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TABLES FOR THE STEP-BY-STEP INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS OF THE FIRST ORDER

By

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March 25, 1963

Technical Report No. 406

Cruft Laboratory
Harvard University
Cambridge, Massachusetts
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The research reported in this document was supported by Grant 21869 of the National Science Foundation. Publication was made possible through support extended to Cruft Laboratory, Harvard University, by the Navy Department (Office of Naval Research), the Signal Corps of the U. S. Army, and the U. S. Air Force under ONR Contract Nonr-1866(32). Reproduction in whole or in part is permitted for any purpose of the United States Government.

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Harvard University
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A study is made of the step-by-step integration of ordinary differential equations of the first order by means of formulas obtained from the Gregory-Newton backward interpolating formula. Tables of relevant constants are presented.
Consider the ordinary differential equation of the first order

\[ y' = f(y, x) \]  

which is to be integrated step-by-step over \( x = a \) to \( b \). A natural method for accomplishing this integration is a predictor-corrector process based upon a suitable finite difference interpolating formula.

Let \( x_0 \) be a tabular point within \((a, b)\) and assume that \( y \) is known at the points \( x_j = x_0 - jh \) \((j = 0, 1, \ldots, \frac{x_0 - a}{h})\). One can then write for \( y' \) the approximation to it which is provided by the Gregory-Newton backward interpolating formula

\[ y' = \sum_{j=0}^{J} \frac{1}{j!} (u + j - 1) [j] \Delta^j f_{-j} + h^{J+1} \frac{1}{(J+1)!} (u+J) [J+1] (J+1) (\xi) \]  

where \( u = (x - x_0)/h \), \( \Delta^j f_{-j} \) is the \( j \)th forward difference of \( y' \) about \( x_{-j} \), \( x_{-j} \leq \xi \leq x_0 \), and \((u - t)^{[j]}\) is the factorial polynomial

\[ (u - t)^{[j]} = (u - t) (u - t - 1) \cdots (u - t - j + 1) \]  

which possesses the expansion

\[ (u - t)^{[j]} = \sum_{k=0}^{j} S^j_k u^{j-k} \]  

where the \( S^j_k \) are the generalized Stirling numbers of the first kind [1].

The formula (2) can be integrated in two fashions. In the first it is assumed that \( y_0, y_{-1}, \ldots, y_{-J} \) are accurately known and that a prediction of \( y_1 = y(x_1) \) is desired:
TR406

\[ y(x_1) = y_0 + h \sum_{j=0}^{J} \beta_j \Delta_j f_{-j} + E_j \]  \hspace{1cm} \text{PREDICTOR} \hspace{1cm} (4)

where the error \( E_j \) is given by

\[ |E_j| \leq h^{J+2} \max \beta_{j+1} |f^{(J+1)}| \]  \hspace{1cm} (5)

and

\[ \beta_j = \frac{1}{j!} \int_0^1 (u+j-1)^{[j]} \, du \]  \hspace{1cm} (6a)

\[ = \frac{1}{j} \sum_{p=0}^{j} \frac{1}{j+1-p} S_p^j \]  \hspace{1cm} (6b)

\[ = \frac{N_j}{L(j) j!} \]  \hspace{1cm} (6c)

where \( L(j) \) is the least common denominator of \( \frac{1}{1}, \frac{1}{2}, \ldots, \frac{1}{j+1} \).

In the second method it is assumed that \( y_{-1}, \ldots, y_{-J} \) are accurately known, that \( y_0 \) is approximately known, and that a corrected value of \( y_0 \) is desired:

\[ y(x_0) = y_{-1} + \sum_{j=0}^{J} \beta_j^* \Delta_j f_{-j} + E_j^* \]  \hspace{1cm} \text{CORRECTOR} \hspace{1cm} (7)

where the error \( E_j^* \) is given by

\[ |E_j^*| \leq h^{J+2} |\beta_{j+1}^*| |f^{(J+1)}|_{\text{max}} \]  \hspace{1cm} (8)
Table I

\( \mathbf{N}_j, \mathbf{N}_j^*, \) and \( L(j)j! \)

