

Optimal Order of One-Point and Multipoint Iteration

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ABSTRACT. The problem is to calculate a simple zero of a nonlinear function f by iteration. There is exhibited a family of iterations of order 2^{n-1} which use n evaluations of f and no derivative evaluations, as well as a second family of iterations of order 2^{n-1} based on $n - 1$ evaluations of f and one of f' . In particular, with four evaluations an iteration of eighth order is constructed. The best previous result for four evaluations was fifth order.

It is proved that the *optimal* order of one general class of multipoint iterations is 2^{n-1} and that an upper bound on the order of a multipoint iteration based on n evaluations of f (no derivatives) is 2^n .

It is conjectured that a multipoint iteration without memory based on n evaluations has optimal order 2^{n-1} .

KEY WORDS AND PHRASES: computational complexity, iteration theory, optimal algorithms, nonlinear equations, multipoint iterations

CR CATEGORIES: 5.10, 5.15, 5.29

1. Introduction

We deal with iterations for calculating simple zeros of a scalar function f . This problem is a prototype for many nonlinear numerical problems [11]. Newton-Raphson iteration is probably the most widely used algorithm for dealing with such problems. It is of second order and requires the evaluation of f and f' , that is, it uses two evaluations. Consider an iteration consisting of two successive Newton-Raphson iterates (composition of iterates). This iteration has fourth order and requires four evaluations, two of f and two of f' . More generally, an iteration composed of n Newton iterates is of order 2^n and requires n evaluations of f and n evaluations of f' , that is, $2n$ evaluations.

We shall show that an iteration of order 2^{n-1} may be constructed from just n evaluations of f . We exhibit a second type of iteration which requires $n - 1$ evaluations of f and one evaluation of f' to achieve order 2^{n-1} .

In particular, with four evaluations we construct an iteration of eighth order. The best previous result [10, p. 196] for four evaluations was fifth order.

Newton-Raphson iteration is an example of a one-point iteration. The basic optimality theorem for one-point iteration states that an analytic one-point iteration which is based on n evaluations is of order at most n . (This theorem was first stated by Traub [9; 10, Sec. 5.4]; we give an improved proof here.) We *conjecture* that a multipoint iteration based on n evaluations has optimal order 2^{n-1} . We prove that the optimal order of one important family of multipoint iterations is 2^{n-1} and that an upper bound on the order of

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multipoint iteration based on n evaluations of f is 2^n . This upper bound is close to the conjectured optimal order of 2^{n-1} .

To compare various algorithms, we must define efficiency measures based on speed of convergence (order), cost of evaluating f and its derivatives (problem cost), and the cost of forming the iteration (combinatory cost). We analyze efficiency in another paper [5]. We confine ourselves here to iterations *without memory*, deferring the analysis of iterations with memory to a future paper.

We summarize the results of this paper. The class of problems and algorithms studied in this paper is defined in Section 2. Particular families of iterations are defined in Sections 3–5. The optimality theorem for one-point iterations is proven in Section 6. An optimal order theorem for one general class of multipoint iterations and an upper bound for the order of a second class are proven in Section 7. A general conjecture is stated in Section 8. Section 9 contains a small numerical example. The Appendix gives ALGOL programs for forming two families of multipoint iterations.

2. Definitions

We define the ensemble of problems and algorithms. Let $D = \{f \mid f \text{ is a real analytic function defined on an open interval } I_f \subset R \text{ which contains a simple zero } \alpha_f \text{ of } f \text{ and } f' \text{ does not vanish on } I_f\}$.

Let Ω denote the set of functions ϕ which maps every $f \in D$ to $\phi(f)$ with the following properties:

1. $\phi(f)$ is a function mapping $I_{\phi, f} \subset I_f$ into $I_{\phi, f}$ for some open subinterval $I_{\phi, f}$ containing α_f .

2. $\phi(f)(\alpha_f) = \alpha_f$.

3. There exists an open subinterval $I_{\phi, f}^0 \subset I_{\phi, f}$ containing α_f such that if $x_{i+1} = \phi(f)(x_i)$ then $\lim_{i \rightarrow \infty} x_i = \alpha_f$ whenever $x_0 \in I_{\phi, f}^0$.

