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OPTIMAL ORDER AND EFFICIENCY FOR ITERATIONS  
WITH TWO EVALUATIONS

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### ABSTRACT

The problem is to calculate a simple zero of a non-linear function  $f$ . We consider rational iterations without memory which use two evaluations of  $f$  or its derivatives. It is shown that the optimal order is 2. This settles a conjecture of Kung and Traub that an iteration using  $n$  evaluations without memory is of order at most  $2^{n-1}$ , for the case  $n = 2$ .

Furthermore we show that any rational two-evaluation iteration of optimal order must use either two evaluations of  $f$  or one evaluation of  $f$  and one of  $f'$ . From this result we completely settle the question of the optimal efficiency, in our efficiency measure, for any two-evaluation iteration without memory. Depending on the relative cost of evaluating  $f$  and  $f'$ , the optimal efficiency is achieved by either Newton iteration or the iteration  $\psi$  defined by

$$\psi(f)(x) = x - \frac{f^2(x)}{f(x+f(x)) - f(x)} .$$

## 1. INTRODUCTION

We deal with optimal iteration for calculating a simple zero of a scalar function  $f$  of one variable, which is a prototypical problem of analytic computational complexity (Traub [72]). Early work on this problem appears in Traub [61,64] while recent results are due to Brent, Winograd and Wolfe [73], Hindmarsh [72], Kung and Traub [73a,73b], Rissanen [71] and Wozniakowski [73]. Surveys of recent advances are given by Traub [73a,73b]. In this paper we consider only iterations without memory.

Kung and Traub [73b] observe that a reasonable efficiency measure of an iteration  $\varphi$  with respect to  $f$  should be defined as

$$(1.1) \quad e(\varphi, f) = \frac{\log_2 p(\varphi)}{v(\varphi, f) + a(\varphi)}$$

where  $p(\varphi)$  is the order of convergence of  $\varphi$ ,  $v(\varphi, f)$  is the evaluation cost and  $a(\varphi)$  is the combinatory cost. For a given  $f$  we are interested in finding an upper bound on  $e(\varphi, f)$  and hopefully obtaining an iteration which attains this upper bound. To bound  $e(\varphi, f)$  we must know the dependence of  $p(\varphi)$ ,  $v(\varphi, f)$ , and  $a(\varphi)$  on  $n$ , the number of evaluations.

Let  $P_n$  denote the maximal order achievable by an iteration using  $n$  evaluations. Kung and Traub [73a] conjecture that, for iterations without memory,

$$(1.2) \quad P_n \leq 2^{n-1}, \quad n = 1, 2, \dots$$

In this paper we study rational two-evaluation iterations without memory. We settle the conjecture for  $n = 2$ . We could define and analyze rational one-evaluation iterations without memory and prove the conjecture for  $n = 1$ . Since the proof follows from straightforward modifications of our theorems, we shall

only indicate these modifications in passing. (This is done after Theorem 4.2.) However, the techniques we use here are suitable for small values of  $n$  only. It seems to us that the proof of the conjecture for general  $n$  will require the development of new techniques.

Furthermore, we show (Theorem 4.1) that for any rational two-evaluation iteration  $\varphi(f)(x)$  one of the two evaluations must be of  $f$  at the point  $x$ . A straightforward modification of this theorem proves that any "locally" convergent iteration requires the evaluation of  $f$  at  $x$ . In Theorem 4.3 we show that the second evaluation of a rational two-evaluation iteration of order  $\geq 2$  must be of either  $f$  or  $f'$  at  $x + O(f(x))$ .

Let  $E_2(f)$  denote the optimal efficiency achievable by a rational two-evaluation iteration without memory. We show that in our efficiency measure, given by (1.1),

$$E_2(f) = \max\left(\frac{1}{c(f)+c(f')+2}, \frac{1}{2c(f)+5}\right).$$

Depending on the relative cost of evaluating  $f$  or  $f'$ , this upper bound is achieved by either Newton iteration

$$(1.3) \quad \gamma(f)(x) = x - \frac{f(x)}{f'(x)}$$

or the iteration  $\psi$ ,

$$(1.4) \quad \psi(f)(x) = x - \frac{f^2(x)}{f(x+f(x)) - f(x)}.$$

The iteration  $\psi$  is derived by Traub [64, Section 8-4]. It may also be derived as a special case of Steffensen iteration [33].

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Basic concepts are introduced in Section 2. In Section 3 we outline the proof of optimal order for  $n = 2$ , with the details given in the following section. Optimal efficiency is studied in the final section.

## 2. BASIC CONCEPTS

Let  $D = \{f \mid f \text{ is a real analytic function defined in an open interval } I_f \subset \mathbb{R} \text{ (the set of real numbers) which contains a simple zero } \alpha_f \text{ of } f \text{ and } f' \text{ does not vanish on } I_f.\}$

Let  $\varphi$  be a function which maps every  $f \in D$  to  $\varphi(f)$  with the following properties:

1.  $\varphi(f)$  is a function mapping  $I_{\varphi, f} \subset I_f$  into  $I_{\varphi, f}$  for some open subinterval  $I_{\varphi, f}$  containing  $\alpha_f$ .
2.  $\varphi(f)(\alpha_f) = \alpha_f$ .
3. There exists an open subinterval  $I_{\varphi, f}^0 \subset I_{\varphi, f}$  containing  $\alpha_f$  such that if  $x_{i+1} = \varphi(f)(x_i)$  then  $\lim_{i \rightarrow \infty} x_i = \alpha_f$  whenever  $x_0 \in I_{\varphi, f}^0$ .
4. There exist functions  $U_0, U_1, U_2$  and non-negative integers  $h, k$  such that

