ON NUMERICAL APPLICATIONS OF EXCLUDING THEOREMS

By

F. KÁLOVICS and Z. ERDÉLYI

Mathematical Institute of Technical University for Heavy Industry
3515 Miskolc, Egyetemváros

(*Received May 6, 1982*)

The paper gives a new method for finding the global minimum in a finite n-dimensional interval.

1. Excluding-theorems

Theorem 1.1 Let $f: D \subset R^n \to R^m$ and assume that

$$\|f(x) - f(a)\|_2 \leq K_1 \|x-a\|_1 + K_2 \|x-a\|_1^2,$$

where $x, a \in D$; $K_1 = K_1(a)$, $K_2 = K_2(a) > \emptyset$; $\|\cdot\|_1$ and $\|\cdot\|_2$ are arbitrary norms on R^n and R^m, respectively. Then

$$\|\alpha - a\|_1 \geq \sqrt{\|f(a)\|_2/K_2 + (K_1/2K_2)^2} - K_1/2K_2; \quad \forall\, a, \alpha \in D \quad \text{and} \quad f(\alpha) = \emptyset.$$

Proof. We can obtain the result from solving a quadratic inequality [2]. The fixed symbols are as follows:

$x = [x_1, x_2, \ldots, x_n]$, x^T: the transpose of x;
$\|B\| = \max_i \sum_k |b_{ik}|$, where $B = [b_{ik}]$ is a real, finite matrix;
$T = T(a, h) = \{x: a-h \leq x \leq a+h;\ h > \emptyset;\ a, h, x \in R^n\}$ is an interval (rectangle) in R^n with centre a and radius h (R^n is canonically ordered).

Theorem 1.2 Assume that $f: R^n \to R^1$ is twice-continuously differentiable on $T(a, h)$ and $f(a) \neq \emptyset$. If

$$r_i = \left(\sqrt{4nK\,|f(a)| + \|f'(a)\|^2} - \|f'(a)\|\right)/2nK; \quad i = 1, 2, \ldots, n;$$

and

$$K > \emptyset,5 \sup_{x \in T} \|f''(x)\|,$$

then $\alpha \notin T(a, h) \cap T(a, r)$; $\quad \forall f(\alpha) = \emptyset$.

Proof. From Taylor formula

$$f(x) = f(a) + f'(a)(x-a)^T + \emptyset{,}5\,(x-a) f''(\xi)(x-a)^T; \quad (x, \xi \in T(a, h)),$$

and thus

$$|f(x) - f(a)| < \|f'(a)\| \cdot \|(x-a)^T\| + nK\,\|(x-a)^T\|^2; \quad \forall\, x \neq a.$$

Hence from Theorem 1.1

$$\|(\alpha-a)^T\| > \sqrt{|f(a)|/nK+(\|f'(a)\|/2nK)^2} - \|f'(a)\|/2nK =$$
$$= \left(\sqrt{4nK\,|f(a)|+\|f'(a)\|^2} - \|f'(a)\|\right)/2nK; \quad \forall f(\alpha)=\emptyset \quad \text{and} \quad \alpha\in T(a,h).$$

Theorem 1.3 Assume that $f_j: R^n \to R^1$ $(j = 1, 2, \ldots, m)$ are twice-continuously differentiable on $T(a, h)$, and let $f: R^n \to R^1$ be defined by $f(x) = \sum_j |f_j(x)|$, $f(a) \neq \emptyset$. If

$$r_i = \left(\sqrt{4nK\cdot f(a)+(\sum \|f_j'(a)\|)^2} - \sum \|f_j'(a)\|\right)/2nK; \quad i = 1, 2, \ldots, n$$

and

$$K > \emptyset, 5 \sum \sup_{x\in T} \|f_j''(x)\|,$$

then $\alpha \notin T(a, h) \cap T(a, r)$; $\forall f(\alpha) = \emptyset$.

