

Numerical Integration with Lie-Series and Result Verification

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Keywords: ODEs, Result Verification, Interval Methods

Introduction

In the present work, a method is presented for determining a verified upper bound on the global error of solutions of systems of ordinary differential equations. Here, the requirement is that the integration method for solving the system is given not only as a sequence of numbers referred to discrete times, but as a whole differentiable function, approximating the exact solution over an appropriate time interval. Integration methods under consideration include Taylor expansion based methods, like Lie series integration [1, 2] or neural networks based methods like physics informed neural networks [4].

Suppose some approximate solution $\tilde{x}(t)$ for $t \in I \subseteq \mathbb{R}$ on some open interval I is given, meeting the above requirements. The approximation solves the system of ordinary differential equations $\dot{x} = F(x)$ with $x \subseteq \mathbb{R}^n$ and some initial condition $x(t_0) = x_0$ where the global error of the approximate solution is unknown. Then in the following a method is presented, which computes afterwards a certified upper bound for the global error of the calculated solution. The global error is calculated either for the whole Interval I or at least for some open interval $I' \subseteq I$ containing $t_0 \in I'$.

Basic properties

The presented method is based on the calculation of the difference $\dot{\tilde{x}}(t) - F(\tilde{x}(t))$ which can, according to the requirements, be executed on the whole interval I . This difference represents some kind of local error and can be controlled by the integration method. It determines the accuracy of the approximation for each $t \in I$. In order to derive an upper bound for the global error, write $\tilde{x}(t) = \tilde{x}_0 + \int_{t_0}^t \dot{\tilde{x}}(\tau) d\tau$ with $\tilde{x}_0 = \tilde{x}(t_0)$, which can be written, since the approximation is demanded to be differentiable. It follows for the global error at time t :

$$\begin{aligned} |x_i(t) - \tilde{x}_i(t)| &\leq \int_{t_0}^t |\dot{x}_i(\tau) - \dot{\tilde{x}}(\tau)| d\tau + |x_{0_i} - \tilde{x}_{0_i}| \\ &\leq \max_{\tau \in [t_0, t]} \{|\dot{x}_i(\tau) - \dot{\tilde{x}}(\tau)|\} \cdot (t - t_0) + |x_{0_i} - \tilde{x}_{0_i}| \end{aligned}$$

for $i = 1, 2, \dots, n$ and $t \in I$. Finally, the equations of motion can be applied and gives

$$|\dot{x}_i(t) - \dot{\tilde{x}}(t)| \leq |F_i(x(t)) - F_i(\tilde{x}(t))| + |\dot{\tilde{x}}_i(t) - F_i(\tilde{x}(t))|$$

with the first term representing a recursion term and the second term controlled by the integration method.

Main results

To resolve the recursion, rewrite the above inequalities in the form $|\dot{x}_i(t + \Delta t) - \dot{\tilde{x}}(t + \Delta t)| - |\dot{x}_i(t) - \dot{\tilde{x}}(t)| \leq \Delta t \cdot \max_{\tau \in [t, t + \Delta t]} \{|F_i(x(\tau)) - F_i(\tilde{x}(\tau))|\} + \Delta t \cdot \max_{\tau \in [t, t + \Delta t]} \{|\dot{\tilde{x}}_i(\tau) - F_i(\tilde{x}(\tau))|\}$ by introducing a small time interval Δt with $[t, t + \Delta t] \subseteq I$. Applying Taylor's formula gives the right hand side $\Delta t \cdot \max_{\substack{\tau \in [t, t + \Delta t] \\ \Theta \in [0, 1]}} \left\{ \sum_k \left| \frac{\partial F_i}{\partial x_k}(x(\tau) + \Theta \cdot (\tilde{x}(\tau) - x(\tau))) \right| \cdot |x_k(\tau) - \tilde{x}_k(\tau)| \right\} + \Delta t \cdot \max_{\tau \in [t, t + \Delta t]} \{|\dot{\tilde{x}}_i(\tau) - F_i(\tilde{x}(\tau))|\}$. Introducing the global error function $\varepsilon_i(t) = |x_i(t) - \tilde{x}_i(t)|$ and the error function of the method $\varepsilon_{0_i}(t) = |\dot{\tilde{x}}_i(t) - F_i(\tilde{x}(t))|$, then executing the limit $\Delta t \rightarrow 0$ gives the differential inequality $\dot{\varepsilon}_i(t) \leq \sum_k \max_{\underline{\xi} \in B_{\underline{\varepsilon}(t)}(x(t))} \left\{ \left| \frac{\partial F_i}{\partial x_k}(\underline{\xi}) \right| \right\} \cdot$

