Properties of a Local Linearization scheme for the numerical integration of ODEs

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Abstract

Some features of a Local Linearization scheme for the numerical integration of Ordinary Differential Equations (ODEs) are studied. It is demonstrated that this one-step explicit scheme has the following properties: 1) consistency; 2) local and global truncation errors of third and second order, respectively; 3) exactitude of the numerical integration for linear ODEs, including linear stiff equations; 4) A-stability; 5) regularity for some classes of ODEs; 6) any trajectory of an ODE near a hyperbolic equilibrium point can be adequately approximated by the orbit of the LL scheme for sufficiently small step length. In particular, the stable and unstable manifolds of the discretization converge to their continuous counterparts; 7) for any ODE with a hyperbolic periodic trajectory the map of the LL scheme has an invariant closed curve that converges to the continuous trajectory with a shift of phase; and 8) any trajectory of an ODE near a stable periodic trajectory can be adequately approximated by a stable invariant curve of the LL scheme for sufficiently small step length.

1 Introduction

Over the last years the Local Linearization (LL) method for the numerical integration of Stochastic Differential Equations (SDEs) has been the subject of a number of papers, e.g., [4, 13, 17, 18, 21, 22]. Extensive simulation studies carried out in these works have demonstrated that the LL schemes show high numerical stability, remarkable computational efficiency and moderate order of convergence.

The LL method can also be applied to SDEs with zero diffusion coefficients, i.e., to Ordinary Differential Equations (ODEs). In this setting, a crucial characteristic of the LL method is that it can be derived from the first order Taylor expansion of the vector field of the ODE [4, 19], in contrast to standard numerical integration methods (e.g., Euler, Runge-Kutta methods, etc. [5]) which are

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based on Taylor expansions of the solution. Following the LL method, a number of integration schemes have been constructed, such as schemes with fixed or adaptive step size, schemes with exact or approximate Jacobian matrix, etc. [14, 19]. Preliminary simulation studies [14, 19] have revealed that such schemes for ODEs have similar properties as LL schemes for SDEs.

The goal of the present paper is to theoretically support some of these simulation results obtained from the use of a non-adaptive LL scheme with exact Jacobian matrix. Special emphasis is given to the connection between the dynamics of the differential equation and the map of the LL scheme.

The paper is organized as follows. In Section 2 the LL scheme is presented. Section 3 deals with the local and global truncation errors of the scheme. Section 4 studies its accuracy and stability in the case of linear ODEs. Finally, the last section deals with the behavior of the scheme near steady states of differentiable systems when the discretization step tends to zero.

2 The Local Linealization scheme

Let

$$\mathbf{x}'(t) = \mathbf{f}(\mathbf{x}(t)),\ t \geq t_0 \in \mathbb{R},\ \mathbf{x}(t_0) = \mathbf{x_0} \in \mathbb{R}^m \tag{1}$$

be an m-dimensional autonomous system of ODE, for which there exists a unique solution. In addition, suppose that the function $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ is differentiable.

The LL method for the numerical integration of this ODE is defined through of the solution of the linear ODEs resulting from the local (piecewise) linearization of the right member of (1).

Specifically, let $h > 0$ be the step-size of the time discretization, $s \geq t_0$ be a fixed time instant, and $\mathbf{y}_s \in \mathbb{R}^m$ a point close to $\mathbf{x}(s) \in \mathbb{R}^m$. Consider the truncated first order Taylor expansion of the function $\mathbf{f}$ at the point $\mathbf{y}_s$,

$$\mathbf{f}(\mathbf{y}(t)) \approx \mathbf{A}(s)\mathbf{y}(t) + \mathbf{a}(s),$$

where $\mathbf{A}(s) = \mathbf{f}'(\mathbf{y}_s)$, $\mathbf{a}(s) = \mathbf{f}(\mathbf{y}_s) - \mathbf{f}'(\mathbf{y}_s)\mathbf{y}_s$, and $t \in [s, s+h]$.

Using this expansion, the linear ODE

$$\mathbf{y}'(t) = \mathbf{A}(s)\mathbf{y}(t) + \mathbf{a}(s),\ \mathbf{y}(s) = \mathbf{y}_s, \tag{2}$$

is obtained as an approximation to equation (1) for $t \in [s, s+h]$. Therefore, the solution of (2) at the point $t = s + h$ [1],

$$\mathbf{y}(s+h) = \exp(\mathbf{A}(s)h)\{\mathbf{y}(s) + \int_0^h \exp(-\mathbf{A}(s)u)du\ \mathbf{a}(s)\}, \tag{3}$$

gives an approximation to the solution of original ODE (1) at this point.

Using expressions (28) and (57) (see Appendixes A and D) it is obtained that

$$\int_0^h \exp(-\mathbf{A}(s)u)du\ \mathbf{A}(s) = -(\exp(-\mathbf{A}(s)h) - \mathbf{I}). \tag{4}$$

Thus, expression (3) can be written as

$$\mathbf{y}(s+h) = \mathbf{y}(s) + h\boldsymbol{\phi}(\mathbf{y}(s), h), \tag{5}$$

where

$$\boldsymbol{\phi}(\mathbf{y}(s), h) = R(\mathbf{y}(s), h)\mathbf{f}(\mathbf{y}(s)), \tag{6}$$

and

$$\mathbf{R}(\mathbf{y}(s), h) = \frac{1}{h}\int_{\mathbf{0}}^{h} \exp(u\mathbf{f}'(\mathbf{y}(s)))du \tag{7}$$

are, respectively, an m-dimensional vector and an $m \times m$ matrix. For purposes to be pursued in the following sections, it is convenient to define $\mathbf{R}(\mathbf{y}(s), 0) = \mathbf{I}$, where $\mathbf{I}$ is the $m \times m$ identity matrix.

The LL scheme that approximates the solution of (1) is defined by the iterative computation of the expression (5),

$$\mathbf{y}(t_{n+1}) = \mathbf{y}(t_n) + h\boldsymbol{\phi}(\mathbf{y}(t_n), h), \tag{8}$$

at the discrete times $t_n = t_0 + nh$, $n = 0, 1, 2...$, starting from $\mathbf{y}(t_0) = \mathbf{x_0}$.

The numerical scheme (8) can also be straightforward obtained from the LL numerical scheme for SDEs by regarding the ODEs as SDEs with zero diffusion coefficients (see, e.g., [4]). For details about the numerical evaluation of the expression (8), see Appendix C.

3 Rate of convergence

Henceforth the solutions of (1) and (8) will be denoted by $\mathbf{x}(t; \mathbf{x_0})$ and $\mathbf{y}(t; \mathbf{y_0})$, respectively. Notations and rules of matrix calculus, as presented in [16], will be widely used in what follows (see Appendix D for details).

Proposition 1 *The LL scheme is consistent, i.e.,* $\boldsymbol{\phi}(\mathbf{u}, 0) = \mathbf{f}(\mathbf{u})$ *for all* $\mathbf{u} \in \mathbb{R}^m$.

Proof. Indeed, $\boldsymbol{\phi}(\mathbf{u}, .)$ is a continuous function with $\boldsymbol{\phi}(\mathbf{u}, 0) = \mathbf{f}(\mathbf{u})$. For details, see Proposition 18 and assertion *ii)* of Proposition 17 in Appendix B. ■

Denote by L_{n+1} and E_{n+1} the local and global truncation errors at t_{n+1} , i.e.,

$$L_{n+1} = \|\mathbf{x}(t_{n+1}; \mathbf{x_0}) - \mathbf{x}(t_n; \mathbf{x_0}) - h\boldsymbol{\phi}(\mathbf{x}(t_n; \mathbf{x_0}), h)\|$$

and

$$E_{n+1} = \|\mathbf{x}(t_{n+1}; \mathbf{x_0}) - \mathbf{y}(t_{n+1}; \mathbf{x_0})\| .$$

Proposition 2 *Suppose that*

$$\|\mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v})\| \leq \lambda_0 \|\mathbf{u} - \mathbf{v}\| \tag{9}$$

for all $\mathbf{u}, \mathbf{v} \in \mathbb{R}^m$ *;* $\mathbf{f}$ *is twice differentiable on* $\mathbb{R}^m$ *;* $(\mathbf{f} \circ \mathbf{x}(., \mathbf{x_0})) \in \mathcal{C}^1([t_0, T], \mathbb{R}^m)$*; and*

$$\left\|\mathbf{f}''(\mathbf{u})\right\| \leq K_2 \tag{10}$$

for all $\mathbf{u} \in \mathbb{R}^m$ *. Then*

$$L_{n+1} \leq Mh^3$$

for $t_{n+1} \leq T$*, where* $M = \frac{1}{2} K_0^2 K_2 \exp((2K_1 + \lambda_0)h)$*,* $K_0 = \max\limits_{t \in [t_0, T]} \|\mathbf{f}(\mathbf{x}(t; \mathbf{x_0}))\|$*, and* $K_1 = \max\limits_{t \in [t_0, T]} \|\mathbf{f}'(\mathbf{x}(t; \mathbf{x_0}))\|$*.*

Proof. Let $\mathbf{c} = \mathbf{x}(t_n; \mathbf{x_0})$, and let $\mathbf{u}$, $\mathbf{v}$ be, respectively, solutions of the equations

$$\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t)),\ \mathbf{u}(t_n) = \mathbf{c} \tag{11}$$

and

$$\mathbf{v}'(t) = \mathbf{g}(\mathbf{v}(t)),\ \mathbf{v}(t_n) = \mathbf{u}(t_n),$$

where $t \in [t_n, t_{n+1}]$ and $\mathbf{g}(\mathbf{z}) = \mathbf{f}(\mathbf{c}) + \mathbf{f}'(\mathbf{c})(\mathbf{z} - \mathbf{c})$ for $\mathbf{z} \in \mathbb{R}^m$.

