On the error bounds for the ordinary differential equations of the first order

Shoichi Seino

Saburo Minato

1. Introduction

When we deal with a differential equation of any type, it frequently happens that its solution is not expressible in closed form, and even if a given differential equation possesses a closed form solution in terms of known functions, it [also happens that the solution is represented by little tabulated functions.

In these cases, a numerical approach is the most convenient way for solving the differential equation. Many methods are available for solving it numerically, so it is important for us to choose the best one among them. An index of it is the error, for the error analysis gives a qualitative basis for an estimation of the computation value and it serves to give the guarantee of accuracy for a computed solution. When we get some approximate solution of the differential equation, we wish to know something about the size of the error. But the estimation of the error is so complicated that it is hard to get a practical and efficient estimate.

W. Uhlmann in Hamburg developes the error bound function, corresponding to the error, of the system of the ordinary differential equations of the first order, considering some kind of "majorant".

On the other hand, G. G. Dahlquist in Stockholm is working in the same line and he introduces the concept of majorant functions in his essential step.

We are interested in both methods, but unfortunately the [publications referring to them are little, consequently numerical experiments on practical examples are needed before successful use of it. Especially on latter method, the algorithms are not yet completely specified, as he says.

We shall compare the Uhlmann's method with some rude one of the estimation of the error bounds of the above type of the differential equation.

For simplicity we shall ignore rounding error in obtaining the following error estimates, i.e., we estimate only the inherent or truncation errors. Rounding error will, of course, be propagated throughout the calculation, but we take the view that, knowing an upper bound for the inherent error from one of the estimate, we can calculate with a number of decimal sufficient to ensure that the rounding error remain within this bound. In principle it would not be difficult to derive similar estimates for the rounding errors.

2. Efficient error bound

We consider the initial value problems of a system of s ordinary differential equations of the first order

(2.1)
$$y_i' = f_i(x, y_1(x), \dots, y_s(x)), \quad y_i(x_0) = y_{i_0} \quad (i = 1, 2, \dots, s),$$

where the functions f_i possess (r+1)-th continuous partial derivatives with respect to (s+1) variables.

We set $x_n = x_0 + nh$ (h is the step length, $n = 0, 1, \dots, N+1$). In the following the existence of the solution will be assumed. We calculate approximate values y_{in} to the values $y_i(x_n)$ of the exact solutions at the points x_n by the way of the r-th order Adams interpolation method for $m+1 \le n \le N+1$ ($m \ge r-1$).

We abbreviate f_{in} to $f_i(x_n, y_{in}, \dots, y_{sn})$.

Let $P_{in}(x)$ be the polynomial of degree r such that $P_{in}(x_k) = f_{ik}$ $(k=n+1-r, \dots, n+1)$, then

$$y_{i,n+1} = y_{in} + \int_{X_n}^{X_{n+1}} P_{in}(t) dt.$$

For $x_n \leq x \leq x_{n+1}$ (n = m, ..., N) we define the functions $y_i^{(x)}$;

(2.2)
$$y_i * (x) = y_{in} + \int_{X_n}^X P_{in}(t) dt,$$

and the defect $d_i(x)$:

$$d_{i}(\mathbf{x}) = \mathbf{y}_{i} * \mathbf{I}(\mathbf{x}) - f_{i}(\mathbf{x}, \mathbf{y}_{1} * (\mathbf{x}), \cdots, \mathbf{y}_{s} * (\mathbf{x})).$$

From (2.2)

$$d_i(x) = P_{in}(x) - f_i(x, y_1^*(x), \dots, y_s^*(x)), \quad \text{for } x_n \leq x \leq x_{n+1}.$$

We calculate the bound d_{iM} of $|d_i(x)|$.

Owing to the fact the functions $y_i^*(x)$ and $f_i(x, y_i^*(x), \dots, y_s^*(x))$ are i(r+1)-th continuously differentiable, there exist (r+1)-th continuously differentiable functions defined in the interval $[x_{n+1}-r, x_{n+2}]$ such that

$$\begin{split} g_i(x) &= f_i(x, y_1 \text{ tr}(x), \cdots, y_s \text{ tr}(x)) & \text{ for } x_n \leq x \leq x_{n+1} \\ g_i(x_k) &= f_{ik} & \text{ for } k = n+1-r, \cdots, n+2. \end{split}$$

and

where

By the well-known formula on interpolation polynomial,

$$|d_{i}(x)| \leq M_{r+1} h^{r+1} \cdot Max |g_{i}^{(r+1)}(x)| \text{ for } x_{n} \leq x \leq x_{n+1}(n=m, \cdots, N),$$

$$M_r = \max_{\substack{r-1 \leq t \leq r}} \frac{(t-1)(t-2)\cdots(t-r)}{r!}.$$

We define the error $\varepsilon_i(x)$ such that

$$\varepsilon_i(\mathbf{X}) = \mathbf{y}_i'(\mathbf{X}) - \mathbf{y}_i(\mathbf{X}),$$

and we put the initial error bound E_i : $|\varepsilon_i(x_m)| \leq E_i$.