Proof. Obviously exist $p_1, p_2, \ldots, p_m$ $(p_j = \emptyset$ or $1)$ so that

$$f(x) \geq F(x) = \sum_j (-1)^{p_j} f_j(x), \quad \text{and} \quad f(a) = F(a).$$

If now Theorem 1.2 is applied to $F(x)$, and it is used that

$$\sqrt{\|f(a)\|_2/K_2+(K_1/2K_2)^2} - K_1/2K_2$$

is a monotone diminishing function of K_1 and K_2 [2], then the proof is complete.

Theorem 1.4 Assume that $f_j: R^n \to R^1$ $(j = 1, 2, \ldots, m)$ are twice-continuously differentiable on $T(a, h)$, and let $f: R^n \to R^1$ be defined by $f(x) = \max_j |f_j(x)|$, $f(a) \neq \emptyset$. If

$$r_i = \left(\sqrt{4nKf(a)+\|f_{j*}'(a)\|^2} - \|f_{j*}'(a)\|\right)/2nK; \quad i = 1, 2, \ldots, n;$$
$$K > \emptyset, 5 \sup_{x\in T} \|f_{j*}''(x)\| \quad \text{and} \quad f_{j*}(a) = f(a),$$

then $\alpha \notin T(a, h) \cap T(a, r)$; $\forall f(\alpha) = \emptyset$.

Proof. By Theorem 1.2 the proof is evident.

2. A method for finding the global minimum

The following problem is given:

$$g(x) = \min, \quad b \leq x \leq c, \quad b, c, x \in R^n.$$

Suppose now that

$$m \leq \min_{b\leq x\leq c} g(x) \leq M$$

and one of the Theorems 1.2–1.4 can be applied to g with $T(a, h) = T\left((b+c)/2, (c-b)/2\right)$.

We can describe the steps of our method as follows.

(1) We examine the realization of $f(x, d) \equiv g(x) - d$ in the case of $d = \emptyset{,}5(m+M) = \tilde{d}$ and $x \in T(a, h)$. Suppose first that $f(x, \tilde{d}) > \emptyset$, $\forall x \in T$; i.e. $\min g > \tilde{d}$. (Of course it is a provisional condition only.) In this case (at such a level $\tilde{d}$), first in the centre of $\tilde{T} = T\left(a, \tilde{d}; h, \frac{M-m}{2}\right) \in R^{n+1}$ one of the Theorems 1.2–1.4 is applied to $f(x, d)$ (see Fig. 1.).

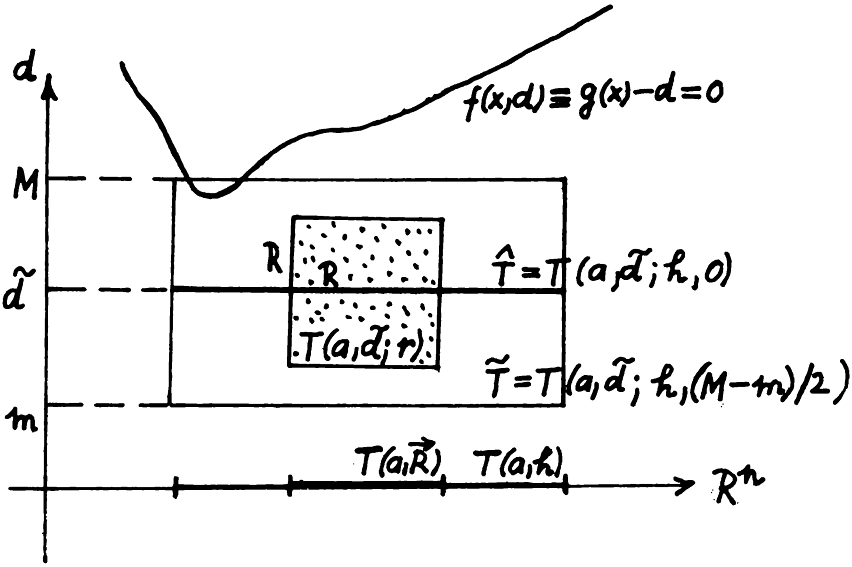

Fig. 1.