(i)  $U_0: \mathbb{R} \rightarrow \mathbb{R}$  is a rational function,

(ii)  $U_1: \mathbb{R}^2 \rightarrow \mathbb{R}$  is defined formally by

$$(2.1) \quad U_1(x, y) = \sum_0^{\ell} a_i(x) y^i$$

where  $a_i: \mathbb{R} \rightarrow \mathbb{R}$  is a rational function and  $a_i$  is not identically equal to zero for some  $i > 0$ ,

(iii)  $U_2: \mathbb{R}^3 \rightarrow \mathbb{R}$  is defined formally by

$$(2.2) \quad U_2(x, y, z) = x + \frac{\sum_0^m b_{i,j}(x) y^i z^j}{\sum_0^n c_{i,j}(x) y^i z^j}$$

where  $b_{i,j}, c_{i,j}: R \rightarrow R$  are rational functions and either  $b_{i,j}$  or  $c_{i,j}$  is not identically equal to zero for some  $(i,j)$  with  $j > 0$ ,

(iv) for all  $f \in D$ ,

$$(2.3) \quad \varphi(f)(x) = U_2(x, f^{(h)}(z_0), f^{(k)}(z_1)),$$

where

$$(2.4) \quad z_0 = U_0(x),$$

$$(2.5) \quad z_1 = U_1(x, f^{(h)}(z_0)).$$

We say  $\varphi$  is a rational two-evaluation iteration without memory, and let  $\Omega_2$  denote the set of all such  $\varphi$ 's.

For  $\varphi \in \Omega_2$  it can be shown (Theorem 4.1) that  $U_0(x) \equiv x$  and  $h = 0$ .

Hence by (2.3) and (2.4),

$$(2.6) \quad \varphi(f)(x) = x + \frac{\sum_0^m b_{i,j}(x) f^i(x) (f^{(k)}(z_1))^j}{\sum_0^n c_{i,j}(x) f^i(x) (f^{(k)}(z_1))^j}.$$

By (2.1) and (2.5),

$$(2.7) \quad f^{(k)}(z_1) = f^{(k)}(x) + f^{(k+1)}(x) \left( \sum_0^{\ell} a_i f^i(x) - x \right) + \frac{1}{2} f^{(k+1)}(x) \left( \sum_0^{\ell} a_i f^i(x) - x \right)^2 + \dots$$

Substituting the righthand side of (2.7) for  $f^{(k)}(z_1)$  in (2.6) we can express  $\varphi(f)(x)$  formally in terms of  $x, f(x), f^{(k)}(x), f^{(k+1)}(x), \dots$ .

Hence we can define functions  $\lambda_i: R \rightarrow R$  such that



$$(2.8) \quad \varphi(f)(x) = \sum_{-\infty}^{\infty} \lambda_i(x) f^i(x)$$

where  $\lambda_i(x)$  depend explicitly on  $x$ ,  $f^{(k)}(x)$ ,  $f^{(k+1)}(x), \dots$ , but not on  $f(x)$ .

It is often desirable to express  $\varphi(f)(x)$  by (2.8). We call the righthand side of (2.8) the canonical form of  $\varphi(f)(x)$ .

By the Taylor series expansion of  $\varphi(f)(x)$  at  $\alpha_f$  we can easily show that there exists a non-negative integer  $p(\varphi)$  such that for any  $f \in D$ ,

$$\lim_{x \rightarrow \alpha_f} \frac{\varphi(f)(x) - \alpha_f}{(x - \alpha_f)^{p(\varphi)}} = S(\varphi, f)$$

exists for a constant  $S(\varphi, f)$  and  $S(\varphi, f) \neq 0$  for at least one  $f \in D$ . We define  $p(\varphi)$  as the order of convergence (order) of  $\varphi$ .

We assume that one arithmetic operation takes one unit time. Let  $c(f^{(i)})$  denote the time needed to evaluate  $f^{(i)}$ ,  $i = h, k$ . Let  $a(\varphi)$  denote the time to compute  $\varphi(f)(x)$  from  $x$  not counting the time to evaluate  $f^{(h)}$  and  $f^{(k)}$ . We define the efficiency of  $\varphi \in \Omega_2$  with respect to  $f \in D$  as

$$e(\varphi, f) = \frac{\log_2 p(\varphi)}{c(f^{(h)}) + c(f^{(k)}) + a(\varphi)} .$$

(See Kung and Traub [73b].)

We could easily define iteration without memory in a more general setting and some of our theorems would still hold. We have chosen here to limit our scope because we wish to focus on optimal efficiency. This is settled by Theorem 5.1 where the hypothesis of rational two-evaluation iteration is crucial. Furthermore, we wish to avoid complicating the proofs. Specifically, Theorem 4.1 holds for iterations satisfying properties 2 and 3. Theorem 4.2

can be proven for analytic iterations. (See Traub [64, Section 5.1] and Kung and Traub [73a, Theorem 6.1].) Furthermore, Theorem 4.4 can be proven for analytic two-evaluation iterations if infinite series are used in (2.1) and (2.2).