4. For any ϕ , there exist nonnegative integers k, d_0, \dots, d_{k-1} , and functions $u_{j+1}(y_0; y_1^0, \dots, y_{d_0+1}^0; \dots, y_1^j, \dots, y_{d_j+1}^j)$ of $1 + \sum_0^j (d_j + 1)$ variables for $j = -1, \dots, k - 1$ such that, for all $f \in D$,

$$\phi(f)(x) = z_k, \quad (2.1)$$

where

$$\begin{aligned} z_0 &= u_0(x), \\ z_{j+1} &= u_{j+1}(x; f(z_0), \dots, f^{(d_0)}(z_0); \dots; f(z_j), \dots, f^{(d_j)}(z_j)), \quad j = 0, \dots, k - 1. \end{aligned} \quad (2.2)$$

The assumption that $f \in D$ is needed for theorems dealing with a class of iterations. Any particular ϕ can be applied to f having only a certain number of derivatives.

In (2.2) we assume $u_0(x) \equiv x$. In another paper [6], we prove that if $\phi \in \Omega$ and if $u_0(x)$ is continuous, then $u_0(x)$ must be identically equal to x .

If $\phi \in \Omega$, ϕ is called an *iteration without memory*, since if the sequence $\{x_i\}$ is generated by $x_{i+1} = \phi(f)(x_i)$, x_{i+1} is computed using information only at the current point x_i . In this paper we limit ourselves to iterations without memory.

We classify iterations without memory. If k is the nonnegative integer in (2.1), then we say ϕ is a k -point iteration. In particular, if $k = 1$, we call ϕ a *one-point iteration* and if $k > 1$ and the value of k is not important, we call ϕ a *multipoint iteration*. (Similar definitions of one-point and multipoint iteration are given in [9; 10, Sec. 1.22].)

If there exists $p(\phi)$ such that for any $f \in D$,

$$\lim_{x \rightarrow \alpha_f} [(\phi(f)(x) - \alpha_f)/(x - \alpha_f)^{p(\phi)}] = S(\phi, f)$$

exists for a constant $S(\phi, f)$ and $S(\phi, f) \neq 0$ for at least one $f \in D$, then ϕ is said to have *order of convergence* (order) $p(\phi)$ and asymptotic error constant $S(\phi, f)$.

This is perhaps the simplest definition of order of convergence. The results of this paper hold, with suitable modifications, for weaker definitions of order [7], but we feel that use of these definitions would obscure the proofs without substantially strengthening the results.

Let $v_i(\phi)$ denote the number of evaluations of $f^{(i)}$ used to compute $\phi(f)(x)$. Then $v(\phi) = \sum_{i \geq 0} v_i(\phi)$ is the total number of evaluations required by $\phi(f)(x)$ per step.

To simplify notation, we often use α, ϕ, p, v_i, v instead of $\alpha_f, \phi(f)(x), p(\phi), v_i(\phi), v(\phi)$, if there is no ambiguity.

The following two examples illustrate the definitions.

Example 2.1. (Newton-Raphson Iteration) $\phi(f)(x) = x - f(x)/f'(x)$. This is a one-point iteration with $v_0 = 1, v_1 = 1, v = 2$, and $p = 2$.

Example 2.2. $z_0 = x, z_1 = z_0 - f(z_0)/f'(z_0)$,

$$\phi(f)(x) = z_2 = z_1 - \{f(z_1)f(z_0)/[f(z_1) - f(z_0)]^2\} \cdot [f(z_0)/f'(z_0)].$$

This is a two-point iteration with $v_0 = 2, v_1 = 1, v = 3$, and $p = 4$. (See Section 5.)

3. A Family of One-Point Iterations

For $f \in D$, let F be the inverse function to f . For every n , define $\gamma_j(f): I_f \rightarrow R, j = 1, \dots, n$, as follows: $\gamma_1(f)(x) = x$ and for $n > 1$,

$$\gamma_{j+1}(f)(x) = \gamma_j(f)(x) + [(-1)^j/j!] \cdot [f(x)]^j \cdot F^{(j)}(f(x)) \tag{3.1}$$

for $j = 1, \dots, n - 1$. Note that $F^{(j)}(f(x))$ can be expressed in terms of $f^{(i)}(x)$ for $i = 1, 2, \dots, j$. It is easy to show that, for example,

$$\gamma_1 = x, \quad \gamma_2 = \gamma_1 - f(x)/f'(x), \quad \gamma_3 = \gamma_2 - [f''(x)/2f'(x)][f(x)/f'(x)]^2.$$

The family $\{\gamma_n\}$ has been thoroughly studied [10, Sec. 5.1]. Its essential properties are summarized in

THEOREM 3.1. *Let γ_n be defined by (3.1). Then for $n > 1$, (1) $\gamma_n \in \Omega$, and γ_n is a one-point iteration; (2) $p(\gamma_n) = n$, (3) $v_i(\gamma_n) = 1, i = 0, \dots, n - 1, v_i(\gamma_n) = 0, i > n - 1$. Hence $v(\gamma_n) = n$.*

Thus γ_n requires the evaluation of f and its first $n - 1$ derivatives. In Section 6 we shall show that, under a mild smoothness condition on the iteration, every one-point iteration of order n requires the evaluation of at least f and its first $n - 1$ derivatives.

