ON MAXIMIZING FUNCTIONS BY FIBONACCI SEARCH

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1. INTRODUCTION

The search for a local maximum of a function $f(x)$ involves a sequence of function evaluations, i.e., observations of the value of $f(x)$ for a fixed value of x. A sequential search scheme allows us to evaluate the function at different points, one after the other, using information from earlier evaluations to decide where to locate the next ones. At each stage, the smallest interval in which a maximum point of the function is known to lie is called the *interval of uncertainty*.

Most of the theoretical search procedures terminate the search when either the interval of uncertainty is reduced to a specific size or two successive estimates of the maximum are closer than some predetermined value. However, an additional termination rule which surprisingly has not received much attention by theorists exists in most practical search codes, namely the number of function evaluations cannot exceed a predetermined number, which we denote by N.

A well-known procedure designed for a fixed number of function evaluations is the so-called Fibonacci search method. This method can be applied whenever the function is unimodal and the initial interval of undertainty is finite. In this paper, we propose a two-stage procedure which can be used whenever these requirements do not hold. In the first stage, the procedure tries to bracket the maximum point in a finite interval, and in the second it reduces this interval using the Fibonacci search method or a variation of it developed by Witzgall.

2. THE BRACKETING ALGORITHM

A function f is *unimodal* on $[a,b]$ if there exists $a \leq \overline{x} \leq b$ such that $f(x)$ is strictly increasing for $a \leq x < \overline{x}$ and strictly decreasing for $\overline{x} < x \leq b$. It has been shown (Avriel and Wilde [2], Kiefer [6]) that the Fibonacci search method guarantees the smallest final interval of uncertainty among all methods requiring a fixed number of function evaluations. This method and its variations (Avriel and Wilde [3], Beamer and Wilde [4], Kiefer [6], Oliver and Wilde [7], Witzgall [10]) use the following idea:

Suppose y and z are two points in $[a,b]$ such that $y < z$, and f is unimodal, then

$$f(y) < f(z) \quad \text{implies} \quad y \leq \overline{x} \leq b,$$
$$f(y) > f(z) \quad \text{implies} \quad a \leq \overline{x} \leq z, \quad \text{and}$$
$$f(y) = f(z) \quad \text{implies} \quad y \leq \overline{x} \leq z.$$

Thus the property of unimodality makes it possible to obtain, after examining $f(y)$ and $f(z)$, a smaller new interval of uncertainty. When it cannot be said in advance that f is unimodel, a similar idea can be used.

Suppose that $f(x_1)$, $f(x_2)$, and $f(x_3)$ are known such that

(1) $\qquad x_1 < x_2 < x_3 \quad \text{and} \quad f(x_2) \geq \max\{f(x_1), f(x_3)\},$

then a local maximum of f exists somewhere between x_1 and x_3. Evaluation of the function at a new point x_4 in the interval (x_1, x_3) will reduce the interval of uncertainty and form a new set of three points x_1', x_2', x_3' satisfying equation (1):

Suppose $x_1 < x_4 < x_2$, then if $f(x_4) \geq f(x_2)$ let $x_1' = x_1$, $x_2' = x_4$, $x_3' = x_2$, and if $f(x_4) < f(x_2)$ let $x_1' = x_4$, $x_2' = x_2$, and $x_3' = x_3$. Similarly for $x_2 < x_4 < x_3$, if $f(x_4) > f(x_2)$ then let $x_1' = x_2$, $x_2' = x_4$, $x_3' = x_3$, and if $f(x_4) < f(x_2)$ then let $x_1' = x_1$, $x_2' = x_2$, $x_3' = x_4$.

When applying quadratic approximation methods, the new point x_4 is chosen as the maximum point of a quadratic function which approximates f. The assumption behind this method is that f is nearly quadratic, at least in the neighborhood of its maximum. However, when the number of function evaluations is fixed in advance, this method may terminate with an interval of uncertainty which is long relative to the initial one.

The quadratic approximation algorithm of Davies, Swann, and Campey [5] includes a subroutine that finds three equally spaced points satisfying equation (1). A more general method developed by Rosenbrock [8] can serve as a preparatory step for a quadratic approximation algorithm (Avriel [1]).

We now describe the search for points satisfying equation (1) in a general form that allows further development of our algorithm. The input data includes the function f, the number of evaluations N, and a set of positive numbers α_i, $i = 3, \ldots, N$.

