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EXTRAPOLATION METHOD FOR NUMERICAL CALCULATION OF THE DERIVATIVE OF THE ANALYTICAL FUNCTION AND ITS ERROR ESTIMATE

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1. INTRODUCTION

Let $T(h)$ be the numerical approximation of an exact problem T, defined by $\lim_{n \to 0} T(h) = T$ and obtained for some discrete parameter h. The following idea of improving $T(h)$ originates from Richardson: For various h_i, $i = 0, 1, 2, \ldots, m$, calculate $T(h_i)$ and construct the interpolation polynomial $T_m(h)$ through points $(h_i, T(h_i))$, the value $T_m(0)$ being taken as an approximate value for T.

The assumption for the numerical application of this extrapolation method is the existence of an asymptotic expansion

$$T(h) \approx \tau_0 + \tau_1 h^{\gamma_1} + \ldots + \tau_k h^{\gamma_k} + R_{k+1}(h) h^{\gamma_{n+1}} \tag{1}$$

where $|R_{k+1}(h)| \leqq M_{k+1}$ for all $h > 0$, $0 < \gamma_1 < \ldots < \gamma_{k+1}$ and $\tau_0, \ldots, \tau_k$ do not depend on h. STETTER [4] proved the existence of such expansions for a very general class of discretization algorithms for non-linear functional equations (e.g. initial and boundary value problems for both ordinary and partial differential equations, integral equations and integro-differential equations).

2. DESCRIPTION OF THE METHOD

The difference quotient

$$T(h) = \frac{f(x + h) - f(x - h)}{2h} \tag{2}$$

of an analytical function $f(x)$ is of the form [1]

$$(3) \qquad T(h) = f'(x) + h^2 \frac{f^{III}(x)}{3!} + h^4 \frac{f^{V}(x)}{5!} + h^6 \frac{f^{VII}(x)}{7!} + \dots,$$

whereby

$$\lim_{h \to 0} T(h) = f'(x).$$

$T(h)$ in (3) has the form (1) and thus we can use Richardson's idea outlined in the introduction. The choice of the interpolation polynomial of n-th degree is closely connected with the properties of the remainder $f'(x) - T(h)$. It is seen from relation (3) that this remainder is an even function of h and therefore we take for $P_n(h)$ the polynomial in h^2. This polynomial has to assume the same values as function $T(h)$ at the points of the zero sequence $\{h_k\}_{k=0}^{m}$. If we denote

$$T_0^{(k)} = T(h_k), \quad k = 0, 1, \dots, m,$$

then from the Lagrange interpolation formula we get for this polynomial for $h = 0$ the expression

$$(4) \qquad T_m^{(0)} \approx P_{2m}(0) = \sum_{k=0}^{m} T_0^{(k)} \prod_{\substack{i=0 \\ i \neq k}}^{m} \frac{h_i^2}{h_i^2 - h_k^2}.$$

The extrapolation for the argument $h = 0$ may be performed by the advantageous Neville-Aitken algorithm from which, by simple recurrent relations, we obtain without knowing the coefficients of the Lagrange polynomial its value at an arbitrary point. Relation (4) is recurrently calculated by means of the so called T-scheme

$$(5) \qquad \begin{array}{ccccc}
T_0^{(0)} & & & & \\
 & T_1^{(0)} & & & \\
T_0^{(1)} & & T_2^{(0)} & \cdot & \\
 & T_1^{(1)} & \cdot & \cdot & \\
T_0^{(2)} & \cdot & \cdot & & T_m^{(0)} \\
\cdot & \cdot & \cdot & \cdot & \\
\cdot & \cdot & T_2^{(m-2)} & & \\
\cdot & T_1^{(m-1)} & & & \\
T_0^{(m)} & & & &
\end{array}$$

in which $T_m^{(0)} \approx T(0)$ and the s-th column $(s = 2, 3, \dots, m)$ is calculated from $(s - 1)$ by

$$(6) \qquad T_s^{(k)} = \frac{h_k^2 T_{s-1}^{(k+1)} - h_{k+s}^2 T_{s-1}^{(k)}}{h_k^2 - h_{k+s}^2}, \qquad \begin{array}{l} k = 0, 1, \dots, m, \\ s = 0, 1, \dots, m - k. \end{array}$$