4. A Family of Multipoint Iterations

We construct a family of multipoint iterations, $\{\psi_n\}$, which require the evaluation of f at n points, no evaluation of derivatives of f , and for which $p(\psi_n) = 2^{n-1}$.

For every n , define $\psi_j(f): I_{\psi_j, f} \subset I_f \rightarrow I_{\psi_j, f}, j = 0, \dots, n$, as follows: $\psi_0(f)(x) = x$ and for $n > 0$,

$$\left. \begin{aligned} \psi_1(f)(x) &= x + \beta f(x), \beta \text{ a nonzero constant,} \\ &\vdots \\ \psi_{j+1}(f)(x) &= Q_j(0), \end{aligned} \right\} \tag{4.1}$$

for $j = 1, \dots, n - 1$, where $Q_j(y)$ is the inverse interpolatory polynomial for f at $f(\psi_k(f)(x)), k = 0, \dots, j$. That is, $Q_j(y)$ is the polynomial of degree at most j such that $Q_j(f(\psi_k(f)(x))) = \psi_k(f)(x), k = 0, \dots, j$.

The $\psi_j(f), j = 1, \dots, n$, are well defined if

$$\psi_j(f)(I_{\psi_j, f}) \subset I_{\psi_j, f}, \quad j = 1, \dots, n. \tag{4.2}$$

That (4.2) holds for $I_{\psi_j, f}$ sufficiently small will be part of the proof of Theorem 4.1.

It is easy to show that, for example,

$$\begin{aligned} \psi_0 &= x, \quad \psi_1 = \psi_0 + \beta f(\psi_0), \quad \psi_2 = \psi_1 - \beta f(\psi_0)f(\psi_1)/[f(\psi_1) - f(\psi_0)], \\ \psi_3 &= \psi_2 - f(\psi_0)f(\psi_1)/[f(\psi_2) - f(\psi_0)] \\ &\quad \cdot \{(\psi_1 - \psi_0)/[f(\psi_1) - f(\psi_0)] - (\psi_2 - \psi_1)/[f(\psi_2) - f(\psi_1)]\}. \end{aligned}$$

An ALGOL program (Program 1) is given in the Appendix for computing ψ_n for $n \geq 4$.

Our interest in the family of iterations $\{\psi_n\}$ is due to the properties proved in

THEOREM 4.1. *Let ψ_n be defined by (4.1). Then for $n > 1$, (1) $\psi_n \in \Omega$, and ψ_n is an n -point iteration, (2) $p(\psi_n) = 2^{n-1}$, (3) $v_0(\psi_n) = n$, $v_i(\psi_n) = 0$, $i > 0$. Hence $v(\psi_n) = n$.*

PROOF. We want to show that, for $f \in D$,

$$\lim_{x \rightarrow \alpha} (\psi_n - \alpha)/(x - \alpha)^{2^{n-1}} = S(\psi_n, f), \quad n = 1, 2, \dots \quad (4.3)$$

for constants $S(\psi_n, f)$. The proof is by induction on n . Since $\lim_{x \rightarrow \alpha} (\psi_1 - \alpha)/(x - \alpha) = 1 + \beta f'(\alpha)$, (4.3) holds for $n = 1$. Assume that (4.3) holds for $n = 1, \dots, m - 1$. From general interpolatory iteration theory [10, Ch. 4], we know that

$$\lim_{x \rightarrow \alpha} [(\psi_m - \alpha)/\prod_{0 \leq n < m} (\psi_n - \alpha)] = Y_m(f), \quad (4.4)$$

where $Y_m(f) = (-1)^{m+1} F^{(m)}(0)/(m![F'(0)]^m)$ and F is the inverse function of f . From (4.4) and the induction hypothesis,

$$\begin{aligned} \lim_{x \rightarrow \alpha} [(\psi_m - \alpha)/(x - \alpha)^{2^{m-1}}] &= \lim_{x \rightarrow \alpha} [(\psi_m - \alpha)/\prod_{0 \leq n < m} (\psi_n - \alpha)] [(\psi_0 - \alpha)/(x - \alpha)] \\ &\quad \cdot \prod_{1 \leq n < m} [(\psi_n - \alpha)/(x - \alpha)^{2^{n-1}}] \\ &= Y_m(f) \prod_{1 \leq n < m} S(\psi_n, f). \end{aligned}$$

Hence $S(\psi_m, f) = Y_m(f) \prod_{1 \leq n < m} S(\psi_n, f)$ and this completes the induction.