### 3. OUTLINE OF THE PROOF OF OPTIMAL ORDER

Since the proofs of the following section are rather detailed, we summarize the ideas and results here.

In our definition of rational two-evaluation iteration without memory,  $\varphi(f)(x)$ , we permit any two evaluations of  $f$  or its derivatives at any two points. In Theorems 4.1 and 4.3 we cut down the "search space" of evaluations. In Theorem 4.1 we show that one of the evaluations must be of  $f$  itself at the point  $x$ . In Theorem 4.3 we show that the second evaluation of a rational two-evaluation iteration of order  $\geq 2$  must be of either  $f$  or  $f'$  at the point  $x + O(f(x))$ . Thus the only rational two-evaluation iterations of order  $\geq 2$  are those using either

- (i) two evaluations of  $f$ , or
- (ii) one evaluation of  $f$  and one of  $f'$ .

In Theorem 4.2 we study the functions  $\lambda_i(x)$  occurring in the canonical form of the iteration  $\varphi$ ,

$$\varphi(f)(x) = \sum_{i=-\infty}^{\infty} \lambda_i(x) f^i(x).$$

It is easy to check that the iterations  $\gamma$  and  $\psi$ , defined by (1.3) and (1.4) respectively, both have order 2 and canonical form

$$(3.1) \quad x - \frac{1}{f'(x)} f(x) + O(f^2(x)),$$

In Theorem 4.2 we show that any iteration with order  $\geq 2$  has canonical form of the type given in (3.1) and that any iteration of order  $\geq 3$  has canonical form of type given by

$$(3.2) \quad x - \frac{1}{f'(x)} f(x) - \frac{f''(x)}{2(f'(x))^3} f^2(x) + O(f^3(x)).$$

(The formulas for  $\lambda_1(x)$  for iterations of arbitrary order were established by Traub [64, Section 5.1] in a somewhat different setting. See also Kung and Traub [73a, Theorem 6.1].)

The main result on optimal order is given in Theorem 4.4 which states that a rational two-evaluation iteration without memory has order at most two. The proof uses a "comparison series" technique first exploited by Traub [61], [64, especially Theorems 5.2, 5.3 and Chapter 9] and also by Kung and Traub [73a, Theorem 6.1]. We compare the canonical form of a rational two-evaluation iteration with the canonical form given by (3.2) and show these forms must be different. Hence the order is less than 3 and since order is an integer in our setting, this implies the order is at most 2.

4. OPTIMAL ORDER

Theorem 4.1

If  $\varphi \in \Omega_2$  then  $U_0$  is an identity function and  $h = 0$ .

Remark. Although in Section 2 it was assumed that  $U_0$  is rational, the proof of this theorem requires only that  $U_0$  be continuous.

Proof

Let  $\varphi \in \Omega_2$ ,  $f \in D$  and  $x \in I_{\varphi, f}^0$ . Define

$$(4.1) \quad \begin{cases} z_0(x) = U_0(x), \\ y_0^h(x) = f^{(h)}(z_0(x)), \\ z_1(x) = U_1(x, y_0^h), \\ y_1^k(x) = f^{(k)}(z_1(x)). \end{cases}$$

Then by (2.3),

$$\varphi(f)(x) = U_2(x, y_0^h(x), y_1^k(x)).$$

Therefore

$$(4.2) \quad \alpha_f = \varphi(f)(\alpha_f) = U_2(\alpha_f, y_0^h(\alpha_f), y_1^k(\alpha_f)).$$

Suppose that  $U_0(x) \neq x$ . Then there exists  $w_0 \in R$  such that  $U_0(w_0) \neq w_0$ . By the continuity of  $U_0$ , there exists an open interval  $I_0$  containing  $w_0$  such that  $U_0(w) \neq w$  for all  $w \in I_0$ . Choose  $f \in D$  such that  $\alpha_f = w_0$ . We shall show that

$$\varphi(f)(w) = w$$

for all  $w \in I_0 \cap I_{\varphi, f}^0$ ,  $w \neq w_0$ . Define  $z_0(w)$ ,  $y_0^h(w)$ ,  $z_1(w)$  and  $y_1^k(w)$  by setting  $x = w$  in (4.1). Then by (2.3),

$$(4.4) \quad \varphi(f)(w) = U_2(w, y_0^h(w), y_1^k(w)).$$

Since  $z_0(w) = U_0(w) \neq w$  and it is without loss of generality in assuming  $w \neq z_1(w)$ , there exists a polynomial  $q$  such that

$$\begin{cases} q(w) = 0, \\ q'(w) = 1, \\ q^{(h)}(z_0(w)) = y_0^h(w), \\ q^{(k)}(z_1(w)) = y_1^k(w). \end{cases}$$

Obviously,  $q \in D$  and  $\alpha_q = w$ . By (4.2) with  $f$  replaced by  $q$ ,

$$(4.5) \quad w = U_2(w, y_0^h(w), y_1^k(w)).$$

Equations (4.4) and (4.5) imply that  $\varphi(f)(w) = w$  for all  $w \in I_0 \cap I_{\varphi, f}^0$ .

This is a contradiction since for any  $x_0 \in I_{\varphi, f}^0$  such that  $x_0 \neq \alpha_f$ ,  $\varphi(f)(x_0) = x_0$ , which does not converge to  $\alpha_f$ .