For example from Theorem 1.2 we get

$$R = r_i = \left(\sqrt{4nK(g(a)-\tilde{d}) + (\|g'(a)\|+1)^2} - (\|g'(a)\|+1)\right)/2nK,$$

where $i = 1, 2, \ldots, n+1$ and

$$K > \emptyset{,}5 \sup_{x \in T} \|g''(x)\|.$$

(Hereby it is known that $f(x, \tilde{d}) > R$, i.e. $g(x) > \tilde{d} + R$; $\forall x \in T(a, h) \cap T(a, \vec{R})$, $\vec{R} = \{R, \ldots, R\}$). If $R < \|h^T\|$, then we cover the set $T(a, h) \setminus T(a, \vec{R})$ with sets (rectangles)

$$T_k = T_k\big(a_1, \ldots, a_{k-1}, a_k - (h_k+R)/2, a_{k+1}, \ldots, a_n; R, \ldots, (h_k-R)/2, h_{k+1}, \ldots, h_n\big),$$

$$T_k' = T_k'(a_1, \ldots, a_{k-1}, a_k + (h_k+R)/2, a_{k+1}, \ldots, a_n; R, \ldots, (h_k-R)/2, h_{k+1}, \ldots, h_n), \quad h_k - R > \emptyset, \quad k = 1, 2, \ldots, n.$$

The number of the covering rectangles is between 2 and $2n$ (see Fig. 2.).

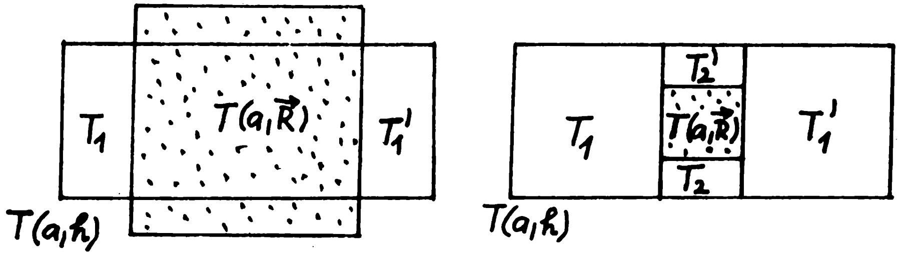

Fig. 2.

We continue the examination of level $\tilde{d}$ with T_1 (if $h_1-R>\emptyset$). If $\hat{T}_1$ can not be excluded in one step, then T_1 must be divided, too. After a finite number of steps the entire $\hat{T}$ will be excluded (Fig. 3.).

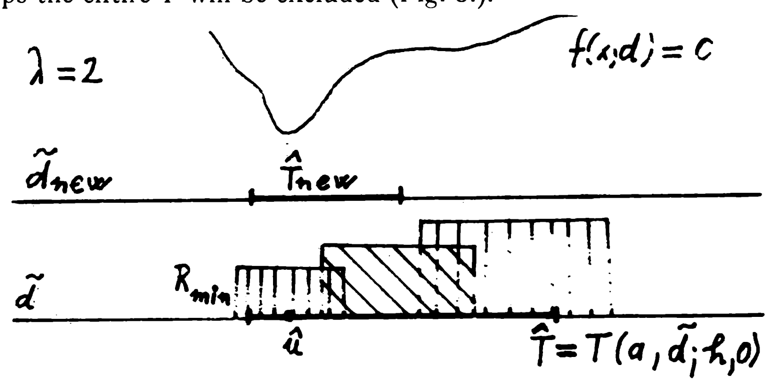

Fig. 3.

Let $R_{\min}$ be the minimum of the computed values R. If $R_{\min}\geq\delta$ (δ is a technical constant), then

$$m:=\tilde{d}+R_{\min}\quad\text{and}\quad M:=\min\{M;\tilde{d}+f_{\min}\},$$

where $f_{\min}$ is the minimum of the computed values $f(x,d)$ on the level $\tilde{d}$. We shall denote such a level $\tilde{d}$ as "type a". If $R_{\min}<\delta$ ("type c"), then $m:=m$ and $M:=\tilde{d}$.

