1 Probabilistic Methods

Several methods have been developed to integrate an Ordinary Differential Equation (ODE) numerically (...). If a deterministic solver is employed, the error introduced by the numerical method is however difficult to quantify (...). In the frame of statistical analyses, quantifying the impact on the uncertainty of the solution due to the numerical approximation is of the utmost importance (...). Therefore, a new class of probabilistic numerical methods have been recently proposed [2] (...).
Let us consider $f\colon \mathbb{R}^d \to \mathbb{R}^d$ and the following ODE

$$\begin{aligned} \frac{\mathrm{d}u(t)}{\mathrm{d}t} &= f(u), \quad t \in (0, T], \\ u(0) &= u_0, \qquad u_0 \in \mathbb{R}^d. \end{aligned} \tag{1}$$

Integrating numerically (1) with a deterministic method on a time discretization $t_k = kh, k = 0, \dots, N, T = Nh$ gives a numerical solution $U_k, k = 0, \dots, N$, defined by

$$\begin{aligned} U_{k+1} &= \Psi(U_k), \quad k = 0, \dots, N-1, \\ U_0 &= u_0, \end{aligned} \tag{2}$$

where Ψ defines one step of a deterministic numerical method to integrate (1).
The idea behind probabilistic methods is adding at each step of the numerical integration a noise component, *i.e.*,

$$\begin{aligned} U_{k+1} &= \Psi(U_k) + \xi_k(h), \\ U_0 &= u_0, \end{aligned} \tag{3}$$

where $\xi_k(h)$ are i.i.d. Gaussian random variables.

1.1 Deterministic methods

We choose the method defined in (2) within the class of the Runge-Kutta methods, since they have been extensively analyzed theoretically and numerically, providing results which can be exploited in the following of this work.
In particular, a method of fourth order is the classic explicit Runge-Kutta method (RK4). It is defined by the following Butcher table

0				
1/2	1/2			
1/2	0	1/2		
1	0	0	1	
	1/6	1/3	1/3	1/6

1.2 Method derivation (M. motivation)

1.3 Strong convergence

In this section we prove a result about strong convergence of the method defined in (3). The following discrete Gronwall lemma is needed in the proof.

Proposition 1.1 (Discrete Gronwall Lemma)**.** *Let y_n be a nonnegative sequence and C_1, C_2 positive constants. If*

$$y_n \leq C_1 + C_2 \sum_{k=0}^{n-1} y_k,$$

then

$$y_n \leq C_1 \exp(nC_2).$$

Two assumptions are necessary to prove the strong convergence result. The first assumption is on the noise model.

Assumption 1.1.

$$\mathbb{E}^h|\xi_k(t)\xi_k(t)^T|_F^2 \leq Kt^{2p+1}.$$

Furthermore, there exists a matrix Q independent of h such that

$$\mathbb{E}^h[\xi_k(h)\xi_h(h)^T] = Qh^{2p+1},$$

where $p \geq 1$.

Let us remark that if $Q = \sigma I$, with I the identity matrix in $\mathbb{R}^{d\times d}$ and $\sigma > 0$, the method (3) can be simulated by

$$U_{k+1} = \Psi_h(U_k) + \sqrt{\sigma}h^{p+\frac{1}{2}}Z_k,$$

where Z_k is a Gaussian random vector with independent entries $Z_{k,i} \sim \mathcal{N}(0,1), i = 1,\dots,d$.
An assumption on the numerical method is needed.

Assumption 1.2. *The function f and a sufficient number of its derivatives are bounded uniformly in $\mathbb{R}^n$ in order to ensure that f is globally Lipschitz and that the numerical flow map Ψ_h has uniform local truncation error of order $q+1$*

$$\sup_{u\in\mathbb{R}^n} |\Psi_t(u) - \Phi_t(u)| \leq Kt^{q+1}.$$

The following result hold.

Proposition 1.2 (Strong Convergence)**.** *Under assumptions 1.1 and 1.2 it follows that there is $K > 0$ such that*

$$\sup_{0<kh<T} \mathbb{E}^h|u_k - U_K|^2 \leq Kh^{2\min\{p,q\}}.$$

Furthermore

$$\sup_{0\leq t\leq T} \mathbb{E}^h|u(t) - U(t)| \leq Kh^{\min\{p,q\}}.$$

This result implies that a reasonable choice in p of Assumption 1.1 is $p = q$.

Proof. Given the method in (3) and writing the exact solution of (1) as

$$u_{k+1} = \Phi_h(u_k),$$

one can compute the truncation error $\epsilon_k = \Psi_h(U_k) - \Phi_h(U_k)$, so that

$$U_{k+1} = \Phi_h(U_k) + \epsilon_k + \xi_k(h).$$

Therefore

$$\begin{aligned} e_{k+1} &= u_k - U_k \\ &= \Phi_h(u_k) - \Phi_h(u_k - e_k) - \epsilon_k - \xi_k(h). \end{aligned}$$

Taking the expectation and under Assumption 1.1

$$\mathbb{E}^h|e_{k+1}|^2 = \mathbb{E}^h|\Phi_h(u_k) - \Phi_h(u_k - e_k) - \epsilon_k|^2 + \mathcal{O}(h^{2p+1}).$$

Developing the square and since Φ_h is Lipschitz continuous with constant $(1+Lh)$ and $\epsilon_k = \mathcal{O}(h^{q+1})$ thanks to Assumption 1.2

$$\begin{aligned} \mathbb{E}^h|e_{k+1}|^2 \leq &(1+Lh)^2\mathbb{E}^h|e_k|^2 + \mathbb{E}^h\left|\left(h^{\frac{1}{2}}(\Phi_h(u_k) - \Phi_h(u_k - e_k), h^{-\frac{1}{2}}\epsilon_k\right)\right| \\ &+ \mathcal{O}\left(h^{2q+2}\right) + \mathcal{O}\left(h^{2p+1}\right). \end{aligned}$$

Then, using Cauchy-Schwarz on the inner product

$$\begin{aligned}\mathbb{E}^h|e_{k+1}|^2 &\leq (1+\mathcal{O}(h))\,\mathbb{E}^h|e_k|^2 + \mathcal{O}\left(h^{2q+1}\right) + \mathcal{O}\left(h^{2p+1}\right)\\ &\leq C_1 h\mathbb{E}^h|e_k|^2 + \mathbb{E}|e_k|^2 + \mathcal{O}\left(h^{2q+1}\right) + \mathcal{O}\left(h^{2p+1}\right)\\ &\leq C_1 h\sum_{i=0}^{k}\mathbb{E}^h|e_i|^2 + \mathcal{O}\left(h^{-1}\right)\left(\mathcal{O}\left(h^{2q+1}\right) + \mathcal{O}\left(h^{2p+1}\right)\right)\\ &\leq C_1 h\sum_{i=0}^{k}\mathbb{E}^h|e_i|^2 + \mathcal{O}\left(h^{2q}\right) + \mathcal{O}\left(h^{2p}\right).\end{aligned}$$

Therefore by Proposition 1.1

$$\begin{aligned}\mathbb{E}^h|e_k|^2 &\leq C_2 h^{2\min\{p,q\}}\exp(C_1 kh)\\ &\leq C_2 h^{2\min\{p,q\}}\exp(C_1 T)\\ &\leq Ch^{2\min\{p,q\}}.\end{aligned}$$

□

1.4 Weak convergence

A result of weak convergence can be proved using a technique of *backward error analysis*. The main idea behind this technique is finding a *modified equation* that the numerical method solves exactly or with a higher accuracy than the original equation.
Let us consider (1) and the numerical method (3). Using the Lie derivative notation, it is possible to find the differential operators $\mathcal{L}$ and $\mathcal{L}^h$ such that for all $\varphi \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{R})$

$$\begin{aligned}\varphi(\Phi_h(u)) &= \left(e^{h\mathcal{L}}\varphi\right)(u),\\ \mathbb{E}\varphi(U_1|U_0 = u) &= \left(e^{h\mathcal{L}^h}\varphi\right)(u).\end{aligned} \tag{4}$$