Bracketing Algorithm:

> *Step 1.* Evaluate f at two distinct points. Denote these points by x_1 and x_2 so that $f(x_1) \leq f(x_2)$. Set $k = 3$.

> *Step 2.* Evaluate f at $x_k = x_{k-1} + \alpha_k(x_{k-1} - x_{k-2})$.
> If $f(x_k) \leq f(x_{k-1})$, stop. (A local maximum exists between x_{k-2} and x_k.)
> If $f(x_k) > f(x_{k-1})$, set $k \leftarrow k + 1$.

> *Step 3.* If $k = N + 1$, stop. (The search failed to bracket a local maximum.)
> If $k \leq N$, return to Step 2.

If the algorithm terminates in Step 2, then the function was evaluated $k \leq N$ times and a local maximum was bracketed between x_{k-2} and x_k. The interval of uncertainty may now be further reduced by evaluating the function at $N - k$ new points $x_{k+1}, \ldots, x_N$. Notice that there is already one point, x_{k-1}, in the interval of uncertainty, for which f is known.

3. REDUCTION OF THE INTERVAL OF UNCERTAINTY

In this section, we propose and analyze alternatives for selecting the increment multipliers α_k. Let $F_0 = F_1 = 1$ and $F_n = F_{n-2} + F_{n-1}$, $n = 2, 3, \ldots$, denote the Fibonacci numbers. If either

$$(2) \qquad x_{k-1} = x_{k-2} + \frac{F_{N-k}}{F_{N-k+1}}(x_k - x_{k-2})$$

or

$$(3) \qquad x_{k-1} = x_k - \frac{F_{N-k}}{F_{N-k+1}}(x_k - x_{k-2})$$

then x_{k-1} is one of the two first evaluations in a Fibonacci search with $N - k + 1$ evaluations, on the interval bounded by x_{k-2} and x_k. In this case, $x_{k+1}, \ldots, x_N$ can be chosen as the next points in this Fibonacci search. This choice

guarantees the smallest final interval of uncertainty among all other methods requiring $N - k$ additional evaluations.

If both (2) and (3) do not hold, the next points can be chosen according to Witzgall's algorithm [10]. This algorithm guarantees the smallest final interval of uncertainty in a fixed number of function evaluations when, for some reason, the first evaluation took place at some argument other than the two optimal ones.

We now show how to choose the increment multipliers α_i, $i = 3, \ldots, N - 1$, so that equations (2) or (3), according to our preference, will hold when the bracketing algorithm terminates after $k < N$ evaluations.

Equation (2) implies that

$$x_{k-1} - x_{k-2} = \frac{F_{N-k}}{F_{N-k+1}}[(x_k - x_{k-1}) + (x_{k-1} - x_{k-2})]$$

or

$$\frac{F_{N-k+1}}{F_{N-k}} = \frac{x_k - x_{k-1}}{x_{k-1} - x_{k-2}} + 1 = \alpha_k + 1.$$

Denote the value of α_k which satisfies the above equation by $\alpha_k^{(1)}$, then

$$(4) \qquad \alpha_k^{(1)} = \frac{F_{N-k+1}}{F_{N-k}} - 1 = \frac{F_{N-k-1}}{F_{N-k}} \leq 1.$$

Equation (2) holds for $k < N$ if and only if $\alpha_k = \alpha_k^{(1)}$.

Similarly, equation (3) implies that

$$x_k - x_{k-1} = \frac{F_{N-k}}{F_{N-k+1}}[(x_k - x_{k-1}) + (x_{k-1} - x_{k-2})]$$

or

$$\frac{F_{N-k+1}}{F_{N-k}} = 1 + \frac{x_{k-1} - x_{k-2}}{x_k - x_{k-1}} = 1 + \frac{1}{\alpha_k}.$$

Denote the value of α_k which satisfies this equation by $\alpha_k^{(2)}$, then

$$(5) \qquad \alpha_k^{(2)} = \frac{1}{\alpha_k^{(1)}} = \frac{F_{N-k}}{F_{N-k-1}} \geq 1.$$

Equation (3) holds for $k < N$ if and only if $\alpha_k = \alpha_k^{(2)}$.

