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A method for improving iteration procedures

By IRWIN MANNING
U.S. Naval Research Laboratory, Washington, D.C.

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Abstract. A technique is developed for improving the speed and range of convergence of iteration procedures. The method is shown to include, as special cases, Newton's method and Aitken's δ^2-acceleration process.

1. *Introduction.* This paper discusses algorithms of the type defined below for finding a desired number c, real or complex.

The constant c is defined by the relation

$$c = f(c), \tag{1·1}$$

where $f(x)$ is a continuous single-valued function of x, and we form a sequence $x_0, x_1, x_2, \ldots$ by the rule

$$x_{n+1} = f(x_n) \tag{1·2}$$

starting from a selected x_0, in the hope that $x_n \to c$ as $m \to \infty$. We shall speak of this algorithm as the iteration procedure defined by $f(x)$ and x_0, or simply the iteration procedure $f(x)$.

A fundamental theorem for such algorithms (1) [also quoted in (2)] gives a sufficient condition that the sequence $\{x_n\}$ convergence to c, and gives bounds on the error involved in truncating the sequence at a given stage. It provides a criterion which if satisfied will guarantee that the iteration procedure is a 'good' one. For simplicity suppose $f(x)$ to be differentiable. Then the theorem indicates that we should demand that $|(d/dx)f(x)| < 1$ over an interval including x_0 and c; furthermore, we desire this derivative to be as small as possible over as wide an interval as possible.

This criterion can be understood by picturing the graph of the curve $f(x)$. When x_0 is chosen close to c we have $(x_1 - c) \approx f'(c)\,(x_0 - c)$, and for efficiency we desire that $|f'(c)|$ be as small as possible. (For this case note that $|f'(c)| < 1$ implies $|x_1 - c| < |x_0 - c|$.) If x_0 is chosen far from c we desire that $|x_1 - c|$ be small even though $|x_0 - c|$ is large; this means that the curve $f(x)$ should be flat over the interval between x_0 and c, which in turn requires that $|f'(x)|$ be small throughout the interval.

Imagine two different iteration procedures $f(x)$ and $F(x)$ for the same number $c = f(c) = F(c)$. Using the above criterion of goodness, we shall say that the iteration procedure $F(x)$ is better than $f(x)$ if $|F'(x)| < |f'(x)|$ over an appropriate range of x. We are completely ignoring the important question of the difficulty of evaluating $F(x)$ as compared with $f(x)$. With this understanding, we now go on to formulate a general technique for improving an iteration procedure.

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2. *Technique for improving iteration procedures.* Let $f(x)$ and $g(x)$ be two differentiable iteration procedures for the same c, neither of which need necessarily converge. For any value of μ, the function

$$F(x) = \mu f(x) + (1-\mu) g(x) \tag{2·1}$$

is also an iteration procedure, that is $F(c) = c$. Our plan is to choose μ a function of x in such a way as to make $F'(x)$ small. Given a non-trivial procedure $f(x)$, one can always find a second procedure $g(x)$ with which to explore this technique: for example, $g(x) = x$, x^2/f, f^2/x, and so on.

Differentiating the above, one has

$$F'(x) = [\mu(f'-g') + g'] + \mu'(f-g). \tag{2·2}$$

We now choose μ so as to make the first bracket identically zero, thus forcing $F'(x)$ to be small whenever the second bracket is small

$$\mu(x) = \frac{g'}{g'-f'} \tag{2·3}$$

and

$$F'(x) = \mu'(f-g). \tag{2·4}$$

Now, $f = g$ at c, so

$$F'(c) = 0 \tag{2·5}$$

whenever $\mu'(c)$ is finite; there will then always exist an interval including c in which $|F'(x)|$ is less than one and the procedure converges. We have

$$\mu'(x) = \frac{g'f''-f'g''}{(g'-f')^2} \tag{2·6}$$

and the smaller this quantity the broader the interval in which $F(x)$ will be an efficient procedure. The requirement that $\mu'(c)$ be finite generally means that

$$f'(c) \neq g'(c). \tag{2·7}$$

(If $f' = g'$ one cannot choose a linear combination (2·1) which puts $F' = 0$.) The improved iteration procedure is

$$F(x) = \frac{fg'-gf'}{g'-f'} \tag{2·8}$$

$$= f - \frac{f'}{g'-f'}(g-f) \tag{2·9}$$

$$= g - \frac{g'}{f'-g'}(f-g). \tag{2·10}$$

The fact that $F'(c)$ is zero means that $F(x)$ is of second order (3). From the Taylor expansion

$$F(x) = F(c) + F'(c)(x-c) + \tfrac{1}{2}F''(c)(x-c)^2 + \ldots \tag{2·11}$$

we see that if the error $|x_0-c|$ of x_0 is small (of order ϵ), then the error of x_1 is of order ϵ^2

$$|x_1-c| = \tfrac{1}{2}|F''(c)| \,.\, |x_0-c|^2. \tag{2·12}$$

The efficiency in the immediate neighbourhood of c is thus measured by

$$F''(c) = \left.\frac{g'f''-f'g''}{f'-g'.}\right|_{x=c}. \tag{2·13}$$

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3. *The case $g = x$.* For the choice $g = x$ the improvement of the previous section becomes

$$F(x) = \mu f(x) + (1-\mu)x \tag{3·1}$$

and $F(x)$ corresponds to averaging, with relative weight $\mu(x)$, the successive iterates given by $f(x)$. We find

$$F = \frac{f - xf'}{1-f'} \tag{3·2}$$

$$= x - \frac{f-x}{f'-1}. \tag{3·3}$$

The requirement that μ' be finite

$$\mu'(x) = \frac{f''}{(1-f')^2} \tag{3·4}$$

generally means that $f' \neq 1$ over the range of interest.