Next, we shall show that  $h = 0$ . Suppose that  $h \geq 1$ . Consider any  $f \in D$  and any  $w \in I_{\varphi, f}^0$ . Then if  $h = 1$  we define a polynomial  $q$  such that

$$\begin{aligned} q(w) &= 0, \\ q^{(h)}(w) &= f^{(h)}(w), \\ q^{(k)}(z_1(w)) &= f^{(k)}(z_1(w)), \end{aligned}$$

and if  $h > 1$  we define  $q$  such that

$$\begin{aligned} q(w) &= 0, \\ q'(w) &= 1, \\ q^{(h)}(w) &= f^{(h)}(w), \\ q^{(k)}(z_1(w)) &= f^{(k)}(z_1(w)). \end{aligned}$$

Clearly, in either case,  $q \in D$  and  $\alpha_q = w$ . Therefore we can again show that  $\varphi(f)(w) = w$  for all  $w \in I_{\varphi, f}^0$ . This is a contradiction. ■

To simplify notation, in the rest of the paper we shall often write  $f^{(i)}$ ,  $\lambda_i$ ,  $a_i$ ,  $b_{i,j}$ ,  $c_{i,j}$  for  $f^{(i)}(x)$ ,  $\lambda_i(x)$ ,  $a_i(x)$ ,  $b_{i,j}(x)$ ,  $c_{i,j}(x)$ , respectively.

Recall that for  $\varphi \in \Omega_2$  we can express  $\varphi(f)(x)$  by its canonical form, i.e.,

$$(4.6) \quad \varphi(f)(x) = \sum_{-\infty}^{\infty} \lambda_i(x) f^i(x).$$

Theorem 4.2

1. If  $p(\varphi) \geq 2$  then  $\lambda_i = 0$  for  $i < 0$ ,

$$\lambda_0 = x \text{ and } \lambda_1 = -\frac{1}{f'}.$$

2. If  $p(\varphi) \geq 3$  then  $\lambda_i = 0$  for  $i < 0$ ,

$$\lambda_0 = x \quad \lambda_1 = -\frac{1}{f'} \quad \text{and} \quad \lambda_2 = -\frac{f''}{2f'^3}.$$

Proof

We shall only prove the second part of the theorem. The first part may be proven analogously.

Define an iteration  $\hat{\varphi}$  such that for any  $f \in D$ ,

$$(4.7) \quad \hat{\varphi}(f)(x) = x - \frac{f}{f'} - \frac{f''}{2f'^3} f^2.$$

It is well known that  $p(\hat{\varphi}) = 3$ . (For example, see Traub [64, Section 5.1].)

Define

$$(4.8) \quad T(f)(x) = \frac{\varphi(f)(x) - \hat{\varphi}(f)(x)}{f^3}.$$

Then by (4.6) and (4.7),

$$(4.9) \quad T(f)(x) = \sum_{-\infty}^{-1} \lambda_i f^{i-3} + (\lambda_0 - x) f^{-3} + (\lambda_1 + \frac{1}{f'}) f^{-2} + (\lambda_2 + \frac{f''}{2f'^3}) f^{-1} + \sum_3^{\infty} \lambda_i f^{i-3}.$$

Suppose that  $p(\varphi) \geq 3$ . Then, since  $p(\hat{\varphi}) = 3$ , (4.8) implies that

$$\lim_{x \rightarrow \alpha_f} T(f)(x) < \infty$$

for all  $f \in D$ . Hence it follows from (4.9) that

$$\lambda_i = 0 \text{ for } i < 0, \lambda_0 = x, \lambda_1 = -\frac{1}{f'}, \text{ and } \lambda_2 = -\frac{f''}{2f'^3}. \quad \blacksquare$$

From Theorems 4.1 and 4.2 we can immediately prove the conjecture (1.2) for  $n = 1$  as follows: Let  $\varphi(f)(x)$  be a rational one-evaluation iteration without memory. Then by a straightforward modification of Theorem 4.1 the evaluation must be of  $f$  at  $x$ . Hence

$$\varphi(f)(x) = H(x, f(x))$$

for some rational function  $H: \mathbb{R}^2 \rightarrow \mathbb{R}$ . It follows that the canonical of  $\varphi$  cannot be given by

$$x - \frac{1}{f'(x)} f(x) + O(f^2(x)).$$

Therefore, by Theorem 4.2,  $p(\varphi) < 2$ . Since  $p(\varphi)$  is an integer, we have  $p(\varphi) \leq 1$ . This proves the conjecture (1.2) for  $n = 1$ .



Theorem 4.3.

Let  $\varphi \in \Omega_2$  and  $p(\varphi) \geq 2$ . Then

1.  $k = 0$  or  $1$ ,
2.  $a_0$  is an identity function.

Proof

1. Suppose that  $k \geq 2$ . Then by (2.7) and (2.8) it is clear that  $\lambda_1(x)$  does not depend on  $f'(x)$  explicitly. Hence by Theorem 4.2,  $p(\varphi) < 2$ . Thus we have shown the first part of the theorem.

2. Assume that  $a_0(x) \neq x$ . Then the set  $\{x | a_0(x) = x\}$  has measure zero.

Note that

$$(4.10) \quad f^{(k)}(z_1) = f^{(k)}(a_0(x)) + f^{(k+1)}(a_0(x))(a_1(x)f(x) + a_2(x)f^2(x) + \dots) + \dots$$

Suppose that  $p(\varphi) \geq 2$ .