Let

$$\begin{aligned} \varepsilon &= \sup_{t \in [t_n, t_{n+1}]} \left\|\mathbf{v}'(t) - \mathbf{f}(\mathbf{v}(t))\right\| \\ &= \sup_{t \in [t_n, t_{n+1}]} \|\mathbf{g}(\mathbf{v}(t)) - \mathbf{f}(\mathbf{v}(t))\| . \end{aligned}$$

From the Taylor formula with Lagrange rest for functions defined on Banach spaces [6] it is obtained that

$$\varepsilon \leq \frac{1}{2} \sup_{t \in [t_n, t_{n+1}]} \left\{ \sup_{\boldsymbol{\xi} \in [\mathbf{c}, \mathbf{v}(t)]} \left\|\mathbf{f}''(\boldsymbol{\xi})\right\| \ \ \|\mathbf{v}(t) - \mathbf{c}\|^2 \right\} . \tag{12}$$

Since

$$\begin{aligned} \|\mathbf{v}(t) - \mathbf{c}\|^2 &= \| \ (t - t_n) \ \boldsymbol{\phi}(\mathbf{c}, t - t_n) \ \|^2 \\ &\leq \Big(\int_0^{t - t_n} \exp(s \left\|\mathbf{f}'(\mathbf{c})\right\|) \|\mathbf{f}(\mathbf{c})\| \, ds \Big)^2 \\ &\leq \exp(2 \left\|\mathbf{f}'(\mathbf{c})\right\| \ (t - t_n)) \ \ \|\mathbf{f}(\mathbf{c})\|^2 \ (t - t_n)^2 \end{aligned}$$

then

$$\varepsilon \leq K_0^2 K_2 \exp(2hK_1) \frac{h^2}{2}$$

where $K_0 = \max\limits_{t \in [t_0, T]} \|\mathbf{f}(\mathbf{x}(t; \mathbf{x_0}))\|$, and $K_1 = \max\limits_{t \in [t_0, T]} \|\mathbf{f}'(\mathbf{x}(t; \mathbf{x_0}))\|$.

The Fundamental Inequality in [11] for the equation (11) implies that

$$\|\mathbf{u}(t) - \mathbf{v}(t)\| \leq \frac{\varepsilon}{\lambda_0} \left(\exp(\lambda_0(t - t_n)) - 1\right)$$

for $t \in [t_n, t_{n+1}]$. By the mean value theorem,

$$(\exp(\lambda_0(t - t_n)) - 1) \leq \lambda_0 \exp(\lambda_0(t - t_n))(t - t_n).$$

Thus,

$$\|\mathbf{u}(t) - \mathbf{v}(t)\| \leq \varepsilon \exp(\lambda_0(t - t_n))(t - t_n) \tag{13}$$

for $t \in [t_n, t_{n+1}]$.

Taking into account that $\mathbf{v}(t) \equiv \mathbf{x}(t_n; \mathbf{x_0}) - (t - t_n)\boldsymbol{\phi}(\mathbf{x}(t_n; \mathbf{x_0}), t - t_n)$ and $\mathbf{u}(t) \equiv \mathbf{x}(t; \mathbf{x_0})$, and substituting t by t_{n+1} in inequality (13), the assertion of the theorem is obtained. ■

The latter proposition provides an estimate of the local truncation error of the LL scheme under a weak continuity assumption but requiring a strong bound condition (condition (10)). In the next proposition the local truncation error is estimated without imposing this bound condition but under a stronger continuity assumption.

Proposition 3 *Let* $\mathbf{f}$ *be twice differentiable on* $\mathbb{R}^m$ *and* $(\mathbf{f} \circ \mathbf{x}(., \mathbf{x_0})) \in \mathcal{C}^2([t_0, T], \mathbb{R}^m)$. *Then*

$$L_{n+1} \leq Mh^3$$

for $t_{n+1} \leq T$, *where*

$$M = \max_{\theta \in [t_0, T]} \frac{W(\theta)}{6}, \tag{14}$$

and

$$W(\theta) = \left\|\mathbf{x}'''(\theta; \mathbf{x_0})\right\| + \exp(h \left\|\mathbf{f}'(\mathbf{x}(\theta; \mathbf{x_0}))\right\|) \left\|\mathbf{f}'(\mathbf{x}(\theta; \mathbf{x_0}))\right\|^2 \left\|\mathbf{x}'(\theta; \mathbf{x_0})\right\|.$$

Proof. Let $\mathbf{c} = \mathbf{x}(t_n; \mathbf{x_0})$, and let $\mathbf{u}$, $\mathbf{v}$ be solutions of

$$\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t)),\ \mathbf{u}(t_n) = \mathbf{c} \tag{15}$$

and

$$\mathbf{v}'(t) = \mathbf{g}(\mathbf{v}(t)),\ \mathbf{v}(t_n) = \mathbf{u}(t_n), \tag{16}$$

respectively, where $t \in [t_n, t_{n+1}]$ and $\mathbf{g}(\mathbf{z}) = \mathbf{f}(\mathbf{c}) + \mathbf{f}'(\mathbf{c})(\mathbf{z} - \mathbf{c})$ for $\mathbf{z} \in \mathbb{R}^m$.

From equations (15) and (16), using the rules of the matrix differential calculus (see Appendix D) it can be shown that

$$\mathbf{u}'(t_n) = \mathbf{f}(\mathbf{c}),$$

$$\mathbf{v}'(t_n) = \mathbf{g}(\mathbf{c}) = \mathbf{f}(\mathbf{c}),$$

$$\mathbf{u}''(t_n) = \mathbf{f}'(\mathbf{c})\mathbf{f}(\mathbf{c}),$$
$$\mathbf{v}''(t_n) = \mathbf{g}'(\mathbf{c})\mathbf{g}(\mathbf{c}) = \mathbf{f}'(\mathbf{c})\mathbf{f}(\mathbf{c}),$$
$$\mathbf{u}'''(t) = (\mathbf{f}^\top(\mathbf{u}(t)) \otimes \mathbf{I})\mathbf{f}''(\mathbf{u}(t))\mathbf{f}(\mathbf{u}(t)) + (\mathbf{f}'(\mathbf{u}(t)))^2\mathbf{f}(\mathbf{u}(t)), \tag{17}$$
$$\mathbf{v}'''(t) = (\mathbf{g}'(\mathbf{v}(t)))^2\mathbf{g}(\mathbf{v}(t)) = (\mathbf{f}'(\mathbf{c}))^2(\mathbf{f}(\mathbf{c}) + \mathbf{f}'(\mathbf{c})(\mathbf{v}(t) - \mathbf{c})). \tag{18}$$

Applying the Taylor formulae with Lagrange rest [6] to the function $\mathbf{u}(t) - \mathbf{v}(t)$ it is obtained that

$$\begin{aligned}\|\mathbf{u}(t) - \mathbf{v}(t)\| &= \| \mathbf{u}(t) - \mathbf{v}(t) - \mathbf{u}(t_n) - \mathbf{v}(t_n) + (\mathbf{u}'(t_n) - \mathbf{v}'(t_n))(t - t_n) \\ &\quad + \frac{(\mathbf{u}''(t_n) - \mathbf{v}''(t_n))}{2}(t - t_n)^2 \ \| \\ &\leq \sup_{\theta \in [t_n, t_{n+1}]} \frac{1}{6} \left\|\mathbf{u}'''(\theta) - \mathbf{v}'''(\theta)\right\| (t - t_n)^3 \\ &\leq \sup_{\theta \in [t_n, t_{n+1}]} \frac{1}{6}(\left\|\mathbf{u}'''(\theta)\right\| + \left\|\mathbf{v}'''(\theta)\right\|)(t - t_n)^3. \end{aligned} \tag{19}$$

From (18) and (4) it follows that

$$\begin{aligned}\left\|\mathbf{v}'''(\theta)\right\| &= \| \ (\mathbf{f}'(\mathbf{c}))^2 \ (\mathbf{f}(\mathbf{c}) + (\theta - t_n)\mathbf{f}'(\mathbf{c})\boldsymbol{\phi}(\mathbf{c}, \theta - t_n)) \ \| \\ &= \| \ (\mathbf{f}'(\mathbf{c}))^2 \exp(\mathbf{f}'(\mathbf{c})(\theta - t_n))\mathbf{f}(\mathbf{c}) \ \| \\ &\leq \left\|\mathbf{f}'(\mathbf{c})\right\|^2 \exp(h \left\|\mathbf{f}'(\mathbf{c})\right\|) \|\mathbf{f}(\mathbf{c})\| \end{aligned} \tag{20}$$

for $\theta \in [t_n, t_{n+1}]$.

Since $(\mathbf{f} \circ \mathbf{u}) \in \mathcal{C}^2([t_0, T], \mathbb{R}^m)$, expression (17) and inequality (20) imply that $\|\mathbf{u}'''(\theta)\|$ and $\|\mathbf{v}'''(\theta)\|$ are bounded functions for all $\theta \in [t_n, t_{n+1}]$.

Finally, the assertion of the theorem follows from the inequalities (19) and (20) since $\mathbf{u}(t) \equiv \mathbf{x}(t; \mathbf{x_0})$ and $\mathbf{v}(t) \equiv \mathbf{x}(t_n; \mathbf{x_0}) - (t - t_n)\boldsymbol{\phi}(\mathbf{x}(t_n; \mathbf{x_0}), t - t_n)$. ■

The next proposition provides an estimate of the global truncation error of the LL scheme.

Proposition 4 *Suppose that* $(\mathbf{f} \circ \mathbf{x}(., \mathbf{x_0})) \in \mathcal{C}([t_0, T], \mathbb{R}^m)$,

$$\|\mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v})\| \leq \lambda_0 \|\mathbf{u} - \mathbf{v}\|, \tag{21}$$

$$\left\|\mathbf{f}'(\mathbf{u}) - \mathbf{f}'(\mathbf{v})\right\| \leq \lambda_1 \|\mathbf{u} - \mathbf{v}\|, \tag{22}$$

and

$$\left\|\mathbf{f}'(\mathbf{u})\right\| \leq \beta_1 \tag{23}$$

for all $\mathbf{u}, \mathbf{v} \in \mathbb{R}^m$. *Then*

$$E_{n+1} \leq K \ L_{n+1} \frac{1}{h}$$

for $t_{n+1} \leq T$, *where* K *is a positive constant.*

Proof. For simplicity, denote $\mathbf{x}(t_n;\mathbf{x_0})$ and $\mathbf{y}(t_n;\mathbf{x_0})$ by $\mathbf{x}_n$ and $\mathbf{y}_n$, respectively. Thus,

$$\begin{aligned} E_{n+1} &= \|\mathbf{x}_{n+1} - \mathbf{y}_n - h\boldsymbol{\phi}(\mathbf{y}_n, h)\| \\ &\leq L_{n+1} + E_n + R_n, \end{aligned} \tag{24}$$

where L_{n+1} is the local truncation error at t_{n+1} , and

$$\begin{aligned} R_n &= \|h\boldsymbol{\phi}(\mathbf{x}_n, h) - h\boldsymbol{\phi}(\mathbf{y}_n, h)\| \\ &= \left\| \int_0^h \exp(u\mathbf{f}'(\mathbf{x}_n))\{\mathbf{f}(\mathbf{x}_n) - \exp(-u(\mathbf{f}'(\mathbf{x}_n) - \mathbf{f}'(\mathbf{y}_n)))\mathbf{f}(\mathbf{y}_n)\}du \right\| \\ &\leq \int_0^h \left\|\exp(u\mathbf{f}'(\mathbf{x}_n))\right\| \left\|\mathbf{I} - \exp(-u(\mathbf{f}'(\mathbf{x}_n)) - \mathbf{f}'(\mathbf{y}_n)))\right\| \|\mathbf{f}(\mathbf{x}_n)\| \, du \\ &\quad + \int_0^h \left\|\exp(u\mathbf{f}'(\mathbf{x}_n))\right\| \left\|\exp(-u(\mathbf{f}'(\mathbf{x}_n)) - \mathbf{f}'(\mathbf{y}_n)))\right\| \|\mathbf{f}(\mathbf{x}_n) - \mathbf{f}(\mathbf{y}_n)\| \, du, \end{aligned}$$

where $\mathbf{I}$ denotes the identity matrix.