As a simple illustration, consider the problem of finding

$$c = \sqrt{N} \tag{3·5}$$

with N a given number. The iteration procedure

$$f_1(x) = N/x \tag{3·6}$$

will never converge. The above improvement technique yields

$$F_1(x) = \frac{2Nx}{N+x^2}. \tag{3·7}$$

For any positive N and finite, positive x_0, this improved procedure always converges, as can be seen as follows: examination of the graph of $F'(x)$ shows that $|F'(x)| < 1$ for $x > x_a$, with $x_a \approx 0{\cdot}4859\sqrt{N}$. But $F(x)/x > 1$ whenever $x < c$; using this fact one easily shows that, even if x_0 or x_1 is less than x_a, one eventually arrives at an x_n in the iteration sequence for which the previously mentioned theorem (1) is satisfied (with x_n and x_{n+1} playing the role of x_0 and x_1).

By comparing their graphs of $F'(x)$, one finds that F_1 above is slightly better than the more familiar iteration procedure (3)

$$F_2(x) = \tfrac{1}{2}[x + (N/x)]; \tag{3·8}$$

this latter corresponds to the F of equation (3·1) with $f = N/x$ and $\mu = \frac{1}{2}$. (We stress again that in this paper we are ignoring the important criterion of relative ease of calculation.)

Suppose that the number sought is defined by a relation of the form

$$\phi(c) = 0. \tag{3·9}$$

Then, for

$$f(x) = x + \phi(x) \tag{3·10}$$

the above improvement (3·1) becomes

$$F(x) = x + \mu\phi(x) \tag{3·11}$$

$$= x - \frac{\phi(x}{\phi'(x)}, \tag{3·12}$$

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which is just Newton's method (1), (3). Thus, the improvement technique here put forward can be viewed as simply a generalization of Newton's method. (The procedure of section 2 for determining $\mu(x)$, when applied to equation (3·11), leads to a simple derivation of Newton's method.)

4. *On Aitken's acceleration process.* The improvement (3·3) of the previous section replaces the sequence $\{x_n\}$ by the accelerated sequence $\{y_n\}$, where $\{x_n\}$ is generated by $f(x)$ and $\{y_n\}$ by $F(x)$

$$y_n = x_n - \frac{x_{n+1}-x_n}{f'(x_n)-1}. \tag{4·1}$$

Instead of evaluating $f'(x)$, one might choose to approximate it as follows: The Taylor expansion of $f(x)$ at x_n is

$$f(x) = f(x_n)+f'(x_n)(x-x_n)+\tfrac{1}{2}f''(x_n)(x-x_n)^2+\ldots. \tag{4·2}$$

Putting $x=x_{n+1}$, we find

$$f'(x_n) \approx \frac{x_{n+2}-x_{n+1}}{x_{n+1}-x_n}, \tag{4·3}$$

providing that the series (4·2) can be truncated at the second term. Substituting this approximation into the above result, we obtain

$$y_n = x_n - \frac{(x_{n+1}-x_n)^2}{x_{n+2}-2x_{n+1}+x_n}, \tag{4·4}$$

which is just Aitken's δ^2-acceleration process (3), (4). In addition to requiring that $f' \neq 1$, our derivation indicates that this process also requires that the series (4·2) can be truncated at the second term; this usually implies the condition

$$|f''(x_n)(x_{n+1}-x_n)| \ll 2|f'(x_n)|. \tag{4·5}$$

In particular, we cannot have $f'(c) = 0$.

Our derivation of Aitken's process suggests an improvement which eliminates the restriction (4·5): substitute into the procedure (4·1) the approximation to $f'(x)$ found by keeping the quadratic term in the Taylor series (4·2)

$$f'(x_n) = \frac{(x_{n+2}-x_{n+1})(x_n-x_{n-1})^2-(x_{n+1}-x_0)^3}{x_{n+1}-2x_n+x_{n-1}}. \tag{4·6}$$

This procedure will require, in addition to $f' \neq 1$, that $f(x)$ not be of third or higher order.

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REFERENCES

(1) COLLATZ, I. *Handbuch der Physik*, vol. II, p. 370 (Berlin, 1955).
(2) MANNING, I. *Phys. Rev.* **139** (1965), B 495–500.
(3) HARTREE, D. R. *Numerical analysis*, Chap. 9 (London, 1958).
(4) HARTREE, D. R. *Proc. Cambridge Philos. Soc.* **45** (1948), 230.

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