Case 1: ( $k = 0$ ).

Since  $\varphi(f)(\alpha_f) = 0$  and  $f(\alpha_f) = 0$ , by (4.10) we have

$$\alpha_f = \alpha_f + \frac{\sum_0^m b_{0,j}(\alpha_f)(a_0(\alpha_f))^j}{\sum_0^m c_{0,j}(\alpha_f)f(a_0(\alpha_f))^j}.$$

Therefore

$$\sum_0^m b_{0,j}(\alpha_f)f(a_0(\alpha_f))^j = 0$$

for all  $f \in D$ . This implies that

$$(4.11) \quad b_{0,j}(x) \equiv 0, \quad j = 0, \dots, m.$$

Let  $r$  be the largest integer such that

$$b_{r,j}(x) \equiv 0, \quad j = 0, \dots, m.$$

Then by (4.11)  $r \geq 0$ . Clearly,  $r < m$ . Note that

$$\sum_0^m b_{i,j}(x) f^i(x) f^j(z_1) = f^{r+1}(x) B(f)(x),$$

where  $B(f)(x) = \sum_{\substack{0 \leq j \leq m \\ 0 \leq i \leq m-r-1}} b_{i+r+1,j}(x) f^i(x) f^j(z_1)$ . By Theorem 4.2, it is clear that

$$\varphi(f)'(\alpha_f) = 0.$$

This implies that

$$(4.12) \quad 1 + \frac{(r+1) f^r(\alpha_f) f'(\alpha_f) B(f)(\alpha_f)}{\sum_0^n c_{0,j}(\alpha_f) f(a_0(\alpha_f))^j} = 0.$$

Hence  $r$  must be equal to 0. Note that

$$B(f)(\alpha_f) = \sum_{0 \leq j \leq n} b_{r+1,j}(\alpha_f) f(a_0(\alpha_f))^j.$$

Therefore (4.12) is reduced to

$$(4.13) \quad \sum_{0 \leq j \leq n} [b_{r+1,j}(\alpha_f) f'(\alpha_f) + c_{0,j}(\alpha_f)] f(a_0(\alpha_f))^j = 0$$

for all  $f \in D$ . Since for any real number  $s$  such that  $s \neq a_0(s)$  and any real numbers  $u, v$  there exists  $f \in D$  such that

$$f(s) = 0, \text{ i.e., } \alpha_f = s,$$

$$f'(s) = u,$$

$$f(a_0(s)) = v,$$

by (4.13),

$$\sum_{0 \leq j \leq n} [b_{r+1,j}(s)u + c_{0,j}(s)]v^j = 0$$

holds for any  $s, u, v$  such that  $s \neq a_0(s)$ . Therefore

$$b_{r+1,j}(x) \equiv c_{0,j}(x) \equiv 0, \quad j = 0, \dots, m.$$

This contradicts the definition of  $r$ .

Case 2: (k = 1)

In this case, we substitute  $f'(a_0(x)) + f''(a_0(x)) (a_1(x)f(x) + a_2(x)f(x)^2 + \dots)$  for  $f'(z_1)$ . Then following the same procedure used in Case 1, we obtain

$$(4.14) \quad \sum_{0 \leq j \leq n} [b_{r+1,j}(\alpha_f) f'(\alpha_f) + c_{0,j}(\alpha_f)] f'(a_0(\alpha_f))^j = 0$$

rather than (4.13) for all  $f \in D$ . By the same reasoning as used before we get a contradiction. ■

The main result on optimal order is given by

Theorem 4.4

If  $\varphi$  is a rational two-evaluation iteration without memory then  $p(\varphi) \leq 2$ .

Proof

Suppose that  $p(\varphi) \geq 3$ . By Theorem 4.3,  $k = 0$  or  $1$  and  $z_1 = x + a_1 f + a_2 f^2 + \dots$ . Hence

$$(4.15) \quad f(z_1) = (1+a_1 f')f + (a_2 f' + \frac{a_1^2}{2} f'')f^2 + \dots,$$

$$(4.16) \quad f'(z_1) = f' + (a_1 f + a_2 f^2 + \dots)f'' + (a_1 f + a_2 f^2 + \dots)^2 \frac{f'''}{2} + \dots$$

$$= f' + a_1 f''f + (a_2 f'' + \frac{a_1}{2} f''')f^2 + \dots$$

Hence if we substitute the righthand sides of (4.15) and (4.16) for  $f(z_1)$  and  $f'(z_1)$ , respectively, then we can define  $v_i$  and  $\mu_i$  as follows:

$$\sum_0^{\infty} v_i f^i = \begin{cases} \sum_0^m b_{i,j} f^i f(z_1)^j & \text{if } k = 0, \\ \sum_0^m b_{i,j} f^i f'(z_1)^j & \text{if } k = 1. \end{cases}$$

and

$$\sum_0^{\infty} \mu_i f^i = \begin{cases} \sum_0^n c_{i,j} f^i f(z_1)^j & \text{if } k = 0, \\ \sum_0^n c_{i,j} f^i f'(z_1)^j & \text{if } k = 1. \end{cases}$$