Now let us see the case $\min g\leq\tilde{d}$. In this case, after a finite number of "excluding steps" $R<\delta$ or $f(x,d)<\emptyset$ at the point in question. If $R=R_{\min}<\delta$ ("type c"), then again $m:=m$ and $M:=\tilde{d}$. If $f(x,d)=f^-<\emptyset$ ("type b"), then $m:=m$ and $M:=\tilde{d}+f^-$.

(2) After examination of the level $\tilde{d}$ the first approximation u of the solution (solutions) is as follows. In case "type a" let u be the first point x, where $R(x)=R_{\min}$, but in cases "type b" and "type c" let u be the final examined point.

(3) With the new values of m and M we repeat the examination to $T(a,h)\cap T(u,\lambda\vec{R}_{\min})$ (for "type a"), or to $T(a,h)$ (for "type b" and "type c"). λ will be discussed in Theorems 2.1 and 2.2; $\vec{R}_{\min}=\{R_{\min},\ldots,R_{\min}\}$.

(4) If $M-m<\varepsilon$, then the process is finished.

Theorem 2.1 Let α the unique solution of our problem. Then $u\to\alpha$, $\forall\, M=g(\alpha)$, $\varepsilon=\emptyset$, $\delta=\emptyset$, $m<M$ and "$\lambda=\infty$".

Proof. Now each level becomes "type a" since $M=g(\alpha)$, $m<M$, $\delta=\emptyset$ and "$\lambda=\infty$". Hence from $\varepsilon=\emptyset\Rightarrow m, \tilde{d}\to M=g(\alpha)\Rightarrow R_{\min}\to\emptyset$ (since $\emptyset<R_{\min}<(M-m)\cdot\emptyset{,}5)\Rightarrow f(u,\tilde{d})=g(u)-\tilde{d}\to\emptyset$ (by each Theorems 1.2–1.4) $\Rightarrow g(u)\to M=g(\alpha)\Rightarrow u\to\alpha$ (since $g(x)$ is continuous on $T(a,h)$ and α is unique solution of the problem).

Remarks. (1) If $M\neq g(\alpha)$ but ε and δ are sufficiently small positive numbers, then $u(=u_i)$ is a sufficiently good approach of α with the "naive method" ($\lambda=\infty$).

(2) We can obtain also certainly convergent modifications of our method for $M=g(\alpha)$

(i) if in place of $T(a,h)\cap T(u,\lambda\vec{R}_{\min})$ we use $T(a,h)\cap(\cup\, T^*(x,\vec{R}))$, where $T^*(x,\vec{R})$ is an exluding set (cube) with $R<M-\tilde{d}$ already used in the process (see Fig. 3.);

(ii) if $R_{\min}\geq M-\tilde{d}$, then $\lambda:=2\lambda$ and we examine the level $\tilde{d}$ again;

(iii) if $m=g(\alpha)$ ([1], [4]).

Theorem 2.2 Let α be the unique solution of our problem. If Theorem 1.2 can be applied to g, then $u\to\alpha$, $\forall\, M=g(\alpha)$, $\varepsilon=\emptyset$, $\delta=\emptyset$, $m<M$ and

$$\lambda\geq(nKR_{\min}+\|g'(u)\|)/|g'_{\alpha u}(\xi)|\,,$$

where $g'_{\alpha u}(\xi)$ is the derivative of g in the direction $u-\alpha$ ($u\neq\alpha$) and in the point $\xi=\alpha+\vartheta(u-\alpha)$, $\emptyset<\vartheta<1$.

