Interval of effective time-step size for the numerical computation of nonlinear ordinary differential equations

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ABSTRACT
The computational uncertainty principle states that the numerical computation of nonlinear ordinary differential equations (ODEs) should use appropriately sized time steps to obtain reliable solutions. However, the interval of effective step size (IES) has not been thoroughly explored theoretically. In this paper, by using a general estimation for the total error of the numerical solutions of ODEs, a method is proposed for determining an approximate IES by translating the functions for truncation and rounding errors. It also illustrates this process with an example. Moreover, the relationship between the IES and its approximation is found, and the relative error of the approximation with respect to the IES is given. In addition, variation in the IES with increasing integration time is studied, which can provide an explanation for the observed numerical results. The findings contribute to computational step-size choice for reliable numerical solutions.

KEYWORDS
ordinary differential equations; interval of effective step size; computational uncertainty principle; integration time; relative error

ARTICLE HISTORY
Received 10 April 2016
Revised 28 April 2016
Accepted 6 May 2016

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1. Introduction

Many works have shown the time-step sensibility of nonlinear dynamical systems. Li, Zeng, and Chou (2000, 2001) and Li (2000) proposed the computational uncertainty principle (CUP) for nonlinear systems of ordinary differential equations (ODEs) under a finite machine precision. The CUP states that using different time-step sizes usually results in different effective computation times (ECTs) and that the maximal ECT (MECT), achieved using the optimal step size (OS), gives the best result. Wang and Huang (2006) focused on Lorenz systems, and reported that the maximum prediction time sensitively relies on the time-step size under certain conditions. Teixeira, Reynolds, and Judd (2007) found the time-step size to affect not only Lorenz systems but also a quasi-geostrophic model. Liu et al. (2015) studied the Global/Regional Assimilation and Prediction System mesoscale numerical forecast, and gave a preliminary explanation of the applicability of OS theory to complicated partial differential equations (PDEs).

The CUP presented by Li, Zeng, and Chou (2000, 2001) theoretically explained the time-step sensibility of nonlinear ODEs, which has been cited by many other researches (Hu and Chou 2004; Li and Wang 2008; Liu et al. 2015; Wang, Li, and Li 2012; Wang, Liu, and Li 2014). In particular, based on the CUP, Wang, Li, and Li (2012) deduced a general ECT function of step size, which explained the experimental formulae proposed by Teixeira, Reynolds, and Judd (2007).

Through a large number of numerical experiments, Li, Zeng, and Chou (2000) introduced the concept of the interval of effective step size (IES) of ODEs. Presenting the IES profiles obtained from numerical results (Figure 1), Li, Zeng, and Chou (2001) suggested that numerical solutions are reliable when step sizes belong to the IES. In such cases, if we know the theoretical formulae of lower and upper bounds of the IES corresponding to a certain error tolerance, it will guide the choices of effective step sizes in computations. However, there has been little relevant prior research in this regard.

This paper explores the IES for nonlinear ODEs based on the studies of Li, Zeng, and Chou (2000, 2001). Let $U_t = [h_{t,1}, h_{t,2}]$ denote the IES at integral time $t$ under a
given error tolerance $\delta$. To obtain $U_t^*$, it is necessary to give a general formula of the numerical error $E(t, h)$ for the solutions of nonlinear ODEs. In numerical calculation, $E(t, h)$ is usually composed of three parts: truncation error, which is caused by differential equation discretization (Gear 1971; Stoer and Bulirsch 1993); round-off error, which is due to limitations of computer precision (Li, Zeng, and Chou 2000, 2001); and initial error (Ding and Li 2008a, 2008b, 2012). From Li, Zeng, and Chou (2001, Equations (60) and (83)), it can be shown that

$$\|E(t, h)\| \leq C(t)[E_1(h) + E_2(h) + Ne_{(0)}],$$

(1)

where $E_1(h) = C_1h^{0.5}$ is relevant to the round-off error; $E_2(h) = C_2h^p$ is relevant to the truncation error, and $p$ is the order of the numerical method; $e_{(0)}$ is relevant to the initial error, and

$$C(t) = e^{\delta E(t-1)/\sqrt{C_1}}.$$  

(2)

