NEWTON-COTES QUADRATURES FOR DIGITAL SOLUTION OF DIFFERENTIAL EQUATIONS

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INTRODUCTION

Methods of solving a differential equation by digital computer are neither new nor few. The question of the means of obtaining the solution with a maximum accuracy, a minimum number of computer instructions and storage, and a minimum amount of calculation time consistent with stability of the answer has been the source of extensive investigations. Standard numerical analysis texts give many procedures but these are not the subject of this report.

This report reviews previous works on trapezoidal convolution and Romberg integration for digital solution of differential equations. Numerical examples of solving first order differential equations with above methods are presented. Efforts have been made to improve the accuracy of the solution. Simpson's rule and higher order Newton-Cotes quadratures require ultimately recursive calculations. Only instantly recursive calculations are amenable to Z-transform notation.

It is necessary to note that trapezoidal convolution cannot be carried out readily on a digital computer because of the large number of multipliers, adders, and storage capacity required if the operation is carried out in a parallel scheme or the increasingly long computation times when done serially. This difficulty is by-passed by using recurrence relations.

TRAPEZOIDAL CONVOLUTION

Trapezoidal convolution can be used to solve time-invariant, time-variant, continuous nonlinear, discontinuous nonlinear equations with arbitary initial conditions. There are many ways of utilizing trapezoidal convolution to solve a given differential equation. Each of these is called a program. Three classes of programs are discernible: the multiple-integrator substitution program; the many-single-integrator program; and the single-integrator program. Halijak (4) has generated a multiple-integrator substitution program and a single-integrator program, the recursive program.

Approximate Convolution

The solution of a linear differential equation with constant coefficients has the form of a convolution. The digital computer must approximate convolution on a denumerable set of equally spaced points. The Riemann sum approximation is the one commonly used on digital differential analyzers and finite differences. This first member of the Newton-Cotes quadrature family is by-passed for the trapezoidal quadrature.

The trapezoidal approximation proceeds as follows:

$$\int_0^t f(\tau)\, g\,(t-\tau)\, d\tau = \sum_{k=0}^{n-1} \int_{kT}^{(k+1)T} f(\tau)\, g\,(nT-\tau)\, d\tau \qquad (1)$$

$$\doteq \frac{T}{2} \sum_{k=0}^{n-1} \Big[f(kT)\, g\,(nT-kT) + f(kT+T)\, g\,(nT-kT-T) \Big] \equiv J_n$$

The Z-transform of the sequence $\{J_n\}$ is

$$\sum_{n=0}^{\infty} J_n z^n = T(Z\bar{f})\,(Z\bar{g}) - 0.5T\Big[f(0)Z\bar{g} + g(0)Z\bar{f} \Big] \doteq Z(\bar{\bar{fg}}) \qquad (2)$$

The transform for the Simpson's rule approximation need not be derived because it and higher order quadratures do not yield an algebra under the operations of addition and discrete convolution. The abbreviation of trapezoidal convolution to T-convolution will be employed.

The program for solving a given nth order differential equation is generated by viewing it as the integral equation.

$$y(t) + \int_0^t g(t-\tau)\, y(\tau) d\tau = \int_0^t \frac{(t-\tau)^{n-1}}{(n-1)!} x(\tau) d\tau \qquad (3)$$

where $g(t-\tau)$ is a polynomial of degree $(n-1)$ and $x(\tau)$ is the forcing function. It is evident that the primary task is to find the approximate Z-transforms of $1/s^m$ and $\bar{Y}/s^m$ in order to solve this problem on a digital computer. This can be done appropriately employing equation (2) and the additional starting fact that $Z(1/s) = 1/(1-z)$.

Recursive Program

The recursive program uses a sequence of ascending order differential equations derived from the given differential equation to solve same. Consider the differential equation

$$(D^3 + aD^2 + bD + c)\, y(t) = x(t), \quad D = d/dt,$$

$$y(0) = \dot{y}(0) = \ddot{y}(0) = 0, \quad 0 \leq t < \infty \qquad (4)$$

First, set up the differential equation

$$(D+a)\, y_1(t) = 1, \quad y_1(0) = 0 \qquad (5)$$

The Laplace transform of this D.E. yields after division by s

$$(1 + \frac{a}{s})\, \bar{y}_1 = \frac{1}{s^2}$$

Taking the Z-transform of both sides and employing the approximate Z-transform equation (2), of the convolution $\frac{a}{s}\ \bar{y}_1$ yields

$$Z\bar{y}_1 \doteq \frac{2Tz}{[1-z]\,[(2+aT) - (2-aT)z]} \doteq Z\left(\frac{1}{s(s+a)}\right) \tag{6}$$

The above approximation is now used in the next derivate $y_2(t)$, which satisfies

$$(D^2+aD+b)\ y_2(t) = 1, \quad y_2(0) = \dot{y}_2(0) = 0 \tag{7}$$

Dividing now by $s(s+a)$ and solving yields

$$\begin{aligned} Z\bar{y}_2 &\doteq \frac{T(1+z)}{2(1-z)}\ \frac{2Tz}{(2+aT) - (4-2bT^2)z + (2-aT)z^2} \\ &\doteq Z\left(\frac{1}{s(s^2 + as + b)}\right) \end{aligned} \tag{8}$$

The third derivative yields the complete solution of

$$\begin{aligned} &(D^3 + aD^2 + bD + c)\ y(t) = x(t) \\ &\quad y(0) = \dot{y}(0) = \ddot{y}(0) = 0 \end{aligned} \tag{9}$$

Dividing its Laplace transform by $s(s^2 + as + b)$ and using the previous approximation yields

$$Z\bar{y} \doteq \frac{T^3\ z(1+z)\,[Z\bar{x}-0.5x(0)]}{(2+aT) - (6+aT-2bT^2-cT^3)z + (6-aT-2bT^2+cT^3)z^2 - (2-aT)z^3} \tag{10}$$

Initial conditions other than zero can be introduced at the last step. The approximating recurrence relation is prepared from the transformation:

$$Z\bar{y} \longrightarrow y_n \qquad\qquad z^k Z\bar{y} \longrightarrow y_{n-k} \tag{11}$$

Integrator Substitution Program

The integrator substitution program casts the Laplace transform of the given differential equation into inverse powers of s by a suitable division and substitutes for them definite functions of z. First of all, the approximate sampled values of $t^n/n!$, which corresponds to the transform $1/s^{n+1}$, are found for a large positive integer n. The derivation of the approximate sampled values depends on the fact that the initial value of $t^n/n!$ is zero except for n=0. For non-unity positive integers n, one calculates that

$$Z\left(\frac{1}{s}\cdot\frac{1}{s^n}\right) \doteq TZ\left(\frac{1}{s}\right) Z\left(\frac{1}{s^n}\right) - 0.5\ TZ\left(\frac{1}{s^n}\right) = Z\left(\frac{1}{s^n}\right)\frac{T(1+z)}{2(1-z)} \qquad (12)$$

The above is now used as a descending recurrence relation

$$Z\left(\frac{1}{s}\cdot\frac{1}{s^n}\right) \doteq Z\left(\frac{1}{s^{n-1}}\right)\left[\frac{T(1+z)}{2(1-z)}\right]^2 \doteq Z\left(\frac{1}{s^{n-2}}\right)\left[\frac{T(1+z)}{2(1-z)}\right]^3 \qquad (13)$$

until it stops at

$$Z\left(\frac{1}{s^{n+1}}\right) \doteq Z\left(\frac{1}{s^2}\right)\left[\frac{T(1+z)}{2(1-z)}\right]^{n-1}, \quad n=1,\ 2,\ 3,\ \ldots \qquad (14)$$

Calculating $Z(1/s^2)$ from equation (2) and replacing n by (n-1), yields

$$Z\left(\frac{1}{s^n}\right) \doteq \frac{Tz}{(1-z)^2}\left[\frac{T(1+z)}{2(1-z)}\right]^{n-2}, \quad n=2,\ 3,\ 4,\ \ldots \qquad (15)$$

Of course, the case of the missing integer has the known value

$$Z\left(\frac{1}{s}\right) = \frac{1}{1-z} \qquad (16)$$

which cannot be continued from the previous formula. One should note that for n=1, 2, 3, the approximate Z-transform of $1/s^n$ coincides with the exact Z-transform. The integrator substitution program is at hand when one finds the sampled values of $(1/s^n)\ \bar{f}\ (s)$. When n=1, direct calculation with (2) yields

$$Z\left(\frac{1}{s}\bar{f}\right) \doteq \frac{T(1+z)}{2(1-z)} Z\bar{f} - \frac{Tf(0)}{2(1-z)} \tag{17}$$

When n=2, 3, . . ., direct calculation with equations (15) and (2) yields

$$Z\left(\frac{1}{s^n}\bar{f}\right) \doteq \left[\frac{T^2 z}{(1-z)^2}\right]\left[\frac{T(1+z)}{2(1-z)}\right]^{n-2} \left[Z\bar{f} - 0.5\, f(0)\right] \tag{18}$$

Differentiator Substitution Program

The differentiator substitution program does not require an intermediate Laplace transformation, but does require one more initial condition which is readily obtained from the given initial conditions and differential equation.

The derivation of the new program depends on equations (16) and (17) and the Laplace transforms for $D^n f(t)$. One must deal with two categories of derivatives, the first and the others.

The approximate Z-transform of the first derivative is now obtained. First, take the Laplace transform to obtain

$$\overline{Df(t)} = s\bar{f}(s) - f(0) = \bar{g}(s) \tag{19}$$

Divide by s to obtain

$$\frac{1}{s}\bar{g} = \bar{f} - \frac{1}{s} f(0) \tag{20}$$

Sampling, T-convolution and identification of $g(0) = \dot{f}(0)$ yields

$$\frac{T(1+z)}{2(1-z)} Z\bar{g} - \frac{Tg(0)}{2(1-z)} \doteq Z\bar{f} - \frac{f(0)}{1-z} \tag{21}$$

Solving for $Z\bar{g}$ yields the desired

$$Z\left[Df(t)\right] \doteq \frac{2(1-z)}{T(1+z)} Z\bar{f} - \frac{2f(0) - T\,\dot{f}(0)}{T(1+z)} \tag{22}$$

The next category of derivatives contains those of order two and higher. Starting with

$$\overline{D^n f(t)} = s^n \bar{f}(s) - \sum_{k=0}^{n-1} s^{n-1-k} f^{(k)}(0) = \bar{g}(s),\ n \geq 2 \qquad (23)$$

and dividing by s^n yields

$$\frac{1}{s^n}\bar{g} = \bar{f} - \sum_{k=0}^{n-1} s^{-1-k} f^{(k)}(0) \qquad (24)$$

Taking the approximate Z-transform yields

$$TZ\left(\frac{1}{s^n}\right)\left[Z\bar{g} - 0.5\ g(0)\right] \doteq Z\bar{f} - \sum_{k=0}^{n-1} Z\left(\frac{1}{s^{1+k}}\right) f^{(k)}(0) \qquad (25)$$

Keeping in mind the transition from $1/s$ to $1/s^2$ and noting that $g(0) = f^{(n)}(0)$ yields

$$Z\left(D^n f(t)\right) \doteq \frac{(1-z)^2}{T^2 z}\left[\frac{2(1-z)}{T(1+z)}\right]^{n-2} Z\bar{f} - \frac{1-z}{T^2 z}\left[\frac{2(1-z)}{T(1+z)}\right]^{n-2} f(0)$$

$$- \sum_{k=1}^{n-1}\left[\frac{2(1-z)}{T(1+z)}\right]^{n-k-1} f^{(k)}(0) + 0.5\ f^{(n)}(0),\quad n \geq 2 \qquad (26)$$

The presence of the terms $f^{(1)}(0)$ in equation (22) and $f^{(n)}(0)$ in equation (26) evidence the need for one more initial condition--a very slight penalty for eliminating the intermediate Laplace transformation.

This differentiator substitution program is equivalent to the integrator substitution and recursive program.

IMPROVED TRAPEZOIDAL INTEGRATION FORMULA AND ITS EFFECT ON TRAPEZOIDAL CONVOLUTION

The improvement employs an alternative form of the Euler-Maclaurin formula. Recall that the Taylor series representation of a function with remainder is

$$g(x) = g(0) + xg^{(1)}(0) + \frac{x^2}{2!} g^{(2)}(0) + \frac{x^3}{3!} g^{(3)}(0) + \int_0^x \frac{(x-u)^3}{3!} g^{(4)}(u)du \qquad (27)$$

If the given function is integrated, then lengthy computations involving repeated use of this Taylor series yield

$$\frac{1}{h}\int_0^h g(x)dx = \frac{g_0+g_1}{2} - \frac{h^2}{12}\,\frac{g_0^{(2)} + g_1^{(2)}}{2} + R(h) \tag{28}$$

The remainder R(h) is given by

$$R(h) = \frac{h^4}{4!}\int_0^1 (\lambda - 2\lambda^3 + \lambda^4)\, g^{(4)}(\lambda h)d\lambda \tag{29}$$

Since the polynomial in the integrand is always positive on the interval of integration, the first mean value theorem for estimating integrals can be applied and yields

$$R(h) \leq \frac{h^4}{120}\, g^{(4)}(\theta h) \qquad 0 < \theta < 1 \tag{30}$$

The essential point of this formula is that the added terms involve only the even derivatives of the function at the end points of the interval.

Improved trapezoidal integration utilizes the first two terms of the approximate integral. A lengthy application of this approximation to the convolution of functions f(t) and g(t) yields

$$\begin{aligned} Z(\overline{\overline{fg}}) \doteq T &\left[(Z\bar{f})(Z\bar{g}) - 0.5(f_0\, Z\bar{g} \div g_0\, Z\bar{f})\right] \\ &- \frac{T^3}{12}\left[(Z\bar{f})(Z\bar{\ddot{g}}) - 0.5(f_0\, Z\bar{\ddot{g}} + \ddot{g}_0\, Z\bar{f})\right] \\ &+ \frac{T^3}{6}\left[(Z\bar{\dot{f}})(Z\bar{\dot{g}}) - 0.5(\dot{f}_0\, Z\bar{\dot{g}} + \dot{g}_0\, Z\bar{\ddot{f}})\right] \\ &- \frac{T^3}{12}\left[(Z\bar{\ddot{f}})(Z\bar{g}) - 0.5(\ddot{f}_0\, Z\bar{g} + g_0\, Z\bar{\ddot{f}})\right] \end{aligned} \tag{31}$$

If this formula were used to solve a differential equation, the solution of a recurrence-differential equation would be required. This is a more difficult problem than the original. The impasse can be broken by using the trapezoidal derivative substitution program. However, difficulties can be anticipated because the second derivative introduces points outside the integration interval.