Further we will use the sequence of steps [2]

$$\{h_k\}_{k=0}^m = \{(p/q)^k h\}_{k=0}^m , \tag{7}$$

where h is any initial step and $p < q$ are natural numbers. The relation (6) will now have the form

$$T_s^{(k)} = \frac{q^{2s} T_{s-1}^{(k+1)} - p^{2s} T_{s-1}^{(k)}}{q^{2s} - p^{2s}} . \tag{8}$$

Remark. If $p = 1$, $q = 2$, we get the classical Romberg extrapolation algorithm.

In this way we obtain $T_m^{(0)}$, i.e. the approximate value of the derivative in the form of a linear combination of several values of the differentiated function. Thus

$$f'(x) = \sum_{i=0}^{2m+1} A_i f(x_i) + E(f) , \tag{9}$$

where $x_i \in [x - h_0, x + h_0]$, A_i are coefficients which depend on the choice of points x_i and $E(f)$ is the corresponding remainder. Coefficients A_i in the relation (9) are unknown, they are recurrently obtained by the calculation.

As to the convergence of the T-scheme, we are curious to know whether $\lim_{m\to\infty} h_m = 0$, i.e. $\lim_{m\to\infty} T_0^{(m)} = T(0)$, implies also $\lim_{m\to\infty} T_m^{(0)} = T(0)$. The answer is given by

Theorem. *For an arbitrary sequence of steps* (7) *it holds that*

$$\lim_{m\to\infty} T_m^{(0)} = \lim_{m\to\infty} T_0^{(m)} = T(0) .$$

The proof follows from Theorem 1 in [3].

Remarks. 1. By the described method higher derivatives can also be calculated since for the n-th derivative it holds [2]

$$T_0^{(k)} = \frac{1}{(2h_k)^n} \sum_{i=0}^{n} \binom{n}{i} (-1)^i f(x + nh_k - 2ih_k) = f^{(n)}(x) + O(h^2) . \tag{10}$$

2. Derivatives can be calculated also from higher order difference formulae than $O(h^2)$. In that case the relation (6) or (8) will change.

3. ESTIMATE OF ERROR OF AN n-TH ORDER DERIVATIVE FORMULA FOR $L^2(\mathscr{E}_\varrho)$

The error $E(f)$ committed by the use of formulas of numerical approximation applied to an analytical function f may be estimated [5] in the form $|E(f)| \leq \sigma_E \|f\|$. The quantity σ_E is the norm of the error functional; it depends solely on the approximation rule employed and is independent of the particular function considered. The quantity $\|f\|$ is the norm of f in the Hilbert space of analytic functions and may be estimated from a knowledge of the values of the function in the complex plane.

Let $\mathscr{E}_\varrho$ be an ellipse in the complex plane $z = x + iy$ having foci at the points $(-1, 0)$ and $(1, 0)$. Let a and b denote its semimajor and semiminor axes, respectively, and let the quantity $\varrho = \varrho(a)$ be defined by

$$(11) \qquad \varrho = (a + b)^2\,, \quad a = \tfrac{1}{2}(\varrho^{1/2} + \varrho^{-1/2})\,, \quad b = \tfrac{1}{2}(\varrho^{1/2} - \varrho^{-1/2})\,.$$

By $L^2(\mathscr{E}_\varrho)$ we mean the class of functions $f(z)$ which are analytic inside and on $\mathscr{E}_\varrho$, and for which

$$\|f\|^2_{\mathscr{E}_\varrho} = \iint_{\mathscr{E}_\varrho} |f(z)|^2 \, dx \, dy$$

is finite.

