Random time step probabilistic methods for uncertainty quantification in chaotic and geometric numerical integration

Assyr Abdulle* Giacomo Garegnani†

Abstract

Keywords.

AMS classification subjects.

1 Introduction

2 Prob. methods

Assumption 1. Assumption on the random variables.

3 Technical part

Assumption 2. Assumptions on f and on Ψ_h.

Theorem 1. *Error growth of deterministic RK [1].*

Lemma 1. *For the additive noise method*

$$\mathbb{E}(Y_n \mid Y_{n-j}) = \Psi_h^j(Y_{n-j}) + \mathcal{O}\big((j-1)h^{2p+1}\big) \tag{1}$$

Proof. We prove the result by induction on the index j. First, consider $\mathbb{E}(Y_n \mid Y_{n-1})$, which is trivially

$$\mathbb{E}(Y_n \mid Y_{n-1}) = \mathbb{E}\left(\Psi_h(Y_{n-1}) + \xi_{n-1} \mid Y_{n-1}\right) = \Psi_h(Y_{n-1}). \tag{2}$$

Iterating once and exploiting the properties of conditional expectations, we get

$$\begin{aligned}\mathbb{E}(Y_n \mid Y_{n-2}) &= \mathbb{E}\left(\mathbb{E}(Y_n \mid Y_{n-1}) \mid Y_{n-2}\right)\\ &= \mathbb{E}\left(\Psi_h(Y_{n-1}) \mid Y_{n-2}\right)\\ &= \mathbb{E}\left(\Psi_h(\Psi_h(Y_{n-2}) + \xi_{n-2}) \mid Y_{n-2}\right).\end{aligned} \tag{3}$$

A Taylor expansion, the properties of conditional expectations and Assumption 1 give

$$\begin{aligned}\mathbb{E}(Y_n \mid Y_{n-2}) = \mathbb{E}\Big(&\Psi_h^2(Y_{n-2}) + \mathrm{D}\Psi_h(Y_{n-2})\xi_{n-2}\\ &+ \mathrm{D}^2\Psi_h(Y_{n-2})(\xi_{n-2},\xi_{n-2}) + \dots \mid Y_{n-2}\Big)\\ = \Psi_h^2&(Y_{n-2}) + \mathcal{O}(h^{2p+1}).\end{aligned} \tag{4}$$

*Mathematics Section, École Polytechnique Fédérale de Lausanne (assyr.abdulle@epfl.ch)
†Mathematics Section, École Polytechnique Fédérale de Lausanne (giacomo.garegnani@epfl.ch)

The induction step can then be written as

$$\begin{aligned}\mathbb{E}(Y_n \mid Y_{n-j}) &= \mathbb{E}\left(\mathbb{E}(Y_n \mid Y_{n-j+1}) \mid Y_{n-j}\right) \\ &= \mathbb{E}\left(\Psi_h^{j-1}(Y_{n-j+1}) \mid Y_{n-j}\right) + \mathcal{O}\big((j-2)h^{2p+1}\big) \\ &= \mathbb{E}\left(\Psi_h^{j-1}(\Psi_h(Y_{n-j}) + \xi_{n-j}) \mid Y_{n-j}\right) + \mathcal{O}\big((j-2)h^{2p+1}\big).\end{aligned} \tag{5}$$

Expanding Ψ_h^{n-j} in a Taylor series we get

$$\begin{aligned}\mathbb{E}(Y_n \mid Y_{n-j}) &= \mathbb{E}\left(\Psi_h^{j}(Y_{n-j}) + \mathrm{D}\Psi_h^{j-1}(Y_{n-j})\xi_{n-j} \mid Y_{n-j}\right) + \mathcal{O}\big((j-1)h^{2p+1}\big) \\ &= \Psi_h^{j}(Y_{n-j}) + \mathcal{O}\big((j-1)h^{2p+1}\big),\end{aligned} \tag{6}$$

which proves the desired result. □

Lemma 2. *For the RTS-RK method*

$$\mathbb{E}(Y_n \mid Y_{n-j}) = \dots \tag{7}$$

Proof. Let us first consider the difference between a single step of a fixed time step method with respect to the RTS-RK method. Any Runge-Kutta method of order $q \geq 1$ can be written for any $y \in \mathbb{R}^d$ and $z > 0$ as

$$\Psi_z(y) = y + zf(y) + z^2 R(y), \tag{8}$$

where $R(y)$ is a function depending on the coefficients of the method, on the function f as well as on z. Hence, for a generic random time step H, we have

$$\Psi_H(y) - \Psi_h(y) = (H-h)f(y) + (H^2 - h^2)R(y). \tag{9}$$

Let us now proceed by induction. For the first step we have thanks to the properties of conditional expectations and (9)

$$\begin{aligned}\mathbb{E}(Y_n \mid Y_{n-1}) &= \mathbb{E}(\Psi_{H_{n-1}}(Y_{n-1}) \mid Y_{n-1}) \\ &= \mathbb{E}(\Psi_h(Y_{n-1}) + \Psi_{H_{n-1}}(Y_{n-1}) - \Psi_h(Y_{n-1}) \mid Y_{n-1}) \\ &= \Psi_h(Y_{n-1}) + \mathcal{O}\big(\,\mathbb{E}(H_{n-1}^2 - h^2)\big).\end{aligned} \tag{10}$$

Conditioning with respect to the previous step therefore gives

$$\begin{aligned}\mathbb{E}(Y_n \mid Y_{n-2}) &= \mathbb{E}\left(\mathbb{E}(Y_n \mid Y_{n-1}) \mid Y_{n-2}\right) \\ &= \mathbb{E}\left(\Psi_h(Y_{n-1}) \mid Y_{n-2}\right) + \mathcal{O}\big(\,\mathbb{E}(H_{n-1}^2 - h^2)\big).\end{aligned} \tag{11}$$

Goes on like before... □

Theorem 2. *For the additive noise method*

$$\|\operatorname{Var} Y_n\|_F \leq C_1 t_n h^{2p} + C_2 t_n^4 h^{4p-2}, \tag{12}$$

where C_1, C_2 are positive constants independent of h and n.

