ZASTOSOWANIA MATEMATYKI
APPLICATIONES MATHEMATICAE
VIII (1965)

M. ŻYCZKOWSKI (Kraków)

ON NUMERICAL EVALUATION OF THE MAXIMUM OF A FUNCTION

In many practical applications functions are given only by the table of their numerical values (the finite-difference method of solution of differential equations, experimental data and so on). The aim of the present paper is to give some formulae for evaluating the maximum or minimum and the inflection point of such a function of one real variable; this problem is very important since extreme values are often used for further applications. A numerical determination of the maximum is necessary for the technique of some types of approximation (W. Walter [6], M. Życzkowski [7]). The method may be useful also for functions given explicitly but by such complicated formulae that analytical investigation is practically impossible.

The paper deals only with the derivation of the approximate formulae and no estimation of error will be given, but accuracy will be illustrated by some numerical examples.

Denote the required extreme value of the function $f(x)$ by f_m and the corresponding point x by $\bar{x}$. At first we derive an analytical formula expressing f_m by means of the values of the function and its derivatives at an arbitrary point which is assumed to lie near $\bar{x}$. This arbitrarily chosen point will be denoted by $x = 0$ without loss of generality. Assume that the function is regular and can be expanded in a Maclaurin series

(1) $$f(x) = f(0)+f'(0)x+\tfrac{1}{2}f''(0)x^2+\tfrac{1}{6}f'''(0)x^3+\ldots,$$

and the point $\bar{x}$ lies inside the radius of convergence of this series. In what follows the values of the function and its derivatives at $x = 0$ will be denoted by $f, f', f'', \ldots,$ without argument or index. The first derivative $f'(x)$ is determined by the series

(2) $$f'(x) = f'+f''x+\tfrac{1}{2}f'''x^2+\tfrac{1}{6}f^{\mathrm{IV}}x^3+\ldots$$

The equation determining $\bar{x}$ is of the form $f'(x) = 0$. It may be solved by means of Euler's method ([3]). Namely we invert the series (2) with respect to the variable $u = f'(x) - f'$ (the coefficients being determined by the formulae of Van Orstrand, [5]) and put $f'(x) = 0$ getting

$$(3) \qquad \bar{x} = -\frac{f'}{f''} - \frac{f'''}{2f''^3} f'^2 - \frac{1}{6}\left(\frac{3f'''^2}{f''^5} - \frac{f^{\mathrm{IV}}}{f''^4}\right) f'^3 - \\ - \frac{1}{24}\left(\frac{15f'''^3}{f''^7} - \frac{10f'''f^{\mathrm{IV}}}{f''^6} + \frac{f^{\mathrm{V}}}{f''^5}\right) f'^4 - \dots$$

The convergence of the series (3) depends mainly on the second derivative f'' and deteriorates with the decrease of the absolute value of this derivative. As a rule, however, the second derivative is sufficiently large in the neighbourhood of the maximum or the minimum. Several error estimations are given in [3]. After the substitution of (3) into (1) we determine the required extreme value $f(\bar{x}) = f_m$ by the formula

$$(4) \qquad f_m = f - \frac{1}{2f''} f'^2 - \frac{f'''}{6f''^3} f'^3 - \frac{1}{24}\left(\frac{3f'''^2}{f''^5} - \frac{f^{\mathrm{IV}}}{f''^4}\right) f'^4 - \\ - \frac{1}{120}\left(\frac{15f'''^3}{f''^7} - \frac{10f'''f^{\mathrm{IV}}}{f''^6} + \frac{f^{\mathrm{V}}}{f''^5}\right) f'^5 - \dots$$

Practically no shifting of the axis x is necessary for using this formula. Such a shifting must be carried out when (3) is used.

The degree of convergence of the series obtained will be illustrated by the following example. Determine the maximum of the function $f(x) = \sin x$ assuming the values of the function and their derivatives at the point $x = \arccos 0{,}1 = 84°15'39''$ to be known. Namely we have $f = 0{,}994988$, $f' = 0{,}1$, $f'' = -0{,}994988$, $f''' = -0{,}1$ and so on. The numerical calculations are as follows:

$$\begin{aligned} f_m = \;& 0{,}994988 \\ & \underline{+0{,}005025} \\ & 1{,}000013 \\ & \underline{-0{,}000017} \\ & 0{,}999996 \\ & \underline{+0{,}000004} \\ & 1{,}000000; \end{aligned}$$

thus four terms of the series ensure the accuracy of six decimal places. The withdrawal of the "starting point" from $\bar{x}$ causes, of course, the convergence to deteriorate; taking the values at $x = 60° = \pi/3$ as known, we obtain from the first four terms of (4) $f_m = 1{,}00235$ with an error of 0,24 per cent — but for many applications even this error may be treated as negligible.