From (4.3) one can easily show that $\psi_j(f)$, $j = 2, \dots, n$, satisfies (4.2) for $I_{\psi_j, f}$ sufficiently small and hence is well defined. It can be verified that $\psi_n \in \Omega$.

It is not difficult to show that $S(\psi_n, f) \neq 0$ for some $f \in D$. Therefore, $p(\psi_n) = 2^{n-1}$. The fact that $v_0(\psi_n) = n$, $v_i(\psi_n) = 0$, $i > 0$ follows from the definition of ψ_n . Q.E.D.

The iteration ψ_2 is second order and is based on evaluations of f at x and $x + \beta f(x)$. This iteration is given by Traub [10, Sec. 8.4]. The iteration ψ_n uses n evaluations of f and is of order 2^{n-1} . For $n > 2$, no iterations with these properties were previously known.

5. A Second Family of Multipoint Iterations

We now construct a second family of multipoint iterations, $\{\omega_n\}$, such that $p(\omega_n) = 2^{n-1}$ and $v(\omega_n) = n$. However, ω_n requires the evaluation of f at $n - 1$ points and the evaluation of f' at one point.

For every n , define $\omega_j(f) : I_{\omega_j, f} \subset I_f \rightarrow I_{\omega_j, f}$, $j = 1, \dots, n$, as follows: $\omega_1(f)(x) = x$ and for $n > 1$,

$$\left. \begin{aligned} \omega_2(f)(x) &= x - f(x)/f'(x), \\ \vdots \\ \omega_{j+1}(f)(x) &= R_j(0), \end{aligned} \right\} \quad (5.1)$$

for $j = 2, \dots, n - 1$, where $R_j(y)$ is the inverse Hermite interpolatory polynomial of degree at most j such that

$$R_j(f(x)) = x, \quad R_j'(f(x)) = 1/f'(x), \quad R_j(f(\omega_k(f)(x))) = \omega_k(x), \quad k = 2, \dots, j. \quad (5.2)$$

One can prove that $\omega_j(f)$, $j = 2, \dots, n$, are well defined for $I_{\omega_j, f}$ sufficiently small. It is easy to show that, for example,

$$\begin{aligned} \omega_1 &= x, \quad \omega_2 = \omega_1 - f(\omega_1)/f'(\omega_1), \\ \omega_3 &= \omega_2 - \{f(\omega_1)f(\omega_2)/[f(\omega_1) - f(\omega_2)]\}^2 \cdot [f(\omega_1)/f'(\omega_1)]. \end{aligned}$$

An ALGOL program (Program 2) is given in the Appendix for computing ω_4 for $n \geq 4$.

The basic properties of the family of iterations $\{\omega_n\}$ is stated in the following theorem. The proof is omitted since it is similar to the proof of Theorem 4.1.

THEOREM 5.1. *Let ω_n be defined by (5.1). Then for $n \geq 2$, (1) $\omega_n \in \Omega$, and ω_n is an $(n - 1)$ -point iteration, (2) $p(\omega_n) = 2^{n-1}$, (3) $v_0(\omega_n) = n - 1$, $v_1(\omega_n) = 1$, $v_i(\omega_n) = 0$, $i > 1$. Hence $v(\omega_n) = n$.*

It is straightforward to show that

$$S(\psi_n, f)/S(\omega_n, f) = [1 + \beta f'(\alpha)]^{2^{n-2}}. \tag{5.3}$$

If ψ_n is used, β should be chosen if possible so that $1 + \beta f'(\alpha)$ is small.

The iteration ω_3 uses two evaluations of f and one of f' and $p(\omega_3) = 4$. Another iteration with these properties is defined by Ostrowski [8, App. G] and a geometrical interpretation is given by Traub [10, Sec. 8.5]. King [3] gives a family of fourth-order methods based on two evaluations of f and one of f' . Jarratt [2] constructs a fourth-order iteration based on one evaluation of f and two of f' . The iteration ω_n uses $n - 1$ evaluations of f and one of f' and $p(\omega_n) = 2^{n-1}$. For $n > 3$, no iterations with these properties were previously known.

6. The Optimal Order of One-Point Iterations

By imposing a mild smoothness condition we can prove that one-point iterations of order n require the evaluation of f and at least its first $n - 1$ derivatives. No such requirement holds for multipoint iterations. For example, the multipoint iteration ψ_n defined in Section 4 has order 2^{n-1} but requires no derivative evaluation.