In particular, $\mathcal{L} = f\cdot\nabla$ and the explicit definition of $\mathcal{L}^h$ is not needed in this scope.
We now introduced a modified ODE

$$\frac{\mathrm{d}\hat{u}}{\mathrm{d}t} = f^h(\hat{u}),$$

and a modified SDE

$$\mathrm{d}\tilde{u} = f^h\tilde{u}\,\mathrm{d}t + \sqrt{h^{2p}Q}\,\mathrm{d}W\,, \tag{5}$$

where p has been introduced in Assumption 1.1. We rewrite the solution of these equations in terms of Lie derivatives as for (4) introducing the differential operators $\hat{\mathcal{L}}$ and $\tilde{\mathcal{L}}$, *i.e.*,

$$\begin{aligned}\varphi\left(\hat{u}(h)|\hat{u}(0) = u\right) &= \left(e^{h\hat{\mathcal{L}}^h}\varphi\right)(u),\\ \varphi\left(\tilde{u}(h)|\tilde{u}(0) = u\right) &= \left(e^{h\tilde{\mathcal{L}}^h}\varphi\right)(u).\end{aligned}$$

Therefore,

$$\begin{aligned}\hat{\mathcal{L}}^h &= f^h\cdot\nabla,\\ \tilde{\mathcal{L}}^h &= f^h\cdot\nabla + \frac{1}{2}h^{2p}Q : \nabla^2,\end{aligned}$$

where $\tilde{\mathcal{L}}^h$ is the *generator* of (5). (... all the passages to get to (28) in [2] ...).

Assumption 1.3. *The function f in (1) is in $\mathcal{C}^\infty$ and all its derivatives are uniformly bounded in $\mathbb{R}^n$. Furthermore, f is such that for all functions φ in $\mathcal{C}^\infty(\mathbb{R}^n, \mathbb{R})$*

$$\begin{aligned}\sup_{u\in\mathbb{R}^n}\left|e^{h\mathcal{L}}\varphi(u)\right| &\leq (1+Lh)\sup_{u\in\mathbb{R}^n}|\varphi(u)|\,,\\ \sup_{u\in\mathbb{R}^n}\left|e^{h\mathcal{L}^h}\varphi(u)\right| &\leq (1+Lh)\sup_{u\in\mathbb{R}^n}|\varphi(u)|\,,\end{aligned}$$

for some $L > 0$.

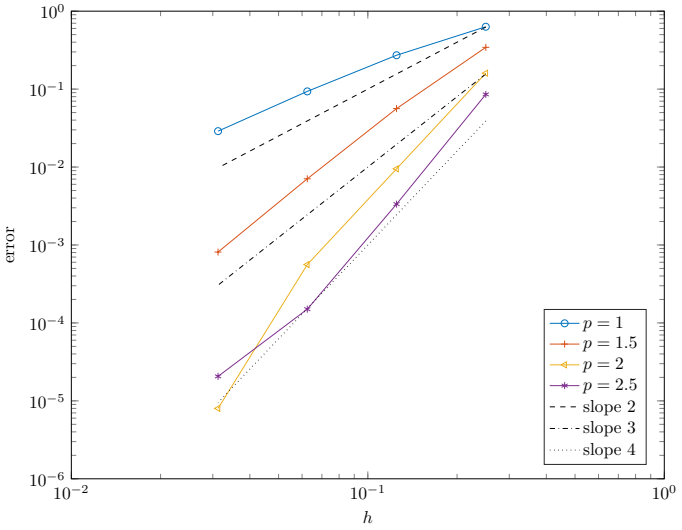

Figure 1: Weak order of convergence of (3) applied to (6).

We can now state the following result about weak convergence.

Proposition 1.3. *Consider the numerical method* (3) *and Assumptions 1.1, 1.2 and 1.3. Then for any function* φ *in* $\mathcal{C}^\infty$ *endowed with the properties of Assumption 1.3,*

$$\left|\varphi(u(T)) - \mathbb{E}^h\left(\varphi(U_k)\right)\right| \leq Kh^{\min\{2p,q\}}, \quad kh = T,$$

and

$$\left|\mathbb{E}\varphi(\tilde{u}(T)) - \mathbb{E}^h\left(\varphi(U_k)\right)\right| \leq Kh^{2p+1}, \quad kh = T,$$

with u *and* $\tilde{u}$ *solutions of* (1) *and* (5).

Proof. proof in [2]. □

1.4.1 Numerical verification of weak order

Let us consider for (1) the FitzHugh-Nagumo model, defined by

$$\begin{aligned} \frac{\mathrm{d}x_1}{\mathrm{d}t} &= c\left(x_1 - \frac{x_1^3}{3} + x_2\right), \\ \frac{\mathrm{d}x_2}{\mathrm{d}t} &= -\frac{1}{c}(x_1 - a + bx_2), \end{aligned} \tag{6}$$

where $a, b, c \in \mathbb{R}$. In particular, we choose $a = 0.2, b = 0.2, c = 3$. We provide the system with the initial condition $x_1(0) = -1, x_2(0) = 1$. We integrate numerically this equation with (3), using RK4 as Ψ. Therefore, Assumption 1.2 holds with $q = 4$. Moreover, we consider Q in Assumption 1.1 to be $Q = \sigma I$ with $\sigma = 0.1$. We approximate the solution up to time $T = 10$ with p in Assumption 1.1 equal to $1, 1.5, 2, 2.5$ and h vary in the range $0.25/(2^i), i = 0, \ldots, 3$. We approximate $\mathbb{E}^h\left(\varphi(U_k)\right)$ using a Monte Carlo simulation over 50000 trajectories and compare it with the solution computed on a fine grid to obtain an estimation of the weak error. Results (Figure 1) show that the predicted order $\min\{2p, q\}$ applies in this example. In particular, since $q = 4$, it is possible to notice that no difference in order is detected between the cases $p = 2$ and $p = 2.5$.

1.5 Multi-level Monte Carlo

In this section, we will explain how to apply the Multi-level Monte Carlo method (MLMC) in this frame. Consider the approximation U_k given by (3) to the solution $u(t)$ of (1). Given φ a function in $\mathcal{C}^\infty$, let us denote by $Z = \mathbb{E}(\varphi(U_N)), Nh = T$ the expectation of the numerical solution at final

time. If a standard Monte Carlo method over M realizations of the numerical solution is applied, the only accessible quantity is

$$\hat{Z} = \frac{1}{M} \sum_{i=1}^{M} \varphi\left(U_N^{(i)}\right),$$

where the index i is referred to the i-th trajectory. Therefore, the quantity $\hat{Z}$ is an unbiased estimator of Z. Then, the Mean Square Error (MSE) of $\hat{Z}$ is given by

$$\begin{aligned} \mathrm{MSE}(\hat{Z}) &= \mathbb{E}\left(\hat{Z} - \varphi\left(u(T)\right)\right)^2 \\ &= \mathrm{Var}\left(\hat{Z}\right) + \left(\mathbb{E}\left(\hat{Z} - \varphi\left(u(T)\right)\right)\right)^2 \\ &= \frac{C_1}{M} + C_2 h^{2\min\{2p,q\}}, \end{aligned} \tag{7}$$

where we have used Proposition 1.3 with C_1, C_2 positive constants. If we introduce as a measure for the error

$$e = \sqrt{\mathrm{MSE}\left(\hat{Z}\right)},$$

then in order to have $e = \mathcal{O}(\varepsilon)$, with ε fixed, one has to set

$$h = \mathcal{O}\left(\varepsilon^{1/\min\{2p,q\}}\right), \quad M = \mathcal{O}(\varepsilon^{-2}).$$

If we measure the cost as the product between the number of timesteps and the number of trajectories, we find easily that in this case

$$\mathrm{cost} = \mathcal{O}\left(\varepsilon^{-2-1/\min\{2p,q\}}\right).$$

The idea of MLMC is introducing an *hierarchical sampling*, introducing levels $l = 0, \ldots, L$, which have time step $h_l = T/N^l$ with $N_l = 2^l$. For each level, the number of trajectories is variable and is denoted by M_l. The estimator of Z is then constructed as

$$\bar{Z} = \sum_{l=0}^{L} \frac{1}{M_l} \sum_{i=1}^{M_l} \left(\varphi_l^{(i)} - \varphi_{l-1}^{(i)}\right), \quad \varphi_l^{(i)} = \varphi\left(U_{N_l}^{(i)}\right).$$

The values $\varphi_l^{(i)}$ are constructed under two assumptions

1. $\varphi_l^{(i)}$ and $\varphi_{l-1}^{(i)}$, with $\varphi_{-1} := 0$, are constructed using the same Brownian path,
2. $\varphi_l^{(i)}, \varphi_{l-1}^{(i)}$ and $\varphi_l^{(j)}, \varphi_{l-1}^{(j)}$ are independent for $i \neq j$.

