

OPTIMAL SOLUTION OF NONLINEAR EQUATIONS

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Abstract.

We survey recent worst case complexity results for the solution of nonlinear equations. Notes on worst and average case analysis of iterative algorithms and a bibliography of the subject are also included.

1. INTRODUCTION.

We study the approximate solution of the equation $f(x) = 0$ and also the problem of computing the topological degree of f . It is assumed that f belongs to the class of smooth functions F defined on a real interval or on the unit simplex or on the unit cube in m dimensions. The information on f consists in general of n values of arbitrary linear functionals which are computed sequentially (adaptively). The topological degree or an approximation to α , a zero of f , is constructed by an algorithm which uses these evaluations.

Several classes of functions F and the two error criteria are studied to determine whether or not it is possible to find an approximation to α which satisfies the error criterion to within a specified tolerance ϵ . The topological degree is computed exactly for the class of Lipschitz functions.

Complexity, i.e., the minimal cost of solving these problems, or lower and upper bounds on the complexity are found, and information and algorithms are developed which solve the problem with cost close to the complexity.

In Sections 2, 3 and 4 we include some history and list recent complexity results for the worst case setting. In Section 5 we exhibit future directions of research, and in Sections 6 and 7 include notes on worst and average case analysis of iterative algorithms.

2. OVERVIEW AND BRIEF HISTORY.

In this section we discuss the worst case setting for the solution of nonlinear equations. We consider here algorithms which use general sequential information and whose error and cost are defined by the worst case performance. Sections 2–5 deal with non-iterative algorithms.

There are numerous papers in this area where optimal or nearly optimal algorithms are found. A partial list includes Booth (1967), Chernousko (1968), Eichhorn (1968), Gross and Johnson (1959), Hyafil (1977), Kiefer (1953, 1957), Micchelli and Miranker (1975), Sikorski (1982, 1984b), Sikorski and Woźniakowski (1983) and Sukharev (1976), who considered the scalar case, and Boulton and Sikorski (1984, 1985a, 1985b, 1985c), Nemirovsky and Yudin (1983), Majstrovskij (1972), Sikorski (1984a) and Todd (1978) who consider the multivariate case. We include here papers dealing with computing extrema since this problem is closely related to zero finding.

We briefly recall some of the results. The first results may be found in the Master's thesis of J. Kiefer, Kiefer (1953). He considers the search for the maximum in the class of scalar unimodal functions. The information is the values of f at n points. He proves that Fibonacci search is the optimal information and the optimal algorithm.

In the 1960's people worked on classes of functions which were convex or unimodal and obtained optimal algorithms for approximating zeros of functions and also derivatives; see Gross and Johnson (1959), Booth (1967), Chernousko (1968) and Eichhorn (1968).

Gross and Johnson consider the solution of scalar nonlinear equations for the class of convex continuous functions changing sign at the endpoints of an interval. The information is sequential function evaluations. They study optimal evaluation points and optimal algorithms.

Booth studies location of zeros of derivatives, Chernousko the search for a zero in the class of scalar functions with bounded difference quotients and Eichhorn the search for the maximum or a zero in the class of unimodal or monotone nonincreasing functions.

In the 1970's the focus shifted to classes of functions with bounded derivatives. Examples here include the work of Micchelli and Miranker (1975) on "envelope methods", Sukharev (1976) on Lipschitz functions and Majstrovskij (1972) on optimality of Newton's method.

An important contribution is the work of Nemirovsky and Yudin (1983). They study the multivariate minimization problem and are interested in finding the minimal number $N(\epsilon)$ of function or derivative evaluations in order to determine ϵ -approximation to the extremum in the residual sense. The authors find sharp estimates for $N(\epsilon)$ for classes of convex and strongly convex functions as well as for nonconvex smooth functions defined on convex and/or compact set G of dimension n . For example $N(\epsilon) \simeq n \ln \frac{1}{\epsilon}$ for the convex class and $N(\epsilon) \simeq (\frac{1}{\epsilon})^{n/k}$ for the nonconvex class of k -times continuously differentiable functions. The authors only occasionally deal with the problem of combining these $N(\epsilon)$ evaluations to compute an approximate solution.