Let ϕ be a one-point iteration. Then from (2.1) and (2.2),

$$\phi(f)(x) = u_1(x, f(x), \dots, f^{(d_0)}(x)),$$

where $u_1(y_0, y_1^0, \dots, y_{d_0+1}^0)$ is a multivariate function of $d_0 + 2$ variables. In this section we drop the superscript on y_j .

The following theorem was first given by Traub [9; 10, Sec. 5.4]. We regard the proof given here as an improvement of Traub's proof.

THEOREM 6.1. *Let ϕ be a one-point iteration of order $p(\phi)$ and let $u_1(y_0, y_1, \dots, y_{d_0+1})$ be analytic with respect to y_1 at $y_1 = 0$. Then $v_i(\phi) \geq 1$, $i = 0, \dots, p(\phi) - 1$, and hence $p(\phi) \leq v(\phi)$.*

PROOF. For $f \in D$, define

$$T(f)(x) = [\gamma_p(f)(x) - \phi(f)(x)]/f^p(x), \tag{6.1}$$

where γ_p is a member of the family of iterations defined in Section 3. To simplify notation, we write f for $f(x)$.

Define σ_i by $\gamma_p = \sum_{i=0}^{p-1} \sigma_i f^i$ where σ_i depends explicitly on $f'(x), \dots, f^{(i)}(x)$ [10, Sec. 5.1]. By the analyticity condition on ϕ , $\phi = \sum_{i=0}^{\infty} \lambda_i f^i$. Therefore from (6.1),

$$T = \sum_{i=0}^{p-1} (\sigma_i - \lambda_i) f^{i-p} - \sum_{i=p}^{\infty} \lambda_i f^{i-p}. \tag{6.2}$$

Since ϕ and γ_p are of order p , (6.1) implies that

$$\lim_{x \rightarrow \alpha_f} T(f)(x) = [S(\gamma_p, f) - S(\phi, f)]/[f'(\alpha_f)]^p < \infty$$

for all $f \in D$. Hence it follows from (6.2) that

$$\sigma_i = \lambda_i, i = 0, \dots, p - 1, \forall f \in D. \tag{6.3}$$

Consider $\sigma_{p-1} = \lambda_{p-1}$. We know that σ_{p-1} depends explicitly on $f'(x), \dots, f^{(p-1)}(x)$ and that the same must be true for λ_{p-1} . Assume $v_j(\phi) = 0$, for some j , $0 < j \leq p - 1$. Then $u_1(y_0, y_1, \dots, y_{d_0+1})$ does not depend on y_{j+1} . This implies that $(\partial^{p-1}/\partial y_1^{p-1}) u_1(y_0, y_1, \dots, y_{d_0+1})$ is independent of y_{j+1} and that $(\partial^{p-1}/\partial y_1^{p-1}) u_1(x, 0, f'(x), \dots,$

$f^{(d_0)}(x)$ is independent of $f^{(j)}(x)$. Hence

$$\lambda_{p-1} = (1/(p - 1)!) (\partial^{p-1}/\partial y_1^{p-1}) u(x, 0, f'(x), \dots, f^{(d_0)}(x))$$

is independent of $f^{(j)}(x)$, which is a contradiction. Therefore $v_i(\phi) \geq 1, i = 1, \dots, p - 1$.

Next we show $v_0(\phi) \geq 1$. Suppose this is false. Then $\lambda_i = 0, i > 0$ and from (6.3), $\sigma_i = 0, i = 1, \dots, p - 1$, which is a contradiction. Q.E.D.

COROLLARY 6.1. *Let γ_n be defined by (3.1). Then γ_n achieves the optimal order of any one-point iteration ϕ for which $v(\phi) = n$ and which satisfies the analyticity condition of the theorem.*

Remark. The analyticity condition is not restrictive. For example, it includes all rational iterations and all iterations defined by simple zeros of polynomials with analytic coefficients.

7. Two Optimal Order Theorems for Multipoint Iterations

We prove an optimal order theorem for one important class of iterations and prove a fairly tight upper bound for the maximal order of a second class of iterations.

Our first class consists of all iterations such that for $j = 0, \dots, k - 1, z_{j+1}$ appearing in (2.2) is given by a Hermite interpolatory iteration based on the points z_0, \dots, z_j . If ϕ belongs to this class, we say it is a *Hermite interpolatory k -point iteration*. The order of ϕ may be computed as follows. From Traub [10, Sec. 4.2],

$$z_{j+1} - \alpha = 0[(z_j - \alpha)^{d_j+1} \dots (z_0 - \alpha)^{d_0+1}]$$

where the d_i are as in (2.2). Hence

$$\phi(f)(x) - \alpha = z_k - \alpha = 0[(x - \alpha)^p],$$

where $p(\phi) = (d_0 + 1) \prod_{j=1}^{k-1} (d_j + 2)$. It is easily verified that

$$v(\phi) = \sum_{j=0}^{k-1} (d_j + 1).$$

We wish to choose k, d_0, \dots, d_{k-1} such that for $v(\phi)$ fixed, $p(\phi)$ is maximized. The choice of k and the d_i are given by