The internal sum in $\bar{Z}$ is a telescopic sum, hence

$$\mathbb{E}(\varphi_L) = \mathbb{E}(\bar{Z}).$$

Then we can compute the MSE of $\bar{Z}$ as

$$\begin{aligned} \mathrm{MSE}(\bar{Z}) &= \mathbb{E}\left(\bar{Z} - \varphi\left(u(T)\right)\right)^2 \\ &= \mathrm{Var}\left(\bar{Z}\right) + \left(\mathbb{E}\left(\bar{Z} - \varphi\left(u(T)\right)\right)\right)^2 \\ &= \mathrm{Var}\left(\bar{Z}\right) + \left(\mathbb{E}\left(\varphi\left(U_{N_L}\right) - \varphi\left(u(T)\right)\right)\right)^2 \\ &= \mathrm{Var}\left(\bar{Z}\right) + \mathcal{O}\left(h_L^{2\min\{2p,q\}}\right). \end{aligned}$$

The variance is then computable as

$$\mathrm{Var}(\bar{Z}) = \sum_{l=0}^{L} \frac{1}{M_l^2} \sum_{i=1}^{M_l} \mathrm{Var}\left(\varphi_l^{(i)} - \varphi_{l-1}^{(i)}\right) = \sum_{l=0}^{L} \frac{V_l}{M_l}.$$

Thanks to Proposition 1.2 it is possible to estimate V_l.

Lemma 1.1. *If φ is Lipschitz continuous then*

$$V_l \leq C h_l^{2\min\{p,q\}},$$

with $C > 0$ is a constant independent of h_l.

Proof. Let us recall that for any random variable Y_1, Y_2, it is true that

$$\mathrm{Var}(Y_1 + Y_2) \leq 2\left(\mathrm{Var}(Y_1) + \mathrm{Var}(Y_2)\right).$$

Let us consider now the case $l = 0$. In this case

$$V_0 = \varphi_0 - \varphi_{-1} = \mathcal{O}(1),$$

as $h_0 = T$. For $l \geq 1$, thanks to the property of the variance above

$$\begin{aligned}\mathrm{Var}(\varphi_l - \varphi_{l-1}) &= \mathrm{Var}\left(\varphi_l - \varphi\left(u(T)\right) + \varphi\left(u(T)\right) - \varphi_{l-1}\right) \\ &\leq 2\left(\mathrm{Var}\left(\varphi_l - \varphi\left(u(T)\right)\right) + \mathrm{Var}\left(\varphi_{l-1} - \varphi\left(u(T)\right)\right)\right)\end{aligned}$$

Then, considering singularly the two terms and denoting by K the Lipschitz constant of φ

$$\begin{aligned}\mathrm{Var}\left(\varphi_l - \varphi\left(u(T)\right)\right) &\leq \mathbb{E}\left(\varphi_l - \varphi\left(u(T)\right)\right)^2 = \mathbb{E}\left(\varphi(U_{N_l}) - \varphi\left(u(T)\right)\right)^2 \\ &\leq K^2 \mathbb{E}\left(U_{N_l} - u(T)\right)^2 \\ &\leq K^2 \mathbb{E}\left|U_{N_l} - u(T)\right|^2 \leq C h_l^{2\min\{p,q\}},\end{aligned}$$

where the last bound is given by Proposition 1.2. □

Therefore, the MSE is given by

$$\mathrm{MSE}(\bar{Z}) = C_1 h_L^{2\min\{2p,q\}} + C_2 \sum_{l=0}^{L} \frac{h_l^{2\min\{p,q\}}}{M_l}.$$

We would like those two terms to balance, therefore we choose M_l as

$$M_l = \frac{h_l^{2\min\{p,q\}} L}{h_L^{2\min\{2p,q\}}},$$

as in this way

$$\mathrm{MSE}(\bar{Z}) = C_1 h_L^{2\min\{2p,q\}} + C_2 \frac{L+1}{L} h_L^{2\min\{2p,q\}} = \mathcal{O}\left(h_L^{2\min\{2p,q\}}\right).$$

Hence, if we use as a measure of the error

$$e = \sqrt{MSE\left(\bar{Z}\right)},$$

and imposing $e = \mathcal{O}(\varepsilon)$ for a fixed ε, we get for the finest time step

$$h_L = \mathcal{O}\left(\varepsilon^{1/\min\{2p,q\}}\right). \tag{8}$$

Let us compute the cost with this choice of the parameters. Defining the cost as the product of the number of time steps and the number of trajectories, we find

$$\mathrm{cost} = \sum_{l=0}^{L} N_l M_l = \sum_{l=0}^{L} \frac{T}{h_l} \frac{h_l^{2\min\{p,q\}} L}{h_L^{2\min\{2p,q\}}}.$$

For a matter of clarity in the computation, we consider three different cases.

Case 1: $q \leq p$

In this case, $\min\{p, q\} = q$ and $\min\{2p, q\} = q$. Therefore

$$\begin{aligned}\text{cost} &= \sum_{l=0}^{L} \frac{T}{h_l} \frac{h_l^{2q} L}{h_L^{2q}} = \frac{TL}{h_L} \sum_{l=0}^{L} \left(\frac{h_l}{h_L}\right)^{2q-1} \\ &= \frac{TL}{h_L} \sum_{l=0}^{L} 2^{(L-l)(2q-1)} = \frac{TL}{h_L} 2^{L(2q-1)} \sum_{l=0}^{L} 2^{-l(2q-1)} \\ &\leq L 2^{2qL} \frac{1}{1-2^{1-2q}} \leq 2L 2^{2qL} = \mathcal{O}\left(L h_L^{-2q}\right),\end{aligned}$$

where we have assumed $q \geq 1$ so that the geometric series converges. Hence, in order to satisfy $e = \varepsilon$ considering that $h_L = T/2^L$ and (8) we can impose

$$L = \left|\log_2 \varepsilon^{1/q}\right|, \tag{9}$$

and therefore the cost can be expressed as

$$\text{cost} = \mathcal{O}\left(\left|\log_2 \varepsilon^{1/q}\right| \varepsilon^{-2}\right).$$

Case 2: $q \geq 2p$

In this case, $\min\{p, q\} = p$ and $\min\{2p, q\} = 2p$. Therefore

$$\begin{aligned}\text{cost} &= \sum_{l=0}^{L} \frac{T}{h_l} \frac{h_l^{2p} L}{h_L^{4p}} = \frac{TL}{h_L^{2p+1}} \sum_{l=0}^{L} \left(\frac{h_l}{h_L}\right)^{2p-1} \\ &= \frac{TL}{h_L^{2p+1}} \sum_{l=0}^{L} 2^{(L-l)(2p-1)} = \frac{TL}{h_L^{2p+1}} 2^{L(2p-1)} \sum_{l=0}^{L} 2^{-l(2p-1)} \\ &\leq \frac{L 2^{2pL}}{h_L^{2p}} \frac{1}{1-2^{1-2q}} = \mathcal{O}\left(L h_L^{-4p}\right),\end{aligned}$$

Hence, in view of (8) we impose as before

$$L = \left|\log_2 \varepsilon^{1/2p}\right|,$$

therefore the final expression of the cost is

$$\text{cost} = \mathcal{O}\left(\left|\log_2 \varepsilon^{1/2p}\right| \varepsilon^{-2}\right).$$

Case 3: $p < q \leq 2p$

In this case, $\min\{p, q\} = p$ and $\min\{2p, q\} = q$. Therefore

$$\begin{aligned}\text{cost} &= \sum_{l=0}^{L} \frac{T}{h_l} \frac{h_l^{2p} L}{h_L^{2q}} = \frac{TL}{h_L^{2q-2p+1}} \sum_{l=0}^{L} \left(\frac{h_l}{h_L}\right)^{2p-1} \\ &= \frac{TL}{h_L^{2q-2p+1}} \sum_{l=0}^{L} 2^{(L-l)(2p-1)} = \frac{TL}{h_L^{2q-2p+1}} 2^{L(2p-1)} \sum_{l=0}^{L} 2^{-l(2p-1)} \\ &\leq \frac{L 2^{2pL}}{h_L^{2q-2p}} \frac{1}{1-2^{1-2q}} = \mathcal{O}\left(L h_L^{2p-2q-2p}\right) = \mathcal{O}\left(L h_L^{-2q}\right).\end{aligned}$$