In addition to these, we define the Lipschitz quotient $L_{ik}(x)$ such that

(2.3)

$$L_{ik}(x) = \frac{f_i(x, y_1(x), \dots, y_{k-1}(x), y_k^*(x), \dots, y_s^*(x)) - f_i(x, y_1(x), \dots, y_k(x), y_{k+1}^*(x), \dots, y_s^*(x))}{y_k^*(x) - y_k(x)}$$

We assume that the functions $L_{ik}(x)$ are continuous and bounded in $x_m \le x \le x_N$, i.e., $l_{ik} \le L_{ik}(x) \le L_{ik}$, $|L_{ik}(x)| \le K_{ik} = Max\{|l_{ik}|, |L_{ik}|\}$.

From (2.1) and (2.3)

$$\varepsilon_i I(\mathbf{x}) = \sum_{k=1}^{s} L_{ik}(\mathbf{x}) \varepsilon_k(\mathbf{x}) + d_i(\mathbf{x}) \quad (i = 1, 2, \cdots, s).$$

Then we have the following [THEOREM I]

If the functions $E_i(x)$ are solutions of the initial value problem

(2.4)
$$E_{i}'(x) = \sum_{\substack{k=1\\k \neq i}}^{s} K_{ik}E_{k}(x) + L_{ii}E_{i}(x) + d_{iM}, \quad E_{i}(x_{in}) = E_{i},$$

then, for $x_m \leq x \leq x_N$,

$$|\varepsilon_i(\mathbf{x})| \leq E_i(\mathbf{x})$$
 (i = 1, 2, ..., s).

PROOF. We put

$$\varepsilon_i(x) = e^{-\alpha(x-x_m)}u_i(x)$$
, for any α such that $\alpha \ge \max_i K_{ii}$

Then we have

$$u_{i}'(x) = \sum_{\substack{k=1\\k\neq i}}^{s} L_{ik}(x)u_{k}(x) + (L_{ii}(x) + \alpha)u_{i}(x) + e^{\alpha(x-x_{m})}d_{i}(x),$$

$$u_i(x_m) = \varepsilon_i(x_m).$$

We consider for $x \ge x_m$ and $i = 1, 2, \dots, s$,

(2.5)
$$z_{i}I(x) = \sum_{\substack{k=1\\k\neq i}}^{s} K_{ik}z_{k}(x) + (L_{ii}+\alpha)z_{i}(x) + e^{\alpha(x-x_{m})}d_{iM}.$$

Each solution of (2.5) is written in the form

$$z_i(x) = z_{io}(x) + \sum_{k=1}^{s} z_k(x_m) z_{ik}(x),$$

where $z_{io}(x)$ is a particular solution of the inhomogeneous equation, $z_{ik}(x)$ are solutions of the homogeneous equation, and $z_{ik}(x_m) = \delta_{ik}$ (i=1,2,...,s; k=0,1,...,s). We wish to show that all the $z_{ik}(x) \ge 0$. To this end we put

$$Z_{ik}^{(0)}(\mathbf{X}) = Z_{ik}(\mathbf{X}_m),$$

and

$$z_{ik}^{(p+1)}(x) = z_{ik}(x_m) + \int_{X_m}^{X} \left\{ \sum_{\substack{j=1\\j\neq i}}^{s} K_{ij} z_{jk}^{(p)}(t) + (L_{ii} + \alpha) z_{ik}^{(p)}(t) + \delta_{ik} e^{\alpha(t - x_m)} d_{iM} \right\} dt.$$

Then we get $\lim_{p\to\infty} z_{ik}^{(p)}(x) = z_{ik}(x)$ by means of the Picard-Lindelöff theorem.

116

By induction, we have $z_{ik}^{(p)}(x) \ge 0$, and it follows that $z_{ik}(x) \ge 0$.

We denote the solutions of (2.5) with conditions $u_{io}(x_m) = \varepsilon_i(x_m)$ and $U_i(x_m) = E_i$ by $u_{io}(x)$ and $U_i(x)$ respectively. In addition, let

$$u_{i,p+1}(x) = \varepsilon_{i}(x_{m}) + \int_{x_{m}}^{x} \left\{ \sum_{\substack{k=1\\k \neq i}}^{s} L_{ik}(t)u_{kp}(t) + (L_{ii}(t) + \alpha)u_{ip}(t) + e^{\alpha(t-x_{m})}d_{i}(t) \right\} dt$$

for $p=0, 1, 2, \cdots$ and $x_m \leq x \leq x_N$.