Then by (2.2),

$$\varphi(f)(x) = x + \frac{\sum_0^{\infty} v_i f^i}{\sum_0^{\infty} \mu_i f^i}.$$

Hence by Theorem 4.2,

$$(4.17) \quad \frac{\sum_0^{\infty} v_i f^i}{\sum_0^{\infty} \mu_i f^i} = -\frac{1}{f'} f - \frac{f''}{2f'^3} f^2 + O(f^3).$$

Suppose that  $\mu_n \neq 0$  and  $\mu_i = 0$  for  $i < n$ . Then by (4.17)

$$(4.18) \quad v_i = 0 \text{ for } i < n+1.$$

$$(4.19) \quad f'v_{n+1} = -\mu_n,$$

$$(4.20) \quad 2f'{}^3v_{n+2} = -\mu_n f'' - 2f'{}^2\mu_{n+1}.$$

Case 1: (k = 0)

It is easy to check that

$$(4.21) \quad \left\{ \begin{array}{l} \mu_0 = c_{0,0}, \\ \mu_1 = c_{1,0} + c_{0,1}(1+a_1f'), \\ \mu_2 = c_{2,0} + c_{1,1}(1+a_1f') + c_{0,2}(1+a_1f')^2 + c_{0,1}(a_2f' + \frac{a_1^2}{2}f''), \\ \mu_3 = c_{3,0} + c_{2,1}(1+a_1f') + c_{1,2}(1+a_1f')^2 + c_{0,3}(1+a_1f')^3 \\ \quad + c_{1,1}(a_2f' + \frac{a_1^2}{2}f'') + 2c_{0,2}(1+a_1f')(a_2f' + \frac{a_1^2}{2}f'') \\ \quad + c_{0,1}(a_3f' + a_1a_2f'' + \frac{a_1^3}{6}f'''), \\ \vdots \end{array} \right.$$

Since  $\mu_n \neq 0$  and  $\mu_i = 0$  for  $i < n$ , by (4.21) one can easily see that

$$(4.22) \quad c_{i,j} = 0 \text{ whenever } i + j < n.$$

Hence,

$$\begin{aligned} \mu_n &= c_{n,0} + c_{n-1,1}(1+a_1f') + \dots + c_{0,n}(1+a_1f')^n, \\ \mu_{n+1} &= c_{n+1,0} + c_{n,1}(1+a_1f') + \dots + c_{0,n+1}(1+a_1f')^{n+1} \\ &\quad + c_{n-1,1}(a_2f' + \frac{a_1^2}{2}f'') + 2c_{n-2,2}(1+a_1f')(a_2f' + \frac{a_1^2}{2}f'') \\ &\quad + \dots + nc_{0,n}(1+a_1f')^{n-1}(a_2f' + \frac{a_1^2}{2}f''). \end{aligned}$$

Similarly, by (4.18), we also have

$$\begin{aligned} v_{n+1} &= b_{n+1,0} + b_{n,1}(1+a_1 f') + \dots + b_{0,n+1}(1+a_1 f')^{n+1}, \\ v_{n+2} &= b_{n+2,0} + b_{n+1,1}(1+a_1 f') + \dots + b_{0,n+2}(1+a_1 f')^{n+2} \\ &\quad + b_{n,1}\left(a_2 f' + \frac{a_1^2}{2} f''\right) + 2b_{n-1,2}(1+a_1 f')\left(a_2 f' + \frac{a_1^2}{2} f''\right) \\ &\quad + \dots + (n+1)b_{0,n+1}(1+a_1 f')^n\left(a_2 f' + \frac{a_1^2}{2} f''\right). \end{aligned}$$

From (4.19),

$$\begin{aligned} (4.23) \quad & b_{n+1,0} f' + b_{n,1}(1+a_1 f') f' + \dots + b_{2,n-1}(1+a_1 f')^{n-1} f' + b_{1,n}(1+a_1 f')^n f' + b_{0,n+1}(1+a_1 f')^{n+1} f' \\ &= -[c_{n,0} + c_{n-1,1}(1+a_1 f') + \dots + c_{0,n}(1+a_1 f')^n]. \end{aligned}$$

By (4.23) it is clear that

$$(4.24) \quad a_1 \neq 0.$$

Also comparing the coefficients of  $f'^{n+2}$ ,  $f'^{n+1}$ ,  $f'^n$  in (4.23), we get

$$(4.25) \quad b_{0,n+1} = b_{1,n} = 0,$$

$$(4.26) \quad b_{2,n-1} = -a_1 c_{0,n}.$$

Comparing the coefficients of  $f''$  in (4.20), we get

$$\begin{aligned} (4.27) \quad & -[b_{n,1} a_1^2 f'^3 + 2b_{n-1,2}(1+a_1 f') a_1^2 f'^3 + \dots + (n-1)b_{2,n-1}(1+a_1 f')^{n-2} a_1^2 f'^3] \\ &= c_{n,0} + c_{n-1,1}(1+a_1 f') + \dots + c_{0,n}(1+a_1 f')^n + c_{n-1,1} a_1^2 f'^2 + 2c_{n-2,2}(1+a_1 f') a_1^2 f'^2 \\ &\quad + \dots + n c_{0,n}(1+a_1 f')^{n-1} a_1^2 f'^2. \end{aligned}$$