Proof. From Theorem 1.2, on the first level $\tilde{d}$

$$R_{\min}=\left(\sqrt{4nK(g(u)-\tilde{d})+(\|g'(u)\|+1)^2}-(\|g'(u)\|+1)\right)/2nK\,,$$

therefore

$$g(u)-\tilde{d}=nKR_{\min}^2+(\|g'(u)\|+1)\,R_{\min}\,.$$

And by $\tilde{d}<g(\alpha)-R_{\min}$ (The first level becomes "type a" since $M=g(\alpha)$, $m<M$, $\delta=\emptyset$. Hence $\tilde{d}+R_{\min}<M=g(\alpha)$.) we get $g(u)-g(\alpha)<nKR_{\min}^2+\|g'(u)\|\,R_{\min}$. But from Lagrange formula

$$g(u)-g(\alpha)\geq|g'_{\alpha u}(\xi)|\;\|(u-\alpha)^T\|>\emptyset,\quad \text{if}\quad u\neq\alpha\,.$$

Hence

$$\|(u-\alpha)^T\|<R_{\min}(nKR_{\min}+\|g'(u)\|)/|g'_{\alpha u}(\xi)|\leq\lambda R_{\min}\,,$$

and we can see that α can be found in the starting rectangle of the new level. (Therefore the new level can be considered as "first level"). The further part of proof is comparable to proof of the Theorem 2.1.

Remarks. (1) $\lim\limits_{\tilde{d}\to g(\alpha)} g'_{\alpha u}(\xi) = \emptyset \not\Rightarrow \lambda \to \infty$.

(2) If in place of $g'_{\alpha u}(\xi)$ we use $g'_{\bar{u}u}(u)$, then the formula of λ is useful also in practice. ($\bar{u}$ and u are approximations of α one after another.)

(3) If $M \neq g(\alpha)$ and only Theorems 1.3 or 1.4 can be applied to g, then we also can give theorems similar to Theorem 2.2.

(4) In the numerical examples we worked with $\lambda = 2$.

3. FORTRAN program of the method and numerical examples

The input parameters of the program are: $n \doteq N$, $\varepsilon \doteq EPS$, $\delta \doteq DEL$, $K \doteq CC$, $m \doteq AH$, $M \doteq FH$, $\lambda \doteq SZ$ and $b_1 \doteq B(1)$, $c_1 \doteq C(1), \ldots, b_n \doteq B(N)$, $c_n \doteq C(N)$. After examination of a level the output parameters are: time, serial number of the level, m, M, GM, number of examined points on the level, $g(u)$, $u_1, u_2, \ldots, u_n$. (Starting value of GM is M and $GM := g(x)$, if $g(x) < GM$.)

The segment RECTANGLE gives data of the next rectangle. The segment FANDDER computes the values of $f(x, d) \doteq F$ and $\|f'(x, d)\| \doteq FD$. We have to exchange F and FD at a new example.

There are two "simplifications" of theory in the program:

(1) if the type of level is "c", then $u := u$.

(2) if the type of level is "a", then $f(u, \tilde{d}) = f_{\min}$ is in place of $R(u) = R_{\min}$, which often gives an identical result and it is more practical.