There is much current research on optimal algorithms for solving nonlinear equations. A precise formulation of the worst case setting is given in Section 3 and selected recent results are stated in Section 4.

3. FORMULATION OF THE PROBLEM.

Let $\alpha(f)$ be a zero of the nonlinear function f and let $x(f)$ be an approximation to $\alpha(f)$. What we mean by approximation is determined by which error criterion we choose. Two commonly used criteria are the root criterion and the residual criterion.

Let $\epsilon > 0$ and a norm $\| \cdot \|$ be given. Then the *root criterion* is defined by

$$(3.1) \quad \|x(f) - \alpha(f)\| \leq \epsilon,$$

and the *residual criterion* is defined by

$$(3.2) \quad \|f(x(f))\| \leq \epsilon.$$

For each of these error criteria we study whether we can compute an approximation to within a tolerance ϵ , for every function f in a class F . This is called the worst case setting.

The information commonly used to solve this problem are evaluations of f and its derivatives. We will, more generally, assume the information consists of linear functionals. Namely, the information on f , $N(f)$, consists of n values of arbitrary linear functionals which are computed sequentially (adaptively):

$$(3.3) \quad N(f) = [L_1(f), \dots, L_n(f)],$$

where the choice of L_i depends on $L_1(f), \dots, L_{i-1}(f)$. If L_i are given a priori the N is called *parallel* or *nonadaptive*, otherwise it is called *sequential* or *adaptive*. It is important to stress that this information is *partial* i.e., there are, in general, many functions sharing the same information. Knowing $N(f)$ we compute $x(f) = \varphi(N(f))$ by an *algorithm* φ which is a mapping

$$(3.4) \quad \varphi : N(F) \rightarrow D,$$

where D is the domain of the functions f . The error of an algorithm φ using N is given by

$$(3.5) \quad e(\varphi, N) = \sup_{f \in F} \|\alpha(f) - \varphi(N(f))\|$$

in the case of the root criterion, and

$$(3.6) \quad e(\varphi, N) = \sup_{f \in F} \|f(\varphi(N(f)))\|$$

in the case of residual criterion.

We next define *problem complexity*.

We assume that functional evaluations cost c and that arithmetic operations and comparisons cost unity.

To compute $\varphi(N(f))$ we must

$$(3.7) \quad \dots \quad \text{Compute } y = N(f),$$

and

$$(3.8) \quad \text{Compute } \varphi(y).$$

Thus the cost of an algorithm φ , $\text{cost}(\varphi, N)$, is given by

$$(3.9) \quad \text{cost}(\varphi, N) = \sup_{f \in F} (\text{cost } N(f) + \text{cost } \varphi(N(f))).$$

The *problem complexity* $\text{comp}(\epsilon)$ is defined as the minimal cost of an algorithm which uses arbitrary information N and computes an approximation $x(f)$ to within tolerance ϵ , i.e.,

$$(3.10) \quad \text{comp}(\epsilon) = \inf \{ \text{cost}(\varphi, N) : \forall \varphi, N : e(\varphi, N) \leq \epsilon \}$$

By optimal information and an optimal algorithm we mean N and φ for which $\text{cost}(\varphi, N) = \text{comp}(\epsilon)$ and $e(\varphi, N) \leq \epsilon$.

4. RECENT RESULTS.

In this section we list some recent complexity results. We conclude that for smooth functions the zero-finding problem with the root criterion is much more difficult than with the residual criterion. For example, for infinitely differentiable real functions with bounded arbitrary semi-norm it is impossible to solve the problem with the root criterion. It is, however, possible to solve it for the residual criterion. Thus additional restrictions on the functions are needed or the use of some nonlinear information is required to obtain positive results for the root criterion for these classes. We show that bisection is an almost optimal complexity algorithm for the class of functions changing sign at the end points of an interval.

We also present recent results on the complexity of computing the topological degree of a mapping, which can be used to determine the existence of a zero of f in a given domain.

Finally, we exhibit some results for the multivariate case, both for the root and residual criteria.

4.1 ROOT CRITERION.

First, we consider the class F of smooth real functions having a real zero:

$$(4.1) \quad F_1 = \{f : [a, b] \rightarrow \mathbb{R}, \exists \alpha : f(\alpha) = 0, f \in C^\infty[a, b], \|f\| \leq 1\},$$

where $\|\cdot\|$ is an arbitrary semi-norm.