From the Finite Increments Inequality [6] and inequalities (22) and (23) it follows that

$$\left\|\mathbf{I} - \exp(-u(\mathbf{f}'(\mathbf{x}_n)) - \mathbf{f}'(\mathbf{y}_n)))\right\| \leq h\lambda_1 \exp(2h\beta_1) \|\mathbf{x}_n - \mathbf{y}_n\|$$

for $u \in [0, h]$. This and the inequalities (21)-(23) imply that

$$R_n \leq hK_1 \|\mathbf{x}_n - \mathbf{y}_n\| = hK_1 E_n,$$

where $K_1 = (h\lambda_1 K_2 + \lambda_0)\exp(3h\beta_1)$ and $K_2 = \max\limits_{t\in[t_0,T]} \|\mathbf{f}(\mathbf{x}(t))\|$.

Substituting this inequality in (24) it is obtained that

$$E_{n+1} \leq L_{n+1} + (1 + hK_1)E_n.$$

By induction the above difference inequality implies that

$$\begin{aligned} E_{n+1} &\leq \frac{((1+hK_1)^n - 1)}{hK_1} L_{n+1} \\ &\leq K\frac{L_{n+1}}{h} \text{ with } K = \frac{(\exp(K_1(T-t_0)) - 1)}{K_1}, \end{aligned}$$

which is the assertion of the theorem. ■

4 Linear Absolute Stability and Stiff Problems

This section deals with some properties of the LL scheme for linear ODEs,

$$\mathbf{x}'(t) = \mathbf{A}\mathbf{x}(t),\ t \geq t_0,\ \mathbf{x}(t_0) = \mathbf{x_0}, \tag{25}$$

where $\mathbf{A}$ is an $m \times m$ matrix independent of t.

Proposition 5 *The LL scheme has zero global truncation error for linear ODEs.*

Proof. This an immediate consequence of Propositions 2 and 4 since $K_2 = 0$ in condition (10). ■

This property means that the discretization of any linear ODE (stiff or not) by means of the LL method yields to a discrete map whose solution coincides with the exact solution. Therefore, the main source of error in the numerical integration of this class of ODEs by means of the LL scheme is the round-off error resulting from the computer arithmetic.

In addition, Proposition 5 yields directly to following.

Proposition 6 *The LL scheme is A-stable.*

This means that the region of absolute stability of the LL scheme (i.e. the set of values λh for which the fixed point of the LL scheme at the origin of the linear system $\mathbf{x}'(t) = \lambda\mathbf{x}(t)$ is stable) contains the whole left half of the complex plane (i.e., it consists of all λh with $Re(\lambda) < 0$ and $h > 0$) [7, 15].

5 Phase portraits near steady states

This section deals with the link between the steady states in an ODE and those in the map of the LL scheme.

Proposition 7 *Any equilibrium point of the ODE (1) is a fixed point of the LL map (8).*

Proof. It follows since $\mathbf{f}(\mathbf{x}) = 0$ implies that $\boldsymbol{\phi}(\mathbf{x}, h) = 0$ for all $\mathbf{x}$ and h. ■

A numerical scheme is said to be regular if no fixed point (called a ghost or spurious fixed point) occurs in the map of the scheme that is not an equilibrium point of the ODE [7, 12].

Proposition 8 *Let $\lambda_1(\mathbf{u}),..,\lambda_p(\mathbf{u})$ be the p distinct eigenvalues of $\mathbf{f}'(\mathbf{u})$, $p \leq m$. The following assertions hold:*

i) The LL scheme with step-size h is regular if $\lambda_i(\mathbf{u})h \neq \pm 2\pi n\sqrt{-1}$ for all $\mathbf{u} \in \mathbb{R}^m$, $i = 1,..,p$, and $n = 1, 2, ...$

ii) For a given step-size h, the unique ghost points of the LL scheme are the points $\mathbf{u} \in \mathbb{R}^m$ such that $\mathbf{f}(\mathbf{u}) \neq 0$, $\lambda_i(\mathbf{u})h = \pm 2\pi n\sqrt{-1}$ for some $1 \leq i \leq p$ and $n = 1, 2...$, and in addition $\mathbf{f}(\mathbf{u})$ is in the null space of matrix $\mathbf{R}(\mathbf{u}, h)$ defined by the expression (7).

Proof. A numerical scheme as (8) is said to be regular if the equality $\mathbf{y}(t_{n+1}) = \mathbf{y}(t_n)$ is equivalent to $\mathbf{f}(\mathbf{y}(t_n)) = 0$. A point $\mathbf{y}(t_n) \in \mathbb{R}^m$ is called a ghost fixed point of a numerical scheme if $\mathbf{f}(\mathbf{y}(t_n)) \neq 0$ and $\mathbf{y}(t_{n+1}) = \mathbf{y}(t_n)$. From these definitions and the assertion *iii)* of Proposition 17 in Appendix B the Proposition 8 is obtained. ■

Proposition 8 implies that the LL scheme is regular for one-dimensional ODEs, and more generally for any ODE whose vector field $\mathbf{f}$ has symmetric Jacobian matrix $\mathbf{f}'$ at every $\mathbf{u} \in \mathbb{R}^m$, since in such case $\mathbf{f}'$ have no complex eigenvalues.

Without loss of generality, let 0 be a hyperbolic equilibrium point of the equation (1). Let $X_s, X_u \subset \mathbb{R}^m$ be the stable and unstable subspaces of the linear vector field $\mathbf{f}'(0)$ such that $\mathbb{R}^m = X_s \oplus X_u$, $(\mathbf{x}_s, \mathbf{x}_u) = \mathbf{x} \in \mathbb{R}^m$ and $\|\mathbf{x}\| = \max\{\|\mathbf{x}_s\|, \|\mathbf{x}_u\|\}$. It is well-known that the local stable and unstable manifolds at 0 may be represented as $M_s = \{(\mathbf{x}_s, p(\mathbf{x}_s)) : \mathbf{x}_s \in K_{\varepsilon,s}\}$ and $M_u = \{(q(\mathbf{x}_u), \mathbf{x}_u)) : \mathbf{x}_u \in K_{\varepsilon,u}\}$, respectively, where the functions $p : K_{\varepsilon,s} = K_\varepsilon \cap X_s \to K_{\varepsilon,u} = K_\varepsilon \cap X_u$ and $q : K_{\varepsilon,u} \to K_{\varepsilon,s}$ are as smooth as $\mathbf{f}$, and $K_\varepsilon = \{\mathbf{x} \in \mathbb{R}^m : \|\mathbf{x}\| \leq \varepsilon\}$ for $\varepsilon > 0$.

Proposition 9 *Let $\mathbf{f} \in \mathcal{C}^2(\Omega)$, where Ω is a bounded neighborhood of 0, and $\mathbf{f}''$ be a Lipschitz function on Ω. Then there exist constants C, ε, ε_0, $h_0 > 0$ such that the local stable M_s^h and unstable M_u^h manifolds of the LL map at 0 are of the form*

$$M_s^h = \{(\mathbf{x}_s, p^h(\mathbf{x}_s)) : \mathbf{x}_s \in K_{\varepsilon,s}\} \text{ and } M_u^h = \{(q^h(\mathbf{x}_u), \mathbf{x}_u) : \mathbf{x}_u \in K_{\varepsilon,u}\},$$

where $p^h = p + O(h^2)$ uniformly in $K_{\varepsilon,s}$, and $q^h = q + O(h^2)$ uniformly in $K_{\varepsilon,u}$. Moreover, for any $\mathbf{x_0} \in K_\varepsilon$ and $h \leq h_0$, there exists $\mathbf{z_0} = \mathbf{z_0}(\mathbf{x_0}, h) \in K_{\varepsilon_0}$ satisfying

$$sup\{\|\mathbf{x}(t_n; \mathbf{x_0}) - \mathbf{y}(t_n; \mathbf{z_0})\| : \mathbf{x}(t; \mathbf{x_0}) \in K_\varepsilon \text{ for } t \in [t_0, t_n]\} \leq Ch^2. \tag{26}$$

Correspondingly, for any $\mathbf{z_0} \in K_\varepsilon$ and $h \leq h_0$, there exists $\mathbf{x_0} = \mathbf{x_0}(\mathbf{z_0}, h) \in K_{\varepsilon_0}$ that fulfils (26), where the sup is taken over all n satisfying $\mathbf{y}(t_j; \mathbf{z_0}) \in K_\varepsilon$,

$j = 0, .., n.$

In order to prove the above proposition the following lemma is useful.

Lemma 10 *Let $\Sigma \subset \mathbb{R}^m$ be an invariant set for the flow of (1). Let K and Ω be, respectively, a compact and a bounded open set such that $\Sigma \subset K \subset \Omega$. If $\mathbf{f} \in \mathcal{C}^2(\Omega)$ and $\mathbf{f}''$ is a Lipschitz function on Ω then it is hold that:*

i) $\boldsymbol{\phi} \to \mathbf{f}$ as $h \to 0$ uniformly in K,

ii) $\boldsymbol{\phi}' \to \mathbf{f}'$ as $h \to 0$ uniformly in K

and

iii) $\|(\mathbf{x}(h;\mathbf{x_0}) - \mathbf{x_0})/h - \boldsymbol{\phi}(\mathbf{x_0}, h)\| = O(h^2)$ uniformly in $\mathbf{x_0} \in K$.