Now we pass to finite differences. Formulae for derivatives in terms of finite differences may be found in many text-books and monographs, but probably the most complete and convenient ones are given in a book by Sh. E. Mikeladze ([4], p. 276). We find there the expressions for the derivatives of the first, second, etc. up to the tenth order in terms of differences up to the eleventh or to the twelfth inclusive. Namely we have

$$\begin{aligned} hf' &= \mu\delta f - \tfrac{1}{6}\mu\delta^3 f + \tfrac{1}{30}\mu\delta^5 f - \tfrac{1}{140}\mu\delta^7 f + \ldots, \\ h^2 f'' &= \delta^2 f - \tfrac{1}{12}\delta^4 f + \tfrac{1}{90}\delta^6 f - \ldots, \\ h^3 f''' &= \mu\delta^3 f - \tfrac{1}{4}\mu\delta^5 f + \tfrac{7}{120}\mu\delta^7 f - \ldots, \\ h^4 f^{\mathrm{IV}} &= \delta^4 f - \tfrac{1}{6}\delta^6 f + \ldots, \\ &\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \end{aligned} \tag{5}$$

where δf, $\delta^2 f$, $\delta^3 f\ldots$ denote the successive differences (the odd ones taken inside the interval, the even ones — at the pivotal points), μ is the averaging operator, namely

$$\mu\delta f = \frac{\delta f_{\frac{1}{2}} + \delta f_{-\frac{1}{2}}}{2}, \tag{6}$$

and h is the distance between the pivotal points (interval); this distance is without special meaning inasmuch as after substitution into (4) it is simply cancelled.

The substitution of (5) into (4) yields the required general formula, expressing the maximum or the minimum of the function, f_m, by its finite differences, i. e. by the values at some equally spaced points:

$$\begin{aligned} f_m = f &- \frac{(\mu\delta f - \frac{1}{6}\mu\delta^3 f + \ldots)^2}{2(\delta^2 f - \frac{1}{12}\delta^4 f + \ldots)} - \frac{(\mu\delta^3 f - \ldots)(\mu\delta f - \frac{1}{6}\mu\delta^3 f + \ldots)^3}{6(\delta^2 f - \frac{1}{12}\delta^4 f + \ldots)^3} - \\ &- \frac{[3(\mu\delta^3 f - \ldots)^2 - (\delta^2 f - \frac{1}{12}\delta^4 f + \ldots)(\delta^4 f + \ldots)](\mu\delta f - \frac{1}{6}\mu\delta^3 f + \ldots)^4}{24(\delta^2 f - \frac{1}{12}\delta^4 f + \ldots)^5} - \ldots \end{aligned} \tag{7}$$

An especially simple formula will be obtained for the approximation of the function $f(x)$ by the parabola of the second degree. Into (7) we substitute $\delta^3 f = \delta^4 f = \ldots = 0$, getting the formula in the closed form

$$f_m \approx f - \frac{(\mu\delta f)^2}{2\delta^2 f} = f_0 - \frac{(f_1 - f_{-1})^2}{8(f_{-1} - 2f_0 + f_1)}, \tag{8}$$

where f_{-1}, f_0 and f_1 denote the values of the function at the three neighbouring points; the middle point should be chosen so as to lie nearest $\bar{x}$ to keep the approximation error as small as possible.

Approximating the given function by a parabola of a higher degree, we get the final formula not in a closed form but as a series. For instance, having five pivotal points at our disposal, we can calculate the differences up to the fourth (thus replacing the function by the polynomial of the fourth degree) and

$$f_m \approx f - \frac{(\mu\delta f - \frac{1}{6}\mu\delta^3 f)^2}{2(\delta^2 f - \frac{1}{12}\delta^4 f)} - \frac{\mu\delta^3 f(\mu\delta f - \frac{1}{6}\mu\delta^3 f)^3}{6(\delta^2 f - \frac{1}{12}\delta^4 f)^3} - \ldots, \tag{9}$$

or, expressing the differences in terms of the given values of the function, denoted here by f_{-2}, f_{-1}, f_0, f_1 and f_2,

$$\begin{aligned} f_m \approx f_0 &- \frac{(-f_2+8f_1-8f_{-1}+f_{-2})^2}{24(-f_2+16f_1-30f_0+16f_{-1}-f_{-2})} - \\ &- \frac{(f_2-2f_1+2f_{-1}-f_{-2})(-f_2+8f_1-8f_{-1}+f_{-2})^3}{12(-f_2+16f_1-30f_0+16f_{-1}-f_{-2})^3} - \ldots \end{aligned} \tag{10}$$

