CONSERVATION HAMILTONIAN RTS-RK

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1. Mean Hamiltonian. Consider the Hamiltonian $E\colon \mathbb{R}^d \to \mathbb{R}$ and the ODE

$$y' = J^{-1}\nabla Q(y), \quad y(0) = y_0. \tag{1}$$

Applying a symplectic Runge Kutta method identified by its numerical flow Ψ, we have that the modified equation is still Hamiltonian and there exist functions E_j, $j = 2, \ldots$, such that

$$\tilde{Q}(y) = Q(y) + hQ_2(y) + h^2Q_3(y) + \ldots, \tag{2}$$

where h is the time step. The series in (2) does not converge, hence we consider the truncation after N terms

$$\tilde{Q}(y) = Q(y) + hQ_2(y) + \ldots + h^{N-1}Q_N(y). \tag{3}$$

Moreover, if q is the order of convergence for Ψ, we have that $E_i \equiv 0$ for $i = 2, \ldots, q$, hence

$$\tilde{Q}(y) = Q(y) + h^qQ_{q+1}(y) + \ldots + h^{N-1}Q_N(y). \tag{4}$$

Let us assume that E is analytic in a neighbourhood of y_0 and denoting $f = J^{-1}\nabla E$ that there exist positive constants R and M such that $\|f(y)\| \leq M$ for all $y \in B_{2R}(y_0) \subset \mathbb{R}^d$. Let us moreover introduce the constants μ and κ given by

$$\mu = \sum_{i=1}^{s} |b_i|, \quad \kappa = \max_{i=1,\ldots,s} \sum_{j=1}^{s} |a_{ij}|, \tag{5}$$

where $\{b_i\}_{i=1}^s$ and $\{a_{ij}\}_{i,j=1}^s$ are the coefficients of the Runge-Kutta method. Finally, let us introduce the constant $\eta = \max\{\kappa, \mu/(2\log 2 - 1)\}$. Denoting by $\tilde{\varphi}_{N,t}(y)$ the flow of the equation corresponding to $\tilde{E}$, we have that the local error satisfies [1, Theorem IX.7.6]

$$\|\Psi_h(y_0) - \tilde{\varphi}_{N,h}(y_0)\| \leq h\gamma M e^{-I_0/h}, \tag{6}$$

for all $h \leq I_0/4$, where $I_0 = R/(eM\eta)$ and $\gamma = e(2 + 1.65\eta + \mu)$.

[...]

Lemma 1.1. *Assume there exists a function $g\colon \mathbb{R}_+ \to (1, +\infty)$ such that $H_i \leq g(h)h$ almost surely. Then under the assumption ...,*

$$\mathbb{E}\,\tilde{Q}(Y_n) - \tilde{Q}(y_0) = \mathcal{O}\big(e^{-I_0/(2g(h)h)}\big), \tag{7}$$

$$\mathbb{E}\,Q(Y_n) - Q(y_0) = \mathcal{O}\big(h^q\big), \tag{8}$$

over exponentially long time intervals $nh \leq e^{I_0/(2g(h)h)}$.

Proof. We exploit the conservation of $\tilde{E}$ along the trajectories of its corresponding dynamical system, i.e., $\tilde{E}(\tilde{\varphi}_{N,z}(y)) = \tilde{Q}(y)$ for $y \in \mathbb{R}^d$ and $z > 0$ and employ a telescopic sum to obtain

$$\begin{aligned}
\mathbb{E}\,\tilde{Q}(Y_n) - \tilde{Q}(y_0) &= \sum_{j=1}^{n} \mathbb{E}\left(\tilde{Q}(Y_{j-1}) - \tilde{Q}(Y_{j-1})\right)\\
&= \sum_{j=1}^{n} \mathbb{E}\left(\tilde{Q}(Y_{j-1}) - \tilde{Q}(\tilde{\varphi}_{N,H_{j-1}}(Y_{j-1}))\right)\\
&= \sum_{j=1}^{n} \mathbb{E}\,\mathbb{E}\left(\tilde{Q}(Y_{j-1}) - \tilde{Q}\tilde{\varphi}_{N,H_{j-1}}(Y_{j-1})) \mid H_{j-1}\right),
\end{aligned} \tag{9}$$

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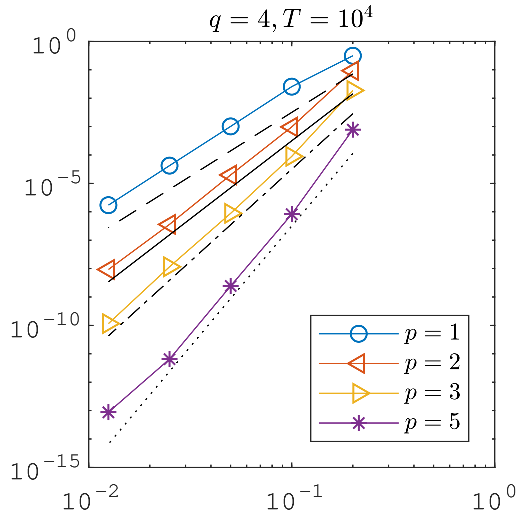

Fig. 1: Convergence of the standard deviation, $h = \{0.2, 0.1, 0.05, 0.025, 0.0125\}$. Reference slopes correspond to $n^{1/2}h^{q+p}$.

where we applied the total expectation with respect to H_{j-1} for the last equality. Then, as E is Lipschitz with constant independent of h and under the assumptions on $\{H_i\}_{i\geq 0}$ and (6) we have

$$
\begin{aligned}
\mathbb{E}\,\tilde{Q}(Y_n) - \tilde{Q}(y_0) &\leq C\sum_{j=0}^{n-1}\mathbb{E}\left(H_j e^{-I_0/H_j}\right) \\
&= Cn\,\mathbb{E}\left(H_0 e^{-I_0/H_0}\right),
\end{aligned} \tag{10}
$$

where the equality is given by the assumption of the random time steps being *i.i.d.* Thanks to the assumption $H_0 \leq g(h)h$ a.s., we have

$$
\mathbb{E}\,\tilde{Q}(Y_n) - \tilde{Q}(y_0) \leq nhe^{-I_0/(g(h)h)}, \tag{11}
$$

which implies the first result. The second result derives then immediately as $Q_{q+1} + hQ_{q+2} + \ldots + h^{N-q-1}Q_N$ is uniformly bounded independently of h. ∎

2. Distribution. Guess by numerics, Figure 1, Kepler system, two-stage Gauss ($q = 4$). Over exponentially long times

$$
\sigma_n = \mathrm{Var}(Q(Y_n))^{1/2} = \mathcal{O}(n^{1/2}h^{q+p}), \tag{12}
$$

REFERENCES

[1] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer Series in Computational Mathematics 31, Springer-Verlag, Berlin, second ed., 2006.