Proof. Let us first remark that since $\operatorname{Var} Y_n$ is symmetric positive definite we have

$$\|\operatorname{Var} Y_n\|_F \leq \operatorname{tr}(\operatorname{Var} Y_n) = \mathbb{E}\|Y_n - \mathbb{E}\, Y_n\|^2. \tag{13}$$

Let us therefore work with the right hand side of the inequality above. By a telescopic sum, we obtain

$$\begin{aligned}&\mathbb{E}\|Y_n - \mathbb{E}\, Y_n\|^2 = \mathbb{E}\|\mathbb{E}(Y_n \mid Y_n) - \mathbb{E}(Y_n \mid y_0)\|^2 \\ &\quad = \mathbb{E}\|\sum_{j=0}^{n-1} \mathbb{E}(Y_n \mid Y_{n-j}) - \mathbb{E}(Y_n \mid Y_{n-j-1})\|^2 \\ &\quad = \sum_{j=0}^{n-1} \mathbb{E}\|\mathbb{E}(Y_n \mid Y_{n-j}) - \mathbb{E}(Y_n \mid Y_{n-j-1})\|^2 \\ &\qquad + 2\sum_{j=0}^{n-1}\sum_{k<j} \mathbb{E}\left(\,\mathbb{E}(Y_n \mid Y_{n-j}) - \mathbb{E}(Y_n \mid Y_{n-j-1}), \mathbb{E}(Y_n \mid Y_{n-k}) - \mathbb{E}(Y_n \mid Y_{n-k-1})\right)\end{aligned} \tag{14}$$

Let us consider the first term. Thanks to Lemma 1, we have

$$
\begin{aligned}
\mathbb{E}(Y_n \mid Y_{n-j}) - \mathbb{E}(Y_n \mid Y_{n-j-1}) &= \Psi_h^j(Y_{n-j}) - \Psi_h^{j+1}(Y_{n-j-1}) + \mathcal{O}\big(jh^{2p+1}\big) \\
&= \Psi_h^j\big(\Psi_h(Y_{n-j-1}) + \xi_{n-j-1}\big) - \Psi_h^{j+1}(Y_{n-j-1}) \\
&\quad + \mathcal{O}\big(jh^{2p+1}\big) \\
&= \mathrm{D}\Psi_h^j(\Psi_h(Y_{n-j-1}))\xi_{n-j-1} \\
&\quad + \mathrm{D}^2\Psi_h^j(\Psi_h(Y_{n-j-1}))(\xi_{n-j-1}, \xi_{n-j-1}) + \mathcal{O}\big(jh^{2p+1}\big).
\end{aligned} \tag{15}
$$

Hence, we get for a constant $C > 0$

$$
\begin{aligned}
\sum_{j=0}^{n-1} \mathbb{E}\|\mathbb{E}(Y_n \mid Y_{n-j}) - \mathbb{E}(Y_n \mid Y_{n-j-1})\|^2 &\leq C \sum_{j=0}^{n} (h^{2p+1} + j^2 h^{4p+2}) \\
&\leq C(t_n h^{2p} + t_n^3 h^{4p-1}).
\end{aligned} \tag{16}
$$

Introducing the notation

$$
P_{j,k} = \mathbb{E}\left(\mathbb{E}(Y_n \mid Y_{n-j}) - \mathbb{E}(Y_n \mid Y_{n-j-1}), \mathbb{E}(Y_n \mid Y_{n-k}) - \mathbb{E}(Y_n \mid Y_{n-k-1}) \right), \tag{17}
$$

we have for $k < j$ thanks to (15) and Assumption 1

$$
\begin{aligned}
P_{j,k} &= \mathbb{E}\left(\mathrm{D}\Psi_h^j(\Psi_h(Y_{n-j-1}))\xi_{n-j-1}, \mathrm{D}\Psi_h^k(\Psi_h(Y_{n-k-1}))\xi_{n-k-1}\right) + \mathcal{O}\big(jkh^{4p+2}\big) \\
&= \mathcal{O}\big(jkh^{4p+2}\big).
\end{aligned} \tag{18}
$$

Therefore, we obtain for a constant $C > 0$

$$
\sum_{j=0}^{n-1} \sum_{k<j} P_{j,k} \leq C t_n^4 h^{4p-2}, \tag{19}
$$

which concludes the proof. □

Theorem 3. *Assumption on local variance mimicking local error $\implies$ global error captured by variance.*

4 Calibration of the probabilistic integrator

- Constant in the error term, need for calibration
- Explanation of the procedure in [2]
- Proposal of a new technique? Proving it works?

5 Adaptive time stepping probabilistic

Is it doable?

6 Inverse problems

Is it possible to have an estimation of variance under posterior measure $\implies$ well-calibrated UQ on the parameter.

7 Numerical experiments

References

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[2] P. R. Conrad, M. Girolami, S. Särkkä, A. Stuart, and K. Zygalakis, *Statistical analysis of differential equations: introducing probability measures on numerical solutions*, Stat. Comput., (2016).