The way to estimate $C_1$ and $C_2$, and details of other parameters, are given in Li, Zeng, and Chou (2001, Equations (60) and (83)). Letting $\delta_1 = \delta/C(t)Ne_{(0)}$ and $\tilde{E}(h) = E_1(h) + E_2(h)$, Equation (1) indicates that $h_{t,1}$ and $h_{t,2}$ should be the solutions of the equation

$$\tilde{E}(h) = \delta_1.$$  

(3)

For a fixed value of $t$, Equation (3) is a nonlinear equation associated with $h$, which can be solved numerically to obtain approximate values of $h_{t,1}$ and $h_{t,2}$ by methods such as fixed-point iteration and Newtonian iteration (Suli and Mayers 2003); however, it is usually hard to provide function expressions for $h_{t,1}$ and $h_{t,2}$ with these methods. This article aims to derive explicit formulae for $h_{t,1}$ and $h_{t,2}$ so as to give a general approximate explicit expression for $U_t$.

2. Method for determining $U_t^*$, an approximation of $U_t$

First, defining $(h_{\text{cross}}, E_{\text{cross}})$ as the intersection of the functions $E_i(h)$ and $E_j(h)$, one gets

$$h_{\text{cross}} = C_{1i}^{\frac{1}{2p}}, \text{ and } E_{\text{cross}} = C_{2i}^\frac{1}{2p},$$

(4)

where $C_{ij} = C_i/C_j$. Besides, Li, Zeng, and Chou (2000, 2001) stated that $\hat{E}(h)$ reaches its minimum $E_{\text{min}}$ when the step size $h$ takes the value of OS, and when the OS denoted by $H$, there are

$$H = \left(\frac{C_{12}}{2p}\right)^{\frac{1}{2p}}, \text{ and } E_{\text{min}} = C_2(2p + 1)\left(\frac{C_{12}}{2p}\right)^{\frac{1}{2p}}.$$  

(5)

Then, we simultaneously translate the functions $E_i(h)$ and $E_j(h)$ so as to move the coordinates of their intersection from $(h_{\text{cross}}, E_{\text{cross}})$ to the lowest point $(H, E_{\text{min}})$ of $\hat{E}(h)$. Let $E_i^*(h)$ and $E_j^*(h)$ denote the translated functions, which are $E_i^*(h) = (1 + 1/2p)E_i(h)$, and $E_j^*(h) = (2p + 1)E_j(h)$. Finally, let $E_i^*(h)$ and $E_j^*(h)$ equal $\delta_1$ respectively to obtain two new equations whose solutions are

$$h_{t,1}^* = \left[\frac{C_1(1 + \frac{1}{2p})}{\delta_1}\right]^2, \text{ and } h_{t,2}^* = \left[\frac{\delta_1}{C_2(2p + 1)}\right]^\frac{1}{2p}.$$  

(6)

Then we regard $U_t^* = [h_{t,1}^*, h_{t,2}^*]$ as the approximation of $U_t$ when $h_{t,1}^* \leq h_{t,2}^*$. Taking the situation of $p = C_1 = C_2 = 1$ as an example, the above process is shown in Figure 2.

3. Relationship between $U_t$ and $U_t^*$

From the above definitions we find: as step size $h$ decreases, $\hat{E}(h)$ initially monotonically decreases to its lowest point $(H, E_{\text{min}})$ before monotonically increasing; $E_i^*(h)$ is a monotonically decreasing function, whereas $E_j^*(h)$ is a monotonically increasing function of $h$, and their intersection is $(H, E_{\text{min}})$; it is easy to prove that when $h < H, E_i^*(h) > \hat{E}(h)$ is always true, and when $h > H, E_j^*(h) > \hat{E}(h)$ is true. Given these, we have:

$$\begin{cases}
\text{When } \delta_1 > E_{\text{min}}, h_{t,1}^* < h_{t,2}^* < H < h_{t,2}^* < h_{t,2}; \\
\text{when } \delta_1 = E_{\text{min}}, h_{t,1}^* = h_{t,2}^* = H = h_{t,2}; \\
\text{when } \delta_1 < E_{\text{min}}, h_{t,1}^* > h_{t,2}^*, \text{ and } h_{t,2}^* \text{ do not exist, and } h_{t,1}^* > h_{t,2};
\end{cases}$$

which does not conform to the definition of $U_t^*$.

