

Bracketing an Optima in Univariate Optimization

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Abstract: In this article, we consider some problems of bracketing an optimum point for a real-valued, single variable function. We show that, no one method, satisfying certain assumptions and requiring a bounded number of function evaluations, can exist to bracket the minimum point of every strongly unimodal function. A similar result is given also for the problem of bracketing the global minimum for multimodal functions. The results extend to some related problems of locating the global minimum point.

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1. Introduction

Consider a single variable real-valued function $f(x): R \rightarrow R$. To find an optima, a minima or a maxima, it is often assumed that, such a point lies in the interval $[a, b]$. Or, in other words, an optima is bracketed in $[a, b]$. The methods of bisection, golden section or Fibonacci search (see, e.g., Bazaraa et al. 2006), for example, for univariate optimization require such an interval. The fact that the optima lies in $[a, b]$ may be deduced from some theoretical or practical

considerations. Otherwise, obtaining such an interval would be the initial problem, which needs to be solved.

We concern ourselves with the problem of finding an interval containing the global minimum point for a real-valued, single variable function. This is an area, which seems to have got little attention in the relevant literature. First, we consider functions, which are strongly unimodal. We show that it is impossible to have a single, exact method, satisfying some very general assumptions, which would require a bounded number function evaluations to give a bracketing interval, for all such functions. A corresponding result is given for the problem of bracketing the global minimum, for multimodal functions. The results given here have some similarity with a result given by Zhu 2004. The author has shown that unconstrained global optimization problem for multivariable, continuous functions in the unbounded domain is undecidable, i.e., such a problem cannot have a solution algorithm. The results given by us are different in the ways that, these are for bracketing for a single variable function, though these can be extended to the problems of locating the global minimum. The result about multimodal functions holds for a bounded domain also. Further, we have a different approach, wherein we make some assumptions about the methods to be used for the given purpose, in the proofs. We deal with a restricted set of methods, not *all* methods. More specifically, we consider only deterministic search methods, which are self-contained. That is, the methods would require no or little prior information about the function and would proceed only according to the information that is obtained by evaluating the function at some points.

The results of this article are given in the next section. This is followed by a discussion on the relevance of such results and some related issues.

2. Observations on Bracketing

2.1. Bracketing for a Unimodal Function

First we consider the problem of bracketing the minimum point for a unimodal function. We make the following assumptions about the functions and methods used.

2.1.1. Assumptions about the Functions

We assume the following for the functions.

- i) The function $f(x): R \rightarrow R$ is defined on $(-\infty, \infty)$ and is finite $(-\infty < f(x) < \infty, -\infty < x < \infty)$ and continuous. It is strongly unimodal, i.e., it has a unique local and global minimum point x^* $(-\infty < x^* < \infty)$, so that $f(x_1) > f(x_2)$ if $x_1 < x_2 \leq x^*$, $f(x_1) > f(x_2)$ if $x_1 > x_2 \geq x^*$, $-\infty < x_1, x_2 < \infty$.

2.1.2. Assumptions about the Method

The method is required to find a finite interval, dependant on the function given, as $[x_1, x_2](-\infty < x_1 < x_2 < \infty)$ which includes the minimum point of the function $f(x)$, i.e., $x_1 \leq x^* \leq x_2$, for any function which satisfies the assumptions in 2.1.1. We consider the methods, which satisfy the following assumptions.

- i) No other information is known at the beginning, except that the function satisfies the assumption in 2.1.1. Subsequently, all information is deduced based on function evaluations at different points. Method proceeds in iterations, in each of which the function is evaluated only at one point and calculations are done with values of points and functional values at such points, evaluated in the current and earlier iterations, if any. In the conclusion of an iteration, either a correct bracketing interval is given or a distinct point, not already evaluated, is selected for next evaluation.