Formula (8) is sometimes insufficiently accurate and the formula (9) or (10) requires the knowledge of the values of the function at as many as five points. Often it is convenient to use the parabola of the third degree, which may be taken through four points. To get an appropriate formula we have to fix the "starting point" inside one of the intervals; then — for an even number of pivotal points — the symmetry of the formula will be ensured. The values of the function $f(x)$ at four equally spaced points will now be denoted by $f_{-\frac{3}{2}}$, $f_{-\frac{1}{2}}$, $f_{\frac{1}{2}}$ and $f_{\frac{3}{2}}$. This time we have to express the values of the function and of its derivatives not at the pivotal point but in the middle of the interval. Thus we apply the formulae (D. R. Hartree [2], p. 62 and 127, L. Fox [1], p. 11)

$$\begin{aligned} f_0 &= \mu f - \tfrac{1}{8}\mu\delta^2 f + \tfrac{3}{128}\mu\delta^4 f - \ldots, \\ hf_0' &= \delta f - \tfrac{1}{24}\delta^3 f + \tfrac{3}{640}\delta^5 f - \ldots, \\ h^2 f_0'' &= \mu\delta^2 f - \tfrac{5}{24}\mu\delta^4 f + \ldots, \\ h^3 f_0''' &= \delta^3 f - \tfrac{1}{8}\delta^5 f + \ldots, \\ h^4 f_0^{\mathrm{IV}} &= \mu\delta^4 f - \ldots, \\ &\ldots\ldots\ldots\ldots\ldots\ldots \end{aligned} \tag{11}$$

which may be deduced in a formal way by multiplying or dividing (5) by the "identity operator" $\mu(1+\frac{1}{4}\delta^2)^{-1/2}$. Odd differences are here taken inside the middle interval and the averaging operator μ has a meaning analogical to (6). Thus, substituting (11) into (4),

$$f_m = \left(\mu f - \frac{1}{8}\mu\delta^2 f + \frac{3}{128}\mu\delta^4 f - \ldots\right) - \frac{(\delta f - \frac{1}{24}\delta^3 f + \ldots)^2}{2(\mu\delta^2 f - \frac{5}{24}\mu\delta^4 f + \ldots)} - \frac{(\delta^3 f - \ldots)(\delta f - \frac{1}{24}\delta^3 f + \ldots)^3}{6(\mu\delta^2 f - \frac{5}{24}\mu\delta^4 f + \ldots)^3} - \ldots \tag{12}$$

Approximating the function $f(x)$ by the parabola of the third degree, passing through four points ($\delta^4 f = \delta^5 f = \ldots = 0$), we get the formulae

$$\begin{aligned} f_0 &\approx \mu f - \tfrac{1}{8}\mu\delta^2 f = \tfrac{1}{16}(-f_{\frac{3}{2}} + 9f_{\frac{1}{2}} + 9f_{-\frac{1}{2}} - f_{-\frac{3}{2}}), \\ hf_0' &\approx \delta f - \tfrac{1}{24}\delta^3 f = \tfrac{1}{24}(-f_{\frac{3}{2}} + 27f_{\frac{1}{2}} - 27f_{-\frac{1}{2}} + f_{-\frac{3}{2}}), \\ h^2 f_0'' &\approx \mu\delta^2 f = \tfrac{1}{2}(f_{\frac{3}{2}} - f_{\frac{1}{2}} - f_{-\frac{1}{2}} + f_{-\frac{3}{2}}), \\ h^3 f_0''' &\approx \delta^3 f = f_{\frac{3}{2}} - 3f_{\frac{1}{2}} + 3f_{-\frac{1}{2}} - f_{-\frac{3}{2}}, \\ f_0^{\mathrm{IV}} &= f_0^{V} = \ldots = 0, \end{aligned} \tag{13}$$

and for the required extreme value f_m

$$f_m \approx \left(\mu f - \frac{1}{8}\mu\delta^2 f\right) - \frac{(\delta f - \frac{1}{24}\delta^3 f)^2}{2\mu\delta^2 f} - \frac{\delta^3 f(\delta f - \frac{1}{24}\delta^3 f)^3}{6(\mu\delta^2 f)^3} - \frac{(\delta^3 f)^2(\delta f - \frac{1}{24}\delta^3 f)^4}{8(\mu\delta^2 f)^5} - \ldots, \tag{14}$$