The improved trapezoidal integration in conjunction with the trapezoidal derivatives leads to the general bilinear form

$$Z(\bar{f}\bar{g}) \doteq \alpha(Z\bar{f})(Z\bar{g}) + \beta Z\bar{f} + \gamma Z\bar{g} + \delta \tag{32}$$

Computation yields

$$\alpha = \frac{T}{6}\left[\frac{-1 + 10z + 6z^2 + 10z^3 - z^4}{z(1+z)^2}\right] \tag{33}$$

$$\beta = Tg_0\left[\frac{3 - 26z - 12z^2 - 14z^3 + z^4}{24z\ (1+z^2)}\right] + T^2\dot{g}_0\left[\frac{3 - 2z + 3z^2}{12\ (1+z)^2}\right] \tag{34}$$

$$\gamma = Tf_0\left[\frac{3 - 26z - 12z^2 - 14z^3 + z^4}{24z\ (1+z^2)}\right] + T^2\dot{f}_0\left[\frac{3 - 2z + 3z^2}{12\ (1+z)^2}\right] \tag{35}$$

$$\delta = \frac{T}{12}\left[\frac{-1 + 7z + z^2 + z^3}{z(1+z)^2}\right] f_0 g_0 - \frac{T^2}{24}\left[\frac{5 - 2z + z^2}{(1+z)^2}\right] f_0\dot{g}_0$$

$$+ \frac{T^3}{48} f_0\ddot{g}_0 - \frac{T^2}{24}\left[\frac{5 - 2z + z^2}{(1+z)^2}\right]\dot{f}_0 g_0$$

$$- \frac{T^3}{6}\left[\frac{z}{(1+z)^2}\right]\dot{f}_0\dot{g}_0 + \frac{T^3}{48}\ddot{f}_0 g_0 \tag{36}$$

Two stumbling blocks are apparent in these formulas: the presence of the factors $1/z$ and $1/(1+z)^2$ which represent a predictor and unbounded function oscillating about zero respectively.

Recall that solution of a differential equation requires knowledge of the sampled values of $1/s^n$ and $(1/s^n)\bar{g}$. The first step is to find $Z(1/s^n)$. It is possible to find $Z(1/s^{n+1})$, $Z(1/s^{n+2})$, and $Z(1/s^{n+3})$ which implies that descending recurrence relations can be found which decrement the exponent by one, two, or three integers. The long series of calculations are not exhibited. However, the recurrence relation which decrements by two integers is the only one which yields the expected exact $Z(1/s^4)$ and $Z(1/s^5)$. This determines which system should be used in the next step.

Calculations of $Z(\bar{g}/s^n)$ produce only two formulas free of $1/(1+z)$ factors. These are

$$Z\left(\frac{1}{s}\,\bar{g}\right) \doteq \frac{T}{2}\left[\frac{1+z}{1-z}\right]\left[\frac{-1+14z-z^2}{12z}\right] Z\bar{g} + \frac{T(1-12z-z^2)}{24z\,(1-z)}\, g_0$$

$$+ \frac{T^2(1+z)}{24(1-z)}\, g_0 + \frac{T^3}{48}\, \ddot{g}_0 \tag{37}$$

$$Z\left(\frac{1}{s^2}\,\bar{g}\right) \doteq \frac{T^2}{12}\left[\frac{1+10z+z^2}{(1-z)^2}\right] Z\bar{g} - \frac{T^2}{12}\,\frac{1+5z}{(1-z)^2}\, g_0 + \frac{T^3}{12}\, z\, \dot{g}_0 \tag{38}$$

The $1/(1+z)$ factor or its powers introduce spurious approximations even for small sampling interval sizes.

Testing the formula for $Z(\bar{g}/s)$ in the differential equation of e^{-t} quickly reveals that this formula is spurious, though for a different reason. The predictor $1/z$ is the source of difficulty.

The formula for $Z(\bar{g}/s^2)$ is satisfactory and is similar to the Boxer-Thaler Z-form operator for second order integration. A test computation in the differential equation for $\sin \omega t$ reveals that the resulting errors are smaller than those obtained using the unimproved integrator substitution program. On the other hand, some test computations on a second order differential equation with non zero coefficient for the first derivative term has revealed that T-convolution yields better approximation than those of Z-form. It is therefore conjectured that equation (38) is best employed in differential equations involving only even order derivatives.

Use of an improved trapezoidal quadrature introduces a maze of possibilities which when traversed yields a lone double integration formula!

ROMBERG INTEGRATION

Romberg Algorithm

Consider the Newton-Cotes formulas of integration.

(1) The trapezoidal approximation of the second order

$$\int_0^1 f(x)dx = \frac{1}{2}(f_0+f_1) - \frac{B_2}{2!} f^{(2)}(\xi), \qquad B_2 = \frac{1}{6} \tag{39}$$

(2) Simpson's rule

$$\int_0^1 f(x)dx = \frac{1}{6}(f_0+4f_{1/2}+f_1) + \frac{1}{2^2}\frac{B_4}{4!} f^{(4)}(\xi), \qquad B_4 = \frac{1}{-30} \tag{40}$$

(3) Gauss formula

$$\int_0^1 f(x)dx = \frac{1}{90}(7f_0 + 32f_{1/4}+12f_{1/2}+32f_{3/4}+7f_1) - \frac{1}{2^5}\frac{B_6}{6!} f^{(6)}(\xi)$$

$$B_6 = \frac{1}{42} \tag{41}$$

where $f_x = f(x)$.

One can observe some disadvantages:

1) The formation of the coefficients is complicated, and it is not easy to obtain a great number of these coefficients nor to calculate them in a recurrent manner;

2) By increasing the number of points for a fixed interval, one needs to calculate again other numerical values;

3) Some of the coefficients become negative for n=8. For n=9 they are all positive, but for $n \geqslant 10$ there are negative coefficients. This tends to produce poor roundoff properties.

As a result, the higher order Newton-Cotes formulas are seldom used. The order of the error terms jumps by 2 in going from an odd number to the next even number, which tends to favor the even-order formulas.

We desire an algorithm which we could apply easily to the digital computer; this algorithm must be such that the coefficients do not appear explicitly; in other words, it will not compel us to calculate the numerical value of the integrand. Romberg's method (10) has this advantage and besides the error terms are not worse than those of the Newton-Cotes formulas. The coefficients are always positive.

To obtain his algorithm, Romberg observed that Simpson's rule is a linear combination of trapezoidal formula:

$$\frac{1}{6}\left(f_0 + 4f_{1/2} + f_1\right) = \frac{4}{3}\left\{\frac{1}{2}\left(\frac{f_0}{2} + \frac{f_{1/2}}{2}\right) + \frac{1}{2}\left(\frac{f_{1/2}}{2} + \frac{f_1}{2}\right)\right] - \frac{1}{3}\left[\frac{f_0}{2} + \frac{f_1}{2}\right] \tag{42}$$

Moreover, the Gauss formula is a linear combination of the Simpson's rule:

$$\frac{1}{90}\left(7f_0 + 32f_{1/4} + 12f_{1/2} + 32f_{3/4} + 7f_1\right)$$
$$= \frac{16}{15}\left[\frac{1}{2}\left(\frac{f_0}{6} + \frac{4f_{1/4}}{6} + \frac{f_{1/2}}{6}\right) + \frac{1}{2}\left(\frac{f_{1/2}}{6} + \frac{4f_{3/4}}{6} + \frac{f_1}{6}\right)\right]$$
$$- \frac{1}{15}\left[\frac{f_0}{6} + \frac{4f_{1/2}}{6} + \frac{f_1}{6}\right]$$

The combination is such that the error terms disappear and the order of error is two degrees higher than that of the Newton-Cotes quadrature. Consequently, starting with trapezoidal sums

$$T_n^{(2)} = \frac{1}{n}\left[\frac{1}{2}f_0 + \sum_{k=1}^{n-1} f_{k/n} + \frac{1}{2}f_1\right]$$

$$n = 1, 2, 4, 8, \ldots \tag{43}$$

Romberg proposes the following algorithm:

$$T_{2n}^{(2m+2)} = T_{2n}^{(2m)} + \frac{T_{2n}^{(2m)} - T_n^{(2m)}}{2^{2m} - 1}$$

where $m = 1, 2, 3, 4, \ldots$

$n = 1, 2, 4, \ldots$ (44)

We can therefore express T_{2n} in function of $T_1^{(2)}$, $T_2^{(2)}$ . . . $T_{2^n}^{(2)}$ using $2^m + 1$ points. For $m = 0, 1, 2$ this algorithm produces formulas which are identical with trapezoidal formula, Simpson's rule, and Gauss formula respectively, but for $n \geq 3$ the resulting formulas are different from the Newton-Cotes formulas.

If we define

$$U_n^{(2)} = \frac{1}{n} \sum_{k=1}^{n} f\left(\frac{2k-1}{2n}\right) \qquad n = 1, 2, 4, 8, \ldots \tag{45}$$

the evaluation of the trapezoidal sums becomes

$$T_{2n}^{(2)} = \frac{1}{2}\left(T_n^{(2)} + U_n^{(2)}\right) \qquad n = 1, 2, 4, \ldots \tag{46}$$

and the higher order terms will be

$$T_{2n}^{(2m+2)} = T_{2n}^{(2m)} + \frac{T_{2n}^{(2m)} - T_n^{(2m)}}{2^{2m} - 1}$$

$m = 1, 2, 3, \ldots$

$n = 1, 2, 4, \ldots$

$n \geq m$ (47)

The whole Romberg algorithm can be shown by the following diagram:

$$
\begin{tikzcd}[column sep=small]
& U_1^{(2)} \arrow[dr] & & U_2^{(2)} \arrow[dr] & & U_4^{(2)} \arrow[dr] & \\
T_1^{(2)} \arrow[rr] \arrow[dr] & & T_2^{(2)} \arrow[rr] \arrow[dl] \arrow[dr] & & T_4^{(2)} \arrow[rr] \arrow[dl] \arrow[dr] & & T_8^{(2)} \arrow[dl] \\
& T_2^{(4)} \arrow[dr] & & T_4^{(4)} \arrow[dl] \arrow[dr] & & T_8^{(4)} \arrow[dl] & \\
& & T_4^{(6)} \arrow[dr] & & T_8^{(6)} \arrow[dl] & & \\
& & & T_8^{(8)} & & &
\end{tikzcd}
$$

Diagonal elements of high order are not necessarily more accurate than those of lower order; this has been first shown by Bauer (1) by means of test calculations.

In the same manner Romberg's second algorithm defines the recurrence formula.

$$U_{2n}^{(2m+2)} = U_{2n}^{(2m)} + \frac{U_{2n}^{(2m)} - U_{n}^{(2m)}}{2^{2m} - 1}$$

$m = 1, 2, 3, \ldots$

$n = 1, 2, 4, \ldots$ (48)

If we elaborate the diagram of T and U, we are able to use the following relations

$$T_{2n}^{(2m)} = \frac{T_n^{(2m)} + U_n^{(2m)}}{2} \qquad (49)$$

$$T_2^{(2m+2)} = \frac{(2^{2m-1}-1)\, T_n^{(2m)} + 2^{2m-1}\, U_n^{(2m)}}{2^{2m} - 1} \qquad (50)$$

$m = 1, 2, 3, \ldots \qquad n = 1, 2, 4, \ldots$

We can also express $T_{2n}^{(2m+2)}$ as a linear combination of $T_1^{(2)}$, $U_1^{(2)}$, $U_2^{(2)} \ldots U_{2n}^{(2)}$ with positive coefficients.

Numerical Example

To illustrate the application of Romberg's integration process, consider a definite integral

$$I = \int_0^1 \frac{\pi}{2} \cos \frac{\pi}{2} x \, dx = \int_0^1 f(x)dx$$

which has exact solution of 1. We first divide the whole interval 0, 1 in eight equal parts, then using equation (45) to calculate U_1, U_2, U_4

$$U_1^{(2)} = f(1/2)$$

$$U_2^{(2)} = \frac{1}{2} \left[f(1/4) + f(3/4)\right]$$

$$U_4^{(2)} = \frac{1}{4} \left[f(1/8) + f(3/8) + f(5/8) + f(7/8)\right]$$

From equation (43)

$$T_1^{(2)} = \frac{1}{2} \left[f(0) + f(1)\right]$$

Then using equation (46) yields

$$T_2^{(2)} = \frac{1}{2} (T_1^{(2)} + U_1^{(2)})$$

$$T_4^{(2)} = \frac{1}{2} (T_2^{(2)} + U_2^{(2)})$$

$$T_8^{(2)} = \frac{1}{2} (T_4^{(2)} + U_4^{(2)})$$

Finally employing equation (47) to generate $T_2^{(4)}$, $T_4^{(4)}$, $T_8^{(4)}$, $T_4^{(6)}$, $T_8^{(6)}$, and $T_8^{(8)}$ successively.

Numerical results are as follows:

$T_1^{(2)} = 0.78539715$

$U_1^{(2)} = 1.1107213$

$T_2^{(2)} = 0.94805920$ $\quad T_2^{(4)} = 1.0022798$

$U_2^{(2)} = 1.0261722$ $\quad U_2^{(4)} = 0.99798920$

$T_4^{(2)} = 0.98711570$ $\quad T_4^{(4)} = 1.0001345$ $\quad T_4^{(6)} = 0.99999150$

$U_4^{(2)} = 1.0064545$ $\quad U_4^{(4)} = 0.99988200$ $\quad U_4^{(6)} = 1.0000081$

$T_8^{(2)} = 0.99678510$ $\quad T_8^{(4)} = 1.0000082$ $\quad T_8^{(6)} = 0.99999980$ $\quad T_8^{(8)} = 0.99999993$

Note that $T_8^{(8)}$ is most accurate.