Of course, if $\epsilon \geq (b - a)/2$, then the midpoint $x(f) = \frac{b+a}{2}$ solves the problem for every f in F . Thus the only interesting case is for $\epsilon < (b - a)/2$. Then Sikorski and Woźniakowski(1983) show

Theorem 4.1. $\text{comp}(\epsilon) = +\infty, \forall \epsilon < \frac{b-a}{2}$. ■

This means that for ϵ less than half of the length of the interval there *exists no* information of the general form (3.3) and *no* algorithm to solve this problem.

A very different result holds when we assume that the functions change sign at the endpoints of an interval. Namely consider the class

$$(4.2) \quad F_2 = \{f : [a, b] \rightarrow \mathbb{R}, f(a) \leq 0, f(b) \geq 0, f \in C^j[a, b]\},$$

where j is an integer, $j = 0, 1, 2, \dots$, or $j = +\infty$. It is known that if the information consists of function evaluations, then the optimal algorithm and information are given by bisection. It is proved in Sikorski (1982) that bisection remains optimal even if the general information of (3.3) is permitted. We have

Theorem 4.2. $\text{comp}(\epsilon) = (c + a_1) \lceil \log \frac{b-a}{\epsilon} \rceil + a_2$, where $a_1 \in [0, 3]$ and $a_2 \in [0, 1]$. ■

The upper bound is realized by bisection information and the bisection algorithm. Thus the bisection algorithm using bisection information enjoys almost minimal complexity. Note that $\text{comp}(\epsilon)$ does not depend on function smoothness. The same result holds for the class of polynomials of unbounded degree assuming the information is continuous, see Sikorski(1984b).

Do similar results hold in the multidimensional case? The analogous assumption to sign change is an assumption on non-zero topological degree(deg). Namely let

$$(4.3) \quad \begin{aligned} F_3 = \{ & f \in C^\infty(\Delta), \Delta - \text{unit triangle in } R^2, \\ & f : \Delta \rightarrow R^2, f \text{ has exactly one zero, which is} \\ & \text{simple, } \deg(f, \Delta, \theta) \neq 0, \theta = (0, 0) \text{ and } \Delta \text{ is} \\ & \text{completely labeled under } f \}. \end{aligned}$$

It turns out that even in the two dimensional case it is impossible to solve this problem. Thus one additional dimension makes the problem noncomputable. Boulton and Sikorski(1984) proved

Theorem 4.3. *If $\epsilon < \text{diam}(\Delta)/2$ then*

$$\text{comp}(\epsilon) = +\infty.$$

■

Thus there *exists no* information and *no* algorithm to solve this problem to within $\epsilon < \text{diam}(\Delta)/2$. In particular, the complexity of all methods which use as information function and/or derivative evaluations *is infinite*. Examples of such methods are continuation and simplicial continuation methods; see Allgower and Georg(1980).

This negative result suggests that additional restrictions on the class of functions or the use of nonlinear information are needed to obtain positive results in the multidimensional case.

4.2 COMPLEXITY OF COMPUTING TOPOLOGICAL DEGREE.

A problem related to zero finding is the computation of topological degree. The crucial property of the degree, expressed by Kronecker's theorem, is the following: if the topological degree of f is not zero on some domain D then the function f has a zero

in D . Thus we can approximate a zero of f by the following algorithm. We start with some domain with nonzero degree. Subdivide this domain, compute the degree, if it is well defined, for the smaller domains, choose a subdomain of nonzero degree, etc. In this way we construct a sequence of domains with decreasing diameters and nonzero degrees. This idea was investigated by many people, see Eiger, Sikorski and Stenger(1984), Harvey and Stenger (1976), Kearfott(1977,1979), Prüfer and Siegbert(1980), Stenger(1975) and Stynes(1979a,1979b,1981). Such an algorithm would not always work, since the degree is not defined if a function has a zero on the boundary of a subdomain. We believe, however, that it would work with high probability. This claim, of course, requires introducing a probability measure into the space of functions ; it will be a topic of future research.