THEOREM 7.1. *Let $d_j \geq 0, k \geq 1$ be integers. Let $v(\phi) = \sum_{j=0}^{k-1} (d_j + 1) = n$ be fixed. Then $p(\phi) = (d_0 + 1) \prod_{j=1}^{k-1} (d_j + 2)$ is maximized exactly when*

$$k = n, \quad d_j = 0, \quad j = 0, \dots, n - 1 \tag{7.1}$$

or

$$k = n - 1, \quad d_0 = 1, \quad d_j = 0, \quad j = 1, \dots, n - 2. \tag{7.2}$$

PROOF. Since $d_j + 1 \leq n, k \leq n$, there are only finitely many cases and the maximum exists. Let the maximum of p be achieved at $\bar{d}_j, j = 0, \dots, \bar{k} - 1$. We show first that $\bar{d}_j = 0, j = 1, \dots, \bar{k} - 1$. Assume that $\bar{d}_r = m, m \geq 1$, for some $r, r = 1, \dots, \bar{k} - 1$. Define $\tilde{d}_j, j = 0, \dots, \bar{k} + m - 1$ as

$$\tilde{d}_j = \bar{d}_j, \quad j = 0, \dots, \bar{k} - 1, \quad j \neq r, \quad \tilde{d}_r = 0, \quad \tilde{d}_j = 0, \quad j = \bar{k}, \dots, \bar{k} + m - 1.$$

Then we can verify that

$$\sum_{j=0}^{\bar{k}+m-1} (\tilde{d}_j + 1) = \sum_{j=0}^{\bar{k}-1} (d_j + 1) = n$$

and

$$(\tilde{d}_0 + 1) \prod_{j=1}^{\bar{k}+m-1} (\tilde{d}_j + 2) > (\bar{d}_0 + 1) \prod_{j=1}^{\bar{k}-1} (\bar{d}_j + 2).$$

This contradiction proves that $\bar{d}_j = 0, j = 1, \dots, \bar{k} - 1$. A similar argument may be used to prove $\bar{d}_0 \leq 1$. If $\bar{d}_0 = 0, \bar{k} = n$ while if $\bar{d}_0 = 1, \bar{k} = n - 1$, which completes the proof. Q.E.D.

COROLLARY 7.1. *Let ϕ be a Hermite interpolatory iteration with $v(\phi) = n$. Then $p(\phi) \leq 2^{n-1}$.*

Note that ψ_n , defined in Section 4, is an instance of (7.1) while ω_n , defined in Section 5, is an instance of (7.2). (Both $\{\psi_n\}$ and $\{\omega_n\}$ are based on inverse interpolation. There are two other families of iterations based on direct interpolation.) Thus we have

COROLLARY 7.2. *Let ψ_n and ω_n be defined by (4.1) and (5.1), respectively. Then ψ_n and ω_n have optimal order for Hermite interpolatory iteration with n evaluations.*

The second theorem of this section gives an upper bound on the order achievable for any multipoint iteration using values of f only (and no derivatives).

THEOREM 7.2. *Let ϕ be a multipoint iteration with $v_0(\phi) = n$, $v_i(\phi) = 0$, $i > 0$. Then $p(\phi) \leq 2^n$.*

PROOF. For $f \in D$, let x_0 be a starting point such that if $x_{i+1} = \phi(f)(x_i)$ then $\lim_{i \rightarrow \infty} x_i = \alpha_f$. From (2.2), for each i , denote $z_{in} = x_i$ and $z_{in+j+1} = u_{j+1}(z_{in}, f(z_{in}), \dots, f(z_{in+j}))$ for $j = 0, \dots, n - 1$. Then

$$\lim_{i \rightarrow \infty} (z_{(i+1)n} - \alpha) / (z_{in} - \alpha)^p = S(\phi, f). \tag{7.3}$$

Hence

$$\lim_{i \rightarrow \infty} (-\log |z_{in} - \alpha|^{1/i}) = p. \tag{7.4}$$

Brent, Winograd, and Wolfe [1, (6.1)] show that there exist an $f \in D$ and a sequence $\{z_i\}$ such that

$$\overline{\lim}_{i \rightarrow \infty} (-\log |z_i - \alpha|)^{1/i} \leq 2. \tag{7.5}$$

By (7.4) and (7.5) it follows that $p \leq 2^n$. Q.E.D.