The complete FORTRAN 19ØØ program of the process (F and FD belong to the first example) is as follows.

```
      MASTER GMIN
      DIMENSION A(1ØØ, 6), H (1ØØ, 6), IND (1ØØ),
     1R (1ØØ), X(6), U(6), B(6), C(6), HH(6)
999   READ (5, 111) N, EPS, DEL, CC, AH, FH, SZ
      IF (N.EQ.Ø) STOP
      READ (5, 112) (B(I), C(I), I = 1, N)
111   FORMAT (IØ, 6FØ.Ø)
112   FORMAT (12FØ.Ø)
      WRITE (1Ø, 121) N, EPS, DEL, CC, SZ
      WRITE (1Ø, 122) (B(I), C(I), I = 1, N)
      WRITE (1Ø, 123)
121   FORMAT (3H N=, I2, 6H  EPS=, F7.5, 6H  DEL=
     1,F7.5, 5H  CC=, F6.2, 5H  SZ =, F6.2)
122   FORMAT (11H INTERVALS:, 6 (2H [,F6.2,1H, , F6.2, 2H];))
123   FORMAT(//78H      TIME    LEVEL   UNDER M   UP
     1PER M          GM   POINTS        G(U)      POINT U:/)
```

```
      DO 1 I = 1,N
      U(I), A(1,I) = (B(I)+C(I))/2
  1   HH(I) = (C(I)-B(I))/2
      CALL FANDDER(U,Ø., UF, FDERN)
      GM = FH
      L,KEM = Ø
 22   CALL TIME(TT)
      WRITE (1Ø, 124) TT, KEM, AH, FH, GM, L, UF, (U(I), I = 1,N)
124   FORMAT (1X, A8, I8, 3F1Ø.4,I8, F1Ø.4,12X, 6F9.3)
      IF(FH-AH. LT.EPS) GO TO 999
      D = (AH+FH)/2
      NI, L, IND(1) = 1
      RMIN, FMIN = 1.E2Ø
      KEM = KEM+1
      DO 2 I = 1,N
  2   H(1,I) = HH(I)
 26   DO 3 I = 1,N
  3   X(I) = A(NI,I)
      CALL FANDDER(X, D, F, FDERN)
      IF (F.GE.Ø) GO TO 21
      DO 5 I = 1,N
  5   U(I) = X(I)
      GM, FH, UF = D+F
      GO TO 22
 21   IF (F.GE.FMIN) GO TO 23
      DO 4 I = 1,N
  4   U(I) = X(I)
      FMIN = F
      UF = D+FMIN
 23   R(NI) = (SQRT (4*N*CC*F+FDERN**2)-FDERN)
     1/(2*N*CC)
      IF (R(NI).LT.DEL) GO TO 24
      IF (R(NI).LT.RMIN) RMIN = R(NI)
      CALL RECTANGLE (N, NI, A, H, IND, R)
      IF (NI.EQ.Ø)GO TO 25
      L = L+1
      GO TO 26
 25   AH = D+RMIN
      DO 9 I = 1,N
      RK = AMIN1 (SZ*RMIN, U(I)-B(I))
      RN = AMIN1 (SZ*RMIN,C(I)-U(I))
      HH(I) = (RK+RN)/2
  9   A(1,I) = (2*U(I)+RN-RK)/2
      IF (D+FMIN.GE.FH)GO TO 27
      FH = D+FMIN
```

```
27    IF (D+FMIN.GE.GM)GO TO 22
      GM = D+FMIN
      GO TO 22
24    FH = D
      GO TO 27
      END

      SUBROUTINE RECTANGLE (N, NI, A, H, IND, R)
      DIMENSION A(1ØØ,6), H(1ØØ,6), IND(1ØØ), R(1ØØ)
62    KE = (IND(NI)+1)/2
      KI = 1-4*KE+2*IND(NI)
      HS = (H(NI,KE)-R(NI))/2
      IF(HS.LE.Ø)GO TO 61
      NN = NI
      NI = NI+1
      S = (H(NN, KE)+R(NN))/2
      DO 41 I = 1,N
      A(NI,I) = A(NN,I)
41    H(NI,I) = H(NN,I)
      A(NI, KE) = A(NI, KE)+KI*S
      H(NI, KE) = HS
      IND (NN) = IND (NN)+1
      IND (NI) = 1
      IF (KI.GT.Ø) H(NN, KE) = R (NN)
      RETURN
61    IND (NI) = IND (NI)+2
63    IF (IND(NI).NE.2*N+1)GO TO 62
      NI = NI-1
      IF (NI.EQ.Ø) RETURN
      GO TO 63
      END

      SUBROUTINE FANDDER (X, D, F, FD)
      DIMENSION X(6)
      F = X(1)**2-2*X(1)*SIN(X(2))-D
      FD = 1+ABS(2*X(1)-2*SIN (X(2)))+
     1+ABS(2*X(1)*COS (X(2)))
      RETURN
      END
```

We tested our program on an ODRA 13Ø4 computer. Now we show an example for each of Theorems 1.2–1.4. The values $\varepsilon = Ø{,}Ø1$, $\delta = Ø{,}ØØ5$, $\lambda = 2$ are fixed in our examples, and u denotes the final approximation of α.