or

$$f_m \approx \frac{-f_{\frac{3}{2}} + 9f_{\frac{1}{2}} + 9f_{-\frac{1}{2}} - f_{-\frac{3}{2}}}{16} - \frac{(-f_{\frac{3}{2}} + 27f_{\frac{1}{2}} - 27f_{-\frac{1}{2}} + f_{-\frac{3}{2}})^2}{576(f_{\frac{3}{2}} - f_{\frac{1}{2}} - f_{-\frac{1}{2}} + f_{-\frac{3}{2}})} - \frac{(f_{\frac{3}{2}} - 3f_{\frac{1}{2}} + 3f_{-\frac{1}{2}} - f_{-\frac{3}{2}})(-f_{\frac{3}{2}} + 27f_{\frac{1}{2}} - 27f_{-\frac{1}{2}} + f_{-\frac{3}{2}})^3}{10368(f_{\frac{3}{2}} - f_{\frac{1}{2}} - f_{-\frac{1}{2}} + f_{-\frac{3}{2}})^3} - \ldots \tag{15}$$

Formulae of type (12) converge better than these of type (7) if the minimal difference δf is smaller than the minimal mean difference $\mu\delta f$ (in absolute values); otherwise formulae of type (7) converge better.

The accuracy of the proposed approximate formulae will be illustrated by the following example. Determine numerically the maximum of the function $f(x) = -x\ln x$, taking as known the values of this function at $x = 0{,}2$, $0{,}3$, $0{,}4$, $0{,}5$, and $0{,}6$ or at the first four or at the middle three points. Analytically we find without difficulty $\bar{x} = 1/e = 0{,}367879$ and $f_m = 1/e = 0{,}367879$. The values of the function and of the successive differences are listed in table 1.

TABLE 1

The function $f(x) = -x\ln x$ and its successive differences

x	$f(x)$	$\delta f(x)$	$\delta^2 f(x)$	$\delta^3 f(x)$	$\delta^4 f(x)$
0,2	0,321888				
		+39304			
0,3	0,361192		−33980		
		+ 5324		+8714	
0,4	0,366516		−25266		−3585
		−19942		+5129	
0,5	0,346574		−20137		
		−40079			
0,6	0,306495				

The minimal difference is here $|\delta f| = 0{,}005324$, and the minimal mean difference $|\mu\delta f| = 0{,}007309$; these values are of the same order, therefore neither of the formulae (7) and (12) is evidently better than the other.

Apply at first the simplest formula (8), using the three middle points. We obtain

$$f_m \approx 0{,}366516 + \frac{0{,}007309^2}{2\cdot 0{,}025266} = 0{,}367573,$$

thus the error amounts to 0,000306 and does not exceed 0,1 per cent. Approximating the function by the parabola of the fourth degree, (9), we substitute $\mu\delta^3 f = 0{,}006922$, and the convergence is as follows:

$$\begin{aligned} f_m \approx\ & 0{,}366516 \\ & \underline{+0{,}001434} \\ & 0{,}367950 \\ & \underline{-0{,}000045} \\ & 0{,}367905 \\ & \underline{+0{,}000001} \\ & 0{,}367906. \end{aligned}$$

This series is convergent, of course, not to the value $1/e$ but to the maximum of the interpolation polynomial of the fourth degree. The error, however, is very small, and for the first four terms of the series it amounts to 0,000027 only.

As far as the formula (14) is concerned we form here another averaging process. Namely we have $\mu f = 0,363854$ (arithmetic mean of $f(0,3)$ and $f(0,4)$), $\delta f = 0,005324$, $\mu\delta^2 f = -0,029623$, and

$$\begin{aligned} f_m \approx\ & 0,363854 \\ & \underline{+0,003703} \\ & 0,367557 \\ & \underline{+0,000415} \\ & 0,367972 \\ & \underline{+0,000007} \\ & 0,367979; \end{aligned}$$

the error for the first four terms of the series amounts to 0,000100.