Hence the number of levels is given by

$$L = \left|\log_2 \varepsilon^{1/q}\right|,$$

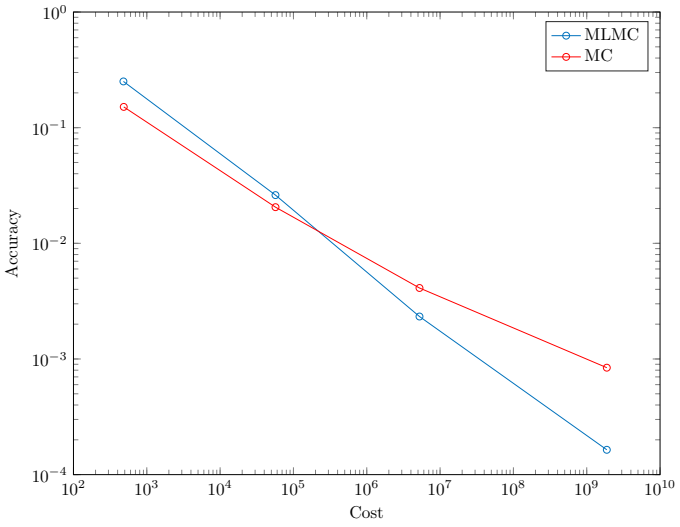

Figure 2: Accuracy of MLMC and standard Monte Carlo for the FitzHug-Nagumo problem with fixed cost.

and the computational cost is given by

$$\text{cost} = \mathcal{O}\left(\left|\log_2 \varepsilon^{1/q}\right| \varepsilon^{-2}\right).$$

Let us remark that in practice the method (3) is tuned so that $p = q$, as in this case neither the strong or the weak order are spoiled by the noise added to the model. Therefore, the first of the three cases presented above is of the highest interest. The plot in Figure **??** shows that in this case MLMC is particularly favorable with respect to Monte Carlo when the integrator has an order q which is small (e.g., $q = 1$).

1.5.1 Numerical example

We consider the Fitzhug-Nagumo problem (6) and we aim to verify the cost of MLMC with respect to standard Monte Carlo for the estimation of the expectation of the solution at final time when applying the numerical method (3). We consider the case $q = p = 1$, using as a deterministic integrator the explicit Euler method. Hence, once a value of accuracy ε is requested, the number of stages L as well as the time steps $h_l, l = 0, \dots, L$, are imposed using (9) and (8). In order to set up the standard Monte Carlo method, we consider the cost obtained in the MLMC simulation, denote by $\hat{C}$ and impose it to be equal for the standard Monte Carlo. In order to obtain a good balance between the error terms in (7) we impose

$$\begin{aligned} \frac{T}{h} M &= \hat{C}, \\ M &= \lceil h^{-2q} \rceil, \end{aligned}$$

thus obtaining for the time step

$$h = \left(\frac{T}{\hat{C}}\right)^{1/(2q+1)}.$$

In this way, the computational cost for MLMC and standard Monte Carlo are imposed to be artificially equal and the two methods can be compared for their weak error with respect to an accurate solution. We impose for MLMC four values of accuracy $\varepsilon = 0.1, 0.01, 0.001, 0.0001$, and apply the aforementioned technique to compare MLMC and Monte Carlo. Results (Figure 2) show that imposing L and $h_l, l = 0, \dots, L$ as above the obtained accuracy in the same order of magnitude as ε. Furthermore, the obtained accuracy is smaller for MLMC than MC if the cost

2 Bayesian inference of parameters

2.1 Bayesian inference - an introduction

(is it necessary?) Introduction of Bayesian inference, concluding with

$$\pi(\theta|d) \propto \mathcal{Q}(\theta)\mathcal{L}(d|\theta)$$

2.2 Bayesian inference of the parameters of an ODE

Let us consider the following initial value problem. Given u_0 a vector in $\mathbb{R}^d$ and a parameter set θ in $\mathbb{R}^p$

$$\begin{aligned} \frac{\mathrm{d}u}{\mathrm{d}t}(t;\theta) &= f(u(t;\theta)), \\ u(0;\theta) &= u_0. \end{aligned} \tag{10}$$

We consider the case in which θ is not known a priori and the problem of estimating its distribution. We consider the set of data d_i in $\mathbb{R}^d$ with $i = 1, \dots, D$ which represents the observed state of the system (10) at a set of time $t_i, i = 1, \dots, D$ in which an observational noise ε is present. We assume that ε is normally distributed with zero mean and a given variance Γ, i.e.,

$$d_i = u(t_i) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \Gamma).$$

If the solution of (10) is computable analytically, then thanks to Bayes theorem we know that once a prior distribution $\mathcal{Q}(\theta)$ is specified, the posterior distribution of θ is given by Bayes' formula and can be expressed as

$$\pi(\theta|d) \propto \mathcal{Q}(\theta)\mathcal{L}(d|u(t;\theta)). \tag{11}$$

Under the hypothesis that the observational error is normally distributed, the likelihood function is easy to compute and is given by

$$\mathcal{L}(d|u(\theta)) \propto \exp\left(\frac{1}{2}\sum_{i=1}^{D}\left(u(t_i;\theta) - d_i\right)^T \Gamma^{-2}\left(u(t_i;\theta) - d_i\right)\right).$$

In many cases, the analytical solution of (10) is not computable in closed form, therefore one replaces the analytical solution with its numerical approximation, which we denote by $U^{h,0}$. We then replace the analytical solution in the ODE, hoping that it does not spoil the quality of the posterior distribution, i.e.,

$$\mathcal{Q}(\theta)\mathcal{L}(d|u(\theta)) \approx \mathcal{Q}(\theta)\mathcal{L}(d|U^{h,0}(t;\theta)).$$

Another approach consists of considering the probabilistic numerical method (3) and a set of realizations of its solution. Let us denote by $U^{h,\sigma}(t,\xi;\theta)$ the numerical solution in this case, where σ represents the amount of uncertainty that is introduced with the method (see Assumption 1.1 and the following remarks). We then replace the likelihood function in (11) integrating over the random variable ξ, thus obtaining the following Bayes' rule

$$\pi(\theta|d) \propto \mathcal{Q}(\theta)\int \mathcal{L}(d|U^{h,\sigma}(t,\xi;\theta))\mathrm{d}\xi.$$

In [2] the authors claim that using the deterministic numerical solution for the purpose of estimating the parameters leads to unreliable posterior distributions, whilst the approximation of $\pi(\theta|d)$ provided by the probabilistic method takes accordingly into account the error introduced by the numerical solution.
In order to draw from the posterior distribution $\pi(\theta|d)$ one has to perform a Markov Chain Monte Carlo method, which is a class of numerical methods for Bayesian inference, briefly introduced in the following section.

Algorithm 1: Metropolis-Hastings algorithm.

Data: $\theta_0, N_{it}, d_i, i = 0, \dots, D$.