From the statements above we know that $U_t^* \subset U_t$ when $\delta_1 > E_{\text{min}}$, and $U_t^* = U_t = (H)$ when $\delta_1 = E_{\text{min}}$; however, when $\delta_1 < E_{\text{min}}$, both $U_t$ and $U_t^*$ are empty sets. These results indicate that $U_t^* \subset U_t$ is always true, which suggests that $U_t^*$ is suitable for serving as an approximate interval $U_t$. In
addition, to obtain a non-empty set \( U^*_t \), we suppose that \( \tilde{\delta}_t \geq E_{\text{min}} \) in the following discussion.

Next, we estimate the error of the approximation \( U^*_t \) with respect to \( U_t \). For this purpose, let \( \Delta_{1,1} = |h_{t,1}^* - h_{t,1}| \) and \( \Delta_{1,2} = |h_{t,2}^* - h_{t,2}| \). Assuming that \( \tilde{\delta}_t \geq E_{\text{min}} \), the relative errors of \( h_{t,1}^* \) and \( h_{t,2}^* \) with respect to \( h_{t,1} \) and \( h_{t,2} \) are respectively

\[
\frac{\Delta_{1,1}}{h_{t,1}} = \left( 1 + \frac{1}{2p} \right)^2 \left( 1 + \frac{h_{t,1}^{p+0.5}}{C_{t,1}} \right)^2 - 1,
\]

and

\[
\frac{\Delta_{1,2}}{h_{t,2}} = 1 - \left( C_{t,2} h_{t,2}^{p+0.5} + 1 \right)^2 (2p + 1)^{-1}.
\]

Obviously, \( h_{t,1} \in [0, H] \) and \( h_{t,2} \in [H, \infty) \) when \( \tilde{\delta}_t \geq E_{\text{min}} \), and when \( h_{t,1} \in [0, H] \), \( \Delta_{1,1}/h_{t,1} \) decreases monotonically with increasing \( h_{t,1} \), and when \( h_{t,2} \in [H, \infty) \), \( \Delta_{1,2}/h_{t,2} \) increases monotonically with increasing \( h_{t,2} \). These lead to

\[
\sup_{0 < h_{t,1} < H} \left| \frac{\Delta_{1,1}}{h_{t,1}} \right| = (1 + 1/2p)^2 - 1, \quad \inf_{h_{t,1} > 0} \left| \frac{\Delta_{1,1}}{h_{t,1}} \right| = 0,
\]

\[
\sup_{H < h_{t,2} < \infty} \left| \frac{\Delta_{1,2}}{h_{t,2}} \right| = 1 - (2p + 1)^{-1/p}, \quad \inf_{H < h_{t,2} < \infty} \left| \frac{\Delta_{1,2}}{h_{t,2}} \right| = 0.
\]

Equation (8) indicates that \( |\Delta_{1,1}/h_{t,1}| \) (or \( |\Delta_{1,2}/h_{t,2}| \)) arrives at its infimum zero when \( h_{t,1} \) (or \( h_{t,2} \)) equals \( H \), and both suprema of \( |\Delta_{1,1}/h_{t,1}| \) and \( |\Delta_{1,2}/h_{t,2}| \) are only relevant to the numerical method order \( p \). Table 1 lists the values of the suprema for \( p \) values of 1 to 10; both of these suprema tend to decrease with increasing \( p \).

**Table 1.** Supremums of relative errors \( |\Delta_{1,1}/h_{t,1}| \) and \( |\Delta_{1,2}/h_{t,2}| \) with different choices of the numerical method order \( p \).

| \( p \) | \( \sup_{0 < h_{t,1} < H} |\Delta_{1,1}/h_{t,1}| \) | \( \sup_{H < h_{t,2} < \infty} |\Delta_{1,2}/h_{t,2}| \) |
|---|---|---|
| 1 | 1.25 | 0.67 |
| 2 | 0.56 | 0.55 |
| 3 | 0.36 | 0.48 |
| 4 | 0.27 | 0.42 |
| 5 | 0.21 | 0.38 |
| 6 | 0.17 | 0.35 |
| 7 | 0.15 | 0.32 |
| 8 | 0.13 | 0.30 |
| 9 | 0.11 | 0.28 |
| 10 | 0.10 | 0.26 |