Consider next the Chebyshev polynomials of the first kind defined by

$$(12) \qquad T_k(z) = \cos\,(k \arccos z)\,, \quad k = 0, 1, \ldots\,.$$

It can be shown that the polynomials

$$(13) \qquad p_k(z) = 2\sqrt{\left(\frac{2k}{\pi}\right)}\,(\varrho^{2k} - \varrho^{-2k})^{-1/2}\, T_k(z)\,, \quad k = 0, 1, \ldots\,,$$

form a complete orthonormal system for $L^2(\mathscr{E}_\varrho)$ with regard to the scalar product

$$\iint_{\mathscr{E}_\varrho} f(z)\,\overline{g(z)}\, dx\, dy = (f, g)\,.$$

If a function $f(z)$ is of class $L^2(\mathscr{E}_\varrho)$, then it can be expanded in a series of Chebyshev polynomials [5]

$$(14) \qquad f(z) = \sum_{k=0}^{\infty} a_k\, p_k(z)\,,$$

where

$$(15) \qquad \sum_{k=0}^{\infty} |a_k|^2 = \|f\|^2_{\mathscr{E}_\varrho} < \infty\,.$$

The series (14) converges uniformly and absolutely in the interior of $\mathscr{E}_\varrho$.

An arbitrary derivative formula of the n-th order is given by the relation

$$(16) \qquad f^n(x)_{x=0} = R_n + E_n(f)$$

where $R_n = \sum_{i=1}^{N} A_i^{(n)} f(x_i^{(n)})$ and, without any loss of generality, it is supposed that the derivative is taken at the point $x = 0$ (the case of an arbitrary point may be handled by means of an appropriate linear transformation). The error $E_n(f)$ involved in the rule R_n is

(17) $$E_n(f) = f^{(n)}(x)_{x=0} - \sum_{i=1}^{N} A_i^{(n)} f(x_i^{(n)}),$$

and it can be estimated for $f(z) \in L^2(\mathscr{E}_\varrho)$ by using (13), (14). Applying the operator E_n to (14), we obtain

$$E_n(f) = \sum_{k=0}^{\infty} a_k E_n(p_k),$$

from where by means of the Schwarz inequality we get the estimate

$$|E_n(f)|^2 \leqq \sum_{k=0}^{\infty} |a_k|^2 \sum_{k=0}^{\infty} |E_n(p_k)|^2 .$$

Let us now denote

(18) $$\sigma_\varrho^2 = \sum_{k=0}^{\infty} |E_n(p_k)|^2 ,$$

then with respect to (15) we obtain

(19) $$|E_n(f)| \leqq \sigma_\varrho \|f\|_{\mathscr{E}_\varrho} .$$

Table 1

$\tau_k^{(1)}$	k	$\tau_k^{(2)}$	k
0	0, 2, 4, ...	0	1, 3, 5, ...
k	1, 5, 9, ...	k^2	2, 6, 10, ...
$-k$	3, 7, 11, ...	$-k^2$	4, 8, 12, ...
$\tau_k^{(3)}$	k	$\tau_k^{(4)}$	k
0	2, 4, 6, ...	0	3, 5, 7, ...
$k^3 - k$	3, 7, 11, ...	$k^4 - 4k^2$	4, 8, 12, ...
$-(k^3 - k)$	5, 9, 13, ...	$-(k^4 - 4k^2)$	6, 10, 14, ...
$\tau_k^{(5)}$	k	$\tau_k^{(6)}$	k
0	4, 6, 8, ...	0	5, 7, 9, ...
$k^5 - 10k^3 + 9k$	5, 9, 13, ...	$k^6 - 20k^4 + 64k^2$	6, 10, 14, ...
$-(k^5 - 10k^3 + 9k)$	7, 11, 15, ...	$-(k^6 - 20k^4 + 64k^2)$	8, 12, 16, ...

The quantity σ_ϱ, which is the norm over $L^2(\mathscr{E}_\varrho)$ of the bounded linear functional E_n, depends only on the ellipse and the derivative rule R_n; but is independent of f, and may therefore be computed once for all. Using (18) and (13) we have for σ_ϱ^2 the expression

$$\sigma_\varrho^2 = \frac{8}{\pi} \sum_{k=0}^{\infty} k(\varrho^{2k} - \varrho^{-2k})^{-1} \left|E_n(T_k(z))\right|^2 .$$