1 Compute $\mathcal{Q}(\theta_0)$ and $\mathcal{L}(d|\theta_0)$;
2 **for** $k = 0, \dots, N_{it}$ **do**
3 Draw ϑ from $q(\theta_k, \cdot)$;
4 Compute the probability $\alpha = \min\left\{1, \frac{\pi(\vartheta|d)q(\theta_k, \vartheta)}{\pi(\theta_k|d)q(\vartheta, \theta_k)}\right\}$;
5 Draw u from $\mathcal{U}(0, 1)$;
6 **if** $\alpha > u$ **then**
7 Accept ϑ, set $\theta_{k+1} = \vartheta$;
8 **else**
9 Set $\theta_{k+1} = \theta$;
10 **end**
11 **end**

2.3 Markov Chain Monte Carlo methods

The Markov Chain Monte Carlo (MCMC) methods are a useful tool for performing Bayesian inference. The main idea behind these methods is creating a chain of guesses of a parameter θ in order to build an approximation of its posterior distribution.
One of the most popular MCMC methods is the Metropolis-Hastings (MH) algorithm [4], presented in pseudo-code in Algorithm 1. In this algorithm, the new guess ϑ of the parameter θ value is drawn from a proposal function $q(\theta_k, \cdot)$ dependent on the current guess θ_k. Then, the new value ϑ is included in the chain as θ_{k+1} with a probability α dependent on the ratio between the posterior distribution evaluated in ϑ and θ, as in line 4 of Algorithm 1. Otherwise, θ_{k+1} is chosen to be equal to θ_k.
Let us remark that if $q(x, y)$ is a symmetric function, then the expression of the probability α at the k-th step simplifies to

$$\alpha = \min\left\{1, \frac{\pi(\vartheta|d)}{\pi(\theta_k|d)}\right\}.$$

This is the case, for example, of a Gaussian proposal distribution, which is a common choice (ADDREF) in case no a priori restriction is imposed on the range of θ.
Let us consider the problem of finding the distribution of the parameter θ defining an ODE. In this case, once the new guess ϑ is generated from the proposal distribution, it is necessary to solve numerically (10) in order to determine the value of the likelihood function. In particular, assuming that the proposal distribution q is symmetric, the value of α at the k-th step in this frame reads in case the deterministic solver is adopted

$$\alpha = \min\left\{1, \frac{\mathcal{Q}(\vartheta)\mathcal{L}(d|U^{h,0}(t;\vartheta))}{\mathcal{Q}(\theta_k)\mathcal{L}(d|U^{h,0}(t;\theta_k))}\right\},$$

while for the probabilistic solver one gets

$$\alpha^{h,\sigma} = \min\left\{1, \frac{\mathcal{Q}(\vartheta)\int \mathcal{L}(d|U^{h,\sigma}(t,\xi;\vartheta))\mathrm{d}\xi}{\mathcal{Q}(\theta_k)\int \mathcal{L}(d|U^{h,\sigma}(t,\xi;\theta_k))\mathrm{d}\xi}\right\}. \tag{12}$$

The integrals in (12) are not trivial to compute, therefore a Monte Carlo approach has to be exploited. In particular, considering M realizations $\{\xi_i\}_{i=1}^{M}$of the random variable ξ, one can approximate the integral of the likelihood as

$$\int \mathcal{L}(d|U^{h,\sigma}(t,\xi;\theta))\mathrm{d}\xi \approx \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}(d|U^{h,\sigma}(t,\xi_i;\theta)). \tag{13}$$

In this way, the probability α is computable and can be used to obtain the distribution of the parameter θ.

2.3.1 An adaptive approach

In the frame of MH algorithms, it is important to have a control on the *acceptance ratio* of the Markov chain, i.e., the number of new guesses that are chosen over the previous value of θ. The acceptance ratio depends on the goodness of the chosen proposal distribution, as if the new guess produced via the proposal distribution have a low probability of being accepted, a low value of acceptance ratio will result from the algorithm. In order to overcome this issue, we choose to adopt the robust adaptive Metropolis-Hastings algorithm (RAM) [8]. Let us consider the case in which the proposal distribution is normal, i.e.,

$$\vartheta = \theta_k + Z, \quad Z \sim \mathcal{N}(0, \Sigma),$$

with a given covariance matrix Σ. It is possible to build a sequence of matrices such that the convergence properties of MH are not spoiled and the acceptance rate is approximately equal to a given value α^*. In particular, we consider for each iteration $n = 1, \dots, N$, the update

$$\vartheta = \theta_k + S_n Z_n, \quad Z_n \sim \mathcal{N}(0, I),$$

with S_n a lower triangular positive definite matrix and I the identity matrix. Then, once the probability α of acceptance has been computed, we update S_n with a lower triangular matrix S_{n+1} satisfying

$$S_{n+1} S_{n+1}^T = S_n \left(I + \eta_n \left(\alpha - \alpha^* \right) \frac{Z_n Z_n^T}{Z_n^T Z_n} \right) S_n^T.$$

Hence, we can compute S_{n+1} as the Cholesky factorization of the right hand side. The sequence $\{\eta_n\}_n$ can be any sequence decaying to zero with n. In this work, we consider

$$\eta_n = n^{-\gamma}, \quad 0.5 < \gamma \leq 1.$$

This algorithm guarantees that the final acceptance rate of MH will be asymptotically equal to the desired value α^* [8].

2.3.2 Noisy pseudo-marginal MCMC

It is crucial to understand whether the approximation of the integrals in (12) influence the convergence of the posterior distribution to the true distribution of θ. Let us denote by $\pi(\theta|d)$ the real posterior distribution of θ, i.e.,

$$\pi(\theta|d) \propto \mathcal{Q}(\theta) \mathcal{L}(d|u(t,\theta)),$$

where u is the exact solution of the equation. Then, let us denote by $\pi^{h,\sigma}(\theta|d)$ the distribution obtained applying MH with the *transition kernel* (define it) induced by the probability $\alpha^{h,\sigma}$. Finally, let us denote by $\pi_N^{h,\sigma}(\theta|d)$ the distribution obtained approximating the integrals with Monte Carlo sums. We can rewrite the probability under the form of a *pseudo-marginal* Metropolis-Hastings (add reference). If one defines the following weights

$$\begin{aligned} W_{\theta,N} &= \frac{1}{N} \frac{\sum_{i=1}^N \mathcal{L}(d|U^{h,\sigma}(t,\xi_i;\theta))}{\int \mathcal{L}(d|U^{h,\sigma}(t,\xi;\theta))\mathrm{d}\xi} \\ &= \frac{1}{N} \sum_{i=1}^N \frac{\mathcal{L}(d|U^{h,\sigma}(t,\xi_i;\theta))}{\int \mathcal{L}(d|U^{h,\sigma}(t,\xi;\theta))\mathrm{d}\xi} \\ &= \frac{1}{N} \sum_{i=1}^N W_\theta^{(i)}, \end{aligned}$$

then the probability of acceptance can be rewritten as

$$\alpha_N^{h,\sigma} = \min \left\{ 1, \frac{\pi(\vartheta|d) W_{\vartheta,N} q(\theta_k, \vartheta)}{\pi(\theta_k|d) W_{\theta_k,N} q(\vartheta, \theta_k)} \right\}.$$

Let us remark that the random variables $W_\theta^{(i)}$ are i.i.d. with the property

$$\mathbb{E}(W_\theta^{(i)}) = 1, \quad i = 1, \dots, N,$$

and in the same way $W_{\theta,N}$ has unitary expectation. The probability can be computed in two different ways

1. the weight $W_{\theta_k,N}$ is not recomputed from the last iteration and only $W_{\vartheta,N}$ is drawn,
2. at each iteration both $W_{\theta_k,N}$ and $W_{\vartheta,N}$ are computed.

The second approach defines a noisy pseudo-marginal Metropolis-Hastings algorithm [1, 5, 6], which requires a double computational cost per iteration, as two Monte Carlo simulation have to be carried out for each MCMC iteration. On the other hand, the value of the likelihood at θ_k could be artificially good due to a particularly favorable set of realizations of ξ. Therefore, the ratio of the posteriors could be small, implying that the chain might remain blocked at the same guess of θ for an arbitrarily large number of iterations. In practice, the noisy approach guarantees a fast mixing, so that even with a double cost per-iteration it is computationally faster than the first approach.

We now consider the convergence of the probability distribution obtained with the noisy pseudo-marginal approach to the real distribution. We consider the total variation distance, which is defined as follow [3]

Definition 2.1. *Given two probability measures ν and μ on a measurable space $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$, the total variation distance between P and Q is defined as*

$$\|\nu - \mu\|_{TV} \coloneqq \sup_{A \in \mathcal{B}(\mathcal{X})} |\nu(A) - \mu(A)|$$

Let us remark that the total variation distance between two probability measures is not often practical to compute. The Hellinger distance is more practical, especially in case the distributions are Gaussian. The Hellinger distance is defined as follows [3].