Proof. From Proposition 18, $\mathbf{f} \in \mathcal{C}^2(\Omega)$ implies that $\boldsymbol{\phi}$ is of class $\mathcal{C}^1$ on $\Omega \times [t_0, T]$. Therefore, $\boldsymbol{\phi}$ is uniformly continuous on the compact set $K \times [t_0, T] \subset \Omega \times [t_0, T]$. Thus,

$$\sup_{\mathbf{z} \in K_\rho} \|\boldsymbol{\phi}(\mathbf{z}, h) - \boldsymbol{\phi}(\mathbf{z}, 0)\| \to 0 \text{ as } h \to 0. \tag{27}$$

Since $\boldsymbol{\phi}(\mathbf{z}, 0) = \mathbf{f}(\mathbf{z})$ for all $\mathbf{z} \in K$ (see Proposition 18 in Appendix B) then the assertion *i)* is obtained from (27).

Likewise, with $\boldsymbol{\phi}'$ instead of $\boldsymbol{\phi}$, *ii)* is obtained.

From Proposition 3,

$$\|(\mathbf{x}(h;\mathbf{x_0}) - \mathbf{x_0})/h - \boldsymbol{\phi}(\mathbf{x_0}, h)\| \leq M(\mathbf{x_0})h^2, \text{ with } \mathbf{x_0} \in K,$$

where $M(\mathbf{x_0})$, defined by (14), depends on $\mathbf{x_0}$.

The function $\mathbf{f}$ is Lipschitz on K since it is of class $\mathcal{C}^2$ on K. $\boldsymbol{\sigma} \in \Sigma$ implies that $\mathbf{x}(t;\boldsymbol{\sigma}) \in \Sigma$ for all t, since Σ is an invariant set [10]. From this and Theorem 112J in [5], it follows that

$$\begin{aligned}
\|\mathbf{x}'(t;\mathbf{x_0})\| &= \|\mathbf{f}(\mathbf{x}(t;\mathbf{x_0}))\| \\
&\leq \|\mathbf{f}(\mathbf{x}(t;\mathbf{x_0})) - \mathbf{f}(\mathbf{x}(t;\boldsymbol{\sigma}))\| + \|\mathbf{f}(\mathbf{x}(t;\boldsymbol{\sigma}))\| \text{ with } \boldsymbol{\sigma} \text{ in } \Sigma \\
&\leq \lambda \|\mathbf{x}(t;\mathbf{x_0}) - \mathbf{x}(t;\boldsymbol{\sigma})\| + \|\mathbf{f}(\mathbf{x}(t;\boldsymbol{\sigma}))\| \\
&\leq \lambda \|\mathbf{x_0} - \boldsymbol{\sigma}\| \ \exp(\lambda(t - t_0)) + \|\mathbf{f}(\mathbf{x}(t;\boldsymbol{\sigma}))\| \\
&\leq 2\lambda \ \exp(\lambda(t - t_0)) \sup_{\mathbf{z} \in K} \|\mathbf{z}\| + \sup_{\mathbf{z} \in K} \|\mathbf{f}(\mathbf{x}(t, \mathbf{z}))\|,
\end{aligned}$$

where λ is the Lipschitz constant for $\mathbf{f}$.

In a similar way it is obtained that $\|\mathbf{f}'(\mathbf{x}(t;\mathbf{x_0}))\|$ and $\|\mathbf{x}'''(t;\mathbf{x_0})\|$ are also bounded by a constant independent on $\mathbf{x_0}$. Therefore, $M(\mathbf{x_0})$ is bounded by a constant independent on $\mathbf{x_0}$, and so *iii)* follows. ■

Proof. of Proposition 9. Since Ω is a bounded neighborhood of the invariant set 0, then there exist a constant $\rho > 0$ and a compact set $K_\rho = \{\mathbf{x} \in \mathbb{R}^m : \|\mathbf{x}\| \leq \rho\} \subset \Omega$ such that Lemma 10 holds with $K = K_\rho$. Furthermore, $\mathbf{f}(\mathbf{x}) = 0$ implies $\boldsymbol{\phi}(\mathbf{x}, h) = 0$ for all h. Thus, the hypotheses of Theorem 3.1 in [2] holds, and so thesis of the Proposition 9 is obtained. ■

Proposition 9 shows that hyperbolic (both stable and unstable) equilibrium points of an ODE are correctly represented in the map of the LL scheme for sufficiently small step length, and that the local stable and unstable manifolds of the discretization converge to those of the continuous system as the step length tends to zero.

Suppose that the system (1) has a hyperbolic closed orbit $\gamma = \{\overline{\mathbf{x}}(t) : t \in [0, T]\}$ of period T in an open bounded set $\Omega \subset \mathbb{R}^m$. Let $\overline{\Omega}$ be the closure of Ω.

Proposition 11 *Let* $\mathbf{f}$ *be a function of class* $\mathcal{C}^3$ *on a neighborhood of* $\overline{\Omega}$*. Then there exist* $h_0 > 0$ *and an open neighborhood* U *of* γ *such that the LL map has an invariant closed curve* $\Gamma_h \subset U$ *for all* $h \leq h_0$*. More precisely, there exist* $T-$*periodic functions* $\overline{\mathbf{y}}_h : \mathbb{R} \to U$ *and* $\sigma_h - 1 : \mathbb{R} \to \mathbb{R}$ *for* $h \leq h_0$*, which are uniformly Lipschitz and satisfy*

$$\overline{\mathbf{y}}_h(t) + h\boldsymbol{\phi}(\overline{\mathbf{y}}_h(t), h) = \overline{\mathbf{y}}_h(\sigma_h(t)), \ t \in \mathbb{R},$$

and

$$\sigma_h(t) = t + h + O(h^3) \ \textit{uniformly for } t \in \mathbb{R}.$$

Furthermore, the curve $\Gamma_h = \{\overline{\mathbf{y}}_h(t) : t \in [0, T]\}$ *converges to* γ *in the Lipschitz norm. In particular,*

$$\max_{t \in \mathbb{R}} \|\overline{\mathbf{x}}(t) - \overline{\mathbf{y}}_h(t)\| = O(h^2)$$

and

$$\sup_{t_1 \neq t_2} \frac{\|(\overline{\mathbf{x}} - \overline{\mathbf{y}}_h)(t_1) - (\overline{\mathbf{x}} - \overline{\mathbf{y}}_h)(t_2)\|}{|t_1 - t_2|} \to 0 \ \textit{as } h \to 0.$$

Proof. Since Lemma 10 holds for the compact set $\overline{\Omega}$, then it also holds for Ω. Moreover, Proposition 18 implies that $\boldsymbol{\phi} \in \mathcal{C}^2(\overline{\Omega} \times [0, h_0])$, so $\boldsymbol{\phi}'$ is Lipschitz on Ω uniformly in h. Therefore, Theorem 2.1 in [3] holds and so the Proposition 11 follows. ■

Proposition 12 *Let* $\mathbf{f}$ *be a function of class* $\mathcal{C}^3$ *on a neighborhood of* $\overline{\Omega}$*. Then the rotation number* ρ_h *of the one-step function* $1 + h\boldsymbol{\phi}(., h)$ *with respect to the invariant curve* Γ_h *is a continuous function of* $h \in [0, h_0]$*, and satisfies*

$$\rho_h = \frac{h}{T} + O(h^3).$$

In particular, there exist $N_0 \in \mathbb{N}$ *and a sequence* h_N , $N \geq N_0$, *such that* $1 + h_N \boldsymbol{\phi}(., h_N)$ *has an orbit*

$$\{\overline{\mathbf{y}}_{h_N}(t_i^N) : t_i = 1, .., N\}$$

of period N *on* Γ_{h_N}. *The following asymptotic relations hold*

$$h_N = \frac{T}{N} + O((\frac{T}{N})^3),$$

$$t_i^N = t_1^N + (i-1)\frac{T}{N} + O((\frac{T}{N})^2), \text{ for } i = 1..N.$$

Proof. Since assertion *iii)* of Lemma 10 holds for the compact set $\overline{\Omega}$, then it holds for Ω. Furthermore, from Proposition 18, $\boldsymbol{\phi} \in \mathcal{C}^2(\Omega \times [0, h_0])$ and $\boldsymbol{\phi}(\mathbf{x}, 0) = \mathbf{f}(\mathbf{x})$ for all $\mathbf{x}$. Therefore, Theorem 4.1 in [3] holds and so the Proposition 12 follows. ■

Propositions 11 and 12 mean that, for h sufficiently small, the map of the LL scheme has a close invariant curve Γ_h , i.e., $(1 + h\boldsymbol{\phi}(., h))(\Gamma_h) = \Gamma_h$, which converges to the periodic orbit γ of continuous system though these curves run out of phase.

The next proposition deals with the behavior of the discrete trajectories of the LL scheme near the invariant curve Γ_h when the ODE (1) has a stable periodic orbit γ. For $\mathbf{x_0}$ in a neighborhood of γ, the following notations will be used:

$$W_h(\mathbf{x_0}) = \{\mathbf{y}(t_n; \mathbf{x_0}) : n \geq 0\}$$

$$w(\mathbf{x_0}) = \{\mathbf{x}(t; \mathbf{x_0}) : t \geq 0\}.$$

Moreover, $d(A, B)$ will denote the Hausdorff distance between two sets A and B, $d(A, B) = max\{\sup_{\mathbf{z} \in A} dist(\mathbf{z}, B), \sup_{\mathbf{z} \in B} dist(\mathbf{z}, A)\}$.

