NOTES ON NUMERICAL ANALYSIS
I. POLYNOMIAL ITERATION

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1. Let $f(x)$ be a real analytic function of the real variable x and α a simple root of the equation $f(x) = 0$. It is well known that a function $\varphi(x)$ can be associated with the equation in many different ways such that

(i) α is a root of the equation $\varphi(x) = x$, i.e. α is a fixed point (invariant point) of the function $\varphi(x)$;

(ii) $$|\varphi'(\alpha)| < 1 .$$

Then it is not difficult to prove that the iteration sequence

$$x_1 = \varphi(x_0) \quad , \quad x_2 = \varphi(x_1) \quad , \ldots , \; x_n = \varphi(x_{n-1}), \ldots$$

will have the root α as its limit if the initial term x_0 is chosen "not too far" from α ; this means that x_0 should be a reasonable approximation to the root.

The speed of the convergence of the iteration sequence will depend roughly on the magnitude of the derivative $\varphi'(x)$ for x near to α ; it will be the greater the smaller $|\varphi'(x)|$ is. Thus it is suggested that the condition (ii) should be replaced by

(iii) $$\varphi'(\alpha) = 0 \quad ,$$

and also that convergence would be further improved by postulating

(iv) $$\varphi''(\alpha) = 0 \; , \; . \; . \; . \; , \quad \varphi^{(k)}(\alpha) = 0 \; .$$

All these conditions can be satisfied.

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A simple and for many numerical purposes suitable choice of $\varphi(x)$ is Newton-Raphson's

$$x - \frac{f(x)}{f'(x)}$$

which satisfies the condition (iii). The convergence of the corresponding iteration is thoroughly discussed by Ostrowski [9]. It may be considered as the first in a series of formulae which successively satisfy the conditions (iv) for increasing natural k (cf. [1]).

An immediate improvement of Newton-Raphson's formula is given by

$$\varphi(x) = x - \frac{f(x)}{f'(x)} + \frac{f(x)^2}{f'(x)} h(x) \qquad \text{(cf. [1], p.268)}$$

where h(x) is an arbitrary function, finite at $x = \alpha$, which can be adapted to the conditions (iv); thus the above mentioned series of formulae can be obtained. This series has the remarkable property that each formula is obtained from the preceding one by simply adding one more term without alterations in the established terms.

If now f(x) is a polynomial one might try to impose on $\varphi(x)$ the condition

(v) $\varphi(x)$ is a polynomial.

C. Domb [3] and A.S. Householder [7], [8] have shown that in addition to the conditions (i), (iii), (iv) also this condition (v) can be satisfied. In the present note a polynomial $\varphi(x)$ will be constructed by another method and this $\varphi(x)$ will be studied in some special cases.

2. It may be assumed that the given polynomial f(x) has only simple roots. This is no restriction because every polynomial with multiple roots can be turned into one having the same roots simple by an elementary division process. Thus the greatest common divisor $(f(x), f'(x)) = 1$. Therefore two polynomials h(x) and $h_1(x)$ can be found such that

$$(1) \qquad h_1(x)f(x) - h(x)f'(x) = 1$$

so that $f(x)$ is a divisor of $1 + h(x)\, f'(x)$.

Now let

$$\varphi(x) = x + f(x)h(x) \; . \tag{2}$$

This is a polynomial and $\varphi(\alpha) = \alpha$. Moreover

$$\varphi'(x) = 1 + f'(x)h(x) + f(x)h'(x) \tag{3}$$

and it is evident that $f(x)$ is a divisor of $\varphi'(x)$; hence $\varphi'(\alpha) = 0$. Thus $\varphi(x)$ satisfies the conditions (i), (iii) and (v).

It may be pointed out that the polynomial $h(x)$ is not uniquely defined; therefore it can be adapted to various additional conditions as will be discussed later on. The most general solution of (1) is given by the polynomials

$$H(x) = h(x) + p(x)f(x) \; , \quad H_1(x) = h_1(x) + p(x)f'(x) \tag{4}$$

where $p(x)$ is an arbitrary polynomial.

So it remains to determine one special solution $h(x)$, $h_1(x)$ of (1). This can always be done by means of the euclidean algorithm which, however, will often be cumbersome with regard to numerical computation. The simplest method to be applied in numerical cases will be the method of unknown coefficients. It is readily seen that if $f(x)$ has the degree m, then the polynomials $h(x)$, $h_1(x)$ of least possible degree have their degrees not greater than $m - 1$ and $m - 2$ respectively.