**Figure 2.** Relation diagram of the IES \( U_t \) and its approximate interval \( U^*_t \).

Notes: The solid curve denotes \( E(h) = h^{-\frac{3}{2}} + h \); the grey solid line denotes \( E(h) = h^{-\frac{3}{2}} \); the black solid line denotes \( E(0) = h; \) the asterisk denotes \( (h_{t,1}, E_{\text{min}}) \); the grey dashed line denotes \( E(h) = 1.5 h^{-\frac{3}{2}} \); the black dashed line denotes \( E(h) = 3 h^{-\frac{3}{2}} \); and the black solid dot denotes \( (H, E_{\text{min}}) \).

**Figure 3.** Schematic representation of the variations in the IES \( U_t \) (solid line) and its approximate interval \( U^*_t \) (dotted line) with increasing integration time \( t \).

**4. Variations in \( U_t \) and \( U^*_t \) with increasing integration time \( t \)**

First, we investigate the variation in \( U^*_t \) with increasing \( t \). Given Equation (6) and considering that \( \tilde{\delta}_t = \delta/C(t) – \text{Ne}_{(0)} \) monotonically decreases with \( t \) (Li, Zeng, and Chou 2001), \( h_{t,1}^* \) increases monotonically and \( h_{t,2}^* \) decreases monotonically with increasing \( t \). That is, as the integral time \( t \) increases, the length of the interval \( U_t^* \) gradually shortens, and eventually becomes a point, which is the OS. This helps to explain the profile shape of the IES in Figure 1.

We next discuss the relationship between \( U_t \) and \( U_t^* \) as \( t \) increases. We denote the MECT by \( T \), and from Li, Zeng, and Chou (2001),

\[
T = \frac{1}{C_t} \ln \left[ \frac{\delta \sqrt{\tilde{C}_t}}{C_t(1 + 1/2p) / \sqrt{H + \text{Ne}_{(0)}}} \right] + t_0.
\]

It is easy to prove that \((\tilde{\delta}_t - \text{E}_{\text{min}})/(T-t) > 0\). From the analysis in section 3, \( U_t^* < U_t \) for \( t < T \), and \( U_t = U_t^* = \{H\} \) for \( t = T \), and both \( U_t \) and \( U_t^* \) are empty sets for \( t > T \). Figure 3 shows a schematic representation of the variations in \( U_t \) and \( U_t^* \) with increasing \( t \).
5. Conclusion and prospection

The unified estimation in Equation (1) for the total error of the numerical solutions for nonlinear ODEs is used here to give a general formula, Equation (6), for determining $U^*_t$, which is an approximation of the IES $U_t$. The analyses given in sections 3 and 4 show that if the error limit $\delta$ satisfies $\delta \geq C(t)(E_{min} + Ne_{op})$, and if the integration time $t$ is not greater than the MECT $T$, there will always be $U^*_t \subseteq U_t$; otherwise, both $U_t$ and $U^*_t$ are empty sets. This result indicates that $U^*_t$ is suitable for approximating the interval $U_t$. In addition, formulae for the relative error of $U^*_t$ with respect to $U_t$ are given, and numerical results suggest that the supremums of the relative errors tend to decrease with increasing numerical method order $p$. Finally, the variation in $U_t$ and $U^*_t$ with increasing integral time $t$ are studied (Figure 3) and used to explain the profile shape of the IES (Figure 1) in Li, Zeng, and Chou (2000).

For the IES, this article only studies nonlinear systems of ODEs. Further research is expected to consider complex PDEs and would aid in choosing an effective step size in numerical computation. In addition, the use of a higher order scheme such as the Taylor Series Method (Wang, Li, and Li 2012) in obtaining a reliable solution could effectively reduce computation time when giving a fixed step size. Thus, the method of applying the IES is not the only choice to compute ODEs.

Disclosure statement

No potential conflict of interest was reported by the authors.

Funding

This study was supported by the National Natural Science Foundation of China [grant numbers 41375110, 11471244].

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