Proposition 13 *Let* γ *be a stable orbit and* $\mathbf{f}$ *be a function of class* $\mathcal{C}^3$ *on a neighborhood of* $\overline{\Omega}$. *Then there exist* h_0, α, β, C, $\rho > 0$, *such that for* $h \leq h_0$ *and* $dist(\mathbf{x_0}, \Gamma_h) \leq \rho$ *the following hold:*

$$dist(\mathbf{y}(t_n; \mathbf{x_0}), \Gamma_h) \leq C \ \exp(-\alpha t_n) \ dist(\mathbf{x_0}, \Gamma_h), \ n \geq 0$$

$$dist(\mathbf{y}(t_n; \mathbf{x_0}), w(\mathbf{x_0})) \leq C(h^2 + min\{h^2 \exp(\beta t_n), \exp(-\alpha t_n)\}), \ n \geq 0.$$

Moreover, for any $\delta > 0$ *there exist* $\rho(\delta)$, $h(\delta) > 0$ *such that*

$$\sup_{n \geq 0} dist(\mathbf{y}(t_n; \mathbf{x_0}), w(\mathbf{x_0})) \leq C h^{2-\delta}$$

for $h \leq h(\delta)$ *and* $dist(\mathbf{x_0}, \Gamma_h) \leq \rho(\delta)$. *Finally,*

$$d(W_h(\mathbf{x_0}), w(\mathbf{x_0})) \to 0 \text{ as } h \to 0$$

uniformly for $dist(\mathbf{x_0}, \gamma) \leq \rho$.

Proof. It can be proved in a similar way as Proposition 11, but using Theorem 3.1 in [3] instead of Theorem 2.1 in [3]. ■

This proposition states the stability of the invariant curve Γ_h and the convergence of the discrete trajectories of the LL scheme to the continuous trajectories of the ODE (1) when the LL scheme start at a point near to the stable periodic orbit γ.

References

[1] L. Arnold, Stochastic Differential Equations, Wiley, 1974.

[2] W.J. Beyn, On the numerical approximation of phase portraits near stationary points, SIAM J. Numer. Anal. 24 (1987) 1095-1113.

[3] W.J. Beyn, On invariant closed curves for one-step methods, Numer. Math. 51 (1987), 103-122.

[4] R. Biscay, J.C. Jimenez, J. Riera and P. Valdes, Local linearization method for the numerical solution of stochastic differential equations, Annals Inst. Statis. Math. 48 (1996), 631-644.

[5] J.C. Butcher, The Numerical Analysis of Ordinary Differential Equations: Runge-Kutta and General Linear Methods, Wiley, 1987.

[6] H. Cartan, Calcul Differentiel. Hermann, Paris, 1967.

[7] J.E. Cartwright and O. Piro, The dynamics of Runge-Kutta Methods, Int. J. Bifurc. & Chaos, 2 (1992), 427-449.

[8] G.H. Golub and C.F. Van Loan, Matrix Computations, 2nd Edition, The Johns Hopkins University Press, 1989.

[9] A. Graham, Kronecker Products and Matrix Calculus: with Applications, Ellis Horwood Limited, 1981.

[10] J. Guckenheimer and P. Holmes, Nonlinear Oscillations, Dynamical Systems, and Bifurcations of Vectors Fields, Springer, 1983.

[11] W. Hurewicz, Lectures on Ordinary Differential Equations. Edicion Revolucionaria, La Habana, 1966.

[12] A. Iserles, Stability and dynamics of numerical methods for nonlinear ordinary differential equations, IMA J. Numer. Anal., 10 (1990), 1-30.

[13] J.C. Jimenez, I. Shoji and T. Ozaki, Simulation of stochastic differential equations through of the Local Linearization method. A comparative study. Submitted to J. Statist. Physcis, 1996.

[14] J.C. Jimenez and L.M. Rodriguez, Numerical integration of ODE through the Local Linearization method: A simulation study. In preparation.

[15] P.E. Kloeden and E. Platen, Numerical solution of stochastic differential equations. Springer-Verlag, Berlin, 1992.

[16] J.R. Magnus and H. Neudecker, Matrix Differential Calculus with Applications in Statistics and Econometrics. John Wiley & Sons, 1988.

[17] T. Ozaki, A bridge between nonlinear time series models and nonlinear stochastic dynamical systems: a local linearization approach, Statistica Sinica, 2 (1992), 113-135.

[18] T. Ozaki, A local linearization approach to nonlinear filtering, Int. J. Control, 57 (1993), 75-96.

[19] L.M. Rodriguez and J.C. Jimenez, Numerical integration of ODEs modelling the evolution of biological systems: the adaptative local linealization scheme with approximate Jacobian" Revista Ciencias Biologica, 29 (1998) 41-43.

[20] W. Rudin, Functional Analysis, McGraw-Hill Book Co., 1973.

[21] I. Shoji and T. Ozaki, Estimation for a continuous time stochastic processes: a new local linearization approach, Res. Memo., No. 524 (1994), The Insti-

tute of Statistical Mathematics, Tokyo. To appear in Stochast. Anal. & Appl.

[22] I. Shoji, Approximation of a continuous time stochastic processes by a local linealization method, Res. Memo. No. 557 (1995), The Institute of Statistical Mathematics, Tokyo. To appear in Math. Comput.

[23] C.F. Van Loan, Computing integrals involving the matrix exponential, IEEE Trans. Autom. Control, AC-23 (1978), 395-404.

6 Appendix A: Some properties of matrix exponential

Proposition 14 *Let* $\mathbf{A}_1$, $\mathbf{A}_2$, $\mathbf{B}$ *be* $m \times m$ *matrices, and* $t \in \mathbb{R}_+$. *Then*

$$\int_0^t \exp(\mathbf{A}_1(t-s))\ \mathbf{B}\ \exp(\mathbf{A}_2 s)ds = \mathbf{L}_m\ \exp(\mathbf{C}t)\ \mathbf{R}_m, \tag{28}$$

where $\mathbf{L}_m = \begin{bmatrix}\mathbf{I}_m\, \mathbf{0}_m\end{bmatrix}$, $\mathbf{R}_m^\top = \begin{bmatrix}\mathbf{0}_m\, \mathbf{I}_m\end{bmatrix}$, $\mathbf{C} = \begin{bmatrix}\mathbf{A}_1 & \mathbf{B} \\ \mathbf{0}_m & \mathbf{A}_2\end{bmatrix}$, $\mathbf{I}_m$ *is the* $m \times m$ *identity matrix, and* $\mathbf{0}_m$ *is the* $m \times m$ *zero matrix.*

Proof. This is a straightforward consequence of Theorem 1 in [23] ■

Proposition 15 *Let* $\mathbf{X}$ *be a matrix of variables,* $\mathbf{Q}$ *be a differentiable* $m \times m$ *matrix function of* $\mathbf{X}$ *and* $t \in \mathbb{R}$. *Then the first derivatives of the matrix exponential* $\exp(\mathbf{Q}(\mathbf{X})t)$ *with respect to variable* t *and* $\mathbf{X}$ *are given by*

$$(\exp(\mathbf{Q}(\mathbf{X})t))'_t = vec(\mathbf{Q}(\mathbf{X})\ \exp(\mathbf{Q}(\mathbf{X})t))) \tag{29}$$

and

$$\exp(\mathbf{Q}(\mathbf{X})t))'_{\mathbf{X}} = \mathbf{L}_{m^2} \exp(M(\mathbf{X})t)\ \mathbf{R}_{m^2}\ \mathbf{Q}'_{\mathbf{X}}(\mathbf{X}), \tag{30}$$

where

$$M(\mathbf{X}) = \begin{bmatrix}\mathbf{I}_m \otimes \mathbf{Q}(\mathbf{X}) & \mathbf{I}_{m^2} \\ \mathbf{0}_{m^2} & \mathbf{Q}^\top(\mathbf{X}) \otimes \mathbf{I}_m\end{bmatrix},$$

and the $m^2 \times m^2$ *matrices* $\mathbf{L}_{m^2}$ *and* $\mathbf{R}_{m^2}$ *are defined as in the previous proposition.*

Proof. (29) is obtained directly by using (57).

Let $\mathbf{E}(\mathbf{X}, t) = \exp(\mathbf{Q}(\mathbf{X})t)$. Using (61), (29) and (60) it is obtained that

$$\begin{aligned}\mathbf{E}''_{t,\mathbf{X}}(\mathbf{X}, t) &= vec(\mathbf{E}''_{\mathbf{X},t}(\mathbf{X}, t)) \\ &= vec(vec(\mathbf{Q}(\mathbf{X})\ \mathbf{E}(\mathbf{X}, t))'_{\mathbf{X}}) \\ &= vec((\mathbf{E}^\top(\mathbf{X}, t) \otimes \mathbf{I}_m)\mathbf{Q}'_{\mathbf{X}}(\mathbf{X}) + (\mathbf{I}_m \otimes \mathbf{Q}(\mathbf{X}))\ \mathbf{E}'_{\mathbf{X}}(\mathbf{X}, t)).\end{aligned} \tag{31}$$

This expression can be rewriting as

$$\mathbf{Y}'_t = vec(\mathbf{U} + \mathbf{R}\mathbf{Y}), \tag{32}$$

where $\mathbf{Y} = \mathbf{E}'_{\mathbf{X}}(\mathbf{X}, t)$, $\mathbf{R} = \mathbf{I}_m \otimes \mathbf{Q}(\mathbf{X})$, and $\mathbf{U} = (\mathbf{E}^\top(\mathbf{X}, t) \otimes \mathbf{I}_m)\mathbf{Q}'_{\mathbf{X}}(\mathbf{X})$.