Error $T_8^{(2)} = -0.0032149$

Error $T_8^{(4)} = 0.0000082$

Error $T_8^{(6)} = -0.0000002$

Error $T_8^{(8)} = -0.00000007$

NEWTON-COTES QUADRATURES FOR DIGITAL SOLUTION OF DIFFERENTIAL EQUATIONS

The use of integral equations to establish existence theorems is a standard device in the theory of differential equations, both ordinary and partial. It owes its efficiency to the smoothing properties of integration, as contrasted with coarsening properties of differentiation. If two functions are close their integrals must be close, whereas their derivatives may be far apart and may not even exist. It follows that a key to the solution of a differential equation lies in the conversion to the proper integral equation.

Trapezoidal Rule

Dahlquist (3) has shown that the trapezoidal rule has the smallest truncation error among all linear multistep methods with a certain stability property. Thus, trapezoidal quadrature's modest accuracy performance is compensated for by better stability.

Consider the vector first-order differential equation

$$\frac{dW}{dt} + Aw = v \tag{51}$$

Integration yields

$$w(t) + A\int_0^t w(\tau)\, d\tau = w_0 + \int_0^t v(\tau)\, d\tau \tag{52}$$

Employing trapezoidal rule yields

$$w_0 = w_0 \tag{53}$$

$$w_1 + \frac{AT}{2}(w_0 + w_1) = w_0 + \frac{T}{2}(v_0 + v_1) \tag{54}$$

$$w_2 + \frac{AT}{2}(w_0 + 2w_1 + w_2) = w_0 + \frac{T}{2}(v_0 + 2v_1 + v_2) \tag{55}$$

Taking differences of adjacent pairs of equations yields the desired recurrence relation

$$w_n - w_{n-1} + \frac{AT}{2}(w_n + w_{n-1}) = \frac{T}{2}(v_n + v_{n-1})$$

or

$$w_n = \frac{1 - \frac{AT}{2}}{1 + \frac{AT}{2}}\, w_{n-1} + \frac{\frac{T}{2}(v_n + v_{n-1})}{1 + \frac{AT}{2}} \tag{56}$$

$$w_n = \alpha w_{n-1} + \beta \qquad n \geq 1 \tag{57}$$

Note that equation (57) is identical with the recurrence relation obtained by applying trapezoidal convolution to equation (51). It is worthwhile to notice that if the coefficients α and β are functions of sampling interval T only, then

$$w_1 = \alpha w_0 + \beta$$
$$w_2 = \alpha w_1 + \beta = \alpha^2 w_0 + \beta + \beta\alpha$$
$$w_3 = \alpha w_2 = \alpha^3 w_0 + \beta + \beta\alpha + \beta\alpha^2$$
$$w_n = \alpha^n w_0 + \beta + \beta\alpha + \beta\alpha^2 + \ldots + \beta\alpha^{n-1}$$
$$w_n = \alpha^n w_0 + \beta\left(\frac{1-\alpha^n}{1-\alpha}\right) \tag{58}$$

which is much more convenient to use than equation (57) because we can obtain the desired value directly without going through step-by-step calculation. When n approaches infinity, w_n converges to

$$\lim_{n\to\infty} w_n = \frac{\beta}{1-\alpha} \tag{59}$$

provided that such limit exists.

The quadrature improvement process due to equation (28) improves the second-order integration formula only. If an additional term such as

$$(g_0^{(4)} + g_1^{(4)})/2$$

were added to the quadrature, then this would improve the fourth-order integration formula, and so on. The contradictory demand that these improved formulas presents--that not only the past but the future values of the unknown solution must be used--effectively blocks improvement of first-order integration formulas. It is natural to turn to the higher order Newton-Cotes quadratures for improvement of this formula.

Simpson's Rule

Another possibility is to improve Simpson's rule by adding higher order terms. Reasoning similar to that employed to derive equation (28) Halijak(6) shows that a more general form of Simpson's rule is

$$\frac{1}{2h}\int_0^{2h} g(x)dx = \frac{g_0 + 4g_1 + g_2}{6} - \frac{h^4}{18}\left[\frac{g_0^{(4)} + 4g_1^{(4)} + g_2^{(4)}}{6}\right] + R(h)$$

$$R(h) \leq \frac{h^6}{1512} g^{(6)}(\theta h) \qquad 0 < \theta < 2 \qquad (60)$$

Employing only the first term gives Simpson's quadrature rule. This result will not be used for accuracy improvement of solutions.

Applying Simpson's rule to the vector first-order differential equation (51) yields

$$w_0 = w_0$$

$$w_1 + \frac{AT}{2}(w_0 + w_1) = w_0 + \frac{T}{2}(v_0 + v_1)$$

$$w_2 + \frac{AT}{3}(w_0 + 4w_1 + w_2) = w_0 + \frac{T}{3}(v_0 + 4v_1 + v_2)$$

$$w_3 + A\left[\frac{T}{2}(w_0 + w_1) + \frac{T}{3}(w_1 + 4w_2 + w_3)\right]$$

$$= w_0 + \left[\frac{T}{2}(v_0 + v_1) + \frac{T}{3}(v_1 + 4v_2 + v_3)\right]$$

Note that two estimates of the same integral are being generated. The first estimate occurs with the odd numbered equations, and this estimate must be started with a trapezoidal integration. The second estimate occurs with the even numbered equations.

Taking differences of adjacent pairs of even numbered equations and odd numbered equations yields the system of equations

$$w_0 = w_0$$

$$w_1 + \frac{AT}{2}(w_0 + w_1) = w_0 + \frac{T}{2}(v_0 + v_1)$$

$$w_n - w_{n-2} + \frac{AT}{3}(w_n + 4w_{n-1} + w_{n-2})$$

$$= \frac{T}{3}(v_n + 4v_{n-1} + v_{n-2}) \qquad \text{for } n \geq 2 \tag{61}$$

Note that a drastic change of systematics has occurred. The calculations are recursive only for $n \geq 2$.

Definition: A system which is recursive after a finite number of values will be called an ultimately recursive calculating system.

Definition: A system which requires only one value to become recursive will be called an instantly recursive calculation system.

It is these that are amenable to Z-transform notation. The most conspicuous example is trapezoidal convolution.

One slight change in the system of equations can improve accuracy. If w_1 can be calculated by an independent method to a greater degree of accuracy than by trapezoidal quadrature, then over all accuracy will be improved. A readily available method is the Taylor series expansion about the time origin. The resulting ultimately recursive system is

$$w_0 = w_0$$

$$w_1 = w_0 + T\dot{w}_0 + \frac{T^2}{2!}\ddot{w}_0 + \frac{T^3}{3!}\dddot{w}_0 + \ldots$$

$$w_n - w_{n-2} + \frac{AT}{3}(w_n + 4w_{n-1} + w_{n-2})$$

$$= \frac{T}{3}(v_n + 4v_{n-1} + v_{n-2}) \quad \text{for } n \geq 2 \tag{62}$$

Following the same procedure we can derive ultimately recursive systems for higher order Newton-Cotes quadratures.

The corresponding integrator substitution program does not exist if the computer memory is limited and computer time must be short.

Functional Iteration

The investigation starts with equation (3). Simpson's rule is then applied and the resulting equations become an instantly recursive system. We shall call this method "the functional iteration method" which will be denoted as ST. From equation (3)

$$y(t) + \int_0^t g(t-\tau)\, y(\tau)\, d\tau = \int_0^t g(t-\tau)\, x(\tau)\, d\tau$$

$$y(t) = -\int_0^t g(t-\tau)\, y(\tau) d\tau + \int_0^t g(t-\tau)\, x(\tau)\, d\tau$$

we generate trapezoidal solution of above equation first. Then the desired functional iteration solution will be obtained by applying Simpson's rule or higher order Newton-Cotes quadratures to the right-hand side of the following equation:

$$\eta(t) = -\int_0^t g(t-\tau)\, y(\tau) d\tau + \int_0^t g(t-\tau)\, x(\tau) d\tau \qquad (63)$$

where $y(\tau)$ is, as mentioned above, the trapezoidal solution.

EMPIRICAL ERROR ANALYSIS

A comparison of the computational errors generated by various sampling sizes when using T-convolution, functional iteration, and higher-order Newton-Cotes quadratures is presented for the following first-order ordinary differential equations,

$$\frac{dy}{dt} + y = 1 \qquad y(0) = 0$$

$$\frac{dy}{dt} + y = 0 \qquad y(0) = 1$$

$$\frac{dy}{dt} + ty = t \qquad y(0) = 2$$

$$\frac{dy}{dt} + y^2 = 1 \qquad y(0) = 0$$

In order to carry out error analysis the following nomenclatures are employed:

$|E_{max}|$ = the largest absolute value of error in the fixed period of computation (0.8 seconds);

T = sampling interval size;

T_c = trapezoidal convolution;

ST = trapezoidal convolution followed by Simpson's rule;

S = Simpson's 1/3 rule;

3/8 = Simpson's 3/8 rule;

G = Gauss' quadrature.

Derivation of Recursive Formulas

The process of derivation of the recursive formula for the differential equation $\frac{dy}{dt} + y = 0$, $y(0) = 0$, will be shown in detail. For the other three cases, only recursive formulas will be presented.

1. $\frac{dy}{dt} + y = 1 \qquad y(0) = 0$ (64)

a) T_c

$$s\bar{y} + \bar{y} = \frac{1}{s}$$

$$\bar{y} + \frac{1}{s}\bar{y} = \frac{1}{s^2}$$

$$Z\bar{y} + Z\left(\left(\frac{1}{s}\right)\bar{y}\right) = Z\left(\frac{1}{s^2}\right)$$

$$Z\bar{y} + \frac{T}{2}\ \frac{1+z}{1-z}\ Z\bar{y} = \frac{Tz}{(1-z)^2}$$

$$(1-z)\ Z\bar{y} + \frac{T}{2}\ (1+z)\ Z\bar{y} = \frac{Tz}{1-z}$$

$$(1 + \frac{T}{2})Z\bar{y} - (1 - \frac{T}{2})zZ\bar{y} = \frac{Tz}{1-z}$$

$$y_n(1 + \frac{T}{2}) - y_{n-1}\ (1 - \frac{T}{2}) = \left\{0,\ T,\ T,\ T,\ .\ .\ .\right\}$$

$$y_0 = \frac{1 + \frac{T}{2}}{1 + \frac{T}{2}}\ y_{-1} + 0 = 0$$

$$y_n = \frac{1 - \frac{T}{2}}{1 + \frac{T}{2}}\ y_{n-1} + \frac{T}{1 + \frac{T}{2}}$$

$$y_n = \frac{2 - T}{2 + T}\ y_{n-1} + \frac{2T}{2 + T} \qquad n \geqslant 1 \tag{65}$$

Note that if we apply the trapezoid rule alone to equation (64), the same recurrence formula as (65) will be obtained.

$$y_t = y_0 + \int_0^t d\tau - \int_0^t y\ d\tau \tag{66}$$

$$y_0 = y_0$$

$$y_1 = y_0 + T - \frac{T}{2}\ (y_0 + y_1) \tag{67}$$

$$y_2 = y_0 + 2T - \frac{T}{2}\ (y_0 + 2y_1 + y_2) \tag{68}$$

Taking the difference of the adjacent formulas we obtain the recurrence formula

$$y_n = y_{n-1} + T - \frac{T}{2}(y_n + y_{n-1})$$

$$y_n = \frac{1 - \frac{T}{2}}{1 + \frac{T}{2}} y_{n-1} + \frac{T}{1 + \frac{T}{2}}$$

$$y_n = \frac{2 - T}{2 + T} y_{n-1} + \frac{2T}{2 + T} \tag{69}$$

which is identical with equation (65). It will be emphasized that when employing the trapezoidal rule alone it is much easier to get recurrence formula than using T-convolution method as far as the first-order ordinary differential equation is concerned, but the same is not true for higher-order ones. In this particular case, the coefficients of y's are the function of T only, so equations (58) and (59) are applicable.

$$y_n = \alpha^n y_0 + \beta\left(\frac{1 - \alpha^n}{1 - \alpha}\right) = \beta\left(\frac{1 - \alpha^n}{1 - \alpha}\right) \tag{70}$$

where $\alpha = \frac{2 - T}{2 + T}$, $\beta = \frac{2T}{2 + T}$

$$\lim_{n \to \infty} y_n = \frac{\beta}{1 - \alpha} = \frac{\frac{2T}{2 + T}}{1 - \frac{2 - T}{2 + T}} = 1 \tag{71}$$

b) ST

$$\eta_0 = y_0$$

$$\eta_2 = y_0 + 2T - \frac{T}{3}(y_0 + 4y_1 + y_2)$$

$$\eta_4 = y_0 + 4T - \frac{T}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + y_4)$$

Taking the difference of the above equations, we get the recurrence formula

$$\eta_n = \eta_{n-2} + 2T - \frac{T}{3}(y_n + 4y_{n-1} + y_{n-2}) \tag{72}$$

$$n = 2, 4, 6, 8, \ldots$$

where y's are trapezoidal solutions.

c) S

$$y_0 = y_0$$

$$y_1 = y_0 + T\dot{y}_0 + \frac{T^2}{2!}\ddot{y}_0 + \frac{T^3}{3!}\dddot{y}_0 + \ldots$$

$$y_2 = y_0 + 2T - \frac{T}{3}(y_0 + 4y_1 + y_2)$$

$$y_4 = y_0 + 4T - \frac{T}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + y_4)$$

$$y_n = y_{n-1} + 2T - \frac{T}{3}(y_n + 4y_{n-1} + y_{n-2})$$

$$y_n = \frac{6T}{3 + T} + \frac{3 - T}{3 + T}y_{n-2} - \frac{4T}{3 + T}y_{n-1} \qquad n \geqslant 2 \qquad (73)$$

Note that instead of using trapezoid formula, Taylor series expansion is employed to estimate the first iterative point, y_1, to improve accuracy.

