An Iterative Method of Numerical Differentiation

By D. B. Hunter

A method of estimating the derivative of a function defined by a table of values is described. The method is similar to those of Aitken and Neville for iterative interpolation, and, like them, can be used with either equally-spaced or unequally-spaced ordinates.

Interpolation

We shall first review Aitken's and Neville's methods of iterative interpolation. Suppose y is a function of x which takes the values $y_0, y_1, y_2, \ldots, y_n$, when $x = x_0, x_1, x_2, \ldots, x_n$. Then, if $i, j, \ldots, p, q$ is any set of distinct integers in the range $(0, n)$, let us denote by

$$y_{i,j,\ldots,p,q}$$

the polynomial of least degree in x which takes the values $y_i, y_j, \ldots, y_p, y_q$ when $x = x_i, x_j, \ldots, x_p, x_q$.

The following relationship holds between these polynomials:

$$y_{i,j,\ldots,p,q} = \frac{1}{x_q - x_i}\begin{vmatrix} y_{i,j,\ldots,p} & x_i - x \\ y_{j,\ldots,p,q} & x_q - x \end{vmatrix} \quad (1)$$

This result is proved, in a rather more general form, by Neville (1934) (p. 92).

Equation (1) can be used as the basis for a number of methods of iterative interpolation. The most familiar are those of Aitken (1932) and Neville (1934).

Aitken's method proceeds by using equation (1) to calculate, from the original ordinates, $y_0, y_1, y_2, \ldots, y_n$ the set of linear approximations $y_{0,1}, y_{0,2}, \ldots, y_{0,n}$. These are used, in turn, to produce the quadratic approximations $y_{0,1,2}, y_{0,1,3}, \ldots, y_{0,1,n}$; and the higher degree approximations are calculated by the same process.

The calculation can be conveniently set out in a table, similar to Table 1 below (in which $n = 4$).

Neville's modification of Aitken's method, which has a number of advantages, is set out in Table 2.

Differentiation

If equation (1) is differentiated, it gives the result:

$$y'_{i,j,\ldots,p,q} = \frac{1}{x_q - x_i}\left\{\begin{vmatrix} y'_{i,j,\ldots,p} & x_i - x \\ y'_{j,\ldots,p,q} & x_q - x \end{vmatrix} + (y_{j,\ldots,p,q} - y_{i,j,\ldots,p})\right\} \quad (2)$$

More generally, if equation (1) is differentiated r times, it gives the result:

$$y^{(r)}_{i,j,\ldots,p,q} = \frac{1}{x_q - x_i}\left\{\begin{vmatrix} y^{(r)}_{i,j,\ldots,p} & x_i - x \\ y^{(r)}_{j,\ldots,p,q} & x_q - x \end{vmatrix} + r(y^{(r-1)}_{j,\ldots,p,q} - y^{(r-1)}_{i,j,\ldots,p})\right\} \quad (3)$$

Table 1

Interpolation by Aitken's Method

y_0					$x_0 - x$
y_1	$y_{0,1}$				$x_1 - x$
y_2	$y_{0,2}$	$y_{0,1,2}$			$x_2 - x$
y_3	$y_{0,3}$	$y_{0,1,3}$	$y_{0,1,2,3}$		$x_3 - x$
y_4	$y_{0,4}$	$y_{0,1,4}$	$y_{0,1,2,4}$	$y_{0,1,2,3,4}$	$x_4 - x$

Table 2

Interpolation by Neville's Method

y_0					$x_0 - x$
y_1	$y_{0,1}$				$x_1 - x$
y_2	$y_{1,2}$	$y_{0,1,2}$			$x_2 - x$
y_3	$y_{2,3}$	$y_{1,2,3}$	$y_{0,1,2,3}$		$x_3 - x$
y_4	$y_{3,4}$	$y_{2,3,4}$	$y_{1,2,3,4}$	$y_{0,1,2,3,4}$	$x_4 - x$