The method may be carried through for a cubic polynomial

$$f(x) = a_0x^3 + a_1x^2 + a_2x + a_3 \qquad (a_0 \neq 0).$$

It is closely related to Sylvester's elimination method for the computation of the discriminant of $f(x)$.

Now let

$$h(x) = b_0x^2 + b_1 x + b_2 \quad , \qquad h_1(x) = c_0x + c_1 \quad .$$

For the five unknown coefficients b_0, b_1, b_2, c_0, c_1 one obtains from (1) a system of five linear equations the first of which is

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$$c_0 = 3b_0 \quad ;$$

making use of this relation in the other equations one obtains the following four equations in the four unknowns b_0, b_1, b_2, c_1 ;

$$\begin{aligned}
a_1 b_0 - 3a_0 b_1 \qquad\qquad + a_0 c_1 &= 0 \\
2a_2 b_0 - 2a_1 b_1 - 3a_0 b_2 + a_1 c_1 &= 0 \\
3a_3 b_0 - a_2 b_1 - 2a_1 b_2 + a_2 c_1 &= 0 \\
- a_2 b_2 + a_3 c_1 &= 1 \quad .
\end{aligned}$$

Their determinant equals

$$-\Delta = 27a_0^2 a_3^2 - 18a_0 a_1 a_2 a_3 + 4a_1^3 a_3 - a_1^2 a_2^2 + 4a_0 a_2^3$$

where Δ is the discriminant of f(x); and $\Delta \neq 0$ because f(x) has only simple roots. The unknown coefficients are given by

$$\begin{aligned}
\Delta \cdot b_0 &= 2a_0(3a_0 a_2 - a_1^2) \\
\Delta \cdot b_1 &= 7a_0 a_1 a_2 - 9a_0^2 a_3 - 2a_1^3 \\
\Delta \cdot b_2 &= 4a_0 a_2^2 - 3a_0 a_1 a_3 - a_1^2 a_2 \\
\Delta \cdot c_1 &= 15a_0 a_1 a_2 - 4a_1^3 - 27a_0^2 a_3 \quad .
\end{aligned}$$

These expressions may be useful for some numerical computations, but they do not seem to lend themselves for the construction of a practical general formula. They become much simpler in the case that $a_0 = 1$, $a_1 = 0$; then

$$\varphi(x) = \frac{1}{\Delta}(6a_2 x^5 - 9a_3 x^4 + 10a_2^2 x^3 - 3a_2 a_3 x^2 - 36a_3^2 x + 4a_2^2 a_3)$$

$$\Delta = -27a_3^2 - 4a_2^3$$

which substantially coincides with Domb's formula (36) in [3]. For a numerical example we refer to this paper.

3. A faster convergence in the iteration will be obtained if one or more of the conditions (iv) is imposed on the polynomial $\varphi(x)$. Indeed putting

(5) $\Phi(x) = x + H(x)f(x) = x + h(x)\, f(x) + p(x)f(x)^2$

one can choose p(x) so that not only $\Phi'(\alpha) = 0$, but also $\Phi''(\alpha) = 0$. By differentiating (5)

$$\Phi'(x) = 1 + h(x)f'(x) + f(x)\Big(h'(x) + 2p(x)f'(x) + p'(x)f(x)\Big)$$

$$= f(x)\Big(h_1(x) + h'(x) + 2p(x)f'(x) + p'(x)f(x)\Big) \quad .$$

In order to have $\Phi'(x)$ divisible by $f(x)^2$ it is only necessary to choose p(x) so that

$$(6) \qquad h_1(x) + h'(x) + 2p(x)f'(x) = q(x)f(x)$$

with a polynomial q(x). With regard to (1) this condition will be satisfied if

$$p(x) = \tfrac{1}{2}\, h(x)\, \Big(h'(x) + h_1(x)\Big) \quad , \quad q(x) = h_1(x)\, \Big(h'(x) + h_1(x)\Big)$$

and by (4)

$$H(x) = h(x) + \tfrac{1}{2}\, h(x)\Big(h'(x) + h_1(x)\Big)\, f(x)$$

$$= h(x)\Big(1 + \tfrac{1}{2}\big(1 + h(x)f'(x)\big) + \tfrac{1}{2}\, h'(x)f(x)\Big)$$

$$= \tfrac{1}{2}\, h(x)\Big(3 + \frac{d}{dx}\, \big(h(x)f(x)\big)\Big)$$

Herewith (5) represents the second in a series of formulae for polynomial iteration.

