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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.

摘要
由于满足计算的不确定性原理，需适当选取时间步长以保证非线性常微分方程组数值解的可靠性，目前尚未见关于有效步长区间的理论结果。本文对于给定的误差限，将方法截断误差与机器舍入误差的相关曲线分别进行平移，从而得到一种确定有效步长近似区间的方法，并推导出近似区间相比于原区间的相对误差公式。另外，研究了有效步长区间随积分时间的变化规律，并对已有的数值结果给出解释。本文所得结论可为数值求解常微分方程组选取有效步长并得到可靠的数值解提供理论支持。

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关键词
常微分方程; 有效步长区间; 不确定性原理; 积分时间; 相对误差

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 (2000) 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 $U_t = [h_{t,1}, h_{t,2}]$ ($h_{t,1} \le h_{t,2}$) denote the IES at integral time t under a

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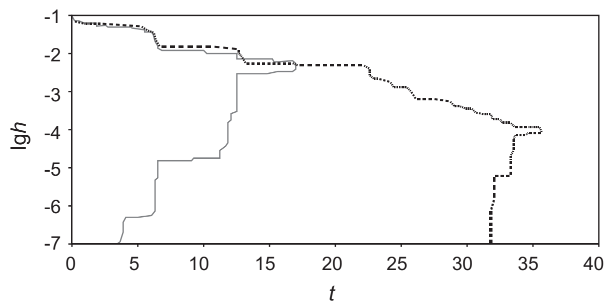

Figure 1. IES profiles obtained using the optimal searching method, when computing the solutions of the *x*-component of the Lorenz equation using the fourth-order Runge–Kutta method for the initial value (5, 5, 10) and $r = 28$ and for 121 different step sizes in the range 10^{-7}–10^{-1}. Source: Li, Zeng, and Chou (2000, Plate I-2(c)).

Notes: Here, the step size h is plotted as a logarithm (to base 10) and time is non-dimensional. The grey solid line is for machine single precision and the black dotted line is for double precision.

given error tolerance δ. To obtain U_t, it is necessary to give a general formula of the numerical error $\boldsymbol{E}(t, h)$ for the solutions of nonlinear ODEs. In numerical calculation, $\boldsymbol{E}(t, h)$ 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

$$\|\boldsymbol{E}(t,h)\| \le C(t)\left[E_1(h) + E_2(h) + Ne_{(0)}\right], \tag{1}$$

where $E_1(h) = C_1 h^{-0.5}$ is relevant to the round-off error; $E_2(h) = C_2 h^p$ is relevant to the truncation error, and p is the order of the numerical method; $e_{(0)}$ is relevant to the initial error, and

$$C(t) = e^{\hat{C}_L \hat{\Gamma}(t-t_0)} / \sqrt{\hat{C}_L}. \tag{2}$$

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 $\tilde{\delta}_t = \delta/C(t) - Ne_{(0)}$ 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

$$\tilde{E}(h) = \tilde{\delta}_t. \tag{3}$$

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 $E_1(h)$ and $E_2(h)$, one gets

$$h_{\text{cross}} = C_{12}^{\frac{1}{p+0.5}}, \text{ and } E_{\text{cross}} = C_2 C_{12}^{\frac{p}{p+0.5}}, \tag{4}$$

where $C_{12} = C_1/C_2$. Besides, Li, Zeng, and Chou (2000, 2001) stated that $\tilde{E}(h)$ reaches its minimum $E_{\min}$ when the step size h takes the value of OS, and when the OS denoted by H, there are

$$H = \left(\frac{C_{12}}{2p}\right)^{\frac{1}{p+0.5}}, \text{ and } E_{\min} = C_2(2p+1)\left(\frac{C_{12}}{2p}\right)^{\frac{p}{p+0.5}}. \tag{5}$$

Then, we simultaneously translate the functions $E_1(h)$ and $E_2(h)$ so as to move the coordinates of their intersection from $(h_{\text{cross}}, E_{\text{cross}})$ to the lowest point $(H, E_{\min})$ of $\tilde{E}(h)$. Let $E_1^*(h)$ and $E_2^*(h)$ denote the translated functions, which are $E_1^*(h) = (1 + 1/2p)E_1(h)$, and $E_2^*(h) = (2p+1)E_2(h)$. Finally, let $E_1^*(h)$ and $E_2^*(h)$ equal $\tilde{\delta}_t$ respectively to obtain two new equations whose solutions are

$$h_{t,1}^* = \left[\frac{C_1\left(1 + \frac{1}{2p}\right)}{\tilde{\delta}_t}\right]^2, \text{ and } h_{t,2}^* = \left[\frac{\tilde{\delta}_t}{C_2(2p+1)}\right]^{\frac{1}{p}}. \tag{6}$$

Then we regard $U_t^* = [h_{t,1}^*, h_{t,2}^*]$ as the approximation of U_t when $h_{t,1}^* \le h_{t,2}^*$. 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, $\tilde{E}(h)$ initially monotonically decreases to its lowest point $(H, E_{\min})$ before monotonically increasing; $E_1^*(h)$ is a monotonically decreasing function, whereas $E_2^*(h)$ is a monotonically increasing function of h, and their intersection is $(H, E_{\min})$; it is easy to prove that when $h < H$, $E_1^*(h) > \tilde{E}(h)$ is always true, and when $h > H$, $E_2^*(h) > \tilde{E}(h)$ is true. Given these, we have:

$$\begin{cases} \text{When } \tilde{\delta}_t > E_{\min}, h_{t,1} < h_{t,1}^* < H < h_{t,2}^* < h_{t,2}; \\ \text{when } \tilde{\delta}_t = E_{\min}, h_{t,1} = h_{t,1}^* = H = h_{t,2}^* = h_{t,2}; \\ \text{when } \tilde{\delta}_t < E_{\min}, h_{t,1} \text{ and } h_{t,2} \text{ do not exist, and } h_{t,1}^* > h_{t,2}^*, \\ \text{which does not conform to the definition of } U_t^*. \end{cases}$$

