OPTIMAL USE OF INFORMATION IN CERTAIN ITERATIVE PROCESSES

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1. Introduction

To approximate numerically a zero α of a real analytic function f,

$$f(\alpha) = 0,$$

iteration is most widely used. We will discuss so-called *k-point stationary iterative processes without memory*, ϕ, defined as follows. Let there exist an interval around α such that for all x_1 in this interval, the following functions ζ_i, $i=2,\ldots,k+1$ are well-defined :

$$z_1 = x_1$$
$$z_2 = \zeta_2(z_1, N(z_1;f))$$
$$z_3 = \zeta_3(z_1,z_2,N(z_1,z_2;f))$$
$$\vdots$$
$$x_2 := \phi(x_1) = z_{k+1} = \zeta_{k+1}(z_1,\ldots,z_k,N(z_1,\ldots,z_k;f)),$$

where

a) x_2 is called the new approximation to α ; we assume that x_2 lies within the same interval a and that the process is converging, i.e. putting $x_1 := x_2$ and repeating the iterative step produces a sequence which converges to α. Also we assume $f'(\alpha) \neq 0$.

b) $N(z_1,\ldots,z_i;f)$ is called the *information set* at

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the points $z_1,\ldots,z_i$ and consists of the set of all evaluations of f and/or its derivatives used at those points when computing z_{i+1}. It is not necessary to give *all* derivatives up to a certain degree at any particular point z_i. Examples of specific N abound in the rest of the paper. Other kinds of information sets can be considered, but are not the topic of this paper ; see for instance Kacewicz [75]. The reader should also be more or less familiar with the work of Woźniakowski [74] [75a].

2. Some known results and conjectures

Definition 2.1.

Let $N(z_1,\ldots,z_k;f)$ be given. We say that $\tilde{f} \equiv f \bmod N$ when for all $f^{(j)}(z_i) \in N$,

$$f^{(j)}(z_i) = \tilde{f}^{(j)}(z_i)$$

As in Woźniakowski [75a] we adopt the following definitions:

Definition 2.2.

The order of iteration $p(\phi)$ is the largest number such that for all f with $f(\alpha) = 0$, for all $\tilde{f} \equiv f \bmod N$ and having a zero $\tilde{\alpha}$ near α, we have

$$\limsup_{x_1 \to \alpha} \frac{|\phi(x_1;N) - \tilde{\alpha}|}{|x_1 - \alpha|^{p(\phi)}} < \infty$$

It can be shown this definition coincides with the usual definition in the literature (e.g. Traub[64]) under weak assumptions on the asymptotical constant

Definition 2.3.

The order of information $p(N)$ is the largest number such that for all f with $f(\alpha) = 0$, for all $\tilde{f} \equiv f \bmod N$ and having a zero $\tilde{\alpha}$ near α, we have

$$\limsup_{x_1 \to \alpha} \frac{|\alpha - \tilde{\alpha}|}{|x_1 - \alpha|^{p(N)}} < \infty$$

Remark that choosing a special f or $\tilde{f} \equiv f \bmod N$ will give upper bounds on these orders, by definition. See also Woźniakowski [75b]. Extensive use will be made of the following two theorems.

Theorem 2.1. (Maximal Order Theorem)

The order $p(\phi)$ is bounded above by $p(N)$ for all ϕ using information N.

Theorem 2.2.

The maximal order is reached for the generalized interpolating methods I_N : $p(I_N) = p(N)$.

For definitions and proofs, see Woźniakowski [75a].

Two kinds of problems arise now.

Problem 1. Given N, compute $p(N)$. (In other words, what is the maximal order achievable with information N).

Problem 2. Given $n = \#N$, the number of elements in N, determine $p_n^* = \max_{\#N=n} \max_{\phi} p(\phi)$, where ϕ uses information N.

Problem 2 is much harder than problem 1. Kung and

Traub conjectured (Kung and Traub [74a]) that

$$(2.3) \qquad P_n^* = 2^{n-1}$$

and exhibited two families of methods which realize this bound for each n. In a later paper, Kung and Traub [74b], they proved (2.3) for n = 1 and 2. Remark that in view of Theorems 2.1 and 2.2, (2.3) is equivalent to

$$Q_n^* = 2^{n-1}$$

where $Q_n^* = \max\limits_{\#N=n} p(N)$.

The conjecture has been settled by Woźniakowski in one very important case.

Definition 2.4.