This could further be improved by choosing instead of p(x) and q(x) another solution of (6) involving an arbitrary polynomial to be adapted to the condition $\Phi'''(\alpha) = 0$, etc. It has, however, often been pointed out that the gain in an increased speed of the convergence of the iteration will be set off by the greater amount of computational work required in the application of the higher degree formulae. They will therefore not be derived. Cf. [3], [7], [8].

4. The formulae (2) and (5) will now be applied to the equation

$$f(x) = x^m - a \quad , \quad a > 0 \quad .$$

It is readily seen that in this case the polynomials

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$$h(x) = -\frac{x}{ma}, \quad h_1(x) = -\frac{1}{a}$$

will be those of lowest degree to solve equation (1); thus for the iteration, according to (2).

$$\varphi_m(x) = \frac{m+1}{m}x - \frac{1}{ma}x^{m+1}. \tag{7}$$

This formula has been given by Hartree [5] and by Domb [3].

To give an idea of its numerical quality let m = 3

$$\varphi_3(x) = \frac{x}{3}\left(4 - \frac{x^3}{a}\right). \tag{7'}$$

For a = 750 we find, beginning with $x_0 = 9$:

$$x_1 = \varphi_3(9) = 9.084, \quad x_2 = \varphi_3(9.084) = 9.0856065$$

which is too large in the sixth decimal because $(9.084)^4$ has been computed as $(82.519)^2$ instead of $(82.519056)^2$ thus showing the disturbing effect on the iteration of a relatively small deviation. The next step, however, puts matters right:

$$x_3 = \varphi_3(9.0856065) = 9.0856030\ldots$$

which is the accurate value of $\alpha = \sqrt[3]{750}$ in all the given figures.

Using (5) one obtains an improved formula for the iteration approximating $\alpha = \sqrt[m]{a}$, viz.

$$\Phi_m(x) = \frac{x}{m^2}\left(\frac{(2m+1)(m+1)}{2} - \frac{2m+1}{a}x^m + \frac{m+1}{2a^2}x^{2m}\right). \tag{8}$$

In particular

$$\Phi_3(x) = \frac{x}{9}\left(14 - \frac{7}{a}x^3 + \frac{2}{a^2}x^6\right),$$

and for a = 750 , $x_0 = 9$:

$$x_1 = \Phi_3(9) = 9.085568, \quad x_2 = \Phi_3(x_1) = 9.08560295\ldots.$$

Finally we consider a seemingly trivial example where m = 1:

$$f(x) = a_0 x - 1, \quad a_0 > 0,$$

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where the function $\varphi(x)$ will define an iteration approximating the number $\alpha = a_0^{-1}$. In this case the two polynomials $h(x) = -a_0^{-1}$, $h_1(x) = 0$ formally satisfy (1); but then the constant function $\varphi(x) = x - a_0^{-1}(a_0 x - 1) = a_0^{-1}$ does not present a useful formula.

But

$$h(x) = -x \ , \quad h_1(x) = -1$$

with regard to (2) yields

$$\varphi_1(x) = 2x - a_0 x^2 \tag{9}$$

(cf. Hartree [5] , (18), Householder [6] , p. 14).

Choosing $p(x) = x$ we obtain by (4)

$$H(x) = a_0 x^2 - 2x$$

and thus by (5)

$$\Phi_1(x) = a_0^2 x^3 - 3a_0 x^2 + 3x \ . \tag{10}$$

These formulae (9) and (10) are certainly not of great practical importance; but they will give instructive examples in the following discussion.

5. <u>The domain of convergence of the iteration</u>. For all applications of the iteration formulae it is important to know where the initial value x_0 of the iteration sequence can be chosen to guarantee convergence of the sequence. This question is easy to decide by a look at a sketch of the graph of the function $\varphi(x) = y$ in a cartesian coordinate system. General theorems in this regard can be formulated (cf. [2] , [4], [10]) ; they are, however, not expedient in the present cases.