d) 3/8

$$y_0 = y_0$$

$$y_1 = y_0 + T\dot{y}_0 + \frac{T^2}{2!}\ddot{y}_0 + \frac{T^3}{3!}\dddot{y}_0 + \ldots$$

$$y_2 = y_0 + (2T)\,\dot{y}_0 + \frac{(2T)^2}{2!}\ddot{y}_0 + \frac{(2T)^3}{3!}\dddot{y} + \ldots$$

$$y_n = y_{n-3} + 3T - 3/8T\,(y_n + 3y_{n-1} + 3y_{n-2} + y_{n-3})$$

$$y_n = \frac{24T}{8 + 3T} + \frac{8 - 3T}{8 + 3T}y_{n-3} - \frac{9T}{8 + 3T}(y_{n-1} + y_{n-2})$$

$$n \geqslant 3 \qquad (74)$$

In this case it is obvious that we need two points to start the recursive formula (74). We shall use the Taylor series to generate necessary initial points.

e) G

$$y_n = y_{n-4} + 4T - \frac{2T}{45}(7y_n + 32y_{n-1} + 12y_{n-2} + 32y_{n-3} + 7y_{n-4})$$

$$y_n = \frac{180T}{45 + 14T} + \frac{45 - 14T}{45 + 14T}\, y_{n-4} - \frac{8T}{45 + 14T}(8y_{n-1} + 3y_{n-2} + 8y_{n-3})$$

$$n \geq 4 \qquad (75)$$

2. $\frac{dy}{dt} + y = 0 \qquad y(0) = 1$

a) T_c

$$y_n = \frac{2 - T}{2 + T}\, y_{n-1} \qquad n \geq 1 \qquad (76)$$

b) ST

$$\eta_n = \eta_{n-2} - \frac{T}{3}(y_n + 4y_{n-1} + y_{n-2})$$

$$n = 2, 4, 6, 8, \ldots \qquad (77)$$

c) S

$$y_n = \frac{3 - T}{3 + T}\, y_{n-2} - \frac{4T}{3 + T}\, y_{n-1} \qquad n \geq 2 \qquad (78)$$

d) 3/8

$$y_n = \frac{8 - 3T}{8 + 3T}\, y_{n-3} - \frac{9T}{8 + 3T}(y_{n-1} + y_{n-2}) \qquad n \geq 3 \qquad (79)$$

e) G

$$y_n = \frac{45 - 14T}{45 + 14T}\, y_{n-4} - \frac{8T}{45 + 14T}(8y_{n-1} + 3y_{n-2} + 8y_{n-3})$$

$$n \geq 4 \qquad (80)$$

3. $\frac{dy}{dt} + ty = t \qquad y(0) = 2$

a) T_c

$$y_n = \frac{2-(n-1)T^2}{2 + nT^2}\, y_{n-1} + \frac{(2n-1)T^2}{2 + nT^2} \qquad n \geq 1 \qquad (81)$$

b) ST

$$\eta_n = \eta_{n-2} + 2(n-1)T^2 - \frac{T^2}{3}\left[ny_n + 4(n-1)y_{n-1} + (n-2)y_{n-2}\right]$$

$$n = 2,\ 4,\ 6,\ 8,\ \ldots \qquad (82)$$

c) S

$$y_n = \frac{6(n-1)T^2}{3 + nT^2} + \frac{3 - (n-2)T^2}{3 + nT^2}\, y_{n-2} - \frac{4(n-1)T^2}{3 + nT^2}\, y_{n-1}, \quad n \geqq 2 \qquad (83)$$

d) 3/8

$$y_n = \frac{12(2n-3)T^2}{8 + 3nT^2} + \frac{8 - 3(n-3)T^2}{8 + 3nT^2}\, y_{n-3}$$

$$- \frac{9T^2}{8 + 3nT^2}\left[(n-1)y_{n-1} + (n-2)y_{n-2}\right] \qquad n \geqq 3 \qquad (84)$$

e) G

$$y_n = \frac{180(n-2)T^2}{45 + 14nT^2} + \frac{45 - 14(n-4)T^2}{45 + 14nT^2}\, y_{n-4}$$

$$- \frac{8T^2}{45 + 14nT^2}\left[8(n-1)y_{n-1} + 3(n-2)y_{n-2} + 8(n-3)y_{n-3}\right]$$

$$n \geqq 4 \qquad (85)$$

4. $\frac{dy}{dt} + y^2 = 1 \qquad y(0) = 0$

a) T_c

$$y_n = \frac{-1 + \sqrt{1 - 2T\left(\frac{T}{2}\, y_{n-1}^2 - y_{n-1} - T\right)}}{T} \qquad n \geqq 1 \qquad (86)$$

b) ST

$$\eta_n = \eta_{n-2} + 2T - \frac{T}{3}\left[y_n^2 + 4y_{n-1}^2 + y_{n-2}^2\right]$$

$$n = 2,\ 4,\ 6,\ 8,\ \ldots \qquad (87)$$

c) S

$$y_n = \frac{-1 + \sqrt{1 - \frac{4T}{3}\left[\frac{T}{3}\left(4y^2_{n-1} + y^2_{n-2}\right) - y_{n-2} - 2T\right]}}{\frac{2T}{3}} \qquad n \geq 2 \tag{88}$$

d) 3/8

$$y_n = \frac{-1 + \sqrt{1 - \frac{3T}{2}\left[\frac{3T}{8}\left(3y^2_{n-1} + 3y^2_{n-2} + y^2_{n-3}\right) - y_{n-3} - 3T\right]}}{\frac{3T}{4}} \qquad n \geq 3 \tag{89}$$

e) G

$$y_n = \frac{-1 + \sqrt{1 - \frac{56T}{43}\left[\frac{2T}{45}\left(32y^2_{n-1} + 12y^2_{n-2} + 32y^2_{n-3} + 7y^2_{n-4}\right) - y_{n-4} - 4T\right]}}{\frac{28T}{45}} \qquad n \geq 4 \tag{90}$$

Results

The error measures for various approximations are presented in Tables 1, 2, 3, 4 and these same error measures are graphed in Figures 1 through 11.

It should be pointed out that the values of error measures are presented with floating point system. For instance,

$$0.112 \text{ E } -05 = 0.112 \times 10^{-5}$$

Table 1. $|e_{max}|$ for $\frac{dy}{dt} + y = 1$, $y(0) = 0$, $t = 0.8$

h	[illegible]-conv	[illegible]	[illegible]	[illegible]/S	S
0.003	.112E-05	.930E-06	.380E-06	.650E-06	.180E-06
0.004	.560E-06	.510E-06	.390E-06	.470E-06	.260E-06
0.005	.980E-06	.130E-06	.140E-06	.440E-06	.260E-06
0.006	.580E-06	.150E-06	.270E-06	.180E-06	.170E-06
0.007	.930E-06	.370E-06	.310E-06	.350E-06	.230E-06
0.008	.142E-05	.690E-06	.150E-06	.230E-06	.130E-06
0.009	.216E-05	.104E-05	.140E-06	.140E-06	.160E-06
0.010	.252E-05	.130E-05	.120E-06	.160E-06	.160E-06
0.012	.369E-05	.194E-05	.140E-06	.190E-06	.180E-06
0.014	.569E-05	.290E-05	.800E-07	.150E-06	.190E-06
0.016	.738E-05	.395E-05	.180E-06	.190E-06	.110E-06
0.018	.947E-05	.492E-05	.150E-06	.140E-06	.140E-06
0.020	.118E-04	.630E-05	.150E-06	.160E-06	.810E-06
0.022	.143E-04	.743E-05	.150E-06	.160E-06	.900E-07
0.024	.170E-04	.892E-05	.130E-06	.150E-06	.120E-06
0.026	.199E-04	.102E-04	.137E-06	.110E-06	.130E-06
0.028	.232E-04	.120E-04	.150E-06	.130E-06	.100E-06
0.030	.267E-04	.137E-04	.140E-06	.150E-06	.130E-06
0.032	.305E-04	.161E-04	.110E-06	.110E-06	.110E-06
0.034	.343E-04	.176E-04	.110E-06	.100E-06	.140E-06
0.036	.386E-04	.202E-04	.110E-06	.100E-06	.120E-06
0.038	.431E-04	.227E-04	.108E-06	.100E-06	.100E-06
0.040	.477E-04	.255E-04	.100E-06	.100E-06	.900E-07
0.042	.527E-04	.277E-04	.130E-06	.100E-06	.110E-06
0.044	.577E-04	.303E-04	.900E-07	.100E-06	.900E-07
0.046	.630E-04	.322E-04	.130E-06	.100E-06	.150E-06
0.048	.684E-04	.344E-04	.100E-06	.900E-07	.110E-06
0.050	.747E-04	.398E-04	.600E-07	.700E-07	.100E-06
0.052	.805E-04	.411E-04	.120E-06	.900E-07	.100E-06
0.054	.862E-04	.426E-04	.600E-07	.110E-06	.100E-06
0.056	.934E-04	.434E-04	.800E-07	.600E-07	.130E-06
0.058	.993E-04	.485E-04	.800E-07	.300E-07	.800E-07
0.060	.107E-03	.546E-04	.140E-06	.400E-07	.100E-06
0.062	.113E-03	.540E-04	.100E-06	.800E-07	.110E-06
0.064	.121E-03	.613E-04	.300E-07	.110E-06	.110E-06
0.066	.132E-03	.683E-04	.800E-07	.600E-07	.900E-07
0.068	.136E-03	.655E-04	.100E-06	.500E-07	.900E-07
0.070	.145E-03	.727E-04	.700E-07	.900E-07	.900E-07
0.072	.154E-03	.802E-04	.900E-07	.100E-06	.100E-06
0.074	.161E-03	.774E-04	.120E-06	.170E-06	.800E-07
0.076	.171E-03	.850E-04	.120E-06	.130E-06	.900E-07
0.078	.181E-03	.938E-04	.150E-06	.140E-06	.600E-07
0.080	.191E-03	.101E-03	.600E-07	.150E-06	.500E-07
0.082	.197E-03	.926E-04	.120E-06	.140E-06	.900E-07
0.084	.208E-03	.101E-03	.900E-07	.180E-06	.110E-06
0.086	.220E-03	.109E-03	.100E-06	.230E-06	.800E-07
0.088	.231E-03	.119E-03	.150E-06	.260E-06	.500E-07

Table 1. (cont.)

T	T-conv	ST	S	3/8	G
0.090	.236E-03	.109E-03	.130E-06	.210E-06	.800E-07
0.092	.249E-03	.118E-03	.110E-06	.240E-06	.100E-06
0.094	.261E-03	.128E-03	.100E-06	.270E-06	.100E-06
0.096	.273E-03	.137E-03	.150E-06	.320E-06	.900E-07
0.098	.286E-03	.148E-03	.220E-06	.380E-06	.800E-07
0.100	.299E-03	.159E-03	.160E-06	.420E-06	.700E-07

Table 2. $|e_n|$ [illegible] $\frac{dy}{dt} + y = 0$, $y(0) = 1$, [illegible] $= 0.5$

T	E-conv	ST	[illegible]	B/S	G	G'
0.003	.500E-06	.101E-05	.600E-06	.100E-06	.150E-06	.150E-06
0.004	.850E-06	.990E-06	.200E-06	.160E-06	.140E-06	.240E-06
0.005	.135E-05	.117E-05	.220E-06	.100E-06	.150E-06	.200E-06
0.006	.140E-05	.115E-05	.140E-06	.130E-06	.130E-06	.150E-06
0.007	.175E-05	.124E-05	[illegible]	.100E-06	.100E-06	.800E-07
0.008	.202E-05	.140E-05	.110E-06	.500E-07	.110E-06	.170E-06
0.009	.273E-05	.173E-05	.150E-06	.900E-07	.700E-07	.120E-06
0.010	.304E-05	.183E-05	.900E-07	.900E-07	.100E-06	.170E-06
0.012	.430E-05	.251E-05	.900E-07	.500E-07	.700E-07	.170E-06
0.014	.613E-05	.340E-05	.150E-06	.600E-07	.500E-07	.250E-06
0.016	.776E-05	.426E-05	.110E-06	.800E-07	.900E-07	.320E-06
0.018	.979E-05	.536E-05	.110E-06	.100E-06	.100E-06	.470E-06
0.020	.121E-04	.659E-05	.130E-06	.100E-06	.600E-07	.700E-06
0.022	.145E-04	.775E-05	.900E-07	.300E-07	.500E-07	.870E-06
0.024	.172E-04	.917E-05	.900E-07	.600E-07	.800E-07	.114E-05
0.026	.201E-04	.105E-04	.110E-06	.700E-07	.800E-07	.147E-05
0.028	.234E-04	.123E-04	.900E-07	.400E-07	.400E-07	.177E-05
0.030	.269E-04	.139E-04	.500E-07	.700E-07	.700E-07	.222E-05
0.032	.307E-04	.164E-04	.120E-06	.300E-07	.500E-07	.265E-05
0.034	.345E-04	.178E-04	.800E-07	.400E-07	.400E-07	.313E-05
0.036	.387E-04	.204E-04	.100E-06	.600E-07	.600E-07	.379E-05
0.038	.433E-04	.229E-04	.800E-07	.500E-07	.500E-07	.444E-05
0.040	.479E-04	.256E-04	.120E-06	.400E-07	.600E-07	.510E-05
0.042	.		.100E-06	.500E-07	.400E-07	.591E-05
0.044	.579E-04	.304E-04	.900E-07	.400E-07	.500E-07	.675E-05
0.046	.631E-04	.324E-04	.100E-06	.300E-07	.500E-07	.809E-05
0.048	.684E-04	.346E-04	.900E-07	.600E-07	.800E-07	.874E-05
0.050	.749E-04	.396E-04	.500E-07	.400E-07	.300E-07	.431E-05
0.052	.806E-04	.413E-04	.100E-06	.500E-07	.500E-07	.111E-04
0.054			.100E-06	.600E-07	.600E-07	.124E-04
0.056	.936E-04	.485E-04	.700E-07	.600E-07	.400E-07	
0.058	.995E-04	.496E-04	.800E-07	.600E-07	.500E-07	.153E-04
0.060	.107E-03	.547E-04	.800E-07	.700E-07	.600E-07	.170E-04
0.062	.113E-03	.549E-04	.700E-07	.900E-07	.700E-07	.187E-04
0.064	.121E-03	.614E-04	.700E-07	.600E-07	.300E-07	.205E-04
0.066	.130E-03	.684E-04	.900E-07	.900E-07	.200E-07	.224E-04
0.068	.136E-03	.657E-04	.800E-07	.100E-06	.200E-07	.245E-04
0.070	.145E-03	.727E-04	.700E-07	.100E-06	.400E-07	.266E-04
0.072	.155E-03	.803E-04	.130E-06	.120E-06	.800E-07	.290E-04
0.074	.161E-03	.775E-04	.130E-06	.110E-06	.300E-07	.313E-04
0.076	.171E-03	.851E-04	.600E-07	.150E-06	.400E-07	.339E-04
0.078	.181E-03	.934E-04	.800E-07	.170E-06	.300E-07	.365E-04
0.080	.191E-03	.101E-03	.600E-07	.100E-06	.400E-07	.393E-04
0.082	.197E-03	.929E-04	.600E-07	.210E-06	.400E-07	.423E-04
0.084	.208E-03	.101E-03	.800E-07	.240E-06	.400E-07	.454E-04
0.086	.220E-03	.109E-03	.130E-06	.260E-06	.500E-07	.487E-04
0.088	.231E-03	.119E-03	.140E-06	.280E-06	.400E-07	.520E-04

[illegible] (cont.)