On the other hand, the solution of (32) is [9]:

$$\mathbf{Y} = \int_0^t \exp(\mathbf{R}(t-\tau))\mathbf{U}(\tau)d\tau.$$

Therefore,

$$\mathbf{E}'_{\mathbf{X}}(\mathbf{X},t)=\int_{\mathbf{0}}^{t}\exp((\mathbf{I}_m\otimes\mathbf{Q}(\mathbf{X}))(t-\tau))\exp((\mathbf{Q}^{\top}(\mathbf{X})\otimes\mathbf{I}_m)\tau)d\tau\ \mathbf{Q}'_{\mathbf{X}}(\mathbf{X}).$$

This and (28) imply (30). ■

Proposition 16 *Let* $\mathbf{X}$ *be a matrix of variables,* $\mathbf{Q}$ *be a differentiable* $m\times m$ *matrix function of* $\mathbf{X}$*, and* $t\in\mathbb{R}_+$*. Then the first derivatives of*

$$\mathbf{I}(\mathbf{X},t)=\int_{\mathbf{0}}^{t}\exp(\mathbf{Q}(\mathbf{X})s)ds \tag{33}$$

with respect to the variables t *and* $\mathbf{X}$ *are given by*

$$\mathbf{I}'_t(\mathbf{X},t)=vec(\exp(\mathbf{Q}(\mathbf{X})t)) \tag{34}$$

and

$$\mathbf{I}'_{\mathbf{X}}(\mathbf{X},t)=\int_{\mathbf{0}}^{t}(\exp(\mathbf{Q}(\mathbf{X})s))'_{\mathbf{X}}ds, \tag{35}$$

where $(\exp(\mathbf{Q}(\mathbf{X})s))'_{\mathbf{X}}$ *is given by (30).*

Proof. Using the expressions (28), (29) and (57) it is obtained that

$$\begin{aligned}(\mathbf{I}(\mathbf{X},t))'_t&=(\mathbf{L}_m\ \exp(\mathbf{C}(\mathbf{X})t)\ \mathbf{R}_m)'_t,\ \text{with}\ \mathbf{C}(\mathbf{X})=\begin{bmatrix}\mathbf{0}_m & \mathbf{I}_m\\ \mathbf{0}_m & \mathbf{Q}(\mathbf{X})\end{bmatrix}\\&=vec(\mathbf{L}_m\ \mathbf{C}(\mathbf{X})\exp(\mathbf{C}(\mathbf{X})t)\ \mathbf{R}_m)\\&=vec(\mathbf{R}_m^{\top}\ \begin{bmatrix}\mathbf{I}_m & \sum_{k=1}^{\infty}(\mathbf{Q}(\mathbf{X}))^{k-1}t^k/k!\\ \mathbf{0}_m & \exp(\mathbf{Q}(\mathbf{X})t)\end{bmatrix}\ \mathbf{R}_m)\\&=vec(\exp(\mathbf{Q}(\mathbf{X})t)).\end{aligned}$$

Thus, (34) follows.

Expression (35) is obtained directly from the Exercise 24 of Chapter 3 in [20]. ■

7 Appendix B: Some properties of the function ϕ

Proposition 17 *Let $t \in [0,T]$, $\mathbf{x}$ be a vector on $\Omega \subset \mathbb{R}^m$, $\mathbf{Q}$ be an $m \times m$ matrix function on Ω, and $\mathbf{E}(\mathbf{x},t) = \exp(\mathbf{Q}(\mathbf{x})t)$. Let $\mathbf{K}(\mathbf{x},t)$ be the $m \times m$ matrix defined by*

$$\mathbf{K}(\mathbf{x},t) = \left\{ \begin{array}{cc} \frac{1}{t}\int_0^t \mathbf{E}(\mathbf{x},u)du & for\ t>0 \\ \mathbf{I}_m & for\ t=0 \end{array} \right\} \tag{36}$$

where $\mathbf{I}_m$ denotes the $m \times m$ identity matrix. Then, the following assertions hold:

i) If $\mathbf{Q} \in \mathcal{C}^2(\Omega, \mathbb{R}^{m\times m})$ then $\mathbf{K} \in \mathcal{C}^2(\Omega \times [0,T], \mathbb{R}^{m\times m})$. Moreover

$$\mathbf{K}'_t(\mathbf{x},t) = \frac{1}{t} vec(\mathbf{E}(\mathbf{x},t) - \mathbf{K}(\mathbf{x},t)), \tag{37}$$

$$\mathbf{K}''_t(\mathbf{x},t) = \frac{1}{t^2} vec(2\mathbf{K}(\mathbf{x},t) + \mathbf{E}(\mathbf{x},t)(\mathbf{Q}(\mathbf{x})t - 2\mathbf{I}_m)), \tag{38}$$

$$\mathbf{K}'_{\mathbf{x}}(\mathbf{x},t) = \frac{1}{t}\int_0^t \mathbf{E}'_{\mathbf{x}}(\mathbf{x},u)du, \tag{39}$$

$$\mathbf{K}''_{\mathbf{x}}(\mathbf{x},t) = \frac{1}{t}\int_0^t \mathbf{E}''_{\mathbf{x}}(\mathbf{x},u)du \tag{40}$$

and

$$\mathbf{K}''_{\mathbf{x},t}(\mathbf{x},t) = \frac{1}{t}(\mathbf{E}'_{\mathbf{x}}(\mathbf{x},t) - \mathbf{K}'_{\mathbf{x}}(\mathbf{x},t)), \tag{41}$$

for $t > 0$. For $t = 0$, $\mathbf{K}'_t(\mathbf{x},0) = \frac{1}{2} vec(\mathbf{Q}(\mathbf{x}))$, $\mathbf{K}''_t(\mathbf{x},0) = \frac{1}{3} vec(\mathbf{Q}^2(\mathbf{x}))$, $\mathbf{K}'_{\mathbf{x}}(\mathbf{x},0) = \mathbf{0}_{m^2,m}$, $\mathbf{K}''_{\mathbf{x}}(\mathbf{x},0) = \mathbf{0}_{m^3,m}$, and $\mathbf{K}''_{\mathbf{x},t}(\mathbf{x},0) = \frac{1}{2}\mathbf{Q}'_{\mathbf{x}}(\mathbf{x})$. Here, $\mathbf{0}_{\alpha\times\beta}$ denotes the $\alpha \times \beta$ zero matrix.

ii) $\mathbf{K}(\mathbf{x},.)$ is a continuous function.

iii) $\mathbf{K}^{-1}(\mathbf{x},t)$ exits for $(\mathbf{x},t) \in \Omega \times [0,T]$ such that $\lambda_i(\mathbf{x})t \neq \pm 2\pi n\sqrt{-1}$ for all $i = 1,..,p$, and $n = 1,2,...$ Here $\lambda_1(\mathbf{x}),..,\lambda_p(\mathbf{x})$ denote the p distinct eigenvalues of $\mathbf{Q}(\mathbf{x})$, and $p \leq m$.

Proof. The expressions (37)-(41) are obtained applying matrix rules of differential calculus (see Appendix D) and Proposition 16.

The continuity order of $\mathbf{Q}$ on Ω implies that the functions (36)-(41) are continuous on $\Omega \times (0,T]$. Thus it remains to prove their continuity just at $t = 0$.

Let $\mathbf{W}^{-1}(\mathbf{x})\mathbf{Q}(\mathbf{x})\mathbf{W}(\mathbf{x}) = diag(\mathbf{J}_1(\mathbf{x}), .., \mathbf{J}_p(\mathbf{x}))$ be the Jordan canonical form of $\mathbf{Q}(\mathbf{x})$, where the $n_i \times n_i$ matrix

$$\mathbf{J}_i(\mathbf{x}) = \begin{bmatrix} \lambda_i(\mathbf{x}) & 1 & 0 & & 0 \\ 0 & \cdot & \cdot & & 0 \\ \cdot & & 0 & \cdot & 1 \\ 0 & & 0 & 0 & \lambda_i(\mathbf{x}) \end{bmatrix}$$

is a Jordan block and λ_i is an eigenvalue of $\mathbf{Q}(\mathbf{x})$ of multiplicity n_i , for $i = 1, .., p$. Then, by using the Jordan Method for computing functions of matrices [8], it is obtained that

$$\exp(u\mathbf{Q}(\mathbf{x})) = \mathbf{W}(\mathbf{x})\mathbf{L}(\mathbf{x}, u)\mathbf{W}^{-1}(\mathbf{x}). \tag{42}$$

Here $\mathbf{L}(\mathbf{x}, u) = diag(\mathbf{L}_1(\mathbf{x}, u), .., \mathbf{L}_p(\mathbf{x}, u))$ is a diagonal matrix and $\mathbf{L}_i(\mathbf{x}, u)$ is an upper triangular matrix defined by

$$[\mathbf{L}_i(\mathbf{x}, u)]_{jk} = \left\{ \begin{array}{cc} u^{k-j} \ \exp(\lambda_i(\mathbf{x})u) & \text{for } k \geq j \\ 0 & \text{for } k < j \end{array} \right\}$$

for any $i = 1, .., p$ and $j, k = 1, .., n_i$.

Substituting (42) in the expressions (36), (37), (38) and (41), it follows that

$$\mathbf{K}(\mathbf{x}, t) = \mathbf{W}(\mathbf{x})\mathbf{A}(\mathbf{x}, t)\mathbf{W}^{-1}(\mathbf{x}), \tag{43}$$

$$\mathbf{K}'_t(\mathbf{x}, t) = vec(\mathbf{W}(\mathbf{x})\mathbf{B}(\mathbf{x}, t)\mathbf{W}^{-1}(\mathbf{x})), \tag{44}$$

$$\mathbf{K}''_t(\mathbf{x}, t) = vec(\mathbf{W}(\mathbf{x})\mathbf{C}(\mathbf{x}, t)\mathbf{W}^{-1}(\mathbf{x})), \tag{45}$$

and

$$\mathbf{K}''_{\mathbf{x},t}(\mathbf{x}, t) = ((\mathbf{W}^{-1}(\mathbf{x}))^\top \otimes \mathbf{W}(\mathbf{x}))\ \mathbf{D}(\mathbf{x}, t)\ (\mathbf{W}^\top(\mathbf{x}) \otimes \mathbf{W}^{-1}(\mathbf{x}))\ \mathbf{Q}'_{\mathbf{x}}(\mathbf{x}). \tag{46}$$

Here

$$\mathbf{A}(\mathbf{x}, t) = \frac{1}{t} \int_0^t \mathbf{L}(\mathbf{x}, u)du,$$

$$\mathbf{B}(\mathbf{x}, t) = \frac{1}{t^2} \int_0^t (\mathbf{L}(\mathbf{x}, t) - \mathbf{L}(\mathbf{x}, u))du,$$

$$\mathbf{C}(\mathbf{x}, t) = \frac{1}{t^3} \int_0^t (2\mathbf{L}(\mathbf{x}, u) + \mathbf{L}(\mathbf{x}, t)(\mathbf{J}(\mathbf{x})t - 2\mathbf{I}_m))du$$

and

$$\mathbf{D}(\mathbf{x}, t) = \frac{1}{t^2} \int_0^t (\int_0^t \mathbf{L}^\top(\mathbf{x}, s) \otimes \mathbf{L}(\mathbf{x}, t - s)ds - \int_0^u \mathbf{L}^\top(\mathbf{x}, s) \otimes \mathbf{L}(\mathbf{x}, u - s)ds)du.$$

Let $\mathbf{1}$ be the unitary vector of m elements. Since for any point $\mathbf{x} \in \Omega$, $\mathbf{A}(\mathbf{x}+\delta\mathbf{1},\delta) \to \mathbf{I}_m$, $\mathbf{B}(\mathbf{x}+\delta\mathbf{1},\delta) \to \frac{1}{2}\mathbf{J}(\mathbf{x})$, $\mathbf{C}(\mathbf{x}+\delta\mathbf{1},\delta) \to \frac{1}{3}\mathbf{J}^2(\mathbf{x})$ and $\mathbf{D}(\mathbf{x}+\delta\mathbf{1},\delta) \to \frac{1}{2}\mathbf{I}_{m^2}$ as $\delta \to 0$, then

$$\mathbf{K}(\mathbf{x}+\delta\mathbf{1},\delta) \to \mathbf{I}_m, \tag{47}$$

$$\mathbf{K}'_t(\mathbf{x}+\delta\mathbf{1},\delta) \to \frac{1}{2}vec(\mathbf{Q}(\mathbf{x})), \tag{48}$$

$$\mathbf{K}''_t(\mathbf{x}+\delta\mathbf{1},\delta) \to \frac{1}{3}vec(\mathbf{Q}^2(\mathbf{x})), \tag{49}$$

and

$$\mathbf{K}''_{\mathbf{x},t}(\mathbf{x}+\delta\mathbf{1},\delta) \to \frac{1}{2}\mathbf{Q}'_{\mathbf{x}}(\mathbf{x}), \tag{50}$$

as $\delta \to 0$.