We begin with the iterative approximation of $\alpha = a_0^{-1}$; with (9) in the form

$$\varphi_1(x) = -a_0(x - \alpha)^2 + \alpha$$

and

$$\varphi_1(0) = 0 \ , \quad \varphi_1(\alpha) = \alpha \ , \quad \varphi_1(2\alpha) = 0$$

$$\varphi_1'(0) = 2 \ , \quad \varphi_1'(\alpha) = 0 \ , \quad \varphi_1'(2\alpha) = -2$$

it is easy to sketch the graph of $y = \varphi_1(x)$ (fig 1, p.105). It cuts the straight line $y = x$ at two points, corresponding to the two fixed points of the function $\varphi_1(x)$, viz. $x = 0$ and $x = \alpha$. The construction carried out under the graph makes it clear that every sequence $x_n = \varphi_1(x_{n-1})$ $(n = 1, 2, \ldots)$ beginning with an x_0 within the open interval $0 < x_0 < 2\alpha$ will have α as its limit. Therefore α is said to be an <u>attractive</u> fixed point of $\varphi_1(x)$. Indeed we note that for $0 < x_0 < \alpha$ the sequence x_n is monotonic increasing. It is bounded above by α and therefore it has a limit. But this limit must be a fixed point of $\varphi_1(x)$; since α is a fixed point and there is no other fixed point between 0 and α, it follows that $\lim x_n = \alpha$. If $\alpha < x_0 < 2\alpha$ then $0 < \varphi_1(x_0) = x_1 < \alpha$; therefore by using x_1 instead of x_0 it follows that also in this case x_n is increasing and has α as limit. We shall not repeat this argument in later examples when it will be used in slightly varied form.

If $x_0 < 0$ or $x_0 > 2\alpha$ then $x_n \rightarrow -\infty$ as $n \rightarrow \infty$. The point $x = 0$ being never approached by a sequence x_n is said to be a <u>repulsive</u> fixed point of $\varphi_1(x)$.

Similarly (10) may be written in the form

$$\Phi_1(x) = a_0^2 (x - \alpha)^3 + \alpha .$$

Fig. 2, p.105, shows a sketch of the graph of this function. It cuts the line $y = x$ in three points, corresponding to the three fixed points $x = 0$, $x = \alpha$, $x = 2\alpha$ of $\Phi_1(x)$. Of these only $x = \alpha$ proves to be attractive and construction and argument employed in the discussion above shows again that for x_0 within the open interval $(0, 2\alpha)$ the sequence $x_n = \Phi_1(x_{n-1})$ is convergent and has α as limit. It is increasing and approaching α from the left side if $0 < x_0 < \alpha$, decreasing if $\alpha < x_0 < 2\alpha$. The points 0 and 2α are repulsive fixed points and for all $x_0 < 0$ and $> 2\alpha$ the sequence x_n tends to $-\infty$ and $+\infty$ respectively as $n \rightarrow \infty$.

It should be noticed that the convergence interval will be the smaller the larger a_0 is. This reflects on the restricted usefulness of the formulae (9) and (10).

6. <u>Convergence of the root iteration defined by (7)</u>. In these cases the situation turns out to be more complicated; essentially different conditions will be found for even and for odd values of m. As prototype of the case of an even m we consider

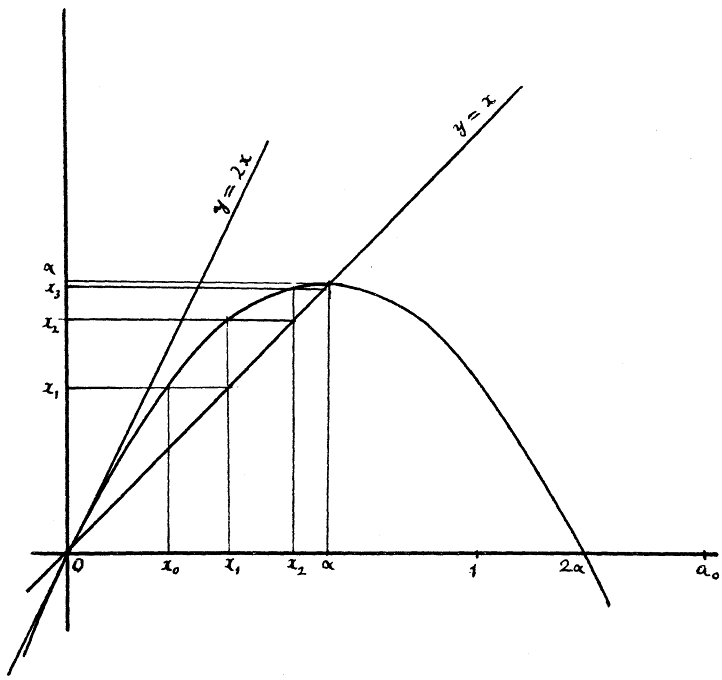

Fig. 1.