[illegible]	P-corr	SI	S	S/8	G	G'
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.5001-07	.5551-04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.[illegible]-07	.5921-04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.[illegible]-07	.6311-04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.[illegible]-07	.6701-04
[illegible]	.1361-03	[illegible]	[illegible]	.4103-06	.2001-07	.7121-04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.5001-07	.7551-04

G' = Simpson's 1/3 rule using trapezoidal rule to approximate starting point [illegible]

Table 3. $|E_{max}|$ for $\frac{dy}{dt} + ay = b$, $y(0) = 1.0$, $b = 2.0$

h	T-conv	E1	3/8	G
0.008	.710E-05	[illegible]	.230E-05	.130E-05
0.009	.550E-05	.150E-04	.200E-05	.120E-05
0.010	.440E-05	.109E-04	.140E-05	.110E-05
0.012	.300E-05	[illegible]	.160E-05	.100E-05
0.014	.370E-05	.470E-05	.130E-05	.100E-05
0.016	.123E-04	[illegible]	.140E-05	.800E-06
0.018	.175E-04	[illegible]	.900E-06	.800E-06
0.020	.237E-04	[illegible]	.900E-06	.600E-06
0.022	.240E-04	[illegible]	.100E-05	.600E-06
0.024	.352E-04	[illegible]	.600E-06	.500E-06
0.026	.419E-04	[illegible]	.800E-06	.500E-06
0.028	.495E-04	.861E-04	.700E-06	.400E-06
0.030	.573E-04	[illegible]	.800E-06	.400E-06
0.032	.650E-04	.900E-04	.900E-06	.400E-06
0.034	.750E-04	[illegible]	.700E-06	.400E-06
0.036	.848E-04	.119E-03		
0.038	.940E-04	.130E-03		
0.040	.104E-03	[illegible]		
0.042	.115E-03	[illegible]		
0.044	.127E-03	.176E-03		
0.046	.139E-03	[illegible]		
0.048	.152E-03	.209E-03		
0.050	.164E-03	.238E-03		
0.052	.178E-03	[illegible]		
0.054	.192E-03	.271E-03		
0.056	.207E-03	.285E-03		
0.058	.226E-03	.310E-03		
0.060	.238E-03	.330E-03		
0.062	.255E-03	.357E-03		
0.064	.271E-03	.379E-03		
0.066	.289E-03	.405E-03		
0.068	.306E-03	.426E-03		
0.070	.325E-03	.450E-03		
0.072	.343E-03	.470E-03		
0.074	.363E-03	.511E-03		
0.076	.383E-03	.530E-03		
0.078	.404E-03	.554E-03		
0.080	.425E-03	.590E-03		
0.082	.446E-03	.624E-03		
0.084	.469E-03	.597E-03		
0.086	.491E-03	.684E-03		
0.088	.514E-03	.707E-03		
0.090	.539E-03	[illegible]		
0.092	.562E-03	.763E-03		
0.094	.586E-03	.815E-03		

Table 3. (cont.)

T	T-conv	ST	3/8	G
0.096	.612E-03	.835E-03		
0.098	.639E-03	.890E-03		
0.100	.665E-03	.947E-03		
0.150	.149E-02	.202E-02		
0.200	.266E-02	.332E-02		

Table 4. $|E_{max}|$ for $\frac{dy}{dt} + y^2 = 1$, $y(0) = 0$, $t = 0.8$

T	T-conv	ST	S	3/8	G
0.003				.921E-03	.263E-03
0.004	.109E-02	.535E-03	.641E-03	.473E-03	.492E-03
0.005	.441E-03	.219E-03	.457E-03	.342E-03	.316E-03
0.006	.450E-03	.182E-03	.367E-03	.207E-03	.265E-03
0.007	.289E-03	.137E-03	.353E-03	.145E-03	.177E-03
0.008	.315E-03	.121E-03	.173E-03	.123E-03	.166E-03
0.009	.184E-03	.800E-04	.142E-03	.733E-04	.102E-03
0.010	.149E-03	.530E-04	.103E-03	.109E-03	.841E-04
0.012	.109E-03	.478E-04	.807E-04	.627E-04	.551E-04
0.014	.669E-04	.275E-04	.775E-04	.386E-04	.514E-04
0.016	.555E-04	.255E-04	.612E-04	.299E-04	.476E-04
0.018	.633E-04	.287E-04	.357E-04	.247E-04	.335E-04
0.020	.550E-04	.261E-04	.392E-04	.167E-04	.235E-04
0.022	.458E-04	.236E-04	.338E-04	.218E-04	.215E-04
0.024	.645E-04	.312E-04	.218E-04	.149E-04	.154E-04
0.026	.453E-04	.225E-04	.163E-04	.100E-04	.212E-04
0.028	.595E-04	.288E-04	.216E-04	.156E-04	.112E-04
0.030	.618E-04	.296E-04	.167E-04	.122E-04	.167E-04
0.032	.598E-04	.302E-04	.143E-04	.140E-04	.996E-05
0.034	.720E-04	.359E-04	.120E-04	.610E-05	.773E-05
0.036	.695E-04	.345E-04	.303E-05	.190E-04	.752E-05
0.038	.729E-04	.373E-04	.117E-04	.679E-05	.563E-05
0.040	.861E-04	.437E-04	.130E-04	.410E-05	.643E-05
0.042	.952E-04	.478E-04	.924E-05	.280E-05	.564E-05
0.044	.107E-03	.532E-04	.111E-04	.667E-05	.363E-05
0.046	.114E-03	.552E-04	.748E-05	.518E-05	.653E-05
0.048	.121E-03	.574E-04	.644E-05	.653E-05	.177E-05
0.050	.131E-03	.661E-04	.875E-05	.495E-05	.492E-05
0.052	.140E-03	.676E-04	.946E-05	.179E-05	.311E-05
0.054	.152E-03	.701E-04	.972E-05	.363E-05	.151E-05
0.056	.160E-03	.784E-04	.559E-05	.217E-05	.296E-05
0.058	.171E-03	.785E-04	.198E-05	.337E-05	.266E-05
0.060	.185E-03	.896E-04	.456E-05	.290E-05	.242E-05
0.062	.197E-03	.883E-04	.308E-05	.117E-05	.306E-05
0.064	.208E-03	.979E-04	.326E-05	.269E-05	.206E-05
0.066	.223E-03	.110E-03	.300E-05	.180E-05	.335E-05
0.068	.234E-03	.105E-03	.174E-05	.328E-05	.302E-05
0.070	.249E-03	.117E-03	.302E-05	.206E-05	.170E-05
0.072	.262E-03	.129E-03	.305E-05	.350E-05	.820E-06
0.074	.279E-03	.123E-03	.258E-05	.193E-05	.238E-05
0.076	.293E-03	.136E-03	.313E-05	.193E-05	.153E-05
0.078	.307E-03	.148E-03	.168E-05	.267E-05	.140E-05
0.080	.323E-03	.152E-03	.241E-05	.141E-05	.148E-05
0.082	.342E-03	.150E-03	.131E-05	.116E-05	.105E-05
0.084	.359E-03	.164E-03	.109E-05	.223E-05	.740E-06
0.086	.376E-03	.178E-03	.280E-05	.243E-05	.102E-05
0.088	.393E-03	.194E-03	.149E-05	.225E-05	.155E-05

Table 4. (cont.)

T	T-conv	ST	S	3/8	G
0.090	.409E-04	.173E-03	.100E-05	.330E-05	.216E-05
0.092	.425E-03	.188E-03	.117E-05	.262E-05	.129E-05
0.094	.446E-03	.204E-03	.930E-06	.253E-05	.930E-06
0.096	.467E-03	.220E-03	.194E-05	.424E-05	.159E-05
0.098	.485E-03	.236E-03	.170E-05	.407E-05	.226E-05
0.100	.507E-03	.254E-03	.176E-05	.472E-05	.110E-05