Here we exhibit lower and upper complexity bounds for the computation of degree in the class of Lipschitz functions. We stress that we compute the degree *exactly*. Let

$$(4.4) \quad F_4 = \{f : C \rightarrow R^n, \|f(x) - f(y)\|_\infty \leq K\|x - y\|_\infty, \|f(x)\| \geq d > 0, \forall x \in \partial C\}$$

where $C = [0, 1]^n$ is the unit cube in R^n . Since the degree is uniquely defined by function values on the boundary of a domain we assume as information the *sequential evaluation of function values* on the boundary ∂C of C . For arbitrary $n, n \geq 2$, we have, Boulton and Sikorski(1985b),

Theorem 4.4. *The complexity of computing degree, $comp(deg)$, is bounded by:*

$$c_{low} \leq comp(deg) \leq c_{up},$$

$$c_{low} \simeq 2n(K/(8d))^{n-1}(c + n),$$

$$c_{up} \simeq 2n(K/(2d))^{n-1}(c + \frac{n^2}{2}(n-1)!),$$

$$\text{whenever } K/(8d) \geq 1.$$

Note that if $K/(2d) < 1$ then the functions in F_4 do not have zeros and therefore the degree is zero for every f . The case $1 \leq K/(2d) < 4$ is open. For the two dimensional case we have the stronger result, see Boult and Sikorski(1985a),

Theorem 4.5. *If $n = 2$ and $K/(4d) \geq 1$ then*

$$\text{comp}(\text{deg}) = 4 \left\lfloor \frac{k}{4d} \right\rfloor (c + a) - 1$$

where $a \in [2, 24]$. ■

In both cases parallel function evaluations are almost optimal information. This information is used by an algorithm due to Kearfott(1979).

These results imply that the topological degree can be computed for small n and/or not too large $K/(2d)$. taking for example $n \leq 5$ and $K/(2d) \leq 10$ the degree can be computed with cost $\leq 10^5(c + 300)$. For large n and/or large $k/(8d)$ the problem is intractable. For example taking $n = 10$ and $K/(8d) = 10^3$ then the lower bound on complexity is $c_{low} \simeq 2 \cdot 10^{28}(c + 10)$.

4.3 RESIDUAL CRITERION.

For the next two classes we show that the complexity of approximating a zero in the residual sense is finite. This contrasts with Theorem 4.1 in which we showed that with the root criterion the complexity is infinite. Namely consider the class F_5 , which contains F_1 from (4.1) with the semi-norm $\|f\| = \|f^{(r)}\|_\infty$, and is defined by

$$(4.5) \quad F_5 = \{f : [a, b] \rightarrow R, f^{(r-1)} \text{ absolutely continuous, } \|f^{(r)}\|_\infty \leq 1 \text{ and } \exists \alpha : f(\alpha) = 0\}.$$

It is proved in Sikorski and Woźniakowski (1983):

Theorem 4.5. $\text{comp}(\epsilon) = \theta(\epsilon^{-1/r})$. ■

It turns out that optimal information is parallel and that the optimal algorithm is easy to implement for small r .

Next we report on the multivariate case. Namely, take Lipschitz class:

$$(4.6) F_6 = \{f : C \rightarrow R^n : \|f(x) - f(y)\|_\infty \leq K\|x - y\|_\infty, \text{ and } \exists \alpha \in C : f(\alpha) = (0, \dots, 0)\},$$

where $C = [0, 1]^n$.

It is proved in Sikorski (1984a):

THEOREM 4.6. $comp(\epsilon) = \theta\left(\left(\frac{K}{2\epsilon}\right)^n\right)$. ■

We also showed that optimal information is parallel and that an optimal algorithm is an easy to implement search procedure. In fact this information and algorithm were already implemented in IMSL library by Aird and Rice (1977) in their ZSRCH routine.

5. FUTURE DIRECTIONS.

We list here a number of directions for future research.

- (i) Optimal information and algorithms in probabilistic and average case models should be studied.
- (ii) For a number of classes that we have investigated, the optimal information is parallel. We wish to obtain general conditions under which parallel information is optimal.
- (iii) For some problems linear information is too weak. Therefore, restricted non-linear information should be investigated.
- (iv) Classes of functions which are piecewise smooth should be considered since these classes arise in practice.
- (v) Optimal information and algorithms should be implemented in software and hardware.