Example 1. The global minimum of $g(x) = x_1^2 - 2x_1 \sin x_2$ we computed in three cases (the solution α is inner point, limit point, extreme point):

b_1	c_1	b_2	c_2	m	M	K	α	u	$g(u)$	time (sec)
−1	2	Ø	2	−4	$g(a)$	3	{1; π/2}	{Ø,991; 1,568}	−Ø,9999	2Ø
2	5	Ø	2	−4	8	6	{2; π/2}	{2,ØØ3; 1,566}	Ø,ØØ66	12
Ø	2	−2	Ø	−4	8	3	{Ø; Ø}	{Ø,ØØ9; −Ø,ØØ5}	Ø,ØØØ2	12

In the first case the "naive method" works for 74 sec.

Example 2. The system of equations

$$\begin{cases} g_1(x) = (x_1-2)x_2 = \emptyset \\ g_2(x) = x_1^2+\sqrt{x_3}+2x_3-14 = \emptyset \\ g_3(x) = x_2x_3-4\,\mathrm{arctg}\,\emptyset{,}5\,x_1 = \emptyset \end{cases} \qquad \begin{cases} -2\le x_1\le 4 \\ -3\le x_2\le 3 \\ 1\le x_3\le 5 \end{cases}$$

has only one single solution $\{2, \pi/4, 4\}$ since $\{\emptyset, \emptyset, (57-\sqrt{113})/8\}\notin T(a, h)$. Here we have computed the global minimum of $g(x) = \sum |g_i(x)|$, for $M = g(\alpha) = \emptyset$, $K = 2$, $m = -16$. We have $m = -16$ by the formula of Theorem 1.3 (after estimation of $\sum \|g_i'(x)\|$), with $R_{\min}\sim\emptyset{,}1\,\|h^T\| = \emptyset{,}3$ (on the first level). The final (1Øth) approximation is:

$$\{2{,}\emptyset\emptyset2;\quad \emptyset{,}786;\quad 3{,}998\}\quad\text{and}\quad g(u) = \emptyset{,}\emptyset\emptyset42\quad(\text{in } 85\text{ sec}).$$

With $m\sim\emptyset$ (or $\lambda\sim 1$ and $m\le -16$) we can get much longer (or much shorter) time. And if we cover $T(a, h)$ by cubes with radius Ø,1 (18ØØØ pc.), then the time is $\sim$4Ø minutes (if in all the centres an excluding-theorem is used).

Example 3. For determining Chebyshev approximation of the table

y	−2	−1	Ø	1	2
z	Ø,6	Ø,9	1,5	1,1	Ø,4

with $z = \dfrac{a}{b+y^2}$,

we shall determine the global minimum of

$$g(x) = \max_i \left|\frac{x_1}{x_2+y_i^2}-z_i\right| .$$

Here we worked with the following data:

$$1\le x_1\le 5,\quad 1\le x_2\le 5,\quad m = -5\quad(\text{by } R_{\min}\sim\emptyset{,}1\,\|h^T\|,\ \text{too}),$$
$$M = 1,\quad K = 5{,}5$$

and

$$\|f'(x, d)\| = x_2^{-1}+x_1x_2^{-2}+1 .$$

Formula of $\|f'\|$ is a rough formula since we always use the "worst" function. The final (7th) approximation of $\alpha = \{3,2\}$ is {3,ØØ4; 2,ØØ2} and $g(u) = \emptyset{,}1\emptyset\emptyset9$ (in 27 sec).

REFERENCES

[1] *Kálovics, F.:* Nemlineáris egyenletrendszerek megoldása érintőparaboloid-módszerrel, NME Közleményei (Miskolc) IV. Sorozat, Természettudományok 23 (1977), 19–33.

[2] *Kálovics, F.:* Globális minimum meghatározása kizárásos módszerrel, Alkalmazott Matematikai Lapok 5 (1979), 269–276.

[3] *Ortega, J. M. and Rheinboldt, W. C.:* Iterative solutions of nonlinear equations in several variables, Academic Press, New York, 1970.

[4] *Szabó, Z.:* Über gleichungslösende Iterationen ohne Divergenzpunkt I–II, Publ. Math. Debreceniensis 20 (1973), 223–233; 21 (1974), 285–293.