Applying the operator E_n to (12), we have

$$\sigma_\varrho^2 = \frac{8}{\pi} \sum_{k=0}^{\infty} k(\varrho^{2k} - \varrho^{-2k})^{-1} \left[\tau_k^{(n)} - \sum_{i=1}^{N} A_i^{(n)} T_k(x_i^{(n)})\right]^2 , \tag{20}$$

where quantities $\tau_k^{(n)}$ $(n = 1, 2, \ldots, 6)$ are given in Table 1 and besides it holds for them

$$\tau_k^{(n)} = 2n\tau_{k-1}^{(n-1)} - \tau_{k-2}^{(n)}, \quad n = 1, 2, \ldots .$$

In Table 2 there are values of σ_ϱ corresponding to a few derivative rules and for the range of values of the parameter ϱ. These values were computed from (20), the algorithm used at the calculation $\sum_{i=1}^{N} A_i^{(n)} T_k(x_i^{(n)})$ being the same as that applied to the calculation of the respective derivative. It must be noted that the basic relation (10) does not change but the choice of the initial step h and the way of its further division affects the knots x_i and coefficients A_i, thus changing the whole derivative rule R_n. In Table 2, therefore, the individual rules are denoted by the initial step h and by values p, q.

In order to use the estimate (19), we have to determine $\|f\|_{\mathscr{E}_\varrho}$ which is different for each function. If it cannot be evaluated directly, it can be estimated [5] either from

$$\|f\|_{\mathscr{E}_\varrho} \leqq \sqrt{(\pi ab)} \max_{z \in \overline{\mathscr{E}}_\varrho} |f(z)| , \tag{21}$$

where $f(z)$ is continuous in the closed ellipse $\overline{\mathscr{E}}_\varrho$, or from

$$\|f\|_{\mathscr{E}_\varrho} \leqq \|f\|_{\mathrm{Ca}} \leqq a \sqrt{(\pi)} \max_{|z| \leqq a} |f(z)| , \tag{22}$$

where C_a is the circle containing $\mathscr{E}_\varrho$ and $f(z)$ is regular in $\overline{C}_a$.

Remark. Quantities σ_ϱ and $\|f\|_{\mathscr{E}_\varrho}$ depend on $\mathscr{E}_\varrho$. Now $\|f\|_{\mathscr{E}_\varrho} = 0$ when $\varrho = 1$ and increases as ϱ increases. On the other hand, σ_ϱ decreases as ϱ decreases. Hence, the best estimate occurs for some intermediate ϱ [5].

The quantities of Table 2 refer to the point $x = 0$. The case of an arbitrary point x_0 is obtained by means of the linear transformation