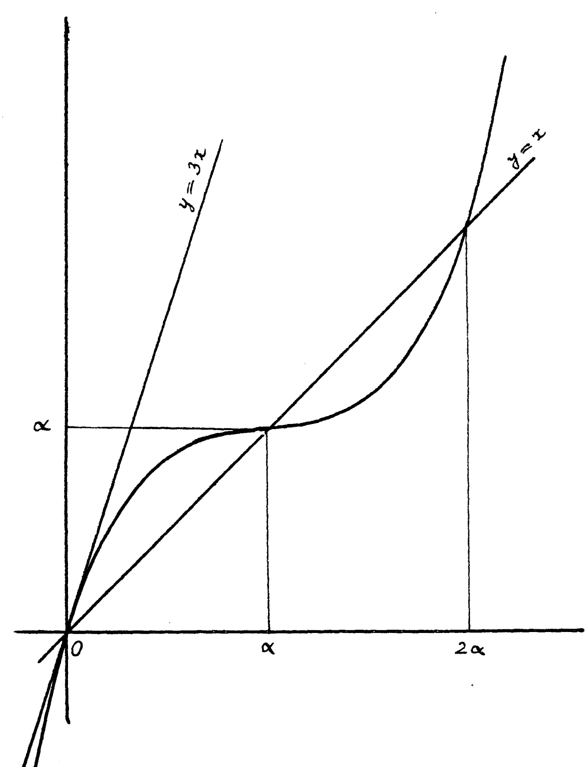

Fig. 2.

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the function

$$\varphi_2(x) = \frac{3}{2}x - \frac{1}{2a}x^3 \quad , \ a > 0 \ , \ \alpha = \sqrt{a} > 0 \ .$$

The graph cuts the x-axis at three points, viz.

$$x = 0 \quad \text{and} \quad x = \pm\ \beta_0 = \pm\ \sqrt{3}\,\alpha \qquad \text{(cf. fig. 3)} .$$

It has its relative maximum and minimum at $x = \alpha$ and $x = -\alpha$ respectively and its point of inflection at $x = 0$ where its gradient equals $\varphi_2'(0) = 3/2$. It cuts the line $y = x$ in three points corresponding to the three fixed points $x = -\alpha$, $x = 0$, $x = \alpha$ of which α and $-\alpha$ are seen to be attractive. These data determine the shape of the graph as shown in fig. 3, p 107.

It is clear that for $0 < x_0 < \alpha\sqrt{3} = \beta_0$ the iteration sequence $x_n = \varphi_2(x_{n-1})$ has α as its limit; it approaches α always from the left side. There is, however, an infinity of other entirely disjoint open convergence intervals consisting of points x_0 for which $x_n \to \alpha$. In order to describe them let

$$\psi(y) = \varphi_2^{-1}(y) \quad (\text{for } |y| > \beta_0 = \alpha\sqrt{3}\ )$$

be the inverse function of $\varphi_2(x)$ which for the given ranges of the variable y is uniquely defined. Put

$$\beta_1 = \psi(-\beta_0) \quad , \quad \beta_2 = \psi(-\beta_1) \quad , \quad \beta_3 = \psi(-\beta_2) \ , \ . \ . \ . \quad .$$

Then the sequence x_n will tend to α if x_0 is a point of any one of the following open intervals

$$I_+ : (0,\ \beta_0),\ (-\beta_1,\ -\beta_0),\ (\beta_1, \beta_2),\ (-\beta_3,\ -\beta_2),\ (\beta_3, \beta_4),\ .\ .\ .$$

Indeed, if $-\beta_1 < x_0 < -\beta_0$, then $x_1 = \varphi_2(x_0)$ is a point of the interval $(0, \beta_0)$, so that the sequence x_n tends to α and $0 < x_n \leqslant \alpha$ if $n \geqslant 2$. Similarly if x_0 lies in (β_1, β_2), then $-\beta_1 < x_1 < -\beta_0$ so that x_2 lies in $(0, \beta_0)$, etc.