Definition 2.2. *If f, g are densities of the measures μ and ν on a measurable space $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$ with respect to a dominating measure λ,*

$$d_H(\mu, \nu) = \left[\int_{\mathcal{X}} \left(\sqrt{f} - \sqrt{g} \right)^2 \mathrm{d}\lambda \right]^{1/2} = \left[2 \left(1 - \int_{\mathcal{X}} \sqrt{fg} \right) \right]^{1/2}.$$

In the Gaussian case, if $\mu = \mathcal{N}(\mu_1, \Sigma_1)$, $\nu = \mathcal{N}(\mu_2, \Sigma_2)$, the Hellinger distance is given by

$$d_H(\mu, \nu)^2 = 1 - \frac{\det(\Sigma_1)^{1/4} \det(\Sigma_2)^{1/4}}{\det\left(\frac{\Sigma_1 + \Sigma_2}{2}\right)^{1/2}} \exp\left(-\frac{1}{8} (\mu_1 - \mu_2)^T \left(\frac{\Sigma_1 + \Sigma_2}{2} \right)^{-1} (\mu_1 - \mu_2) \right).$$

The Hellinger distance is equivalent to the total variation distance with the relation [3]

$$\frac{d_H(\mu, \nu)^2}{2} \leq \|\mu - \nu\|_{TV} \leq d_H(\mu, \nu), \tag{14}$$

hence when the total variation distance will not be computable, we will estimate it using the Hellinger distance. We consider now the distance between the true distribution of θ and the distribution obtained with the noisy-pseudomarginal approach. Let us remark that by the triangular inequality

$$\left\| \pi - \pi_N^{h,\sigma} \right\|_{TV} \leq \left\| \pi - \pi^{h,\sigma} \right\|_{TV} + \left\| \pi^{h,\sigma} - \pi_N^{h,\sigma} \right\|_{TV}.$$

Intuitively, the first term in the sum concerns the numerical accuracy of the numerical method, while the second term concerns the quality of the approximation performed in (13). For the first

term, if θ is a vector of $\mathbb{R}^g$ we remark that thanks to Theorem 1.3 we have

$$\begin{aligned}\left\|\pi - \pi^{h,\sigma}\right\|_{TV} &= C \sup_{A\in\mathcal{B}(\mathbb{R}^g)} \int_A \mathcal{Q}(\theta)\left(\mathcal{L}(d|u(\theta)) - \left(\int \mathcal{L}(d|U^{h,\sigma}(\theta,\xi))\mathrm{d}\xi\right)\right)\mathrm{d}\theta \\ &= C \sup_{A\in\mathcal{B}(\mathbb{R}^g)} \int_A \mathcal{Q}(\theta)\left(\mathcal{L}(d|u(\theta)) - \mathbb{E}^{\xi}\left(\mathcal{L}(d|U^{h,\sigma}(\theta,\xi))\right)\right)\mathrm{d}\theta \\ &\leq C h^{\min\{q,2p\}} \sup_{A\in\mathcal{B}(\mathbb{R}^g)} \int_A \mathcal{Q}(\theta)\mathrm{d}\theta \\ &= C h^{\min\{q,2p\}},\end{aligned}$$

where $\mathbb{E}^{\xi}(\cdot)$ denotes the expectation with respect to the random variable ξ and C is a positive constant independent of h.
For the second term, since the weights $W_{\theta,N}$ are given by arithmetic averages and have unitary expectation, the following result has been shown [5].

Proposition 2.1. *Under appropriate conditions (add them?) there exist* $0 < \delta < 1/6$, $C_\delta > 0$ *and* $N_0 \in N^+$ *such that for all* $N \geq N_0$

$$\left\|\pi^{h,\sigma} - \pi_N^{h,\sigma}\right\|_{TV} \leq C_\delta \frac{\log(N)}{N^{\frac{1}{2}-\delta}}.$$

With the two results above, we can now estimate the convergence with respect to h and N to the true probability distribution in the total variation distance

$$\begin{aligned}\left\|\pi - \pi_N^{h,\sigma}\right\|_{TV} &\leq \left\|\pi - \pi^{h,\sigma}\right\|_{TV} + \left\|\pi^{h,\sigma} - \pi_N^{h,\sigma}\right\|_{TV} \\ &\leq C h^{\min\{q,2p\}} + C_\delta \frac{\log(N)}{N^{\frac{1}{2}-\delta}}.\end{aligned}$$

where C and C_δ are specified above. Hence, defining the error e as

$$e \coloneqq \left\|\pi - \pi_N^{h,\sigma}\right\|_{TV}$$

and imposing it to be equal to $\mathcal{O}(\varepsilon)$ where ε is a desired tolerance we find that the time step h has to satisfy

$$h = \mathcal{O}\left(\varepsilon^{1/\min\{q,2p\}}\right).$$

As far as the number of samples N in $W_{\theta,N}$ is concerned, if we define the function $F_\delta \colon \mathbb{R} \to \mathbb{R}$ as

$$F_\delta(N) \coloneqq \frac{\log(N)}{N^{\frac{1}{2}-\delta}},$$

then its inverse function F_δ^{-1} is given by

$$F_\delta^{-1}(x) = \exp\left(\frac{1}{\gamma} W(\gamma x)\right).$$

where $\gamma \coloneqq \delta - 1/2$ and W is the Lambert function. Therefore, in order to balance the two error terms it is necessary to impose

$$N = \mathcal{O}(F_\delta^{-1}(\varepsilon)).$$

Thus, the computational cost per iteration of the noisy Metropolis-Hastings algorithm is given by

$$\begin{aligned}\text{cost} &= \mathcal{O}(h^{-1}N) \\ &= \mathcal{O}\left(\varepsilon^{-1/\min\{q,2p\}} F_\delta^{-1}(\varepsilon)\right)\end{aligned}$$

Let us remark that the computational cost predicted by this formula is rapidly growing for small values of ε, leading to unaffordable computational times when a precise computation is required.

2.3.3 A MLMC approach

Instead of arithmetic averages, use

$$W_{\theta,\mathrm{MLMC}} = \sum_{l=0}^{L} \frac{1}{M_l} \sum_{i=1}^{M_l} \left(W_l^{(i)} - W_{l-1}^{(i)} \right),$$

where (definition of W_l)

2.3.4 Numerical example

We consider the test equation

$$\begin{aligned} \frac{\mathrm{d}u(t)}{\mathrm{d}t} &= \lambda u(t), \\ u(0) &= 1 \end{aligned}$$

with λ a real negative parameter. If λ is big in absolute value, the equation is stiff. In this experiment, we are not interested in stiff equations, therefore we consider $\lambda = -0.5$. The analytical solution of this equation is known and is given by

$$u(t) = \exp(\lambda t), \quad t > 0.$$

We are interested in verifying the order of convergence of the noisy MH presented in section 2.3.2. We consider the prior distribution to be a Gaussian centered in the true value of the parameter $\bar{\lambda} = -0.5$ with unitary variance. Then, we generate data from the analytical solution at $t = 1$ with a normal disturbance, i.e.,

$$d = \exp(\lambda) + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \Gamma),$$

with $\Gamma = 0.001$. In this way, it is possible to generate the true posterior distribution $\pi(\lambda|d)$ through Bayes' rule

$$\pi(\lambda|d) \propto \mathcal{Q}(\lambda)\mathcal{L}(d|\exp(\lambda)),$$

where the prior distribution is given by

$$\mathcal{Q}(\lambda) = (2\pi)^{-1/2} \exp\left(-\frac{1}{2}(\lambda - \bar{\lambda}) \right),$$

and the likelihood is given by

$$\mathcal{L}(d|\exp(\lambda)) = (2\pi\Gamma)^{-1/2} \exp\left(-\frac{1}{2\Gamma}(\exp(\lambda) - d)^2 \right).$$

Normalizing the product of prior and likelihood, we obtain the true posterior distribution for the parameter λ. We consider now the RAM algorithm for the probabilistic method (3) with explicit Euler as a deterministic solver. We consider $h = \{0.1, 0.05, 0.01\}$ and $N = \{1, 10, 100, 1000, 10000\}$. In this way, we can observe for each value of h the convergence of the posterior distribution $\pi_N^{h,\sigma}$ to the exact distribution. In order to estimate the total variation distance between $\pi_N^{h,\sigma}$ and π we consider the bound given by the Hellinger distance between the normal distributions with the estimate values of mean and variance (14).