$$t = \frac{1}{nh}(x - x_0) ,$$

Table 2

Values of σ_Q

a \ σ_Q	n h p q (1, 0·05, 1, 2)	(1, 0·8, 3, 4)	(1, 1·0, 1, 2)	(2, 0·2, 3, 4)	(2, 0·5, 3, 4)	(2, 0·5, 1, 2)	(3, 0·3, 3, 4)	(3, 0·32, 3, 4)
1·01	2·6695(−3)	2·7455(−8)	8·2507(0)	1·3271(−2)	3·8795(−3)	1·3741(−1)	9·7357(−4)	5·6434(−4)
1·02	3·2921(−4)	2·0629(−8)	3·3664(0)	3·9631(−2)	3·5612(−2)	3·0743(0)	2·1900(−2)	2·0844(−2)
1·03	7·5226(−6)	1·7362(−8)	1·8327(0)	1·9617(−2)	9·9263(−3)	6·7748(−1)	8·9712(−6)	2·9598(−6)
1·04	5·1744(−6)	1·5349(−8)	1·1396(0)	1·0005(−2)	9·0154(−3)	6·1538(−1)	7·5638(−6)	2·0747(−6)
1·05	3·7265(−6)	1·3935(−8)	7·6635(−1)	5·1853(−3)	1·4765(−3)	1·4210(−1)	6·5559(−6)	1·5318(−6)
1·10	1·0437(−6)	1·0136(−8)	1·8328(−1)	3·8875(−3)	1·9419(−4)	4·2758(−1)	3·8558(−6)	5·3034(−7)
1·15	4·0446(−7)	8·1954(−9)	6·6167(−2)	9·8534(−4)	1·5766(−4)	8·7256(−2)	2·6030(−6)	2·8148(−7)
1·20	1·8852(−7)	6·9159(−9)	2·8840(−2)	8·3313(−4)	1·3330(−4)	4·6196(−3)	1·8788(−6)	1·8300(−7)
1·25	1·0108(−7)	5·9816(−9)	1·4092(−2)	7·2139(−4)	1·1542(−4)	4·0038(−3)	1·4150(−6)	1·3139(−7)
1·30	6·1346(−8)	5·2600(−9)	7·4515(−3)	6·4382(−4)	1·0157(−4)	3·5250(−3)	1·0983(−6)	9·9554(−8)
1·40	3·1177(−8)	4·2080(−9)	2·4565(−3)	5·0830(−4)	8·1328(−5)	2·8236(−3)	7·0551(−7)	6·2578(−8)
1·50	2·1195(−8)	3·4739(−9)	9·4355(−4)	4·1982(−4)	6·7171(−5)	2·3325(−3)	4·8162(−7)	4·2325(−8)
1·75	1·2646(−8)	2·3436(−9)	1·3239(−4)	2·8337(−4)	4·5339(−5)	1·5746(−3)	2·1953(−7)	1·9119(−8)
2·00	9·0316(−9)	1·7077(−9)	2·7230(−5)	2·0652(−4)	3·3044(−5)	1·1476(−3)	1·1661(−7)	1·0123(−8)
2·50	5·4436(−9)	1·0360(−9)	2·2387(−6)	1·2530(−4)	2·0048(−5)	6·9626(−4)	4·2925(−8)	3·7181(−9)
3·00	3·6756(−9)	7·0001(−10)	3·1550(−7)	8·4674(−5)	1·3548(−5)	4·7051(−4)	1·9602(−8)	1·6967(−9)
4·00	2·0141(−9)	3·8363(−10)	1·5600(−8)	4·6406(−5)	7·4250(−6)	2·5787(−4)	5·8878(−9)	5·0942(−10)
5·00	1·2740(−9)	2·4267(−10)	1·5798(−9)	2·9354(−5)	4·6967(−6)	1·6312(−4)	2·3559(−9)	2·0381(−10)

Values in the parentheses indicate the power of 10 by which the tabulated values should be multiplied.

which maps the interval $x_0 - nh \leqq x \leqq x_0 + nh$ onto $-1 \leqq t \leqq 1$, i.e. the point $x = x_0$ into $t = 0$. Let the error E_n^* be given for the point $x = x_0$ as follows

$$(23) \qquad E_n^*(f) = f^{(n)}(x)_{x=x_0} - \sum_{i=1}^{N} A_i \, f(x_i) \, .$$

The analogous error for the point $t = 0$ is given by

$$(24) \qquad E_n(f) = f^{(n)}(t)_{t=0} - \sum_{i=1}^{N} A_i f\left(\frac{1}{nh}(x_i - x_0)\right).$$

If function $f(x)$ is analytic on $[x_0 - nh, x_0 + nh]$, then

$$g(t) = f(nht + x_0)$$

is analytic on $[-1, 1]$ and setting $t_i = (1/nh)(x_i - x_0)$, we have

$$E_n^*(f) = g^{(n)}(t)_{t=0} - \sum_{i=0}^{N} A_i \, g(t_i) \, .$$

We have thus obtained

$$E_n^*(f) = E_n(g) \, ,$$

i.e.

$$(25) \qquad |E_n^*(f)| = |E_n(g)| \leqq \sigma_\varrho \|g\|_{\mathscr{E}_\varrho} \, .$$

The σ_ϱ are tabulated values in the $z = x + iy$ plane, and $\|g\|_{\mathscr{E}_\varrho}$ also refers to this plane.

4. NUMERICAL EXAMPLES

Example 1. The calculation of the 1st–5th derivatives of the function $\exp(e^x)$ at points $x = 0$ and 1 with various initial steps. The results obtained are in Table 3. From this Table it is seen that these values depend on the choice of the initial step (in particular for higher derivatives). The question of the most suitable initial step has not yet been solved.