Further it is readily seen that if x_0 lies in one of the complementary open intervals

$$I_- : (-\beta_0,\ 0),\ (\beta_0, \beta_1),\ (-\beta_2,\ -\beta_1),\ (\beta_2, \beta_3),\ .\ .\ .$$

the sequence x_n tends to $-\alpha$ from the right side. These intervals separate the intervals of convergence to $+\alpha$. Because of the increasing slope of the graph, the length of the intervals (β_n, β_{n+1}), $(-\beta_{n+1}, -\beta_n)$ tends rapidly to zero as n increases; nevertheless the two sets I_+ and I_- cover the whole x-axis.

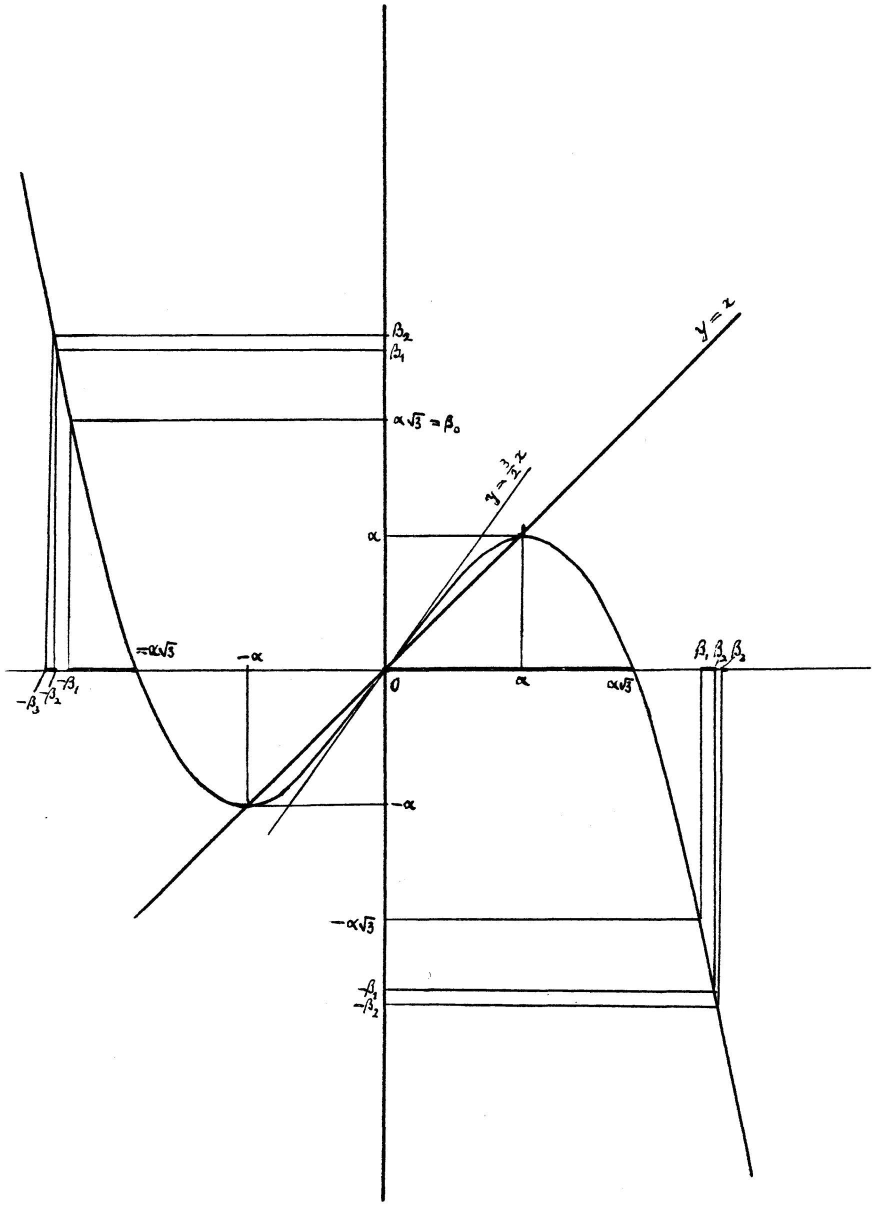

Fig. 3.