2.3.5 A Gaussian filtering approach

An interesting approach for the Bayesian analysis of the parameters of an ODE or of an SDE has been recently proposed in [7]. In this paper, the authors propose a Gaussian filtering approach to solve the differential equation at each step of an MCMC algorithm, avoiding in this way the computationally inefficient Monte Carlo simulation typical of the MCWM approach. The method consists in building at each iteration of the MCMC algorithm a Gaussian approximation of the solution of an SDE, computing the evolution of the mean and variance of a Gaussian distribution with an ODE approach. Let us consider the acceptance probability in a standard MH

$$\alpha = \min \left\{ \frac{\mathcal{Q}(\vartheta)\mathcal{L}(d|\vartheta)}{\mathcal{Q}(\theta_k)\mathcal{L}(d|\theta_k)} \right\}.$$

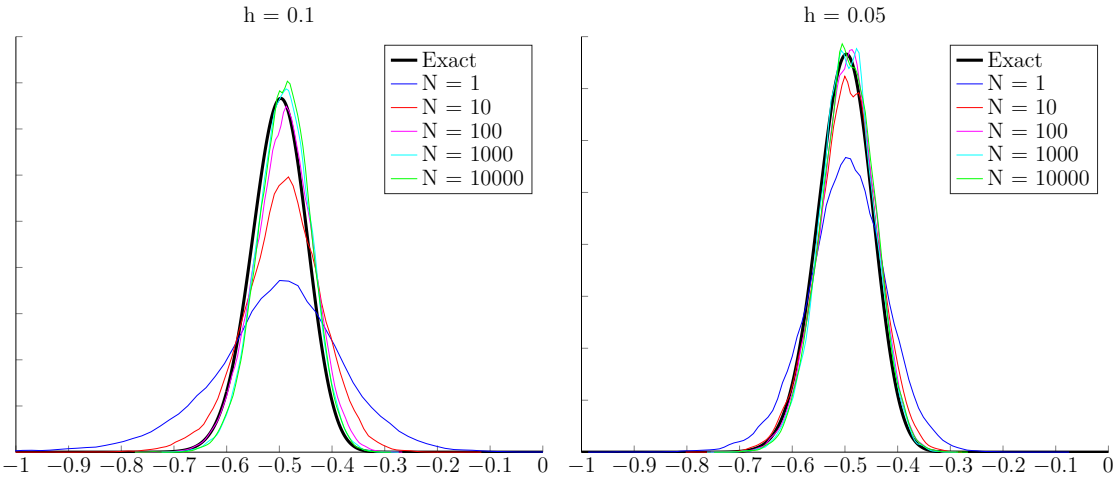

Figure 3: Distribution $\pi_N^{h,\sigma}$ for the different values of h and N.

While the prior distribution is easy to evaluate, the likelihood function is in this case intractable. The pseudo-marginal MCMC approach and its noisy version approximate the likelihood with a Monte Carlo simulation, which can be extremely costly.
Let us consider $f\colon \mathbb{R}^{N_s} \to \mathbb{R}^{N_s}$, $g\colon \mathbb{R}^{N_s} \to \mathbb{R}^{N_s \times N_s}$, W a d-dimensional Wiener process and the following SDE

$$\begin{aligned} \mathrm{d}U(t;\theta) &= f_\theta(U)\mathrm{d}t + g_\theta(U)\mathrm{d}W, \quad 0 < t \leq T, \\ U(0) &= U_0, \end{aligned} \tag{15}$$

where we assume that U_0 is a deterministic initial condition in $\mathbb{R}^{N_s}$ and that the functions f, g depend on a parameter θ of $\mathbb{R}^{N_p}$. Under Assumption 1.1 with $Q = \sigma I$, solving an ODE with the probabilistic method defined in (3) is equivalent to solving numerically (15) for the choice

$$g(U) = G = \sigma h^p I,$$

with I the identity matrix in $\mathbb{R}^{N_s \times N_s}$. Since the method proposed in [7] is applicable to any SDE of the form (15), in the following we formally maintain this more general notation. Let us denote by y_i an observation of the state of (15) at time t_i for $i = 1, \ldots, N_d$, and by Y_i the set of all observations up to time t_i, i.e.,

$$Y_i = \{y_1, y_2, \ldots, y_{i-1}, y_i\}.$$

Let us furthermore assume that y_i is measured from the solution with the following additive noise model

$$y_i = U(t_i) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \Sigma_y).$$

The likelihood appearing in the probability α can be therefore written as

$$\begin{aligned} \mathcal{L}(Y_k|\theta) &= \prod_{i=1}^{k} (2\pi \det(\Sigma_y))^{-k/2} \exp\left(-\frac{1}{2}(U(t_i;\theta) - y_i)^T \Sigma_y^{-1} (U(t_i;\theta) - y_i)\right) \\ &= \prod_{i=1}^{k} \mathcal{L}_i(y_i|\theta). \end{aligned}$$

2.4 Numerical example

We consider the ODE defined in (6) and the problem of determining the values of the parameters $\theta = (a, b, c)^T$ in $\mathbb{R}^3$. We consider as the true value of θ the vector $\bar{\theta} = (0.2, 0.2, 3)$. In order to produce the observations d_i, we consider a reference solution $\bar{u}(t, \bar{\theta})$ produced with a fine time step and its values at $t_i = 1, 2, 3, \ldots, 39$ and then we consider

$$d_i = \bar{u}(t_i, \bar{\theta}) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, 10^{-3} I), \quad i = 1, \ldots, 39,$$

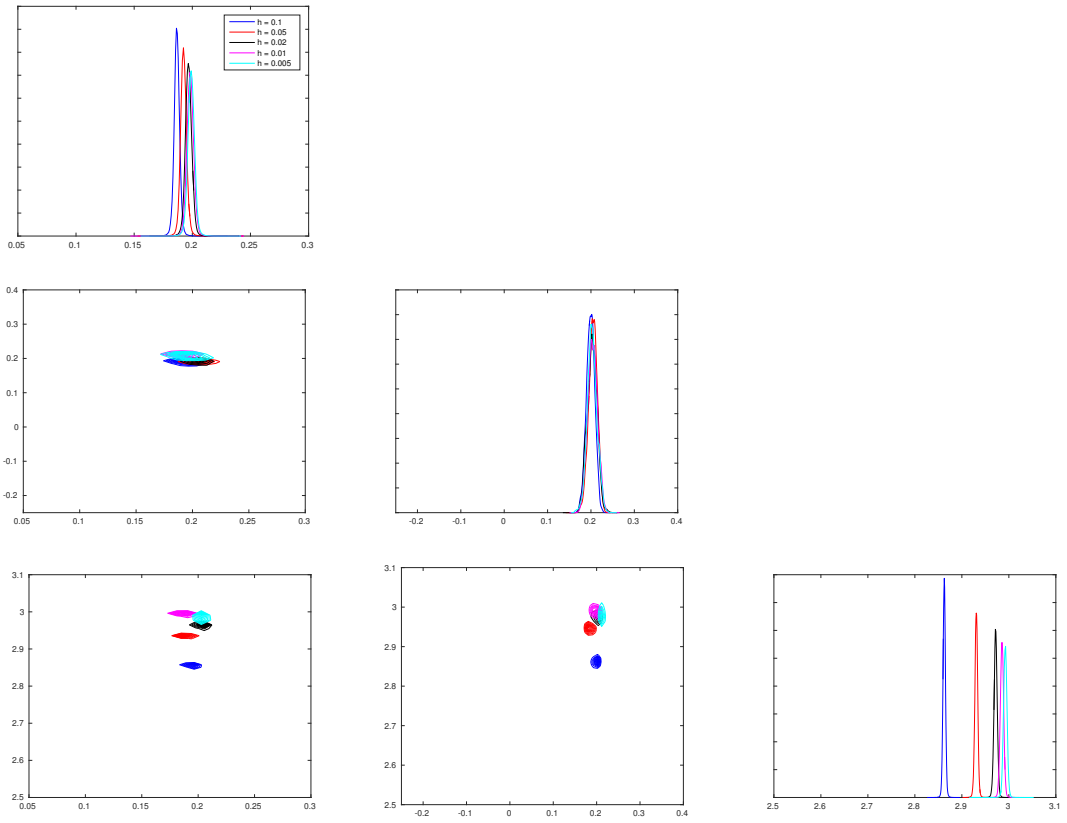

Figure 4: Marginal distributions for θ obtained with the deterministic solver. The posterior distributions are clearly concentrated and mutually singular.

where I is the identity matrix in $\mathbb{R}^{3\times 3}$. Therefore, we consider a diagonal noise with independent normal components having all variance 10^{-3}. We approximate the posterior distribution $\pi(\theta|d)$ with both the deterministic and the probabilistic solvers using time steps h_i in the range $\{0.1, 0.05, 0.01, 0.005\}$. The proposal function $q(x, y)$ for MH is Gaussian, and the prior distribution $\mathcal{Q}(\theta)$ is lognormal with unitary variance and mean $\bar{\theta}$. We consider 10^6 iterations of the MH algorithm for all time steps and in both the deterministic and the probabilistic case. Results show that

- In the deterministic case (Figure 4) the marginals of the posterior distributions show an extremely small variance and are not nested for different time steps. This means that the estimation of parameters is not reliable as it does not account for the error introduced by the numerical approximation of the ODE.
- In the probabilistic case (Figure 5) the results show bigger variances, with posterior distributions which fully account for the numerical approximation. In fact, one can see that for the smaller values of the time step the marginal distributions are more concentrated, while for the big values (e.g. $h = 0.1, 0.05$) the estimation of θ is clearly unreliable, as it is supposed to be due to numerical integration.