Let $d_k = |x_k - x_{k-1}|$, $k = 1, \ldots, N$, denote the search increments, then

$$(6) \qquad d_2 = |x_2 - x_1| \quad \text{and}$$

$$d_k = \alpha_k d_{k-1} = \alpha_k \cdot \alpha_{k-1} \cdot \cdots \cdot \alpha_3 |x_2 - x_1|, \quad k = 3, \ldots, N.$$

Denote the search increments by $d_k^{(1)}$ and $d_k^{(2)}$ when $\alpha_k^{(1)}$ and $\alpha_k^{(2)}$ are chosen, respectively, for $k = 2, \ldots, N - 1$. Then equations (4) and (6) yield

$$d_k^{(1)} = \frac{F_{N-k-1}}{F_{N-k}} \cdot \frac{F_{N-k}}{F_{N-k+1}} \cdot \cdots \cdot \frac{F_{N-4}}{F_{N-3}} \cdot |x_2 - x_1| = \frac{F_{N-k-1}}{F_{N-3}}|x_2 - x_1|,$$

$k = 2, \ldots, N - 1.$

If the bracketing algorithm terminates after $k < N$ evaluations, then the maximum is located in an interval of length

$$|x_k - x_{k-2}| = d_k^{(1)} + d_{k-1}^{(1)} = \frac{F_{N-k-1} + F_{N-k}}{F_{N-3}}|x_2 - x_1| = \frac{F_{N-k+1}}{F_{N-3}}|x_2 - x_1|.$$

This interval is further searched by a Fibonacci search with $N - k + 1$ evaluations (including the one in x_{k-1}) which reduces its length by a factor $(F_{N-k+1})^{-1}$. Consequently, the length of the final interval is

$$\frac{|x_2 - x_1|}{F_{N-3}},$$

independent of k. This length is satisfactorily small in comparison with

$$\frac{|x_2 - x_1|}{F_{N-2}},$$

which can be achieved by $N - 2$ evaluations if f is known to be unimodal with a maximum between x_1 and x_2.

Suppose, however, that the bracketing algorithm terminates after N evaluations without bracketing a local maximum. The total size of the searched interval is

$$\sum_{k=2}^{N-1} d_k^{(1)} = \frac{|x_2 - x_1|}{F_{N-3}}(F_{N-3} + F_{N-4} + \cdots + F_0) = \frac{F_{N-1}}{F_{N-3}}|x_2 - x_1|$$

$$= \left(1 + \frac{F_{N-2}}{F_{N-3}}\right)|x_2 - x_1| \le 3|x_2 - x_1|.$$

In fact, when N is large, this sum approaches $(1 + \tau)|x_2 - x_1|$ where $\tau \cong 1.618$ satisfies $\tau^2 = 1 + \tau$. The cost of obtaining a small final interval in case of success is in searching a relatively small interval and thus increasing the chances that the bracketing algorithm will fail.

This default can be overcome by using $\alpha_k^{(2)}$ rather than $\alpha_k^{(1)}$. In this case,

$$d_k^{(2)} = \frac{F_{N-3}}{F_{N-k-1}}\ \frac{F_{N-k+1}}{F_{N-k}}\ \cdots\ \frac{F_{N-3}}{F_{N-4}}|x_2 - x_1| = \frac{F_{N-3}}{F_{N-k-1}}|x_2 - x_1|,$$

$$k = 2, \ldots, N - 1.$$

The sequence $d_k^{(2)}$ increases with k so that a larger interval is scanned, and it is less likely that the bracketing algorithm will fail. In practice, some of the last increments $d_k^{(2)}$ may be replaced by smaller increments, possibly by $d_k^{(1)}$.

4.   SUMMARY

We suggest a two-stage search procedure for maximizing functions by a fixed number of evaluations. The first stage is a quite standard bracketing subroutine and the second is either the regular Fibonacci search or the modified method of Witzgall. During the first stage, the kth evaluation is at the point x_k calculated from $x_k = x_{k-1} + \alpha_k(x_{k-1} - x_{k-2})$. We suggest three alternatives:

A.   Let $\alpha_k = \alpha_k^{(1)} \le 1$. In case of success, proceed by Fibonacci search to obtain a small final interval.

B.   Let $\alpha_k = \alpha_k^{(2)} > 1$. In case of success, proceed by Fibonacci search.

The chances for success are better than in case A, but the final interval is longer.

C.   Let $\alpha_k > 0$ be arbitrary and proceed by Witzgall's method.

We note that different alternatives may be chosen for different values of k.

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