N is *hermitean* iff for all i, $1 \leq i \leq k$, we have

$$f^{(k)}(z_i) \in N \Rightarrow f^{(k-1)}(z_i) \in N \text{ for all } k > 0.$$

Theorem 2.3. (Woźniakowski [75b])

The conjecture of (2.3) is true if the maximum is taken over hermitean N. We will show later that a partial converse is not true, i.e. that $p(N) = 2^{\#N-1}$ does not imply that N is hermitean.

3. A solution to problem 1 for n = 3

We will prove in this section that $P_3^* = 4$, showing the correctness of the conjecture in this case. Our proof uses special cases of some general results on certain n-evaluations iterations one of which is to be treated in a later paper, namely

Theorem 3.1.

If $N = \{f(z_1), f^1(z_2), \ldots, f^{(n)}(z_{n+1})\}$ then

$$p(N) \leq 2n$$

Note : N is the so-called Abel-987Končarov information.

In the proof of the following lemma and the rest of the paper we assume that at each z_i used in ϕ, some new information is computed. This is not a restriction since otherwise we can substitute the expressions for these z_i in the other ζ_j, obtaining an equivalent iteration (with less points).

Lemma 3.1.

Let ϕ be an iteration using two pieces of information, i.e.

$$z_1 = x_1$$

$$z_2 = \zeta_2(z_1, N(z_1; f))$$

$$x_2 := \phi(x_1) = z_3 = \zeta_3(z_1, z_2, N(z_1, z_2; f)) \text{ with } \#N = 2$$

(By the above convention, ϕ is a 1- or 2-point iteration).

Then, if there exists a (known) constant C, $C \neq 0$ and $C \neq 1$, such that for all f

$$\alpha - z_2 = C(\alpha - z_1) + O(\alpha - z_1)^2, \qquad (3.1)$$

then ϕ cannot be of second order.

Proof : If $C \neq 1$, then from (3.1) we could solve for α :

$$\alpha = \frac{z_2 - C\, z_1}{1 - C} + O(\alpha - z_1)^2$$

And $z_2^* = \frac{z_2 - C z_1}{1 - C}$ would therefore produce a second order approximation to α. Since $P_1^* = 1$, both pieces of information must be used then at z_1, but then ϕ is a one-point iteration, i.e. $z_3 = z_2$ by the convention, and from (3.1) and $C \neq 0$ it follows that ϕ is only of first order.

Theorem 3.2.

$$P_3^* = 4$$

Proof : We prove that $p^*(N) \leq 4$ for all N with $\#N = 3$, where

$$p^*(N) = \max \{p \mid \text{for all } \tilde{f} = f + G,\ G \equiv 0 \bmod N,\ \tilde{f}(\tilde{\alpha}) = 0, \text{ and } G \text{ monic polynomial of degree} < 3, \limsup_{x_1 \to \alpha} \frac{|\alpha - \tilde{\alpha}|}{|x_1 - \tilde{\alpha}|^p} < \infty\}$$

thereby restricting the class of $\tilde{f}$ such that $\tilde{f} \equiv f \bmod N$.

Step 1

We need one evaluation of f at z_1 to assure convergence so N is of the form

$$N = \{f(z_1),\ f^{(i)}(z_2),\ f^{(j)}(z_3)\}$$

(Kung and Traub [74a]).

We will suppose z_2 and z_3 not necessarily different, unless of course i or j equals 0 or $i = j$. It is clear this does not affect the bounds on the optimal order.

Since now G is a monic polynomial of degree < 3, we can take i and $j \leq 2$. Indeed, if i or $j > 3$, $G \equiv 0 \bmod N$ is automatically satisfied ; if

$i < j = 3$, we can interpolate the zero function for this information at z_1 and z_2 with a monic polynomial of degree ≤ 2 - from $P_2^* = 2$ it follows that the optimal order is $2 < 4$, and similarly if $j < i = 3$. If $i = j = 3$ we can even take $G(z) = z - z_1$ in which case the order of information evidently is equal to $1 < 4$.

Remark

The above argument can of course be generalized to any n : it is closely related to the Pólya conditions on the set N, see Woźniakowski [75b], Sharma [72].

Step 2

The different cases for the information N.
With an obvious notation, in the following cases the answer is already known :

Case 1 : $\{f_1, f_2, f_3\}$: Hermitean N, order $\leq 2^{3-1}=4$

Case 2 : $\{f_1, f_2', f_3'\}$: "Brent information with m=0", applying the results of Sec. 4, we find

if $z_1 \neq z_2 : p(N) \leq m+2(k-1)-1=0+4-1=3<4$;
if $z_1 = z_2 : p(N) = m+2(k-1)+1=1+2+1=4$

Case 3 : $\{f_1, f_2', f_3''\}$: "Abel-Goncarov" N, by Theorem 3.1. : order $\leq 2.2 = 4$

Case 4 : $\{f_1, f_2'', f_3''\}$: Take again $G(z)=z-z_1$ as in Step 1 ; order $\leq 1 < 4$ (here the Pólya conditions are not satisfied).