Table 3

Derivatives by Aitken's Method

y_0					$x_0 - x$
y_1	$y'_{0,1}$				$x_1 - x$
y_2	$y'_{0,2}$	$y'_{0,1,2}$			$x_2 - x$
y_3	$y'_{0,3}$	$y'_{0,1,3}$	$y'_{0,1,2,3}$		$x_3 - x$
y_4	$y'_{0,4}$	$y'_{0,1,4}$	$y'_{0,1,2,4}$	$y'_{0,1,2,3,4}$	$x_4 - x$

These results may be used, in conjunction with equation (1), to estimate the derivatives of a function at any point, as well as the value of the function itself. For instance, the first derivative can be calculated, using two tables; the first is like Table 1 or 2, and calculates the function, and the second, to calculate the derivative, is similar to Table 3 (which gives the form to be combined with Table 1). The second column of this table is obtained by using the equation

$$y'_{0,i} = \frac{y_i - y_0}{x_i - x_0} \quad (4)$$

and the later columns can be filled in by using equation (2), taking the values of $y_{j,\ldots,p,q}$ and $y_{i,j,\ldots,p}$ from Table 1.

The extension of the method to estimate higher derivatives, using equation (3), is obvious. The calculation of $y^{(r)}$ requires $r+1$ tables, to calculate, respectively, the values of $y, y', y'', \ldots, y^{(r)}$. If $1 < s \leqslant r$, the table for $y^{(s)}$ contains zeros in columns 2 to s, and the remaining columns are filled in by applying equation (3), taking the values of $y^{(s-1)}_{j,\ldots,p,q}$ and $y^{(s-1)}_{i,j,\ldots,p}$ from the previous table.

Example

As an example, let us estimate the values of y and y', where $y = \sqrt{x}$, for $x = 12\cdot3$, from the following table of square roots.

x	$\sqrt{x}$
10	3·1622 777
11	3·3166 248
12	3·4641 016
13	3·6055 513
14	3·7416 574
15	3·8729 833

We shall use Neville's method. As the calculation proceeds, the more significant digits of the intermediate results tend to become constant; as they do so, they can be omitted from the calculation.

The resulting two tables are given as Tables 4 and 5. These two tables give the results:

$$y = 3\cdot5071\,355$$
$$y' = 0\cdot1425\,664,$$

the last digit being uncertain in each case. Compare with the true results:

$$y = \sqrt{12\cdot3} = 3\cdot5071\,356$$

$$y' = \frac{1}{2\sqrt{12\cdot3}} = 0\cdot1425\,665.$$

Conclusions

It is hoped that the method of differentiation described above will be useful in many applications. Most of the existing methods of numerical differentiation can be used only for tables with equally-spaced ordinates, and are designed to give the derivative either at the tabular points, or midway between them. The method of this paper can be used with either equally-spaced or unequally-spaced ordinates, and can be used to estimate the derivative at any point within the range of the table. On the other hand, the calculation is only slightly simpler when applied to a tabular point, than when applied to a general point. In fact, if the derivative is required at a tabular point x_k, the table corresponding to Table 4 must still be calculated in full, the only simplification being that any approximation $y_{i,j,\ldots,p,q}$ in which k appears among the suffixes can be immediately set equal to y_k, without calculation.

The method has the further disadvantage that it is necessary to estimate y as well as y'. However, in suitable cases, the advantages of the method will outweigh its disadvantages.

Table 4

Calculation of y

3·1622 777						−2·3
3·3166 248	·5172 760					−1·3
3·4641 016	·5083 446	070 049				−0·3
3·6055 513	·5065 365	071 693	1 309			0·7
3·7416 574	·5102 770	070 976	1 382	51		1·7
3·8729 833	·5184 034	074 328	1 311	59	5	2·7

Table 5

Calculation of y'

3·1622 777						−2·3
3·3166 248	·1543 471					−1·3
3·4641 016	·1474 768	419 806				−0·3
3·6055 513	·1414 497	426 551	25 525			0·7
3·7416 574	·1361 061	425 184	25 720	655		1·7
3·8729 833	·1313 259	418 424	25 625	671	64	2·7

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