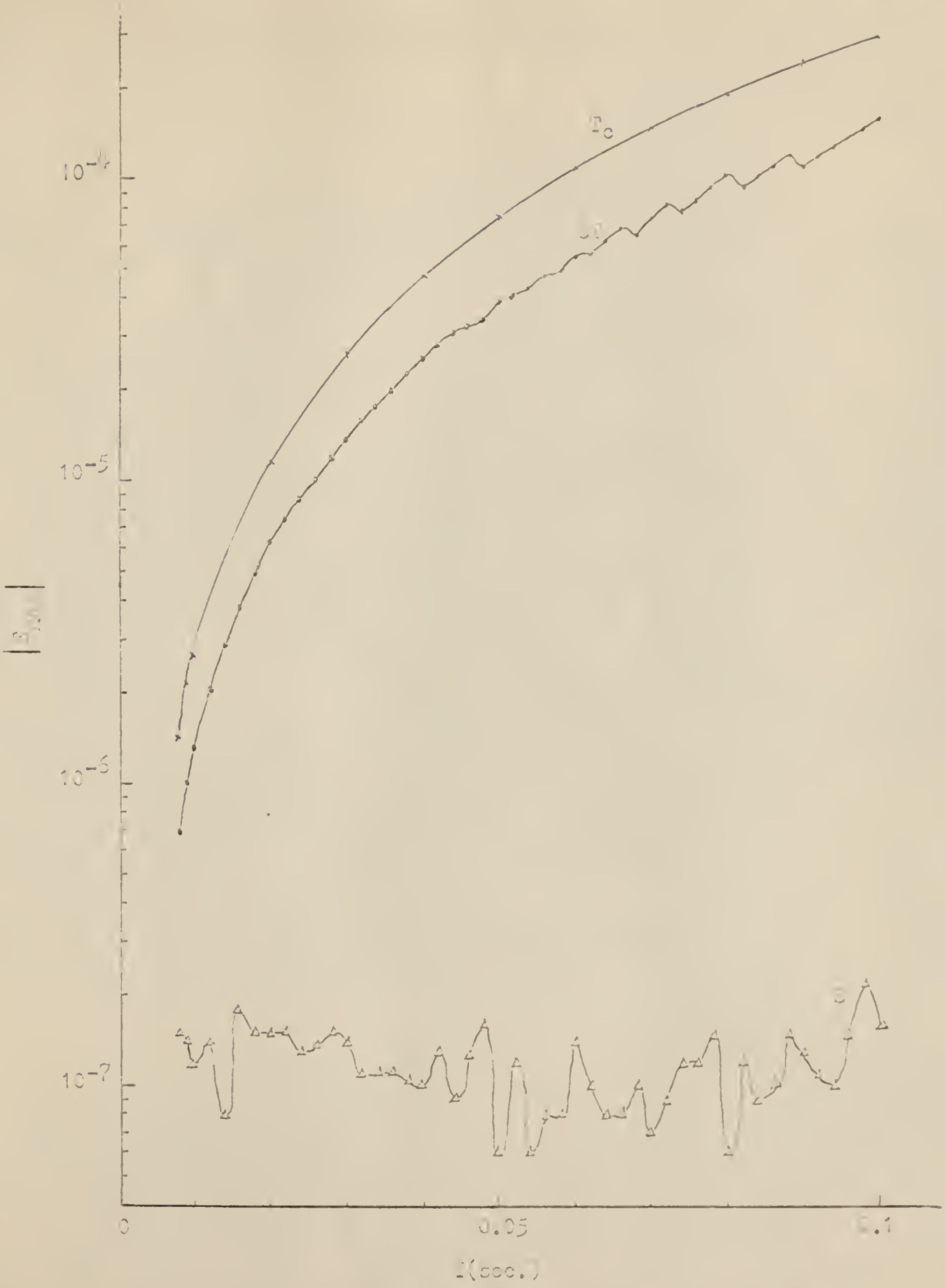

Fig. 1. Error curves of $\frac{dy}{dt} + y = 0$, $y(0) = 0$, $c = 0.0$

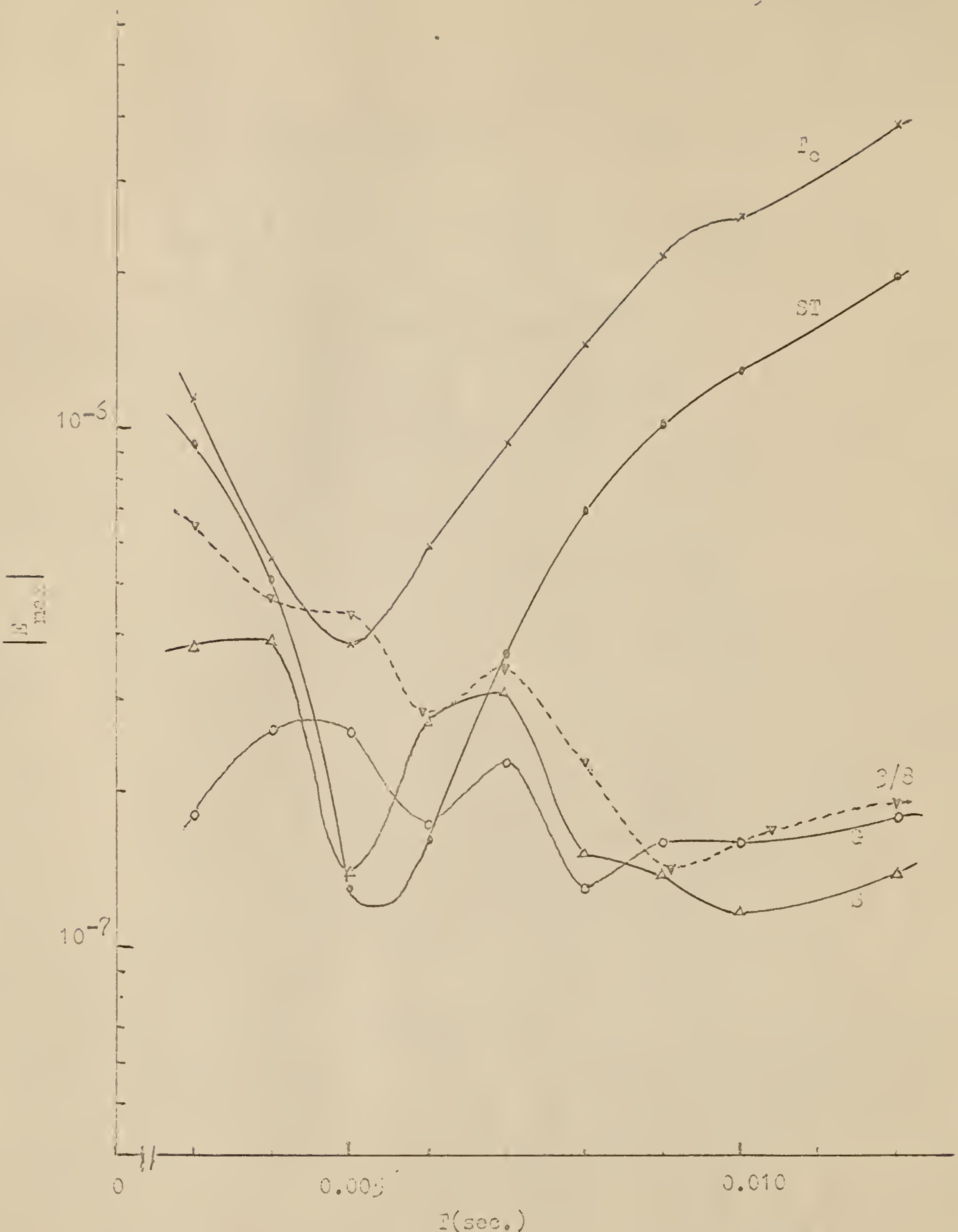

Fig. 2. Error curves of $\frac{dy}{dt} + y = 1$, $y(0) = 0$, $t = 0.5$

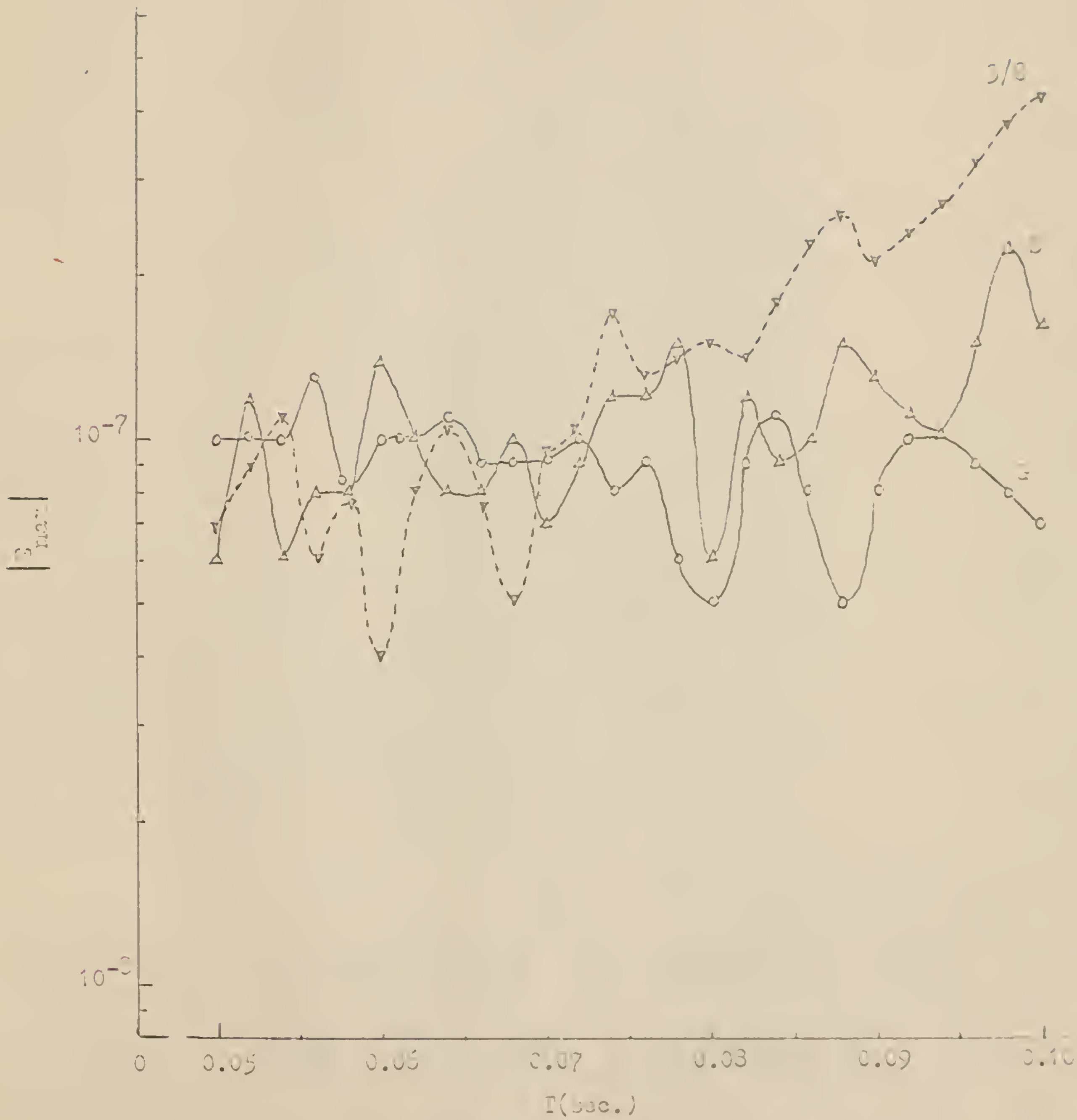

Fig. 3. Error curves of $\frac{dy}{dt} + y = 1$, $y(0) = 0$, $t = 0.6$

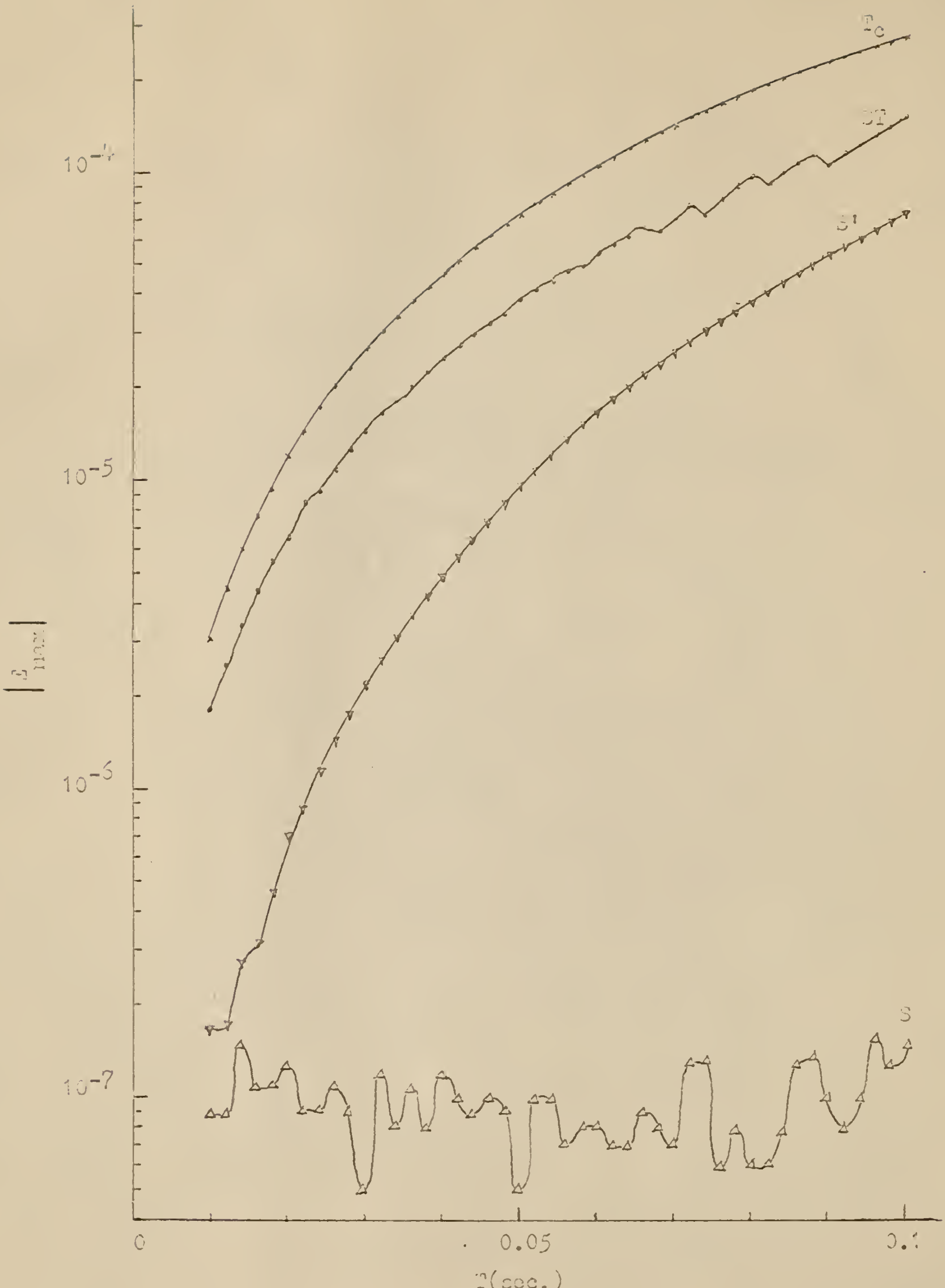

Fig. 4. Error curves of $\frac{dy}{dt} + y = 0$, $y(0) = 0$, $t = 0.8$

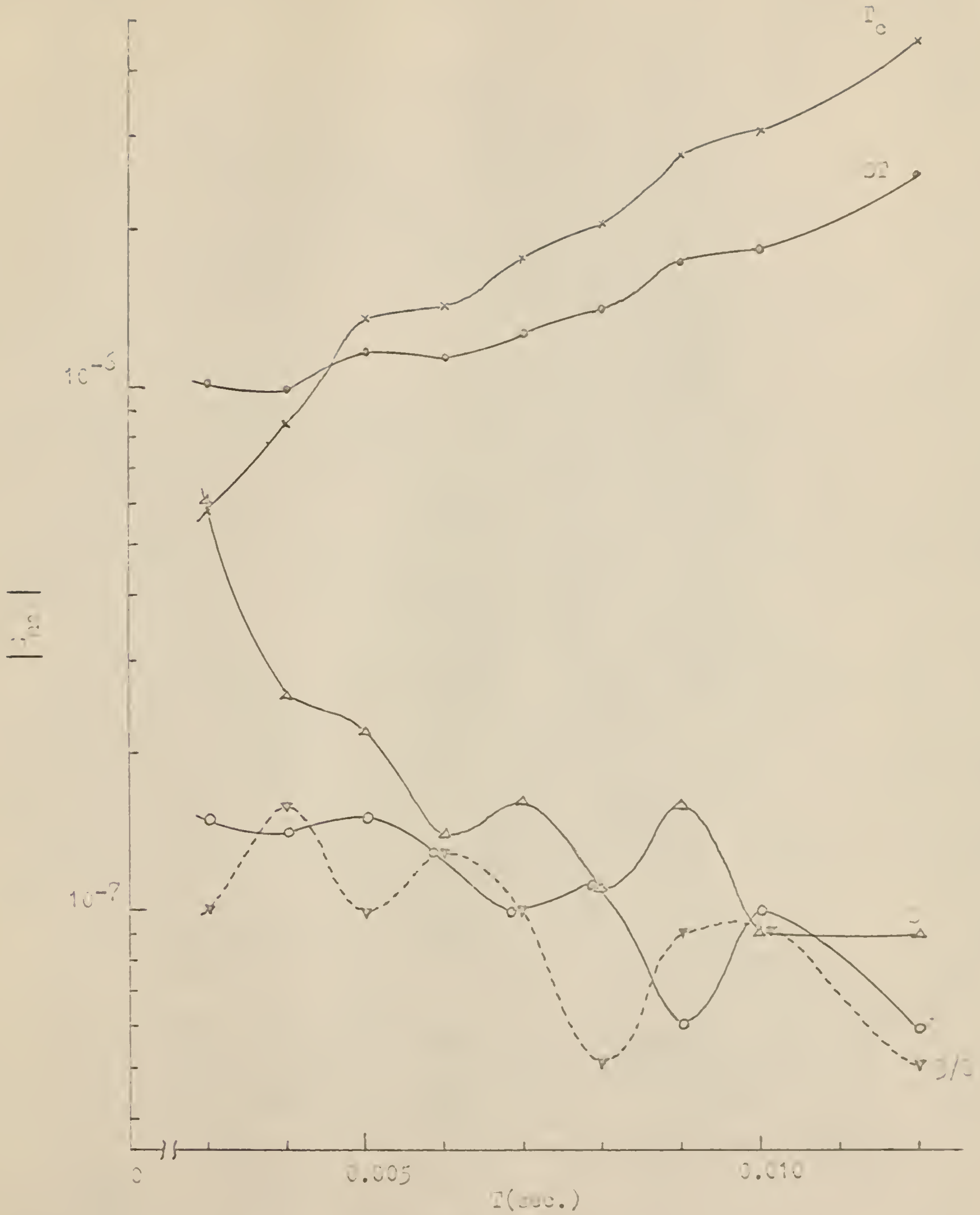

Fig. 5. Error curves of $\frac{dy}{dt} + y = 0$, $y(0) = 1$, $t = 0.3$

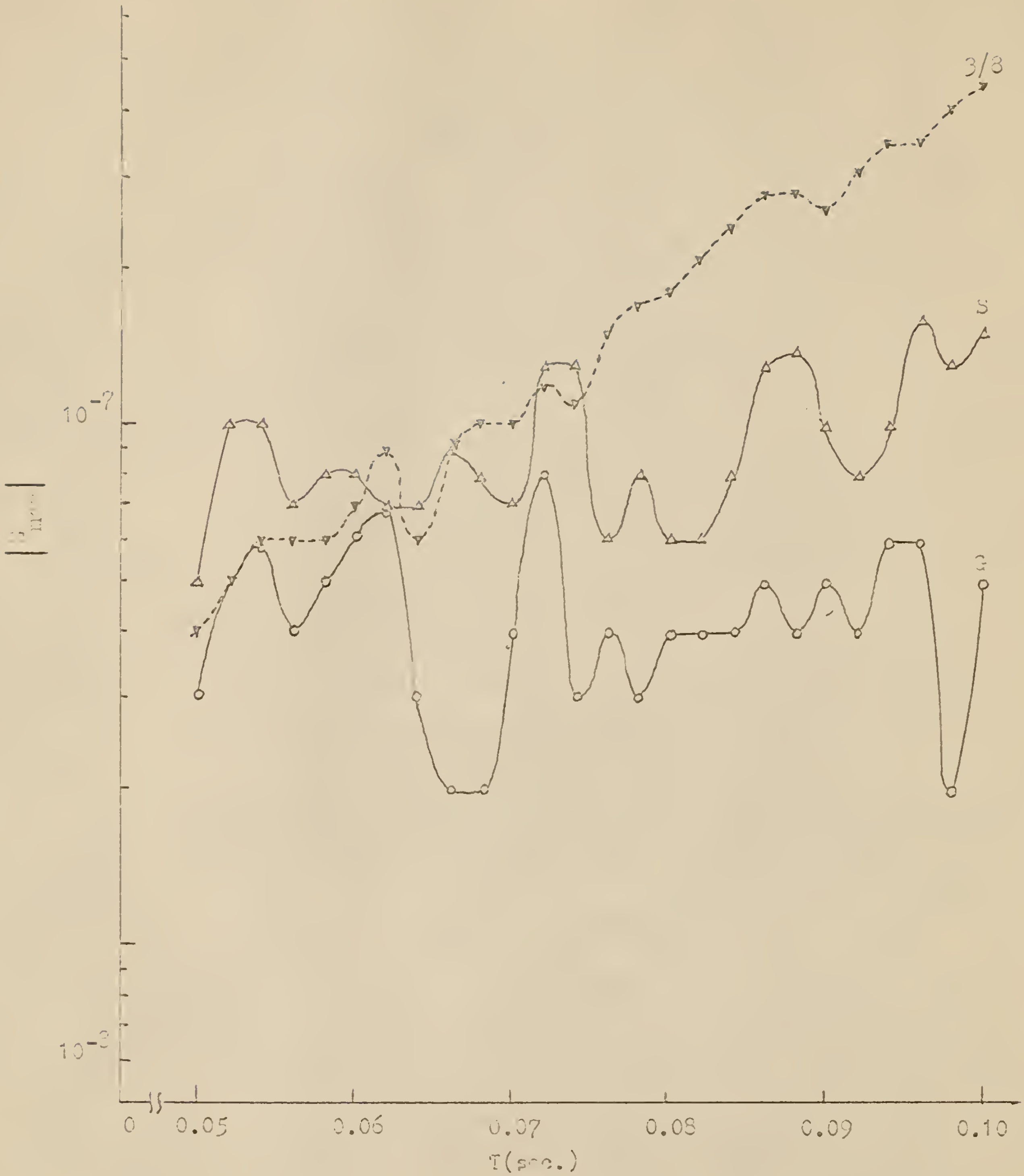

Fig. 6. Error curves of $\frac{dy}{dt} + y = 0$, $y(0) = 1$, $t = 0.8$

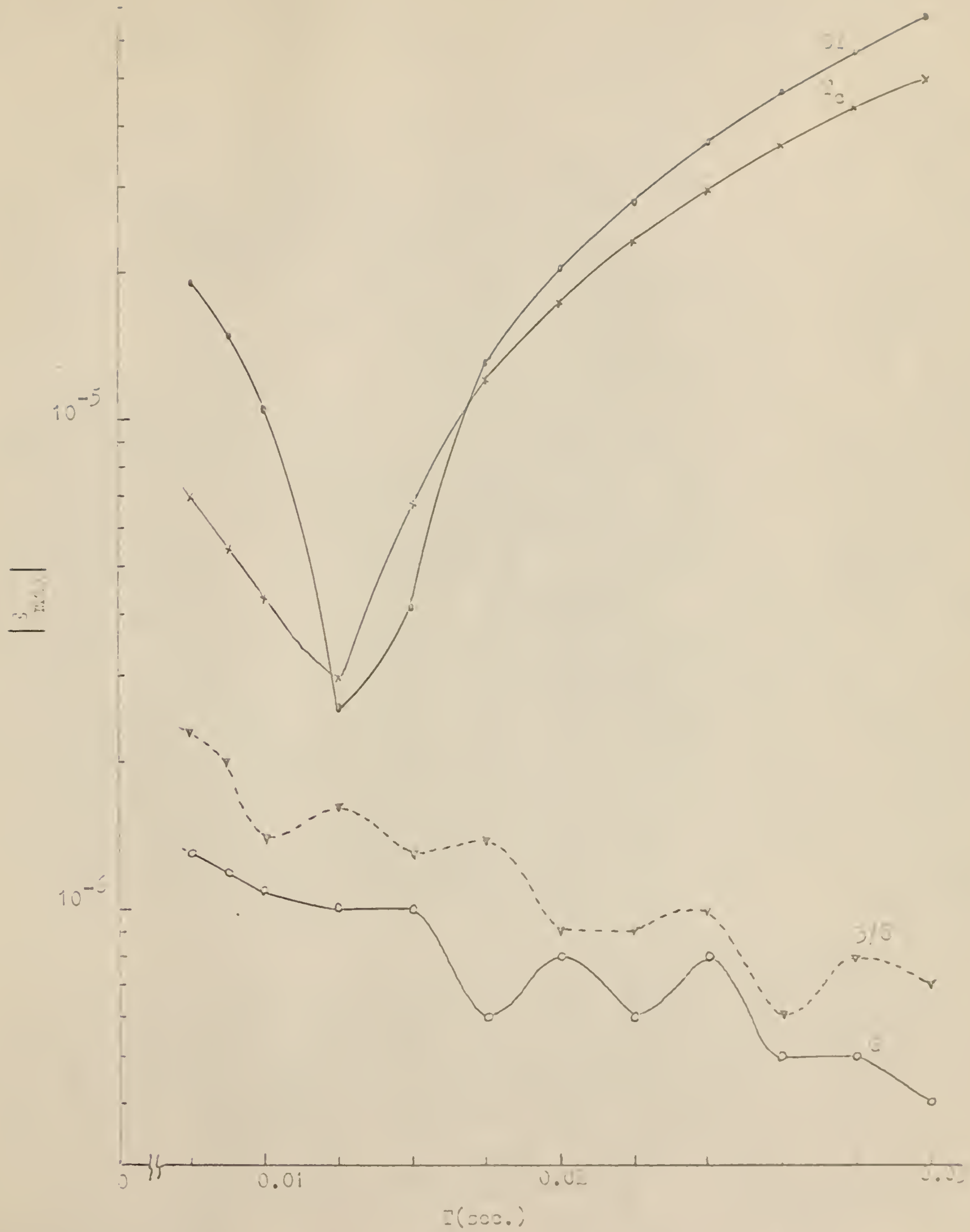

Fig. 7. Error curves of $\frac{dy}{dt} + 5y = t$, $y(0) = 2$, $t = 2.0$

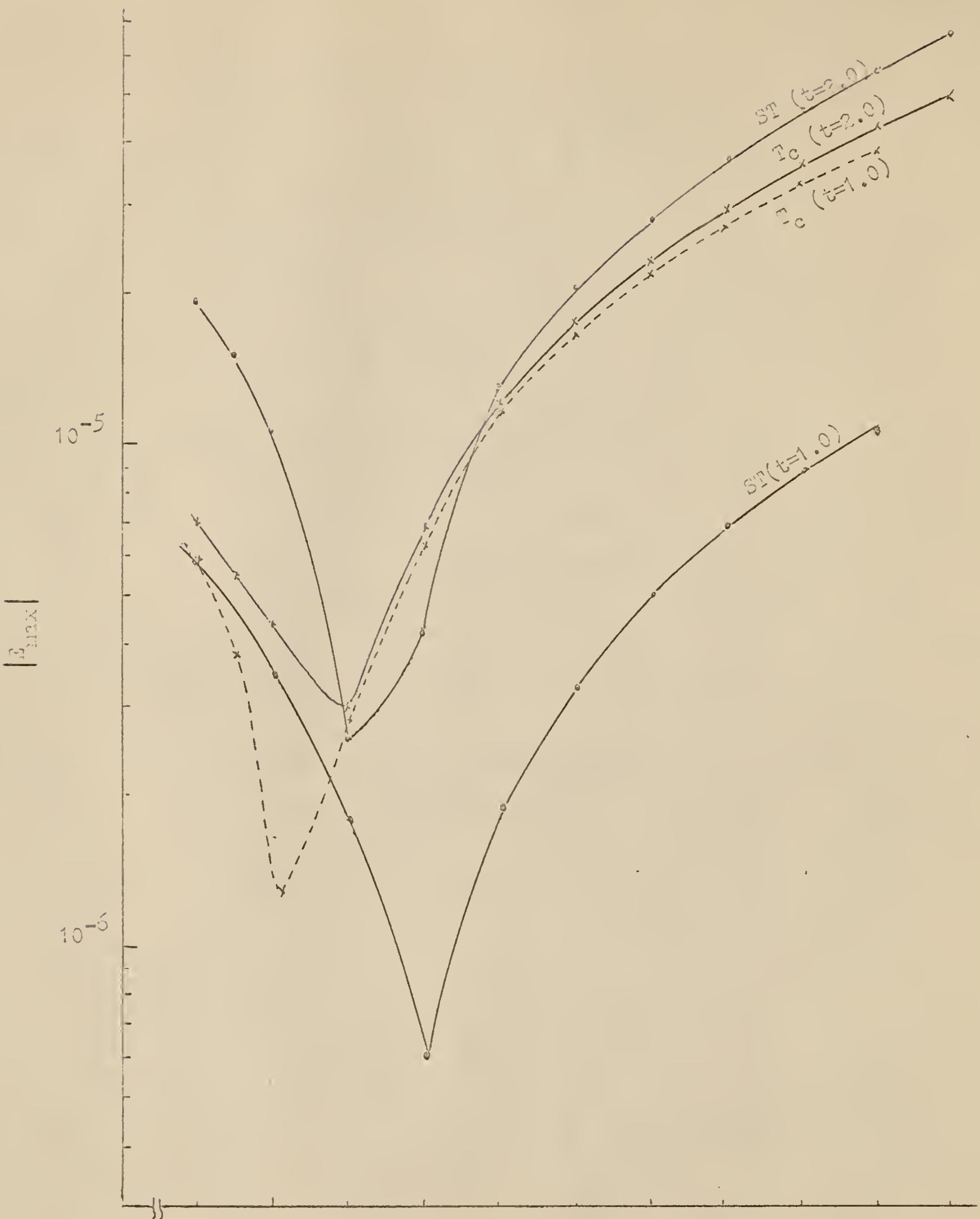

Fig. 8. Error curves showing the degeneration of ST

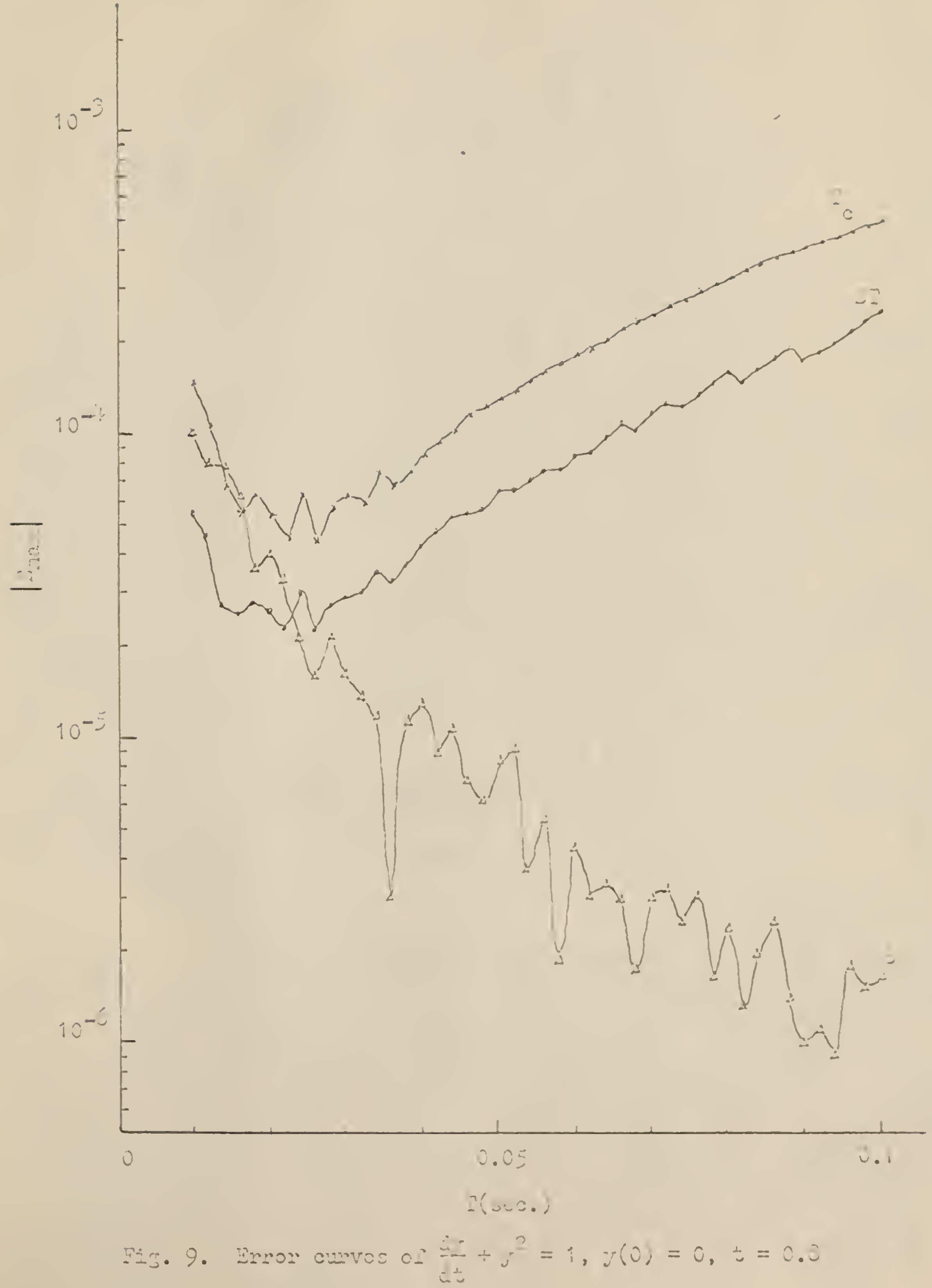

Fig. 9. Error curves of $\frac{dy}{dt} + y^2 = 1$, $y(0) = 0$, $t = 0.8$

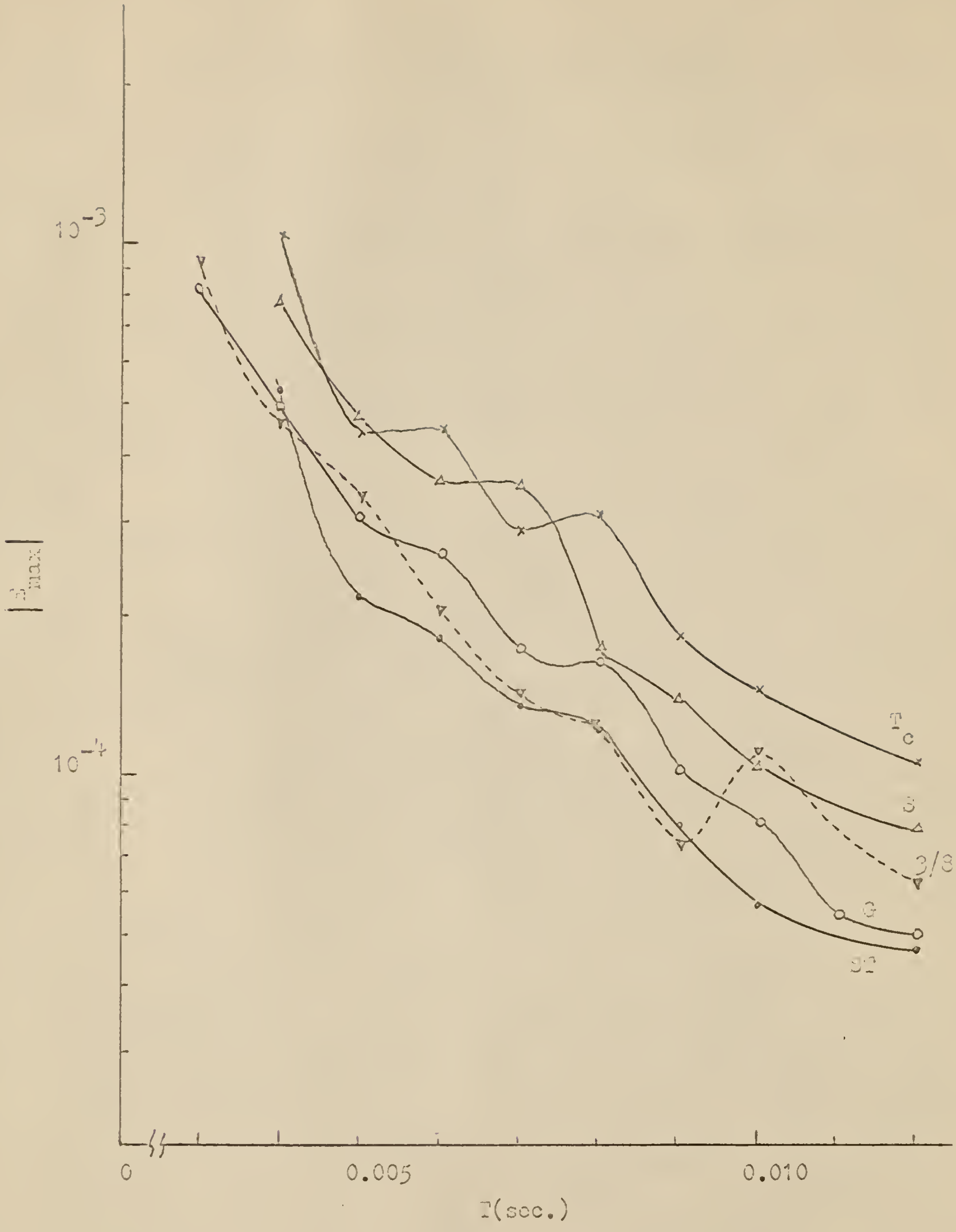

Fig. 10. Error curves of $\frac{dy}{dt} + y^2 = 1$, $y(0) = 0$, $t = 0.8$

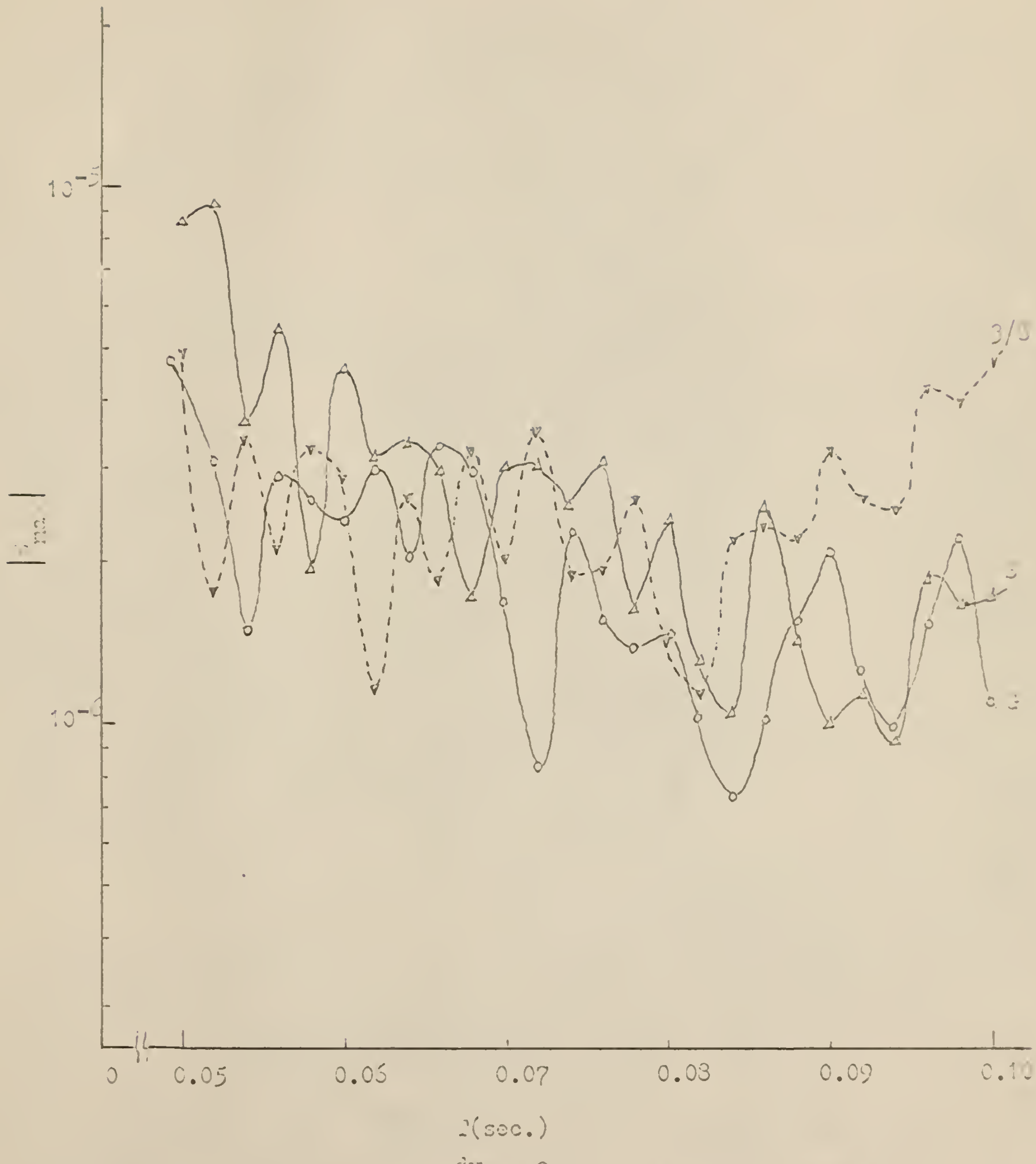

Fig. 11. Error curves of $\frac{dy}{dt} + y^2 = 1$, $y(0) = 0$, $t = 0.8$

DISCUSSION

Investigation of the graphs shows that there exists a sampling interval size which minimizes the largest absolute value of error for the fixed computation duration in T-convolution (T_c) and function iteration (ST). For the case of $\frac{dy}{dt} + y = 0$, $y(0) = 1$, the optimum sampling interval size are not shown but the author has confirmed this by other computation which shows that the optimum interval size falls between 0.002 and 0.003 seconds. There is some heuristic justification for the existence of this minimum error in the T-convolution case. If the interval size is large, then trapezoidal integration generates large errors. If one observes the function of z obtained by the T-convolution process, then the limit as T approaches zero yield a factor $(1-z)^n$ in the denominator, where n is the order of the differential equation being studied. In spite of the exact solution being bounded, unbounded approximating functions then occur when $n \geq 2$ and the errors are correspondingly large.

The minimum error point is a function of computation time t. Referring to Figure 8, one will observe that for T-convolution when computation time, t, increases from 1 second to 2 seconds, the minimum error point moves from $T \doteq 0.01$ to $T \doteq 0.12$. Few examples do not justify any definite conclusion, but from the above example the minimum error point may be the function of the solution time. If one increases the computation time, t, further, one can find the optimum sampling range for minimum error point for the particular differential equation under consideration.