Comparing the coefficients of  $f'^{n+1}$  in (4.27) we get

$$(4.28) \quad (n-1)b_{2,n-1} = -nc_{0,n}a_1.$$

(4.24), (4.26) and (4.28) imply that

$$b_{2,n-1} = c_{0,n} = 0.$$

(4.23) and (4.27) are reduced to

$$(4.29) \quad b_{n+1,0}f' + b_{n,1}(1+a_1f')f' + \dots + b_{3,n-2}(1+a_1f')^{n-2}f' \\ = -[c_{n,0} + c_{n-1,1}(1+a_1f') + \dots + c_{1,n-1}(1+a_1f')^{n-1}],$$

and

$$(4.30) \quad -[b_{n,1}a_1^2f'^3 + \dots + (n-2)b_{3,n-2}(1+a_1f')^{n-3}a_1^2f'^3] \\ = c_{n,0} + \dots + c_{0,n-1}(1+a_1f')^{n-1} + c_{n-1,1}a_1^2f'^2 + \dots + (n-1)c_{1,n-1}(1+a_1f')^{n-2}a_1^2f'^2.$$

Comparing the coefficients of  $f'^{n-1}$  and  $f'^n$  in (4.29) and (4.30), respectively, we get

$$(4.31) \quad b_{3,n-2} = -a_1c_{1,n-1}$$

$$(4.32) \quad (n-2)b_{3,n-2} = -(n-1)c_{1,n-1}a_1.$$

(4.24), (4.31) and (4.32) imply that

$$b_{3,n-2} = c_{1,n-1} = 0.$$

By induction we can show that

$$c_{j,n-j} = 0 \text{ for } j = 0, 1, \dots, n.$$

Therefore,  $\mu_n = 0$ . This is a contradiction.

Case 2. (k = 1)

In this case it is easy to check that

$$(4.33) \left\{ \begin{array}{l} \mu_0 = c_{0,0} + c_{0,1}f' + c_{0,2}f'^2 + \dots, \\ \mu_1 = c_{1,0} + c_{1,1}f' + c_{1,2}f'^2 + \dots + c_{0,1}a_1f'' + 2c_{0,2}a_1f'f'' + 3c_{0,3}a_1f'^2f'' + \dots \\ = (c_{1,0} + c_{1,1}f' + c_{1,2}f'^2 + \dots) + a_1f''(c_{0,1} + 2c_{0,2}f' + 3c_{0,3}f'^2 + \dots), \\ \mu_2 = (c_{2,0} + c_{2,1}f' + c_{2,2}f'^2 + \dots) + a_1f''(c_{1,1} + 2c_{1,2}f' + 3c_{1,3}f'^2 + \dots) \\ + (a_2f'' + \frac{a_1}{2}f''') (c_{0,1} + 2c_{0,2}f' + 3c_{0,3}f'^2 + \dots), \\ \vdots \end{array} \right.$$

Since  $\mu_n \neq 0$  and  $\mu_i = 0$  for  $i < n$ , by (4.33) one can easily see that

$$c_{i,j} = 0 \text{ for } i < n, j = 0, 1, \dots$$

Hence

$$\mu_n = c_{n,0} + c_{n,1}f' + c_{n,2}f'^2 + \dots,$$

$$\mu_{n+1} = (c_{n+1,0} + c_{n+1,1}f' + \dots) + a_1f''(c_{n,1} + 2c_{n,2}f' + 3c_{n,3}f'^2 + \dots).$$

Similarly, by (4.18), we also have

$$v_{n+1} = b_{n+1,0} + b_{n+1,1}f' + b_{n+1,2}f'^2 + \dots,$$

$$v_{n+2} = (b_{n+2,0} + b_{n+2,1}f' + \dots) + a_1f''(b_{n+1,1} + 2b_{n+1,2}f' + 3b_{n+1,3}f'^2 + \dots).$$

Comparing the coefficients of  $f'^i$ ,  $i = 0, 1, \dots$  in (4.19), we get

$$(4.34) \left\{ \begin{array}{l} c_{n,0} = 0, \\ c_{n,j} = b_{n+1,j-1}, j = 1, 2, \dots \end{array} \right.$$

Next, comparing the coefficients of  $f''$  in (4.20), we get



$$\begin{aligned}
 (4.35) \quad & 2a_1 f'^3 (b_{n+1,1} + 2b_{n+2,2} f' + 3b_{n+1,3} f'^2 + \dots) \\
 & = -(c_{n,0} + c_{n,1} f' + c_{n,2} f'^2 + \dots) - 2a_1 f'^2 (c_{n,1} + 2c_{n,2} f' + \dots).
 \end{aligned}$$

Hence, comparing coefficients of  $f'^i$ ,  $i = 0, 1, \dots$  in (4.35), we get

$$(4.36) \quad \begin{cases} c_{n,0} = c_{n,1} = 0 \\ -c_{n,j+1} - 2ja_1 c_{n,j} = 2(j-1)a_1 b_{n+1,j-1}, \quad j = 1, 2, \dots \end{cases}$$

From (4.34) and (4.36) it is trivial to see that

$$c_{n,j} = 0 \text{ for } j = 0, 1, 2, \dots .$$

Therefore,  $\mu_n = 0$ . This is a contradiction. ■

## 5. OPTIMAL EFFICIENCY

### Lemma 5.1

If  $\varphi \in \Omega_2$  and  $\varphi$  uses evaluations of  $f$  and  $f'$  then  $a(\varphi) \geq 2$ .