Example 2. Estimate the error E occuring in evaluating $(d/dx) \exp(e^x)_{x=0}$ $(h = 1, p/q = \frac{1}{2})$ and $(d^2/dx^2) \exp(e^x)_{x=0}$ $(h = 0{\cdot}5, p/q = \frac{3}{4})$. $\exp(e^z)$ is an entire function of z and its therefore of class $L^2(\mathscr{E}_\varrho)$ for all $\varrho > 1$. Now

$$|\exp(e^z)| = \exp\{\mathrm{Re}(e^z)\} = \exp(e^x \cos y) \, .$$

Thus on $\mathscr{E}_\varrho$ we have

$$|\exp(e^z)| \leqq \exp(e^a) \, ,$$

and by (19) and (21) we get

$$(26) \qquad |E_1| < \sqrt{(\pi ab)} \exp(e^a) \, \sigma_\varrho(1, \tfrac{1}{2}) \, .$$

Table 3

h	$p=1,\ q=2$: $\frac{d}{dx}\exp(e^x)_{x=0}$	$p=1,\ q=2$: $\frac{d}{dx}\exp(e^x)_{x=1}$	$p=3,\ q=4$: $\frac{d}{dx}\exp(e^x)_{x=0}$	$p=3,\ q=4$: $\frac{d}{dx}\exp(e^x)_{x=1}$
0·02	2·71828069	41·19353676	2·71828221	41·19353950
0·05	2·71828187	41·19354987	2·71828222	41·19354510
0·40	2·71828185	41·19354987	2·71828172	41·19355488
0·80	2·71028188	41·19356910	2·71828151	41·19355226
1·00	2·71828184	41·19355690	2·71828197	41·19355357
h	$\frac{d^2}{dx^2}\exp(e^x)_{x=0}$	$\frac{d^2}{dx^2}\exp(e^x)_{x=1}$	$\frac{d^2}{dx^2}\exp(e^x)_{x=0}$	$\frac{d^2}{dx^2}\exp(e^x)_{x=1}$
0·02	5·43639913	153·1640430	5·43648859	153·1687293
0·05	5·43651001	153·1689301	5·43654166	153·1688619
0·20	5·43656208	153·1689930	5·49138495	153·1691699
0·40	5·43656212	153·1691240	5·43656155	153·1691604
0·50	5·43655573	153·1691084	5·43656307	153·1692419
h	$\frac{d^3}{dx^3}\exp(e^x)_{x=0}$	$\frac{d^3}{dx^3}\exp(e^x)_{x=1}$	$\frac{d^3}{dx^3}\exp(e^x)_{x=0}$	$\frac{d^3}{dx^3}\exp(e^x)_{x=1}$
0·02	13·5862502	681·454630	13·4580781	675·3334065
0·05	13·5907953	681·509060	13·5907190	681·5012169
0·15	13·5916048	681·643183	13·5912432	681·4960136
0·30	13·5914114	698·600353	13·5913858	681·4997482
0·32	13·5912477	681·497744	13·5913950	681·5008812
h	$\frac{d^4}{dx^4}\exp(e^x)_{x=0}$	$\frac{d^4}{dx^4}\exp(e^x)_{x=1}$	$\frac{d^4}{dx^4}\exp(e^x)_{x=0}$	$\frac{d^4}{dx^4}\exp(e^x)_{x=1}$
0·02	41·1169219	3478·22986	40·7399788	3478·261280
0·05	40·7636666	3481·56985	40·7667530	3484·064740
0·10	40·7670107	3481·61053	40·7760875	3481·825531
0·20	40·7666786	3481·62234	40·7741329	3479·529482
0·25	40·7747991	3478·77254	40·7742379	3478·807739
h	$\frac{d^5}{dx^5}\exp(e^x)_{x=0}$	$\frac{d^5}{dx^5}\exp(e^x)_{x=1}$	$\frac{d^5}{dx^5}\exp(e^x)_{x=0}$	$\frac{d^5}{dx^5}\exp(e^x)_{x=1}$
0·02	140·134945	19551·1774	140·134945	19708·4760
0·05	140·683602	19822·5887	141·108862	19853·9014
0·06	141·167152	19874·2766	141·261202	19855·8304
0·12	141·228155	19874·3518	141·333875	19855·8922
0·20	141·553560	19842·4092	141·343023	19851·7753

The right-hand side of (26) is minimized for $a = 1{\cdot}75$ and yields

$$|E_1| < (2{\cdot}8099)(317{\cdot}3)(1{\cdot}3239 \times 10^{-4}) = 0{\cdot}1180 .$$

The real absolute error is 0·00000001.