$\varepsilon_k(t) + \varepsilon_{0_i}(t)$ for $i = 1, 2, \dots, n$. The tightest upper bound for the global error gives the *information equality*

$$\dot{\underline{\varepsilon}}(t) = M(\underline{x}(t)) \cdot \underline{\varepsilon}(t) + D(\underline{x}(t), \underline{\varepsilon}(t)) \cdot \underline{\varepsilon}(t) + \underline{\varepsilon}_0(t) \quad (1)$$

with the matrices $M(\underline{x}) = (m_{ij}(\underline{x}))$, $m_{ij} = \left| \frac{\partial F_i}{\partial x_j}(\underline{x}) \right|$ and $D(\underline{x}, \underline{\varepsilon}) = (d_{ij}(\underline{x}, \underline{\varepsilon}))$ with $d_{ij}(\underline{x}, \underline{\varepsilon}) = \max_{\xi \in B_{\underline{\varepsilon}}(\underline{x})} \left\{ \left| \frac{\partial F_i}{\partial x_j}(\xi) \right| - \left| \frac{\partial F_i}{\partial x_j}(\underline{x}) \right| \right\}$.

The right hand side of the information equality contains 3 terms. In the limit of vanishing errors, $\varepsilon \rightarrow 0$ and $\varepsilon_0 \rightarrow 0$, only the first term remains. Thus M represents the intrinsic dynamic instability of the underlying dynamis of the system. The generation of error due to the dynamic instability is related to the positive Liapunov exponents [5]. The second term is due to the actual uncertainty and represents error propagation. Even for a absolutely precise method, $\varepsilon_0 \rightarrow 0$, this term still remains. Finally the third term represents the local error created by the integration method.

The information equation is not only of theoretical interest. At first sight, obtaining a certified solution of a system of ODEs needs to solve the additional equation (1) which also needs to be certified. So it seems to be a circular approach. This obstacle can be overcome by calculating a poorer upper bound the following way. First, by interchanging $\underline{x}(t)$ and $\tilde{x}(t)$ when applying Taylor's formula, instead of (1), $\dot{\underline{\varepsilon}}(t) = M(\tilde{x}(t)) \cdot \underline{\varepsilon}(t) + D(\tilde{x}(t), \underline{\varepsilon}(t)) \cdot \underline{\varepsilon}(t) + \underline{\varepsilon}_0(t)$ can be derived. Second, set an a priori upper bound $\underline{\varepsilon}_{max}$ for the global error. This error is used in the second term of the above equation leading to $\dot{\underline{\varepsilon}}(t) = \tilde{M}(\tilde{x}(t)) \cdot \underline{\varepsilon}(t) + \underline{\varepsilon}_0(t)$ with $\tilde{M}(\tilde{x}(t)) = M(\tilde{x}(t)) + D(\tilde{x}(t), \underline{\varepsilon}_{max})$. This equation can be integrated analytically and the solution is $\underline{\varepsilon}(t) = \exp(\int_{t_0}^t \tilde{M}(\tilde{x}(\tau)) d\tau) \cdot \left(\int_{t_0}^t \exp(-\int_{t_0}^{\tau'} \tilde{M}(\tilde{x}(\tau)) d\tau) \cdot \underline{\varepsilon}_0(\tau') d\tau' + \underline{\varepsilon}(t_0) \right)$ which can be solved in a certified way by numerical integration with an interval method [6]. Suppose that the integration method is a Lie series expansion [2]. Then the local error $\underline{\varepsilon}_0(t)$ can be controlled by the order of the Lie series. A certified upper bound for the global error $\underline{\varepsilon}(t)$ at any time $t \in I'$ or a global upper bound on the whole interval I' can be calculated by subdividing the interval I' and calculating an interval enclosure of the

above integral ([6], Section 9.1). By appropriately choosing the subdivision, the enclosure can be sharpened. Finally, with this method it is also possible to determine a time interval $I'' \subseteq I'$, $t_0 \in I''$, with the property that the global error is bound by some a priori given value ε_{max} .

Some well known systems of ODEs are considered and numerical experiments are done to illustrate and validate the method.

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