Functional iteration technique is primarily designed for improvement of accuracy in computation. Test computations show that it surely lowers the maximum error, $|E_{max}|$, for some interval of computation time t, but as t increases further, the rate of increase in $|E_{max}|$ exceeds that of T-convolution and it will become less accurate than that of T-convolution. This accuracy regression property of functional iteration technique is vividly displayed in Figures 7 and 8. In this particular example, when T lies between 0.012 and 0.016, the accuracy of ST is greater than that of T_c, but for $T > 0.016$ or $T < 0.012$ the accuracy is poorer than T_c. Again, there is a problem of estimating optimum sampling range. As in the case of the optimum sampling range for minimum error, one can only assume that one of the deciding factors will be computation time, t. Since the accuracy improvement property of the functional iteration (ST) is not high even if one uses the sampling size, T, in optimum range, unless one can estimate regression point beforehand, one should avoid employing this method.

Generally speaking, application of Simpson's rule and other higher-order Newton-Cotes integration formula in the solution of differential equation gives better results than T-convolution method. Especially when the initial values are estimated as accurately as possible, the solutions are amazingly accurate. The effect of initial values to the accuracy of solution is clearly shown in Figure 4. When trapezoidal rule is used to approximate y_1, the error curve of Simpson's rule is similar to the T-convolution, though $|E_{max}|$ of the former is lower than that of the latter. On the other hand, the adoption of Taylor series in approximation of y_1 gives a much better error characteristic. There is one often overlooked trouble that occurs when Simpson's formula is used to start the chain for the odd-numbered sample points. The result of this jumping two steps ahead is that the accumulated errors at the odd- and even-numbered points are rather independent of each other, especially as the weights attached to the computed integrand values are different. This tends to produce an oscillation. While this oscillation is due to errors committed and hence gives some measure of the accuracy of the results, it can be very annoying.