We easily verify, by induction, that

 $|u_{ip}(\mathbf{x})| \leq U_i(\mathbf{x})$ (i=1,2,...,s; p=0,1,2,...).

Again applying the Picard-Lindelöff theorem,

$$\lim_{p\to\infty} u_{ip}(x) = u_i(x), \text{ and also } |u_i(x)| \leq U_i(x).$$

We put

$$E_i(\mathbf{x}) = e^{-\alpha (\mathbf{x} - \mathbf{x}_m)} U_i(\mathbf{x}),$$

then $E_i(x)$ satisfies (2.4), and

$$|\varepsilon_i(\mathbf{x})| = |u_i(\mathbf{x})e^{-\alpha(\mathbf{x}-\mathbf{x}_m)}| \leq U_i(\mathbf{x})e^{-\alpha(\mathbf{x}-\mathbf{x}_m)} = E_i(\mathbf{x}).$$

Next result will be used later.

[COROLLARY]

For $x_m \leq x \leq x_N$,

$$|\varepsilon(x)| \leq E(x) = \begin{cases} E \cdot e^{(x - x_m)L} + d_M \frac{e^{(x - x_m)L} - 1}{L}, & \text{if } L \neq 0 \\ E + d_M (x - x_m), & \text{if } L = 0. \end{cases}$$

PROOF. Taking i=1 in (2.4), we can prove immediately.

3. Error bound for the improved polygon method

Hereafter we restrict our attention to the first order differential equation

(3.1)
$$y' = f(x, y), \quad y(x_0) = y_0$$

We assume that the function f(x, y)

- (a) is continuous in a domain D of the real (x,y) plane,
- (b) is bounded as $|f(x,y)| \leq M$ for any $(x,y) \in D$,
- (c) satisfies the Lipschitz condition

$$|f(x,y)-f(x,y^*)| \leq K|y-y^*|$$
 for any (x,y) and $(x,y^*) \in D$

(d) possesses bounded derivatives $|\frac{d^kf}{dx^k}|\!\leq\!\!N_k\ (k\!=\!1,2).$

By y_n we denote the approximations of the values $y(x_n)$ of the exact solution of (3.1) at the points x_n $(n=1,2,\cdots)$.

Now we calculate the next y_{n+1} from y_n by the formula

$$y_{n+1} = y_n + hf_{n+\frac{1}{2}},$$

where $h = x_{n+1} - x_n$, $f_{n+\frac{1}{2}} = f(x_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})$, $x_{n+\frac{1}{2}} = x_n + \frac{1}{2}h$, and $y_{n+\frac{1}{2}} = y_n + \frac{1}{2}hf_n$.

The error in the approximate values yn means the quantity

(3.2)
$$\varepsilon_n = y_n - y(x_n).$$

we put
$$\Delta \varepsilon_n = \varepsilon_{n+1} - \varepsilon_n$$

so that

$$d\varepsilon_n = hf(x_{n+\frac{1}{2}}, y_n + \frac{1}{2}hf_n) - \int_{x_n}^{x_{n+1}} F(x)dx$$

with F(x) = f(x, y(x)).

We set

 $(3.3) \qquad \qquad \Delta \varepsilon_n = I_n + h J_n,$

where $I_n = hF(x_{n+\frac{1}{2}}) - \int_{x_n}^{x_{n+1}} F(x) dx$, and $J_n = f(x_{n+\frac{1}{2}}, y_{n+\frac{1}{2}} + \frac{1}{2}hf_n) - f(x_{n+\frac{1}{2}}, y(x_{n+\frac{1}{2}})).$

For the quadrature error In, the next well-known inequality holds:

$$(3.4) |I_n| \leq h^3 N_2/24.$$

Using the Lipschitz condition (c), we obtain

(3.5)
$$|J_n| \leq K |y_{n+\frac{1}{2}} + \frac{1}{2} h f_n - y(x_{n+\frac{1}{2}}) | \leq K \cdot ((1 + \frac{1}{2} h K) |\varepsilon_n| + \frac{1}{8} h^2 N_1).$$

From (3.3), (3.4) and (3.5), it follows that

$$|\varepsilon_{n+1}| \leq |\varepsilon_n| (1+hK+\frac{1}{2}h^2K^2) + \frac{1}{8}h^3(KN_1+\frac{1}{3}N_2).$$

Thus, we obtain the independent error bound from this recursive error estimate. The result obtained is stated in theorem form as follows.