Step 3

Exhaustive checking of the remaining cases. Let us set

$$G(z) = (z-z_1)(z^2+az+b)$$

Case 5 : $\{f_1,f_2,f_3'\}$

Now $G(z) = (z-z_1)(z-z_2)(z-c)$.
The condition $\tilde{f}'(z_3) = 0$ gives

$$(2z_3-z_1-z_2)(z_3-c)+(z_3-z_1)(z_3-z_2) = 0$$

So in general, c is a function of z_1, z_2 and z_3 which itself is also a function of z_1 and z_2. Since $P_2^* = 2$, $\alpha-c$ cannot be of higher order than $(\alpha-z_1)^2$. Therefore
$\tilde{\alpha} - \alpha = O(G(\alpha)) = O(\tilde{f}(\alpha)) = O(\alpha-z_1)(\alpha-z_2)(\alpha-c)$
cannot be of higher order than $(\alpha-z_1)^4$ since $\alpha-z_2$ is at most of order $(\alpha-z_1)$ because $P_1^* = 1$. Thus $p^*(N) \leq 4$ for this N.

Case 6 : $\{f_1,f_2,f_3''\}$

Completely analogous to case 5, the condition at z_3 now is

$$(z_3-c) + (2z_3-z_1-z_2) = 0.$$

Case 7 : $\{f_1,f_2'',f_3\}$

Now $G(z) = (z-z_1)(z-z_3)(z-c)$.
The condition at z_2 : $c = 3z_2 - z_1 - z_3$, again gives that $(\alpha-c)$ is at most of second order in $(\alpha-z_1)$.
Now $(\alpha-z_3)$ is at most of first order in $(\alpha-z_1)$ since the function

$$\tilde{G}(z) = z - z_1$$

interpolates the zero function at the points z_1 and z_2 for the given information. Thus with an obvious notation,

$\tilde{\alpha}(\tilde{G}) - \alpha = \mathcal{O}(\alpha - z_1)$, and by theorem 2.1 and 2.2,

$$(\alpha - z_3) = \mathcal{O}(\alpha - z_1) \text{ at most.}$$

Consequently,

$$\tilde{\alpha}(G) - \alpha = \mathcal{O}(\tilde{f}(\alpha)) = \mathcal{O}(\alpha - z_1)(\alpha - z_3)(\alpha - c)$$

is again at most of order $(\alpha - z_1)^4$.

<u>Case 8</u> : $\{f_1, f_2'', f_3'\}$

This is a permutation of the Abel-Gončarov information. It is an easy consequence of the proof of Theorem 3.1 that also here we have,

$$p(N) \leq 2 - 2 = 4.$$

A direct proof for this case can also be found, and is left to the reader.

<u>Case 9</u> : $\{f_1, f_2', f_3\}$

$G(z) = (z - z_1)(z - z_3)(z - c)$.

Again, $(\alpha - c)$ being of 3rd order or more in $(\alpha - z_1)$ would contradict $P_2^* = 2$, so if $(\alpha - z_3)$ is of order 1 in $(\alpha - z_1)$ we are done. However $(\alpha - z_3)$ and $(\alpha - c)$ cannot be both of second order, since the condition $G'(z_2) = 0$ reads

$$(2z_2 - z_1 - z_3)(z_2 - c) + (z_2 - z_1)(z_2 - z_3) = 0$$

which is easily seen to be equivalent to

$$e_3(\alpha - c) = e_2(2e_1 - 3e_2) - (e_1 - 2e_2)(e_3 + (\alpha - c))$$

where $e_i = \alpha - z_i$; $i=1,2,3$.

Now $e_3(\alpha-c)$ cannot be of order 4 while by lemma 3.1 with $C = \frac{2}{3}$, $e_2(2e_1-3e_2)$ is at most of order 2 and $(e_1-2e_2)(e_3+(\alpha-c))$ is at least of third order. Note that if $2z_2 - z_1 - z_3 = 0$, this case becomes non-poised (Sharma [72]) and the function $G(z) = (z-z_1)(z-z_3)$ interpolates zero with respect to this N, giving a maximal order of 3.

Theorem 3.3.

Hermitean information is not uniquely optimal.

Proof : We exhibit two examples for $n = 3$

a) Consider again case (6) of Theorem 3.2.

We have $G(\alpha) = (\alpha-z_1)(\alpha-z_2)(\alpha-c)$

where $\qquad c = 3z_3 - z_1 - z_2$.