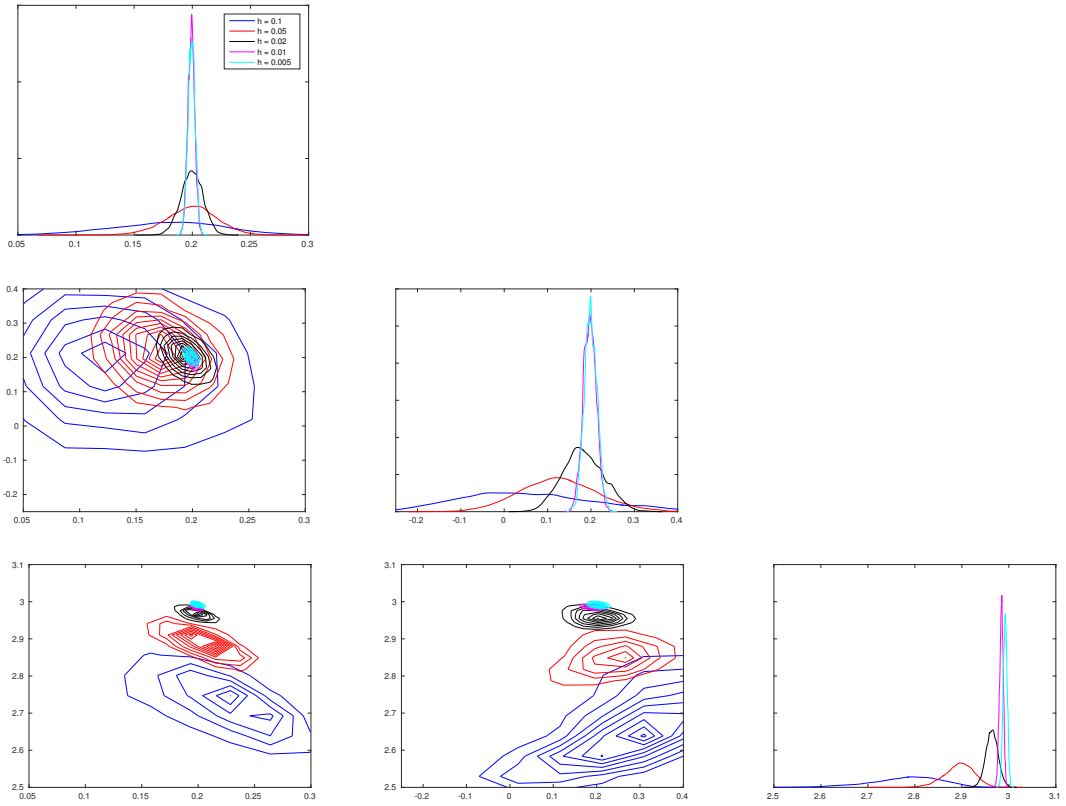

Figure 5: Marginal distributions for θ obtained with the probabilistic solver. The posterior distributions account for the numerical error.

3 Numerical example

Let us consider the Lorenz system, *i.e.*,

$$\begin{aligned}\frac{\mathrm{d}x}{\mathrm{d}t} &= \sigma(y-x),\\ \frac{\mathrm{d}y}{\mathrm{d}t} &= x(\rho-z)-y,\\ \frac{\mathrm{d}z}{\mathrm{d}t} &= xy-\beta z,\end{aligned}$$

where $\sigma = 10, \rho = 28, \beta = 8/3$. We provide the system with initial conditions

$$x(0) = -10, \quad y(0) = -1, \quad z(0) = 40,$$

and integrate the system up to the final time $T = 20$. We choose as deterministic integrator the classic fourth-order Runge-Kutta method, with timestep $h = 0.001$. Results show that the realizations of the numerical solutions obtained with the probabilistic method follow the behaviour of the deterministic method in the first part of the time span and then show a chaotic behaviour, revealing the features of the underlying system. The three components x, y, z of the solution obtained with the deterministic and probabilistic solvers are depicted in Figure 6.

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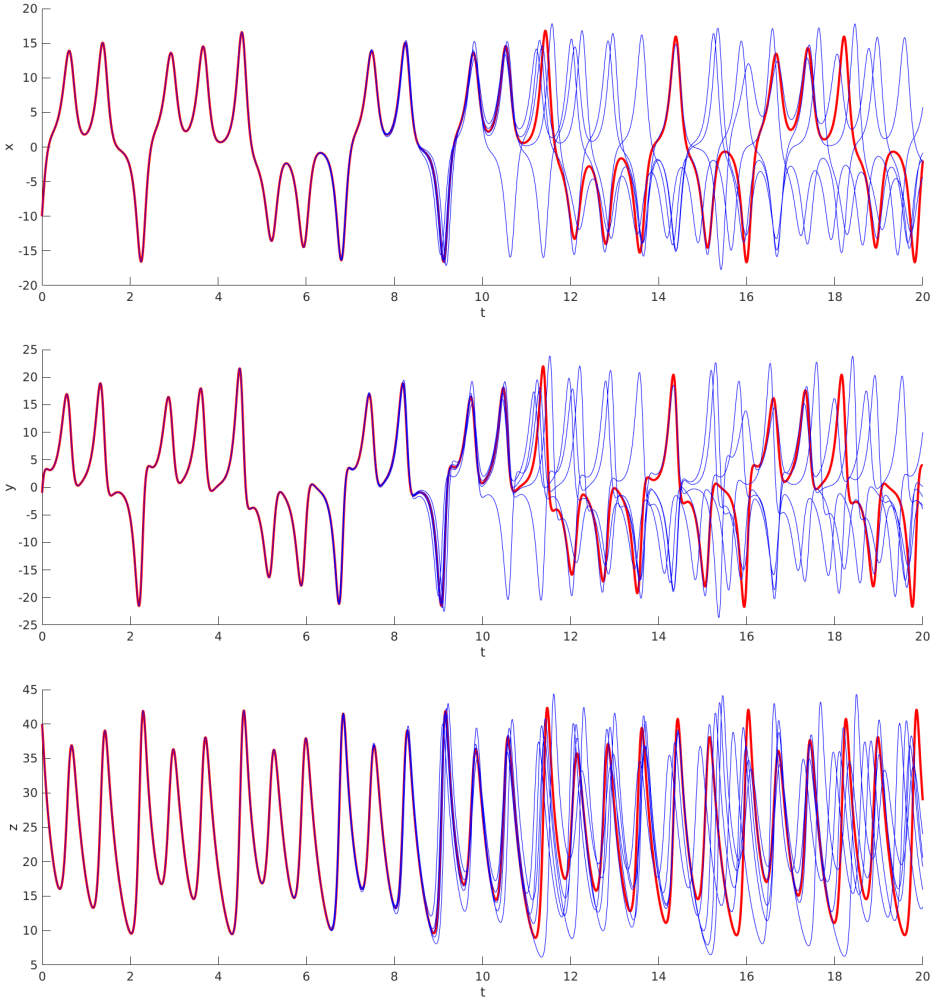

Figure 6: Solution of the Lorenz system obtained with the deterministic solver (red) and realizations of the solution obtained with the probabilistic solver (blue).

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