### Proof

It suffices to show that  $\varphi(f)(x)$  depends explicitly on  $x$ ,  $f(x)$  and  $f'(z_1)$ . Suppose that  $\varphi(f)(x)$  does not depend explicitly on  $x$ . Then

$$\varphi(f)(x) = G(f(x), f'(z_1))$$

for some rational function  $G: \mathbb{R}^2 \rightarrow \mathbb{R}$ . Since  $\varphi(f)(\alpha_f) = \alpha_f$ ,

$$(5.1) \quad G(0, f'(\alpha_f)) = \alpha_f$$

for all  $f \in D$ . Clearly for any real numbers  $s, t$  ( $t \neq 0$ ), there exists  $f \in D$  such that

$$\begin{aligned} \alpha_f &= s, \\ f'(\alpha_f) &= t. \end{aligned}$$

By (5.1) we have

$$G(0, t) = s$$

for all  $(t, s)$  with  $t \neq 0$ . This is a contradiction. ■

### Lemma 5.2

If  $\varphi \in \Omega_2$ ,  $p(\varphi) \geq 2$  and  $\varphi$  uses evaluations of  $f$  only then  $a(\varphi) \geq 5$ .

### Proof

We assume notation used in Case 1 of the proof of Theorem 4.4.

Suppose  $\mu_n \neq 0$  and  $\mu_i = 0$  for  $i < n$ . From (4.23) we can easily see that  $n > 0$ . Note that, by (4.24),  $a_1 \neq 0$ .

Case 1: (n = 1)

By (4.23)

$$c_{1,0} + c_{0,1}(1+af') \neq 0,$$

$$c_{1,0} = -c_{0,1},$$

$$b_{1,1} = b_{0,2} = 0,$$

$$b_{2,0} = -a_1 c_{0,1}.$$

Hence

$$\varphi(f)(x) = x - \frac{a_1 f^2(x) + \dots}{f(z_1) - f(x) + \dots}.$$

Since the higher order terms in  $f(x)$  cannot cancel the terms shown, the theorem is proven for this case.

Case 2: (n = 2)

By (4.23)

$$c_{2,0} + c_{1,1}(1+a_1 f') + c_{0,2}(1+a_1 f')^2 \neq 0$$

$$c_{2,0} + c_{1,1} + c_{0,2} = 0,$$

$$b_{3,0} + b_{2,1} = -c_{1,1} a_1 - 2c_{0,2} a_1,$$

$$b_{2,1} + c_{0,2} a_1 = 0,$$

$$b_{0,3} = b_{1,2} = 0.$$

Hence

$$b_{3,0} = a_1 c_{2,0},$$

$$b_{2,1} = -a_1 c_{0,2},$$

$$b_{2,1} - b_{3,0} = a_1 c_{1,1}.$$

Therefore,

$$(5.2) \quad \varpi(f)(x) = x + \frac{b_{3,0}f^3(x) + b_{2,1}f^2(x)f(z_1) + \dots}{c_{2,0}f^2(x) + c_{1,1}f(x)f(z_1) + c_{0,2}f^2(z_1) + \dots}.$$

Since  $c_{2,0} + c_{1,1}(1+a_1f') + c_{0,2}(1+a_1f')^2 \neq 0$ ,  $b_{3,0}$  and  $b_{2,1}$  cannot both be zero. Then one can easily check from (5.2) that  $a(\varpi) \geq 5$ .

Case 3: ( $n \geq 3$ )

One of  $b_{n+1-j,j}$ ,  $j = 0, \dots, n-1$  must be non-zero. But to compute  $b_{n+1-j,j}f(x)^{n+1-j}f(z_1)^j$  from  $f(x)$  and  $f(z_1)$  requires at least two arithmetic operations. The argument of  $f(z_1)$  requires at least one arithmetic operation. The division takes one arithmetic operation. Also, to combine with  $x$  requires another arithmetic operation. Therefore  $a(\varpi) \geq 5$ . ■

For any  $f \in D$ , define

$$E_2(f) = \sup_{\varpi \in \Omega_2} e(\varpi, f),$$

Then  $E_2(f)$  is the optimal efficiency achievable by a rational two-evaluation iteration without memory with respect to  $f$ . By Theorem 4.4 and Lemmas

5.1 and 5.2, we have

$$(5.3) \quad E_2(f) \leq \max\left(\frac{1}{c(f)+c(f')+2}, \frac{1}{2c(f)+5}\right).$$

Consider Newton iteration  $\gamma$  and the iteration  $\psi$  defined by (1.2) and (1.3), respectively. We have

$$(5.4) \quad e(\gamma, f) = \frac{1}{c(f)+c(f')+2},$$

and

$$(5.5) \quad e(\psi, f) = \frac{1}{2c(f)+5} .$$

From (5.3), (5.4) and (5.5) we have the main result on optimal efficiency.

Theorem 5.1

1. If  $c(f') \leq c(f) + 3$  then

$$E_2(f) = \frac{1}{c(f)+c(f')+2} ,$$

i.e., Newton iteration is optimal.

2. If  $c(f') \geq c(f)+3$  then

$$E_2(f) = \frac{1}{2c(f)+5} ,$$

i.e., the iteration  $\psi$  defined by (1.3) is optimal.

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