In Section 4, we constructed an iteration ψ_n such that $v_0(\psi_n) = n$, $v_i(\psi_n) = 0$, $i > 0$ and $p(\psi_n) = 2^{n-1}$. Hence the upper bound of Theorem 7.2 is within a factor of two of the order of that iteration. We conjecture in the next section that $p = 2^{n-1}$ is optimal.

8. A Conjecture

CONJECTURE 8.1. *Let ϕ be an iteration (with no memory) with $v(\phi) = n$. Then*

$$p(\phi) \leq 2^{n-1}. \tag{8.1}$$

This extends a conjecture of Traub [11] which states (8.1) for $n = 2, 3$.¹

9. Numerical Example

Let $f(x) = x^3 + \ln(1 + x)$ where \ln denotes the logarithm to the natural base. Hence $\alpha = 0$. Starting at $x_0 = 10^{-1}$ and 10^{-2} , we compute x_1 by iterations ψ_n and ω_n , $n = 3, 4, 5$. For comparison we also use as many steps of the Newton-Raphson iteration as necessary to bring the error to about 10^{-16} . Calculations were done in double precision arithmetic on a DEC PDP-10 computer. About 16 digits are available in double precision.

Results are summarized in Examples 1-3. The parameter β that appears in ψ_n was chosen $\beta = -.2$ which makes the asymptotic error constant of ψ_n for this problem near unity. The asymptotic error constants of ω_n , $n = 3, 4, 5$, and the Newton-Raphson iteration are also near unity for this problem. Recall that $p(\psi_n) = p(\omega_n) = 2^{n-1}$ and that for Newton-Raphson iteration, $p = 2$. We expect $x_1 \doteq x_0^p$ to hold and this is numerically verified in the examples. From (5.3), we expect

$$\psi_n(x_0) / \omega_n(x_0) \doteq (.8)^{2^{n-2}}, \tag{9.1}$$

and (9.1) is numerically verified in the examples for $x_0 = 10^{-2}$.

The examples illustrate the advantage of ψ_n and ω_n over the repeated use of Newton-Raphson iteration. Starting with $x_0 = 10^{-1}$, $\omega_5(x_0)$ calculates the zero to "full accuracy"

¹ Note added in proof. Kung and Traub [6] have established this conjecture for $n = 2$.

at a cost of four evaluations of f and one of f' . Four Newton-Raphson iterations are required with a cost of four evaluations of f and four of f' . The difference is significant when the evaluation of f' is expensive. This observation takes only the cost of f' into account. A more complete analysis based on efficiency measure considerations is given by Kung and Traub [5].

Example 1.

x_0	10^{-1}	10^{-2}
$x_1 = \psi_3(x_0)$	$.21 \times 10^{-4}$	$.27 \times 10^{-8}$
$x_1 = \psi_4(x_0)$	$-.80 \times 10^{-9}$	$-.47 \times 10^{-16}$
$x_1 = \psi_5(x_0)$	$-.27 \times 10^{-16}$	

Example 2.

x_0	10^{-1}	10^{-2}
$x_1 = \omega_3(x_0)$	$.30 \times 10^{-4}$	$.42 \times 10^{-8}$
$x_1 = \omega_4(x_0)$	$-.15 \times 10^{-8}$	$-.12 \times 10^{-16}$
$x_1 = \omega_5(x_0)$	$-.24 \times 10^{-16}$	

Example 3. Let $x_{i+1} = \phi(x_i)$, where ϕ denotes Newton-Raphson iteration.

x_0	10^{-1}	10^{-2}
x_1	$-.26 \times 10^{-2}$	$-.48 \times 10^{-4}$
x_2	$-.33 \times 10^{-6}$	$-.11 \times 10^{-8}$
x_3	$-.54 \times 10^{-11}$	$.46 \times 10^{-17}$
x_4	$-.31 \times 10^{-16}$	

Appendix

Program 1 and Program 2, which are adapted from a result of Krogh [4], compute $\psi_n(f)(x)$ (with the parameter β) and $\omega_n(f)(x)$ for $n \geq 4$.