To obtain order 4, this suggests we must have

$$\alpha - c = O(\alpha-z_1)^2, \text{ or}$$

$$(3.1) \qquad z_3 = \frac{z_1+z_2}{3} + \frac{1}{3}\gamma \text{ with } \gamma-\alpha=\theta(\alpha-z_1)^2$$

To find such a γ, take

$$z_1 = x_1$$

$$z_2 = z_1 + f(z_1)$$

and γ the root of the interpolating (1^{st} degree) polynomial at these two points, i.e.

$$\gamma = z_1 - \frac{z_2 - z_1}{f(z_1) - f(z_1)} f(z_1)$$

Then construct z_3 by (3.1) and

$$x_2 := \phi(x_1) := z_4$$

as the root of the (2^{nd} degree) polynomial interpolating f with respect to the information at z_1, z_2 and z_3. This method is easily seen to be of fourth order.

b) Case 3 with $z_1 = z_2$. Now $G(z) = (z-z_1)^2(z-c)$ and $G''(z_3) = 0$ gives $3z_3 = 2z_1 + c$. By taking $z_3 = \frac{2}{3}z_1 + \frac{1}{3}\gamma$ where again $\alpha - \gamma = O(\alpha-z_1)^2$, for example by a Newton-step, it is easy to show that the following method has fourth order :

$$z_1 = x_1 \quad (= z_2)$$
$$z_3 = \frac{2}{3} z_1 + \frac{1}{3} \left(z_1 - \frac{f(z_1)}{f'(z_1)}\right)$$

$x_2 := \phi(x_1) := z_4$ = zero of the second degree polynomial interpolating f with respect to the information at z_1 and z_3.

Remarks

The previous arguments permit the determination of all arrangements of the information ($\#N = 3$) which can give optimal order. They are denoted by their incidence matrices (Sharma [72]) as follows :

A) $\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$ B) $\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ C) $\begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$ D) $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

E) $\begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ F) $\begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}$ G) $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

The cases A) and C) have optimal generalizations for all $n > 3$, it will be shown in a later paper that also case F) can be generalized to a *non-hermitean* optimal case for all n.

4. A solution to a "problem 2" for N = Brent information.

Definition 4.1.

$$N_{m,\ell,k}=\{f(z_1),f'(z_1),\dots,f^{(m)}(z_1)\ ;\ f^{(\ell)}(z_2),\dots,f^{(\ell)}(z_k)\}$$

is called Brent-information, where the z_i are distinct, $m \geq 1$, $k \geq 2$ and $\ell \geq 1$.

Brent has shown the following

Theorem 4.1. (Brent [74])

Assume $\ell \leq m + 1$.

There exist methods using $N_{m,\ell,k}$ of order $m+2k-1$.

We will now prove that the Brent methods make optimal use of the information $N_{m,\ell,k}$ (with respect to order).

Theorem 4.2.

Let $N_{m,\ell,k}$ be as in definition 4.1. Then if $\ell \leq m+1$,

$$p(N) = m + 2k - 1$$

If $\ell > m + 1$, $p(N) = m + 1$.

Proof : A technique is used similar to theorem 3.2. If $\ell > m + 1$, a function $G(z) \equiv 0 \bmod N$ is given by

$$G(z) = (z-z_1)^{m+1}$$

And consequently $|\tilde{\alpha}-\alpha| = O(\tilde{f}(\alpha)) = O(\alpha-z_1)^{m+1}$.

By theorem 2.1 the maximal order is not more than $m + 1$. Methods realizing this order exist and are trivial to find. Thus $p(N) = m + 1$.

If $\ell \leq m + 1$, we construct $G(z)$ as follows.

To satisfy the conditions at $z_2,\ldots,z_k$ we must have

$$G^{(\ell)}(z) = (z-z_1)^{m-\ell+1}(z-z_2)(z-z_3)\ldots(z-z_k)H(z)$$

where $H(z)$ is any (sufficiently regular) function.
Integrating ℓ times,

$$G(z) = \int_{z_1}^{z} (t-z)^{\ell-1}(t-z_1)^{m-\ell+1}(t-z_2)\ldots(t-z_k)H(t)\,dt.$$

According to the remark at (2.2), we obtain an upper bound by choosing a special H.
Take $H(t) = (t-z_2)\ldots(t-z_k)$, making

$$G(z) = \int_{z_1}^{z} (t-z)^{\ell-1}(t-z_1)^{m-\ell+1}[(t-z_2)\ldots(t-z_k)]^2\,dt.$$