The same method may be applied to determine the inflection point of the function $f(x)$. Denote the absciessa of the inflection point by $\bar{\bar{x}}$ and the corresponding value of $f(\bar{\bar{x}})$ by f_i. Instead of (3) we now have

$$\bar{\bar{x}} = -\frac{1}{f'''}f'' - \frac{f^{\mathrm{IV}}}{2f'''^3}f''^2 - \left(\frac{f^{\mathrm{IV}^2}}{2f'''^5} - \frac{f^{\mathrm{V}}}{6f'''^4}\right)f''^3 - \ldots \tag{16}$$

and after the substitution of (16) into (1)

$$f_i = f - \frac{f'}{f'''}f'' - \frac{f'f^{\mathrm{IV}}}{2f'''^3}f''^2 + \left(\frac{1}{3f'''^2} - \frac{f'f^{\mathrm{IV}^2}}{2f'''^5} + \frac{f'f^{\mathrm{V}}}{6f'''^4}\right)f''^3 + \ldots \tag{17}$$

Passing to finite differences we may use (5) or (11). The simplest formula is here obtained for the approximation of the function $f(x)$ by the polynomial of the third degree; thus the formulae (11) are more convenient, as a rule. Assuming $\delta^4 f = \delta^5 f = \ldots = 0$ we get the formula in the closed form

$$f_i \approx \mu f - \frac{1}{12}\mu\delta^2 f - \frac{\delta f \mu\delta^2 f}{\delta^3 f} + \frac{(\mu\delta^2 f)^3}{3(\delta^3 f)^2}. \tag{18}$$

The derivatives may also be expressed in terms of the values of the function $f(x)$, (13), but the final formula will not be quoted here.

References

[1] L. Fox, *The numerical solution of two-point boundary problems*, Oxford 1957.

[2] D. R. Hartree, *Numerical analysis*, Oxford 1958.

[3] J. Łukaszewicz and M. Warmus, *Metody numeryczne i graficzne* (*Numerical and graphical methods*), Warszawa 1956.

[4] Sh. E. Mikeladze, *Численные методы математического анализа* (*Numerical methods of mathematical analysis*), Москва 1953.

[5] C. E. Van Orstrand, *Reversion of power series*, Phil. Mag. 19 (1910), pp. 366-376.

[6] W. Walter, *Über Tschebyscheff—Approximation differenzierbarer Funktionen*, GAMM-Tagung Würzburg, April 1961.

[7] M. Życzkowski, *The "onefold optimum approximation" and some of its applications in mechanics*, Bull. Acad. Polon. Sci., Ser. Sci. Techn., 11 (1963), pp. 199-208.

Received on 23. 4. 1964

M. ŻYCZKOWSKI (Kraków)

OKREŚLANIE EKSTREMÓW FUNKCJI NA DRODZE NUMERYCZNEJ

STRESZCZENIE

Celem pracy jest podanie przybliżonych wzorów, określających ekstremum regularnej funkcji jednej zmiennej lub jej punkt przegięcia, przy znajomości wartości tej funkcji w kilku równomiernie rozłożonych punktach (węzłach). Zagadnienia tego typu występują przy analizie funkcji określonej równaniem różniczkowym całkowanym metodą różnic skończonych, danymi doświadczalnymi itp.

Zastosowano najpierw odwrócenie szeregu potęgowego i określono ekstremum poprzez wartości funkcji i jej kolejnych pochodnych w pewnym punkcie, leżącym blisko tego ekstremum. W dalszym ciągu wyrażono pochodne przez różnice skończone w dwóch wariantach: przyjęto, że punkt wyjściowy jest węzłem interpolacji, wzory (5), lub że leży wewnątrz przedziału, wzory (11). Technikę obliczeń i stopień zbieżności pokazano na przykładzie analizy funkcji $f(x) = -x\ln x$.

М. ЖИЧКОВСКИ (Краков)

ОПРЕДЕЛЕНИЕ ЭКСТРЕМУМА ФУНКЦИИ ЧИСЛЕННЫМ МЕТОДОМ

РЕЗЮМЕ

Целью настоящей работы является получение приближенных формул, с помощью которых можно определить экстремум гладкой функции одной переменной и её точку перегиба, зная значения этой функции в нескольких равномерно распределенных точках (узлах). Задачи этого вида появляются при исследовании функции определенной с помощью дифференциального уравнения, интегрированного методом конечных разностей, функции составленной по экспериментальным наблюдениям и в других случаях.

Сначала применяется обращение степенного ряда и определяеться экстремум по значениям функции и её последовательных производных в некоторой точке близкой к этому экстремум. Далее производные функции выражаются через конечные разности двояким образом: предполагается, что исходная точка является узлом интерполяции - формулы (5) — или же, что она находится внутри интервала - формулы (11). Вычислительная техника и быстрота сходимости иллюстрируются на примере функции $f(x) = -x\ln x$.