[THEOREM II]

Let ε_n be the error defined by (3.2) and E_n^* be the error bound of ε_n , then

$$E_{n}^{*} = \frac{1}{8} b^{2} \left(N_{1} + \frac{N_{2}}{3K} \right) \frac{(1 + hK + \frac{1}{2}h^{2}K^{2})^{n} - 1}{1 + \frac{1}{2}hK}.$$

4. Numerical examples

As the first example, we consider the inital value problem

$$\mathbf{y'} = \mathbf{y} - \mathbf{x}, \quad \mathbf{y}(0) = 2.$$

We compute the values y_n which are the approximations of the exact solution y(x) at the points x_n , using the Lunge-Kutta method of the fourth order with h=0.1. Table I shows the values of the error bounds corresponding to the methods in sec. 2 and 3.

n	Χn	Уn	$d_{\mathbf{M}}$	$E(x_n)$	En*
2 3 4 5 6 7 8 9 10	0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0	2. 421 403 2. 649 858 2. 891 824 3. 148 721 3. 422 118 3. 713 752 4. 025 540 4. 359 601 4. 718 280	$\begin{array}{c} 0.\ 000\ 071\\ 0.\ 000\ 079\\ 0.\ 000\ 087\\ 0.\ 000\ 096\\ 0.\ 000\ 106\\ 0.\ 000\ 117\\ 0.\ 000\ 130\\ 0.\ 000\ 143\\ 0.\ 000\ 158 \end{array}$	$\begin{array}{c} 0.\ 000\ 041\\ 0.\ 000\ 054\\ 0.\ 000\ 071\\ 0.\ 000\ 092\\ 0.\ 000\ 118\\ 0.\ 000\ 151\\ 0.\ 000\ 192\\ 0.\ 000\ 242\\ 0.\ 000\ 304 \end{array}$	$\begin{array}{c} 0.\ 001 \ 007 \\ 0.\ 001 \ 774 \\ 0.\ 002 \ 760 \\ 0.\ 004 \ 007 \\ 0.\ 005 \ 564 \\ 0.\ 007 \ 489 \\ 0.\ 009 \ 851 \\ 0.\ 012 \ 735 \\ 0.\ 016 \ 239 \end{array}$

As another example, let's discuss the initial value problem

 $y' = 2xy, \quad y(2) = 1.$

The approximations y_n are calculated by the second order Adams interpolation method with the step length h=0.01. We represent the result calculated for $E(x_n)$ and $E_n *$ in Table II.

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n	Xn	Уn	d _M	$E(x_n)$	En*
5 10 15 20 25 30 35 40 45 50	$\begin{array}{c} 2.05\\ 2.10\\ 2.15\\ 2.20\\ 2.25\\ 2.30\\ 2.35\\ 2.40\\ 2.45\\ 2.50\end{array}$	$\begin{array}{c} 1.224 \ 461 \\ 1.506 \ 820 \\ 1.863 \ 587 \\ 2.316 \ 377 \\ 2.893 \ 613 \\ 3.632 \ 813 \\ 4.583 \ 710 \\ 5.812 \ 498 \\ 7.407 \ 642 \\ 9.487 \ 869 \end{array}$	$\begin{array}{c} 0.\ 000\ 074\\ 0.\ 000\ 098\\ 0.\ 000\ 130\\ 0.\ 000\ 174\\ 0.\ 000\ 234\\ 0.\ 000\ 315\\ 0.\ 000\ 315\\ 0.\ 000\ 425\\ 0.\ 000\ 577\\ 0.\ 000\ 787\\ 0.\ 001\ 077\\ \end{array}$	$\begin{array}{c} 0.\ 000 \ 004 \\ 0.\ 000 \ 010 \\ 0.\ 000 \ 019 \\ 0.\ 000 \ 034 \\ 0.\ 000 \ 056 \\ 0.\ 000 \ 088 \\ 0.\ 000 \ 135 \\ 0.\ 000 \ 205 \\ 0.\ 000 \ 307 \\ 0.\ 000 \ 455 \end{array}$	$\begin{array}{c} 0.\ 000\ 019\\ 0.\ 000\ 055\\ 0.\ 000\ 122\\ 0.\ 000\ 240\\ 0.\ 000\ 452\\ 0.\ 000\ 829\\ 0.\ 001\ 499\\ 0.\ 002\ 698\\ 0.\ 004\ 860\\ 0.\ 008\ 789 \end{array}$

5. Comment

These examples show that the value of the error bound E(x) introduced by Uhlmann is smaller than E*, and it increases slowly as n does. In comparing other methods it may be sure that the Uhlmann's method is very efficient. His procedure consists in taking the error bound function E(x), corresponding to the error function $\varepsilon(x)$, which is the solution of the first order linear differential equation with constant coefficients. Generally speaking, it is not easy to seek bounds of Lipschitz quotients. Moreover, even if the function E(x) is expressed in exact form, we must calculate the value of it numerically.

When the system of the differential equations is given, the numerical procedure of the error bound function E(x) is more complicated.

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