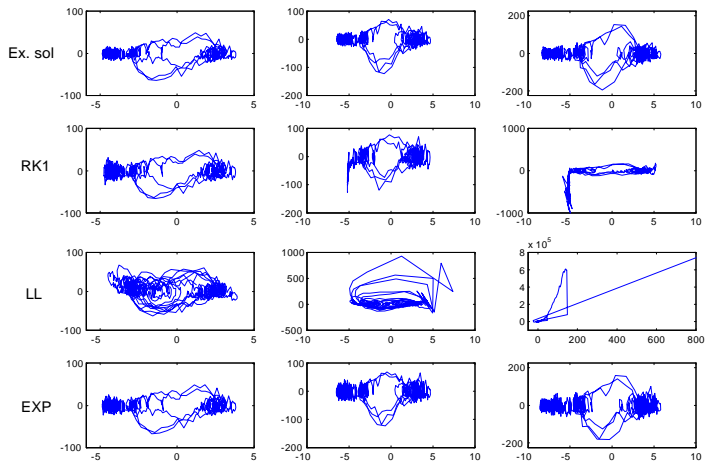
$$\begin{aligned}dx^1 &= x^2 dt, \\dx^2 &= E \left( \left( 1 - (x^1)^2 \right) x^2 - x^1 \right) dt + \sigma d\mathbf{W}_t\end{aligned}$$

$E = 10$ ,  $[t_0, T] = [0, 12]$ ,  $\mathbf{x}(t_0) = (2, 0)$ .

$$\sigma = 200$$



$$\sigma_1 = 100, \sigma_2 = 200, \sigma_3 = 400$$



# References



H. de la Cruz, R.J. Biscay, J.C. Jimenez, F. Carbonell, HOLL methods: An approach for constructing A-stable explicit schemes for SDEs with additive noise, BIT, 50 (2010) 509-539.



J.C. Jimenez, H. de la Cruz, Convergence rate of strong local linearization schemes for SDEs with additive noise, BIT, 52 (2012) 357-382.



D. Higham, X. Mao, C. Yuan, Almost sure and moment exponential stability in the numerical simulation of SDEs, SIAM J. Numer. Anal., 45 (2) (2010) 592-609.



Y. Komori, K. Burrage, A stochastic exponential Euler scheme for simulation of stiff biochemical reaction system, BIT, 10.1007/s10543-014-0485-1 (2014)



G.N. Milstein, M.V. Tretyakov, Stochastic Numerics for Mathematical Physics, Springer, 2004.



C. Shi, Y. Xiao, C. Zhang, The convergence and MS stability of Exponential Euler method for semilinear SDEs, Abstract and Applied Analysis, 10.1155/2012/350407 (2012)