Consider now $G(\alpha) = \tilde{f}(\alpha)$. Transform $G(\alpha)$ to the interval $[-1,+1]$; after some easy calculations we obtain

$$\tilde{f}(\alpha) = K(\alpha-z_1)^{\ell-1}(\alpha-z_1)^{m-\ell+1}(\alpha-z_1)^{2(k-1)}(\alpha-z_1).I(\alpha)$$

where $K \neq 0$ does not depend on α or any of the z_i and where

$$I(\alpha) = \int_{-1}^{+1} (1-\tau)^{\ell-1}(1+\tau)^{m-\ell+1} \prod_{i=2}^{k} \left(\tau+\frac{z_1-z_i}{\alpha-z_1}\right)^2 \alpha d\tau.$$

As is well known, $I(\alpha)$ is minimized when $\prod_{i=2}^{k} \left(\tau + \frac{z_1-z_i}{\alpha-z_1}\right)$ is equal to the $(k-1)^{st}$ monic Jacobi polynomial corresponding to the weight function $(1-\tau)^{\ell-1}(1+\tau)^{m-\ell+1}$.
Then $I(\alpha) \geqslant c$ where c is independent of the z_i.
(See for example G. Natanson : "Konstruktive Funktionentheorie").
So $|\tilde{\alpha}-\alpha| = O(\tilde{f}(\alpha)) = O(\alpha-z_1)^p$

with $p = (\ell-1) + (m-\ell+1) + 2(k-1) + 1$
$= m + 2k - 1.$

Thus $p(N) \leq m + 2k - 1$, but by Brent's theorem and theorem 2.1, we have equality.

Note : The previous theorem was independently discovered by Woźniakowski. A generalization of this theorem is possible.

Theorem 4.3.

Let now $N = \{f(z_1), f'(z_1), \ldots, f^{(m_1)}(z_1)$;
$f^{(\ell)}(z_2), \ldots, f^{(\ell+m_2)}(z_2)$;
$f^{(\ell)}(z_3), \ldots, f^{(\ell+m_3)}(z_3)$;
...
$f^{(\ell)}(z_k), \ldots, f^{(\ell+m_k)}(z_k)\}$ $m_1 \geq 1$,
$\ell \geq 1$.

Then if $\ell > m_1 + 1$, $p(N) = m_1 + 1$, and if $\ell \leq m_1+1$,

$$(4.1) \qquad p(N) \leq 1 + m_1 + 2. \sum_{i=1}^{k} \left[\frac{m_i+1}{2}\right]$$

Proof : The proof runs analogously, with H replaced by

$$H(t) = \prod_{i=2}^{k} (t-z_1)^{\varepsilon_i} \text{ with } \varepsilon_i = \begin{cases} 0 \text{ if } m_i \text{ odd} \\ 1 \text{ if } m_i \text{ even} \end{cases}$$

(The Jacobi polynomial is now of degree $\sum_{i=2}^{k} \left[\frac{m_{i+1}}{2}\right]$)

Remark 4.1.

Let $m_i = 1$ for $i = 2,\ldots,k$. Then $p(N) \leq m + 2k - 1$, so we gain nothing compared to the Brent information case ! In general the order cannot be raised if all m_i are even and we add the pieces of information $f^{(\ell+m_i+1)}(z_i)$ for $i = 2,\ldots,k$.

Remark 4.2.

Contrary to Theorem 4.2 the inequality (4.1) is not yet known to be an equality in general. If all m_i are equal, methods can be constructed by means of so-called "s-polynomials" realizing the bound. For a definition of these, see Ghizetti and Ossicini, "Quadrature Formulae". Again, for details we refer to a forthcoming paper on this subject.

Remark 4.3.

Kung and Traub's conjecture states that the optimal order for a given number of pieces of information will double by adding one extra piece of information. That it is however possible to increase the order more than twofold when it is not optimal, is shown by the following example :

Let $N = \{f(z_1), f'(z_1), f''(z_1) \; ; \; f'(z_2), f''(z_2)\}$.

By theorem 4.3 and remark 4.1 any method using this information must have order at most 5. Adding the element $\{f(z_2)\}$ to N, we get however an information at which allows us to obtain order 12, as is easily shown. Although of course not a counterexample to the conjecture - we believe it is true - it will complicate any possible proof by induction.

Finally, we state without proof the following result, used in the proof of Theorem 3.1 :

Theorem 4.4.

If in Theorem 4.3 $m_1 = 0$ (and consequently, to avoid trivial cases, $l = 1$) the order of information is bounded by

$$p(N) \leq 1 + m_2 + \sum_{i=3}^{k} \left\lfloor \frac{m_i+1}{2} \right\rfloor .$$

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