For the error E_2 also holds

$$|E_2| < \sqrt{(\pi ab)} \exp(e^a)\, \sigma_\varrho(0{\cdot}5, \tfrac{3}{4}) ,$$

from where for $a = 1{\cdot}10$ we get

$$|E_2| < (1{\cdot}2584)(20{\cdot}09)(1{\cdot}9419 \times 10^{-4}) = 0{\cdot}0049 .$$

In this case the real absolute error is 0·00000059.

Table 4

h	$p = 1, q = 2$: $\Gamma'(x)_{x=1}$	$p = 1, q = 2$: $\Gamma'(x)_{x=2}$	$p = 3, q = 4$: $\Gamma'(x)_{x=1}$	$p = 3, q = 4$: $\Gamma'(x)_{x=2}$
0·02	−0·577214861	0·422784155	−0·577215634	0·422784051
0·05	−0·577215040	0·422784929	−0·577215031	0·422784398
0·40	−0·577215342	0·422784266	−0·577215381	0·422784562
0·80	−0·577215605	0·422784247	−0·577215837	0·422784337
1·00	−0·577215517	0·422784313	−0·577215463	0·422784420

h	$p = 1, q = 2$ $\Gamma''(x)_{x=1}$	$p = 3, q = 4$ $\Gamma''(x)_{x=1}$
0·02	1·97814444	1·97785540
0·05	1·97813029	1·97814206
0·20	1·97810884	1·97812159
0·40	1·97811233	1·97812276
0·50	1·97811618	1·97809845

Example 3. Table 4 contains the calculated values of the 1st and 2nd derivatives of the function Γ (x) at the points $x = 1, 2$.

Example 4. Estimate the error E_1 which arises in evaluating $\Gamma'(x)_{x=1}(h = 0{\cdot}8, p/q = \tfrac{3}{4})$. Transferring to the point $z = 0$, we must consider the function

$$g(z) = \Gamma[0{\cdot}8(z + 1{\cdot}25)] .$$

This function is regular in $|z| < 1{\cdot}25$; hence we may take a in the range $1 < a <$

$< 1{\cdot}25$. Now

$$|\Gamma(x + iy)| \leqq \Gamma(x) \quad \text{for} \quad x > 0\,,$$

so that

$$|g(z)| = |\Gamma[0{\cdot}8(x + 1{\cdot}25) + 0{\cdot}8iy]| \leqq \Gamma[0{\cdot}8(x + 1{\cdot}25)]\,.$$

The concavity of the Γ function implies

$$|g(z)| \leqq \max\{\Gamma[0{\cdot}8(a + 1{\cdot}25)]\,,\quad \Gamma[0{\cdot}8(-a + 1{\cdot}25)]\}\,,\quad z \in \mathscr{E}_\varrho\,.$$

Thus we have

$$|E_1| < \sqrt{(\pi ab)}\max\{\Gamma[0{\cdot}8(a + 1{\cdot}25)]\,,\quad \Gamma[0{\cdot}8(-a + 1{\cdot}25)]\}\,\sigma_\varrho$$

from where for $a = 1{\cdot}03$ we get

$$|E_1| < (0{\cdot}8936)\,(5{\cdot}131)\,(1{\cdot}7362 \times 10^{-8}) = 0{\cdot}0000000796\,.$$

The real absolute error is 0·0000000604.

Estimations of the norms in examples 2 and 4 are from [5].

All calculations were carried out by the Danish computer GIER.

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Súhrn

EXTRAPOLAČNÁ METÓDA NUMERICKÉHO VÝPOČTU DERIVÁCIE ANALYTICKEJ FUNKCIE A JEJ ODHAD CHYBY

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Článok opisuje numerickú metódu výpočtu derivácie analytickej funkcie. Sú tabelované tzv. chybové koeficienty pre odhad chyby a ich použitie je demonštrované na niekoľkých príkladoch.

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