6. ITERATIVE MODEL OF COMPUTATION: WORST CASE.

In the 1960's and 1970's most of the research on optimal solution of nonlinear equations was devoted to the *iterative* model. In this model one constructs a sequence of points convergent to a zero of a function and wants to obtain information and an algorithm which guarantee the fastest possible convergence for every function in a given class. Thus, this can be viewed as an asymptotic worst case model with stationary iterative information;

stationary iterative information here means that a fixed set of linear functionals is repeatedly used in generating a sequence of points. Thus, for example, Newton information is evaluations of a function and its derivative on a sequence of points. Research monographs are due to Traub(1964), Ortega and Rheinboldt(1970), and Traub and Woźniakowski(1980, part B). Although our paper is not devoted to the iterative model we present a brief survey of this field.

The study of iterative complexity was initiated by the work of Traub(1961,1964). In his 1964 monograph Traub considers iterations for approximating a simple or multiple zero of a scalar nonlinear function f . The information is the values of f and its derivatives. He introduces the classification of iterations according to the information used as one-point, one-point with memory, multipoint and multipoint with memory. He proves the maximal order theorem for one-point iterations and introduces the idea of interpolatory iteration. He conjectures that memory always adds less than one to order for a one-point iteration. He introduces multipoint iterations and shows that it differs significantly from one-point iteration. He considers several complexity measures.

Woźniakowski(1972-1976) generalizes the problem of maximal order to the multivariate and infinite dimensional cases, establishes the maximal order of interpolatory algorithms for the scalar case and shows that memory does not in general increase order for the multivariate case. He introduces the concept of order of information which provides a general tool for establishing the maximal order of an iteration. He shows that maximal order depends only on information used by an algorithm and not on the structure of the algorithm, see also Traub and Woźniakowski(1976a,1976b,1979,1980a,1980b,1980c). Significant papers on optimal iteration include Brent (1973, 1976a, 1976b), Brent, Winograd and Wolfe (1973), Kacewicz (1976a, 1976b, 1979), Kung (1976) Kung and Traub (1974a,1974b,1976), Meersman (1976a, 1976b), Saari and Simon (1978), Trojan (1980a, 1980b) and Wasilkowski (1980, 1981a, 1981b, 1983).

There is also a very interesting stream of work for the approximate solution of scalar or

multivariate polynomial equations. It is assumed that complete information is available and given by the degree and coefficients of a polynomial. There is a number of interesting papers in that area. Some of them deal with average or probabilistic settings, some of them deal with different models of computation. A partial list includes: Hirsch and Smale (1979), Kim (1985), McMullen (1985), Murota (1982), Renegar (1984,1985a,1985b,1985c), Schönhage (1982), Shub and Smale (1985), Smale (1981,1985) and Wongkew (1985).

7. ITERATIVE MODEL OF COMPUTATION: AVERAGE CASE.

There have been a number of important recent papers on average case algorithmic analysis of iterative methods for computing polynomial zeros.

Pioneering work is due to Shub and Smale(1985) who analyze the average behavior of Newton-type method for approximating zeros of complex polynomials. Also for polynomial zeros Renegar(1984, 1985a,1985b) investigates the simplicial-continuation algorithm due to Kuhn,(Kuhn et al. (1984)), and the multivariate Newton method.

Shub and Smale (1985) show that, on the average, six starts of a modified Newton's method are sufficient to obtain a point z , with $|f(z)| < \epsilon$, at cost proportional to $d(d + \log 1/\epsilon)$ for a complex normalized polynomial f of degree d . Renegar(1984) assumes the normalized Lebesgue measure on the coefficients of complex polynomials and proves that for sets of polynomials of large measure the Kuhn's simplicial algorithm finds a point z with $|f(z)| < \epsilon$ and also $|z - \alpha| < \epsilon$, where $f(\alpha) = 0$, within $O(\log 1/\epsilon)$ steps. In Renegar(1985a, 1985b,1985c) he generalizes these results to the multivariate case.

We believe that a significant area for future research will be to obtain optimal information and algorithms in average case and probabilistic settings.

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