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The separating points $0, \beta_0, -\beta_0, \beta_1, -\beta_1, \ldots, \beta_{k-1}, -\beta_{k-1}$ are the real roots (zeros) of the k times iterated function $\varphi_2^k(x)$ where

$$\varphi_2^1(x) = \varphi_2(x), \quad \varphi_2^2(x) = \varphi_2(\varphi_2(x)), \ldots, \quad \varphi_2^k(x) = \varphi_2(\varphi_2^{k-1}(x)).$$

Indeed

$$\varphi_2^2(\pm\beta_0) = \varphi_2(0) = 0, \quad \varphi_2^2(\pm\beta_1) = \varphi_2(\mp\beta_0) = 0, \quad \ldots \quad .$$

Also note that if x_0 coincides with any one of the β_i, then $x_n \longrightarrow 0$. Thus although 0 is a repulsive fixed point of $\varphi_2(x)$ in the sense of the definition, there are nevertheless iteration sequences (with almost all terms equal to zero) having 0 as limit.

Now it is not difficult to show that for the function $\varphi_m(x)$ of (7) with any even $m = 2r > 0$ the general appearance of the graph is the same as in the case $m = 2$. In fact $\varphi_{2r}(x)$ has exactly three real zeros: $x = 0$ and $x = \pm\beta_0 = \pm(2r+1)^{1/2r}\alpha$, where $\alpha = a^{1/2r}$. The graph cuts the line $y = x$ in three points corresponding to the three real fixed points $x = 0$, $x = \pm\alpha$ of $\varphi_{2r}(x)$, and it has a point of inflexion at 0. Further the points $\beta_n = \varphi_{2r}^{-1}(-\beta_{n-1})$ separate the different convergence intervals in the same way as in the case of $m = 2$. Thus the result of the preceding discussion can be summarized as follows. <u>The limit function</u>

$$\tilde{\varphi}_{2r}(x) = \lim_{n\to\infty} \varphi_{2r}^n(x)$$

<u>assumes only three different values for all real values of the variable</u> x :

$$\tilde{\varphi}_{2r}(x) = \begin{cases} \alpha & \text{if } x \in I_+ \\ 0 & \text{if } x = \pm\beta_n \quad (n = 0, 1, 2, \ldots) \\ -\alpha & \text{if } x \in I_- \, . \end{cases}$$

For all practical computations it seems obvious that x_0 should be selected within the interval $(0, \alpha)$.

Regarding an odd value of m consider first the value $m = 3$. The function $\varphi_3(x)$ as given by (7') has its real zeros at $x = 0$ and $x = \sqrt[3]{4}\,\alpha > 0$ if α represents the real third root of a. The graph passes through 0 with the slope 4/3 and cuts the line $y = x$ in two points, corresponding to the two real fixed points 0 and α of $\varphi_3(x)$; there is no point of inflexion. The maximum is reached for $x = \alpha$. After these indications a sketch of the curve can easily be drawn; it shows that the only convergence interval of the iteration is the open interval $(0, \sqrt[3]{4}\alpha)$.

Similarly it is seen that the iteration with $\varphi_{2r-1}(x)$ has the interval $(0, \beta)$, $\beta = (2r)^{1/2r-1}\alpha$, $\alpha = a^{1/2r-1}$, as its domain of convergence.

7. By the same method the convergence of the iteration with the function $\Phi_m(x)$ of (8) can be investigated. This function has only the one real zero $x = 0$. For the further discussion we distinguish again between even and odd values of m.

If $m = 2r$ the graph cuts the line $y = x$ in five points

$$x = 0, \; x = \pm\alpha = \pm\sqrt[m]{a}, \; x = \pm\alpha_1 = \pm\left(\frac{3m+1}{m+1}\right)^{1/m}\alpha$$

corresponding to the five real fixed points of $\Phi_m(x)$, of which $+\alpha$ and $-\alpha$ are attractive and the others repulsive because $\Phi_m'(\pm\alpha) = 0$, $\Phi_m'(\pm\alpha_1) > 1$, $\Phi_m'(0) > 1$. The function has no extremum; it has two stationary points of inflexion at $x = \pm\alpha$ and one other point of inflexion at $x = 0$. To guarantee convergence of the sequence $x_n = \Phi_m(x_{n-1})$ to the limit $\alpha > 0$ one has to choose x_0 in the interval $(0, \alpha_1)$; for x_0 in $(-\alpha_1, 0)$ the sequence tends to $-\alpha$. For all other $x_0 > \alpha$ and $x_0 < -\alpha$ it tends to $+\infty$ and $-\infty$ respectively.

If $m = 2r + 1$ the graph cuts the line $y = x$ in the three points $x = 0$, $x = \alpha$, $x = \alpha_1$ of which only α represents an attractive fixed point. For convergence of x_n to α one has to choose x_0 in the interval $(0, \alpha_1)$.

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