Furthermore, using (43)-(44) it is obtained that

$$\mathbf{K}'_t(\mathbf{x},0) = \lim_{\delta\to\mathbf{0}} vec(\frac{\mathbf{K}(\mathbf{x},\delta)-\mathbf{K}(\mathbf{x},0)}{\delta}) = \frac{1}{2}vec(\mathbf{Q}(\mathbf{x})),$$

$$\mathbf{K}''_t(\mathbf{x},0) = \lim_{\delta\to\mathbf{0}} vec(\frac{\mathbf{K}'_t(\mathbf{x},\delta)-\mathbf{K}'_t(\mathbf{x},0)}{\delta}) = \frac{1}{3}vec(\mathbf{Q}^2(\mathbf{x})),$$

and

$$\mathbf{K}''_{\mathbf{x},t}(\mathbf{x},0) \equiv (\mathbf{K}'_t(\mathbf{x},0))'_{\mathbf{x}} = \frac{1}{2}\mathbf{Q}'_{\mathbf{x}}(\mathbf{x}).$$

This and the limits (47)-(50) imply that the functions $\mathbf{K}$, $\mathbf{K}'_t$, $\mathbf{K}''_t$, and $\mathbf{K}''_{\mathbf{x},t}$ are continuous on $\Omega \times 0$. Therefore, they are continuous on $\Omega \times [0,T]$.

From (39) and (30) it is obtained that

$$\mathbf{K}'_{\mathbf{x}}(\mathbf{x},t) = \mathbf{L}_{m^2}\ (\frac{1}{t}\int_{\mathbf{0}}^{t} \exp(M(\mathbf{x})u)du)\ \mathbf{R}_{m^2}\ \mathbf{Q}'_{\mathbf{x}}(\mathbf{x}),$$

$$\mathbf{K}''_{\mathbf{x}}(\mathbf{x},t) = ((\mathbf{R}_{m^2}\ \mathbf{Q}'_{\mathbf{x}}(\mathbf{x}))^{\top} \otimes \mathbf{L}_{m^2})\ \mathbf{L}_{4m^4}\ (\frac{1}{t}\int_{\mathbf{0}}^{t} \exp(H(\mathbf{x})u)du)\ \mathbf{R}_{4m^4}$$

$$+(\mathbf{I}_m \otimes \mathbf{L}_{m^2}\ (\frac{1}{t}\int_{\mathbf{0}}^{t} \exp(M(\mathbf{x})u)du)\ \mathbf{R}_{m^2})\ \mathbf{Q}''_{\mathbf{x}}(\mathbf{x}),$$

where the matrix $M(\mathbf{x})$ is defined as in Proposition 15, and the matrix

$$H(\mathbf{x}) = \begin{bmatrix} \mathbf{I}_{2m^2} \otimes M(\mathbf{x}) & \mathbf{I}_{4m^4} \\ \mathbf{0}_{4m^4} & M^{\top}(\mathbf{x}) \otimes \mathbf{I}_{2m^2} \end{bmatrix}.$$

Since, for any continuous matrix function $\mathbf{Q}$ on Ω, function $\mathbf{K}$ is continuous on $\Omega \times (0,T]$ and expression (47) holds then, the functions

$$\frac{1}{t}\int_{\mathbf{0}}^{t} \exp(M(\mathbf{x})u)du \text{ and } \frac{1}{t}\int_{\mathbf{0}}^{t} \exp(H(\mathbf{x})u)du$$

are continuous on $\Omega \times (0,T]$, and

$$\frac{1}{\delta}\int_{\mathbf{0}}^{\delta} \exp(M(\mathbf{x}+\delta\mathbf{1})u)du \to \mathbf{I}_{2m^2},$$

$$\frac{1}{\delta}\int_{\mathbf{0}}^{\delta} \exp(H(\mathbf{x}+\delta\mathbf{1})u)du \to_{8m^4}$$

as $\delta \to 0$. Therefore, $\mathbf{K}'_{\mathbf{x}}$ and $\mathbf{K}''_{\mathbf{x}}$ are continuous on $\Omega \times (0,T]$, and $\mathbf{K}'_{\mathbf{x}}(\mathbf{x}+\delta\mathbf{1},\delta) \to \mathbf{0}_{m^2,m}$ and $\mathbf{K}''_{\mathbf{x}}(\mathbf{x}+\delta\mathbf{1},\delta) \to \mathbf{0}_{m^3,m}$ as $\delta \to 0$. Furthermore, $\mathbf{K}'_{\mathbf{x}}(\mathbf{x},0) = \mathbf{0}_{m^2,m}$ and $\mathbf{K}''_{\mathbf{x}}(\mathbf{x},0) = \mathbf{0}_{m^3,m}$ since $\mathbf{K}(\mathbf{x},0) = \mathbf{I}_m$ for all $\mathbf{x}$. Thus, $\mathbf{K}'_{\mathbf{x}}$ and $\mathbf{K}''_{\mathbf{x}}$ are continuous on $\Omega \times [0,T]$. This completes the proof of assertion *i)*.

Assertion *ii)* follows from the continuity of function $\mathbf{K}$.

On the other hand, for $i = 1,..,p$ and $j = 1,..,n_i$,

$$[\mathbf{A}_i(\mathbf{x},t)]_{jj} = \left\{ \begin{array}{cc} (\exp(\lambda_i(\mathbf{x})t)-1)/(\lambda_i(\mathbf{x})t) & \text{for } \lambda_i(\mathbf{x}) \neq 0 \text{ and } t>0 \\ 1 & \text{otherwise} \end{array} \right\}$$

Therefore, $[\mathbf{A}_i(\mathbf{x},t)]_{jj} \neq 0$ if $\lambda_i(\mathbf{x}) \in \mathbb{R}$. For $\lambda_i(\mathbf{x}) \in \mathbb{C}$, $[\mathbf{A}_i(\mathbf{x},t)]_{jj} = 0$ if $\lambda_i(\mathbf{x})t = \pm 2\pi n\sqrt{-1}$ for some $n = 1,2,...,$ and $[\mathbf{A}_i(\mathbf{x},t)]_{jj} \neq 0$ otherwise. From this and expression (43), the assertion *iii)* follows. ■

Proposition 18 *Let* $\mathbf{x}$ *be a vector in* $\Omega \subset \mathbb{R}^m$ *and* $h \in [0,T]$. *If the function* $\mathbf{f} \in \mathcal{C}^3(\Omega,\mathbb{R}^m)$ *then, the function* $\boldsymbol{\phi}$ *defined as*

$$\boldsymbol{\phi}(\mathbf{x},h) = \left\{ \begin{array}{cc} \frac{1}{h}\int_{\mathbf{0}}^{h} \exp(u\mathbf{f}'(\mathbf{x}))du\ \mathbf{f}(\mathbf{x}) & \textit{for } h>0 \\ \mathbf{f}(\mathbf{x}) & \textit{for } h=0 \end{array} \right\}$$

is of class $\mathcal{C}^2(\Omega \times [0,T],\mathbb{R}^m)$. *Moreover, for* $h>0$

$$\boldsymbol{\phi}'_h(\mathbf{x},h) = (\mathbf{f}^\top(\mathbf{x}) \otimes \mathbf{I}_m)\ \mathbf{R}'_h(\mathbf{x},h),$$

$$\boldsymbol{\phi}''_h(\mathbf{x},h) = (\mathbf{f}^\top(\mathbf{x}) \otimes \mathbf{I}_m)\ \mathbf{R}''_h(\mathbf{x},h),$$

$$\boldsymbol{\phi}'_{\mathbf{x}}(\mathbf{x},h) = (\mathbf{f}^\top(\mathbf{x}) \otimes \mathbf{I}_m)\ \mathbf{R}'_{\mathbf{x}}(\mathbf{x},h) + \mathbf{R}(\mathbf{x},h)\ \mathbf{f}'(\mathbf{x}),$$

$$\begin{aligned}\boldsymbol{\phi}''_{\mathbf{x}}(\mathbf{x},h) = &((\mathbf{R}'_{\mathbf{x}}(\mathbf{x},h))^\top \otimes \mathbf{I}_m)\ (\mathbf{f}^\top(\mathbf{x}) \otimes \mathbf{I}_m)'_{\mathbf{x}} + (\mathbf{I}_m \otimes (\mathbf{f}^\top(\mathbf{x}) \otimes \mathbf{I}_m))\mathbf{R}''_{\mathbf{x}}(\mathbf{x},h) \\ &+((\mathbf{f}'(\mathbf{x}))^\top \otimes \mathbf{I}_m)\mathbf{R}'_{\mathbf{x}}(\mathbf{x},h) + (\mathbf{I}_m \otimes \mathbf{R}(\mathbf{x},h))\mathbf{f}''(\mathbf{x})\end{aligned}$$

and

$$\boldsymbol{\phi}''_{\mathbf{x},h}(\mathbf{x},h) = (\mathbf{f}^\top(\mathbf{x}) \otimes \mathbf{I}_m)\ \mathbf{R}''_{\mathbf{x},h}(\mathbf{x},h) + \mathbf{R}'_h(\mathbf{x},h)\ \mathbf{f}'(\mathbf{x}),$$

where $\mathbf{R}$ *is defined as in (7). For* $h = 0$, $\boldsymbol{\phi}'_h(\mathbf{x},0) = \frac{1}{2}\mathbf{f}'(\mathbf{x})\mathbf{f}(\mathbf{x})$, $\boldsymbol{\phi}''_h(\mathbf{x},0) = \frac{1}{3}(\mathbf{f}'(\mathbf{x}))^2\mathbf{f}(\mathbf{x})$, $\boldsymbol{\phi}'_{\mathbf{x}}(\mathbf{x},0) = \mathbf{f}'(\mathbf{x})$, $\boldsymbol{\phi}''_{\mathbf{x}}(\mathbf{x},0) = \mathbf{f}''(\mathbf{x})$ *and* $\boldsymbol{\phi}''_{\mathbf{x},h}(\mathbf{x},0) = \frac{1}{2}(\mathbf{f}^\top(\mathbf{x}) \otimes \mathbf{I}_m)\mathbf{f}''(\mathbf{x},h) + \frac{1}{2}(\mathbf{f}'(\mathbf{x}))^2$.