<table>
<thead>
<tr>
<th>j</th>
<th>0</th>
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<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
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<td>1</td>
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<tr>
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<td>-1</td>
<td>-1</td>
<td>-3</td>
<td>-38</td>
<td>-135</td>
<td>-4315</td>
<td>-48125</td>
<td>-950684</td>
<td>-7217406</td>
<td>-682590930</td>
</tr>
<tr>
<td>( L(j)j! )</td>
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<td>2</td>
<td>12</td>
<td>72</td>
<td>1440</td>
<td>7200</td>
<td>302400</td>
<td>4233600</td>
<td>101606400</td>
<td>914457600</td>
<td>100590336000</td>
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</table>
and

$$\beta_j^* = \frac{1}{j!} \int_{-1}^{0} (u + j - 1)[j] \, du$$  \hspace{1cm} (9a)$$

$$= \frac{1}{j!} \sum_{p=0}^{j} \frac{(-1)^{j-p}}{j+1-p} \cdot \frac{(-1)^{j-1}}{p} \cdot S_p^j$$  \hspace{1cm} (9b)$$

$$= \frac{S_j^*}{L(j)!}$$  \hspace{1cm} (9c)$$

This corrected value of $y_0$ can itself be used in (7) to obtain what is presumably a still better value of $y_0$, and this process can be repeated indefinitely until it converges to a final value or, in bad cases, is seen to be divergent. The use of (4) to obtain an initial estimate and the repeated use of (7) to improve this value constitutes a well-known predictor-corrector process.

The quantities $\beta_j$ and $\beta_j^*$, as defined by (6a) and (9a), respectively, have been described by Collatz [2] and tabulated by him for $j = 0(1)6$. The increasing use of digital machines - often in double precision - for the integration of differential equations has made a somewhat extended table of these coefficients desirable and the existence now [1] of extensive tables of the $S_k^j$ has made possible the simple computation from (6b) and (9b). Table I presents the results of such an extension; the table entries were checked using the recursion relation [2]

$$\beta_{j+1}^* = \beta_j^* + \beta_{j+1}^*$$  \hspace{1cm} (10)$$
Figure I presents a graph of these coefficients. The $\beta_j$ can be seen to fall off slowly and can be shown, from (6a), to satisfy the inequality

$$\frac{j}{j+1} < \frac{\beta_{j+1}}{\beta_j} < 1 \quad j \geq 0$$  \hspace{1cm} (11a)

which implies that their decline is very slow indeed. The $\beta_j^*$ can be seen to fall off somewhat faster; this is to be expected since, from (6a) and (9a),

$$|\beta_j^*| < \frac{\beta_j^*}{j-1} \quad j \geq 2$$  \hspace{1cm} (11b)

These data point up the intrinsic superiorities of corrector formulas over predictor formulas: (i) that, since $|\beta_j^*| < |\beta_j|$ the series (7) converges faster than the series (4), and (ii) that, since the $\beta_j^*$ decay much faster than the $\beta_j$, the buildup of computational error in the taking of successive differences will, for a given number of terms in the interpolating series, have much less effect on the final answer when a corrector formula is used.

In actual practice the calculation of the several differences is often not carried out. Instead, the differences are expanded as

$$\Delta^j f_{-j} = \sum_{p=0}^{j} \gamma_{pj} f_{-p} \quad (12)$$

and (4) rewritten as

$$y(x_1) = y_0 + h \sum_{j=0}^{J} \left( \sum_{p=0}^{j} \gamma_{pj} \beta_j f_{-p} + E_j \right) \quad (13a)$$
### Table II

<table>
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<tr>
<th>( j )</th>
<th>( \phi(j) )</th>
<th>( \gamma(j) )</th>
</tr>
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<th>( \gamma(p) )</th>
</tr>
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</tr>
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<td>2</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
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<td>4</td>
</tr>
<tr>
<td>4</td>
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<td>5</td>
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</tr>
<tr>
<td>9</td>
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</tbody>
</table>
The calculation of the next value of \( y \) can then be accomplished directly from (13c) or (14c) and the labor of maintaining a difference table thereby eliminated. Tables of \( \delta_p(J) \) and \( \delta^*_p(J) \) have been computed for \( J = 0(1)10 \) and \( p = 0(1)J \) and are given in Tables II and III, respectively; they represent a considerable extension over the existing tables [2, 3] which go at most to \( J = 5^* \). The values of \( \delta_p(J) \) and \( \delta^*_p(J) \) were checked by the relations [2]

*The values of \( a_p(5) \) given in Reference 3 are believed to be in error.
and by having key portions of the computations individually repeated.

The selection of a predictor-corrector pair for a specific problem is by no means simple, it being necessary to choose \( J \) and \( h \) with care to minimize the effects of roundoff and truncation error. However, for modern digital machines operated in double precision, \( J = 10 \) will probably be as large as is profitable since by this point the computing error generated in calculating the \( \Delta^1 f_{-j} \) will be growing much faster than the \( \beta_j^* \) will be decreasing, and the total error due to this cause will normally be at least as important as the truncation error \( E_j^* \). Finally, for suitable \( f(y, x) \), it may be desirable to suspend the common practice of using a low order predictor to obtain an estimate of the next point which can then be improved using a high order corrector; the existence of high order predictors makes the initial use of a high order predictor formula and the suspension of corrector iterations seem attractive where the superior roundoff suppressing properties of a corrector formula are not essential.
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