Program 1

begin

comment This program computes $\psi_n(f)(x)$ (with parameter β) for a given function f and a given value x ;

integer i, k, n ; **real** x, h, r, psi ;

real array $v[0 : n - 1, 0 : n - 1], \text{pi}[0 : n - 1]$;

$v[0, 0] := x$;

$h := \beta \times f(x)$;

$v[0, 1] := v[0, 0] + h$;

$v[1, 1] := h / (f(v[0, 1]) - f(v[0, 0]))$;

$r := v[1, 1] \times f(v[0, 0])$;

$v[0, 2] := v[0, 0] - r$;

$v[1, 2] := r / (f(v[0, 0]) - f(v[0, 2]))$;

$\text{pi}[2] := f(v[0, 0]) \times f(v[0, 1])$;

$v[2, 2] := (v[1, 1] - v[1, 2]) / (f(v[0, 1]) - f(v[0, 2]))$;

$\text{psi} := v[0, 2] + \text{pi}[2] \times v[2, 2]$;

for $k := 3$ **step 1 until** $n - 1$ **do**

begin

$v[0, k] := \text{psi}$;

for $i := 0$ **step 1 until** $k - 1$ **do**

begin

$v[i + 1, k] := (v[i, i] - v[i, k]) / (f(v[0, i]) - f(v[0, k]))$;

end;

$\text{pi}[k] := -f(v[0, k - 1]) \times \text{pi}[k - 1]$;

$\text{psi} := \text{psi} + \text{pi}[k] \times v[k, k]$;

end;

end;

Program 2

```

begin
  comment This program computes  $\omega_n(f)(x)$  for a given function  $f$  and a given value  $x$ ;
  comment  $f'$  is denoted by  $fp$ ;
  integer  $i, k, n$ ; real  $x, n11, \text{omega}, d$ ;
  real array  $v[0 : n - 1, 0 : n - 1], \text{pi}[0 : n - 1]$ ;
   $v[0, 0] := x$ ;
   $v[0, 1] := x$ ;
   $n11 := f(v[0, 0])/fp(v[0, 0])$ ;
   $v[0, 2] := v[0, 0] - n11$ ;
   $d := f(v[0, 0]) - f(v[0, 2])$ ;
   $v[1, 2] := n11/d$ ;
   $v[2, 2] := v[1, 2] \times f(v[0, 2])/d$ ;
   $\text{omega} := v[0, 2] - f(v[0, 0]) \times v[2, 2]$ ;
   $v[1, 1] := n11/f(v[0, 0])$ ;
   $v[2, 2] := -v[2, 2]/f(v[0, 0])$ ;
   $\text{pi}[2] := f(v[0, 0]) \times f(v[0, 0])$ ;
  for  $k := 3$  step 1 until  $n - 1$  do
    begin
       $v[0, k] := \text{omega}$ ;
      for  $i := 0$  step 1 until  $k - 1$  do
        begin
           $v[i + 1, k] := (v[i, i] - v[i, k])/(f(v[0, i]) - f(v[0, k]))$ ;
        end;
         $\text{pi}[k] := -f(v[0, k - 1]) \times \text{pi}[k - 1]$ ;
         $\text{omega} := \text{omega} + \text{pi}[k] \times v[k, k]$ ;
      end;
    end;
  end;

```

REFERENCES

1. BRENT, R., WINOGRAD, S., AND WOLFE, P. Optimal iterative processes for root-finding. *Numer. Math.* 20 (1973), 327-341.
2. JARRATT, P. Some efficient fourth order multipoint methods for solving equations. *BIT* 9 (1969), 119-124.
3. KING, R. R. A family of fourth-order methods for nonlinear equations. *SIAM J. Numer. Anal.* 10 (1973), 876-879.
4. KROGH, F. T. Efficient algorithms for polynomial interpolation and numerical differentiation. *Math. Comp.* 24 (1970), 185-190.
5. KUNG, H. T., AND TRAUB, J. F. Computational complexity of one-point and multipoint iteration. Report, Computer Sci. Dep., Carnegie-Mellon U., Pittsburgh, Pa. To appear in *Complexity of Real Computation*, R. Karp, Ed., American Mathematical Society, Providence, R. I.
6. KUNG, H. T., AND TRAUB, J. F. Optimal order for iterations using two evaluations. Report, Computer Sci. Dep., Carnegie-Mellon U., Pittsburgh, Pa., 1973. To appear in *SIAM J. Numer. Anal.*
7. ORTEGA, J. M., AND RHEINBOLDT, W. C. *Iterative Solution of Nonlinear Equations in Several Variables*. Academic Press, New York, 1970.
8. OSTROWSKI, A. M. *Solution of Equations and Systems of Equations*, 2nd ed. Academic Press, New York, 1966.
9. TRAUB, J. F. On functional iteration and the calculation of roots. Proc. 16th Nat. ACM Conf., 5A-1 (1961), pp. 1-4.
10. TRAUB, J. F. *Iterative Methods for the Solution of Equations*. Prentice-Hall, Englewood Cliffs, N. J., 1964.
11. TRAUB, J. F. Computational complexity of iterative processes. *SIAM J. Comput.* 1 (1972), 167-179.

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