Proof. Let $\mathbf{K}$ and $\mathbf{Q}$ be the functions defined in Proposition 17. According to the expression (6) the function $\boldsymbol{\phi}$ can be rewritten as $\boldsymbol{\phi}(\mathbf{x},h) = \mathbf{R}(\mathbf{x},h)\mathbf{f}(\mathbf{x})$. Taking into account that $\mathbf{R}(\mathbf{x},h) = \mathbf{K}(\mathbf{x},h)$ with $\mathbf{Q}(\mathbf{x}) = \mathbf{f}'(\mathbf{x})$, the derivatives of the function $\boldsymbol{\phi}$ may be obtained by means of matrix rules of differential calculus (see Appendix D) and Proposition 17. Finally, the continuity of the function $\boldsymbol{\phi}$ follows from the continuity of the functions $\mathbf{f}$ and $\mathbf{R}$. ■

8 Appendix C: Computational aspects of the LL numerical scheme

For computational purposes, it is convenient to transform the expression (8) that defines the LL numerical scheme.

The expression (8) can be rewritten as

$$\mathbf{y}(t_{n+1}) = \mathbf{y}(t_n) + \int_0^h \exp(u\mathbf{f}'(\mathbf{y}(t_n)))du\ \mathbf{f}(\mathbf{y}(t_n)). \tag{51}$$

From (28), this can be expressed as

$$\mathbf{y}(t_{n+1}) = \mathbf{y}(t_n) + \mathbf{L}_m\ \exp(\mathbf{C}h)\ \mathbf{R}_m\ \mathbf{f}(\mathbf{y}(t_n)), \tag{52}$$

where the matrix $\mathbf{C}$ is defined as $\mathbf{C} = \begin{bmatrix} \mathbf{0}_m & \mathbf{I}_m \\ \mathbf{0}_m & \mathbf{f}'(\mathbf{y}(t_n)) \end{bmatrix}$, and the matrices $\mathbf{L}_m$ and $\mathbf{R}_m$ are defined as in Appendix A.

To improve the accuracy and efficiency in calculating (52), a further simplification can be made. From Theorem 1 in [23], $\exp(\mathbf{C}h) = \begin{bmatrix} \mathbf{0}_m & \mathbf{G} \\ \mathbf{0}_m & \mathbf{F} \end{bmatrix}$, where $\mathbf{G}$ and $\mathbf{F}$ are $m \times m$ matrices, and thus $\mathbf{L}_m \exp(\mathbf{C}h)\ \mathbf{R}_m = \mathbf{G}$. Therefore, the computation of $\mathbf{L}_m \exp(\mathbf{C}h)\ \mathbf{R}_m$ is reduced to take a block of the matrix $\exp(\mathbf{C}h)$, which avoids matrix multiplications by $\mathbf{L}_m$ and $\mathbf{R}_m$. This allows to use the following expression instead of (52),

$$\mathbf{y}(t_{n+1}) = \mathbf{y}(t_n) + \mathbf{G}\ \mathbf{f}(\mathbf{y}(t_n)). \tag{53}$$

The matrix exponential involved in this expression can be computed by a number of well known algorithms (see e.g. [8]).

An alternative method for computing (51), which is based on the Schur decomposition of matrix functions, is given in [4].

9 Appendix D: Some rules of the matrix algebra and matrix calculus

In this appendix some rules of matrix algebra and calculus are summarized, following [16].

Let $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{D}$ be matrices. Then

$$vec(\mathbf{ABC}) = (\mathbf{C}^\top \otimes \mathbf{A})vec(\mathbf{B}) \tag{54}$$

if the matrix product $\mathbf{ABC}$ exists;

$$(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = (\mathbf{AC} \otimes \mathbf{BD}) \tag{55}$$

if the matrices product $\mathbf{AC}$ and $\mathbf{BD}$ exist;

$$\exp(\mathbf{A} + \mathbf{B}) = \exp(\mathbf{A}) \exp(\mathbf{B}) \tag{56}$$

if $\mathbf{A}$, $\mathbf{B}$ commute and the matrix sum $\mathbf{A} + \mathbf{B}$ is defined;

$$\exp(\mathbf{A}) = \sum_{k=\mathbf{0}}^{\infty} \mathbf{A}^k / k! \tag{57}$$

if $\mathbf{A}$ is a square matrix. This series converges absolute and uniformly in any domain $\|\mathbf{A}\| \leq a$;

$$\exp(\mathbf{A}) \otimes \mathbf{I} = \exp(\mathbf{A} \otimes \mathbf{I}) \tag{58}$$

if $\mathbf{A}$ is a square matrix;

$$\mathbf{I} \otimes \exp(\mathbf{A}) = \exp(\mathbf{I} \otimes \mathbf{A}) \tag{59}$$

if $\mathbf{A}$ is a square matrix. Here, the symbols $^\top$, $\otimes$ and vec denote transpose, Kronecker product and vectorization operators, respectively.

Let $\mathbf{F} : \mathbb{R}^{s \times t} \to \mathbb{R}^{m \times p}$ be a differentiable matrix function. According to the identification theorem for matrix functions, the derivative $\mathbf{F}'(\mathbf{X})$ of $\mathbf{F}(\mathbf{X})$ is the $mp \times st$ matrix defined by

$$d\ vec(\mathbf{F}(\mathbf{X})) = \mathbf{F}'(\mathbf{X})\ d\ vec(\mathbf{X}),$$

where d denotes the differential operator.

Since computations with differentials are relatively easy, the following steps for computing the derivative of a matrix function are recommended: 1) compute the differential of $\mathbf{F}(\mathbf{X})$, 2) vectorize to obtain $d(vec(\mathbf{F}(\mathbf{X}))) = \mathbf{A}(\mathbf{X})d(vec(\mathbf{X}))$, and 3) conclude that $\mathbf{F}'(\mathbf{X}) = \mathbf{A}(\mathbf{X})$.

If $\mathbf{U}$ and $\mathbf{V}$ are matrix functions, $\mathbf{A}$ is a matrix of real constants and λ is a real constant then $d\mathbf{A} = \mathbf{0}$, $d(\lambda\mathbf{U}) = \lambda d\mathbf{U}$, $d(\mathbf{U} \pm \mathbf{V}) = d\mathbf{U} \pm d\mathbf{V}$, $d(\mathbf{UV}) = (d\mathbf{U})\mathbf{V} + \mathbf{U}d\mathbf{V}$, and $d(vec(\mathbf{U})) = vec(d\mathbf{U})$.

Chain Rule: Let $\mathbf{S}$ be a subset of $\mathbb{R}^{n \times q}$ and $\mathbf{F} : \mathbf{S} \to \mathbb{R}^{m \times p}$ be a differentiable function at an interior point $\mathbf{C}$ of $\mathbf{S}$. Let $\mathbf{T}$ be a subset of $\mathbb{R}^{m \times p}$ such that $\mathbf{F}(\mathbf{X}) \in$

$\mathbf{T}$ for all $\mathbf{X} \in \mathbf{S}$, and $\mathbf{G} : \mathbf{T} \to \mathbb{R}^{r\times s}$ be a differentiable function at an interior point $\mathbf{W} = \mathbf{F}(\mathbf{C}) \in \mathbf{T}$. Then the composite function $\mathbf{H} : \mathbf{S} \to \mathbb{R}^{r\times s}$defined by $\mathbf{H}(\mathbf{X}) = \mathbf{G}(\mathbf{F}(\mathbf{X}))$ is differentiable at $\mathbf{C}$, and $\mathbf{H}'_{\mathbf{C}}(\mathbf{C}) = \mathbf{G}'_{\mathbf{W}}(\mathbf{W})\ \mathbf{F}'_{\mathbf{C}}(\mathbf{C})$.

Other derivative rules:

$$(\mathbf{F}(\mathbf{X})\mathbf{G}(\mathbf{X}))'_{\mathbf{X}} = (\mathbf{G}^{\top}(\mathbf{X}) \otimes \mathbf{I}_m)\mathbf{F}'_{\mathbf{X}}(\mathbf{X}) + (\mathbf{I}_q \otimes \mathbf{F}(\mathbf{X}))\mathbf{G}'_{\mathbf{X}}(\mathbf{X}) \tag{60}$$

if $\mathbf{F} : \mathbb{R}^{s\times t} \to \mathbb{R}^{m\times p}$ and $\mathbf{G} : \mathbb{R}^{s\times t} \to \mathbb{R}^{p\times q}$ are differentiable matrix functions;

$$H''_{t,\mathbf{X}}(\mathbf{X}, t) = vec(H''_{\mathbf{X},t}(\mathbf{X}, t)) \tag{61}$$

if $H \in \mathcal{C}^2(\mathbb{R}^{s\times t} \times \mathbb{R}, \mathbb{R}^{s\times t})$. Here $H''_{t,\mathbf{X}}(\mathbf{X}, t) \equiv (H'_{\mathbf{X}}(\mathbf{X}, t))'_t$. .