From the statements above we know that $U_t^* \subset U_t$ when $\tilde{\delta}_t > E_{\min}$, and $U_t^* = U_t = \{H\}$ when $\tilde{\delta}_t = E_{\min}$; however, when $\tilde{\delta}_t < E_{\min}$, both U_t and U_t^* are empty sets. These results indicate that $U_t^* \subseteq U_t$ is always true, which suggests that U_t^* is suitable for serving as an approximate interval U_t. In

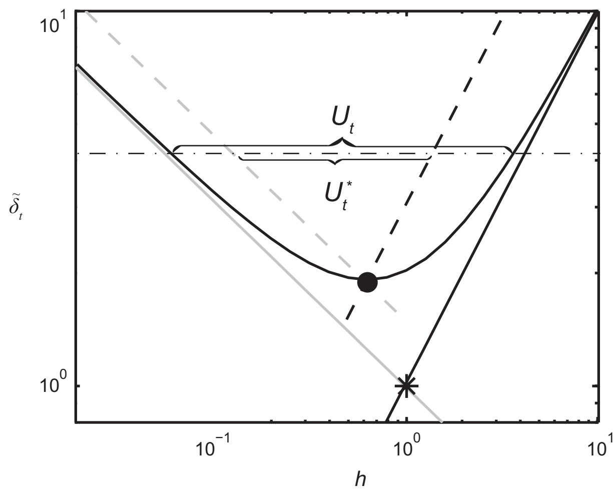

Figure 2. Relation diagram of the IES U_t and its approximate interval U_t^*.

Notes: The solid curve denotes $\tilde{E}(h) = h^{-0.5}+h$; the grey solid line denotes $E_1(h) = h^{-0.5}$; the black solid line denotes $E_2(h) = h$; the asterisk denotes (h_{cross}, E_{cross}); the grey dashed line denotes $E_1^*(h) = 1.5h^{-0.5}$; the black dashed line denotes $E_2^*(h) = 3h$; and the black solid dot denotes (H, E_{min}).

addition, to obtain a non-empty set U_t^*, we suppose that $\tilde{\delta}_t \geq E_{min}$ in the following discussion.

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

$$\left|\Delta_{t,1}/h_{t,1}\right| = \left(1+\frac{1}{2p}\right)^2\left(1+h_{t,1}^{p+0.5}/C_{12}\right)^{-2}-1,$$

$$\text{and } \left|\Delta_{t,2}/h_{t,2}\right| = 1-\left(C_{12}h_{t,2}^{-(p+0.5)}+1\right)^{\frac{1}{p}}(2p+1)^{-\frac{1}{p}}. \qquad (7)$$

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

$$\sup_{0\leq h_{t,1}\leq H}\left|\Delta_{t,1}/h_{t,1}\right| = (1+1/2p)^2-1, \quad \inf_{0\leq h_{t,1}\leq H}\left|\Delta_{t,1}/h_{t,1}\right| = 0,$$

$$\sup_{H\leq h_{t,2}<\infty}\left|\Delta_{t,2}/h_{t,2}\right| = 1-(2p+1)^{-1/p}, \quad \inf_{H\leq h_{t,2}<\infty}\left|\Delta_{t,2}/h_{t,2}\right| = 0. \qquad (8)$$

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

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

p	$\sup_{0\leq h_{t,1}\leq H}\left\|\Delta_{t,1}/h_{t,1}\right\|$	$\sup_{H\leq h_{t,2}<\infty}\left\|\Delta_{t,2}/h_{t,2}\right\|$
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

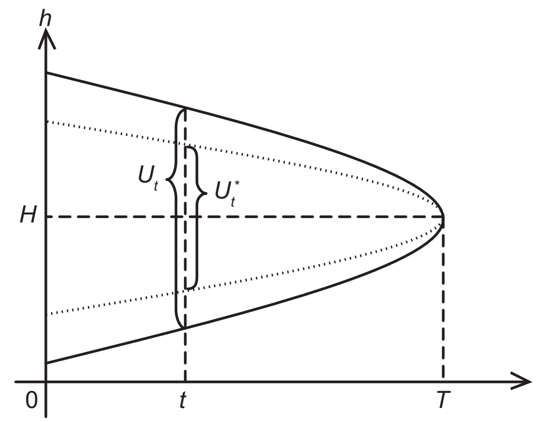

Figure 3. Schematic representation of the variations in the IES U_t (solid line) and its approximate interval U_t^* (dotted line) with increasing integration time t.

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 $\tilde{\delta}_t = \delta/C(t) - Ne_{(0)}$ 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),

$$T = \frac{1}{\hat{C}_L\hat{\Gamma}}\ln\left[\frac{\delta\sqrt{\hat{C}_L}}{C_1(1+1/2p)/\sqrt{H}+Ne_{(0)}}\right]+t_0. \qquad (9)$$

It is easy to prove that $(\tilde{\delta}_t - E_{min})/(T-t) > 0$. From the analysis in section 3, $U_t^* \subset U_t$ for $t < T$, $U_t = U_t^* = \{H\}$ 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 δ satisfies $\delta \geq C(t)(E_{\min} + Ne_{(0)})$, 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.

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