Oscillation is observed in every case of test computations; it is conjectured that for special case of $y' = f(t)$, oscillation may be avoided if we estimate y_2 by Taylor series, then even-numbered point chain only is computed by Simpson's rule and the half Simpson's formula (Hamming, p. 127) is used to produce each odd-numbered point.

Considering that Simpson's second rule and Gauss' formula have to approximate more starting points, that coefficients are more complex, that accuracy improvement effect is about the same as Simpson's rule, higher-order Newton-Cotes quadrature formulas have doubtful performance in digital solution of differential equations.

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NEWTON-COTES QUADRATURES FOR DIGITAL SOLUTION OF DIFFERENTIAL EQUATIONS

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The essential content of this report is metaprogramming for the digital approximation of the solution of first-order differential equations using Newton-Cotes quadratures.

When trapezoidal quadratures are employed, there are two possible programs: the first-order vector differential equation program and the integrator substitution program. These can be succinctly described in Z-transform notation.

Romberg proposes an algorithm for numerical integration which generates high-order integration quadratures by repeated use of linear combinations of trapezoidal quadrature. The coefficients of Romberg quadratures are always positive and the error terms are not worse than those of the Newton-Cotes quadratures. It could be very useful in digital solution of differential equations.

When Simpson's rule or higher-order Newton-Cotes quadratures are employed, the phenomenon of ultimately recursiveness appears in the first-order vector differential equation program, but there is no integrator substitution program possible for high-speed calculation. Z-transform notation must be dropped in ultimately recursive calculations.

Empirical error analysis shows that there exists an optimum sampling range which minimizes the largest absolute value of error for the fixed computation duration in T-convolution (T_c) and function iteration (ST); that as a result of accuracy regression property, ST has only limited use in the solution of differential equations; that Simpson's rule or higher-order Newton-Cotes quadratures has higher accuracy but less stable than T-convolution; that the estimation of starting points plays a vital role in accuracy improvement of the solution of differential equations by higher-order Newton-Cotes quadratures.

In conclusion, if one employs Newton-Cotes quadratures to solve differential equations, one can expect that trapezoidal rule has lower accuracy but higher stability and less computation time while the reverse is true for higher-order quadratures.