Thus, the method generates a sequence of 2-tuples $(x^{(i)}, f(x^{(i)}))$, $i = 1, 2, \dots$, where $x^{(i)}$ denotes the point for evaluation and $f(x^{(i)})$ the functional value at this point at the i -th iteration.

- ii) The selection of the point for first evaluation ($x^{(1)}$) is fixed and same for any function.
- iii) The selection of the point for i -th evaluation, $x^{(i)}$, $i = 2, 3, \dots$, is dependant only on $x^{(j)}$, $f(x^{(j)})$, $j = 1, 2, \dots, i-1$. The output of a bracketing interval also depends only on such values.

So, if for two functions these values are same for $j = 1, 2, \dots, i-1$, the points selected for i -th evaluation for the two functions must be the same. If, in such a case, a bracketing interval is given after $(i-1)$ function evaluations, the same interval would be given as the output for the other function.

- iv) Bracketing is done only with points for which functional values are calculated. That is, the bracketing interval is given as, $[x^{(i)}, x^{(j)}]$, $i, j \in \{1, 2, \dots\}$, $x^{(i)} < x^{(j)}$.

- v) If at any iteration, three points as $x^{(i)} > x^{(j)} > x^{(k)}$ have been evaluated such that, $f(x^{(i)}) \geq f(x^{(j)})$, $f(x^{(k)}) \geq f(x^{(j)})$, in that iteration or earlier, the method must stop with a bracketing interval.

The above assumptions are quite general in nature, and it is not conceivable that any deterministic method which is practicable, does not use more information about the function, would not satisfy such assumptions. Assumption (i) defines an iteration. Assumption (ii) is reasonable because at the start all the information which is known is that the function is strongly unimodal. The same information is known for any input function. Assumption (ii) and (iii) tell about the deterministic nature of the method. By Assumption (iv), bracketing is done only with points at which the function has been evaluated. This assumption, primarily, is to make the analysis simpler. If bracketing is done with points at which the function has not been evaluated, but in a way that satisfies other assumptions, another method can be thought of which is identical

except that at the end extra evaluations are done at the end points of the bracketing interval. By Assumption (v), we consider only “efficient” methods, which do not do unnecessary calculations. No further calculations are done, if a bracketing interval can be determined with points for which the function has been evaluated.

2.1.3. Result regarding such Bracketing

With the above assumptions, we have the proposition as given next.

Proposition 2.1. *There cannot exist a single method, satisfying the assumptions (2.1.2), with which a finite interval as $[x_1, x_2] (-\infty < x_1 < x_2 < \infty)$ containing the minimum point x^* (i.e., $x_1 \leq x^* \leq x_2$) can be determined with a number of function evaluations that is bounded, for every function, satisfying the assumptions (2.1.1).*

Proof. Suppose, there exists such a method which determines an interval as required with maximum N function evaluations, where N is known and independent of the function.

Note that, there must be at least two function evaluations. Consider a function $f(x)$ for which n ($N \geq n \geq 2$) function evaluations are required in the method to give a correct bracketing interval. Recall that $x^{(i)}$ denotes the point for the i -th function evaluation. After $(n-1)$ evaluations, arrange the points in increasing order, $x^{(R(1))} < x^{(R(2))} < \dots < x^{(R(n-1))}$, where i , $R(i) \subset \{1, 2, \dots, n-1\}$, $R(i) \neq R(j)$, if $i \neq j$. It must be the case that, either, $f(x^{(R(1))}) > f(x^{(R(2))}) > \dots > f(x^{(R(n-1))})$; or, $f(x^{(R(1))}) < f(x^{(R(2))}) < \dots < f(x^{(R(n-1))})$. Otherwise, a bracketing interval would be found before n evaluations. We shall consider the first case only, two cases being similar.

Construct a function $g(x)$ as in the following. Let, after n evaluations, $B = \max_{i \in \{1, 2, \dots, n\}} \{x^{(i)}\}$. Take $\Delta A > 0$. The points are arranged in increasing order, after $(n-1)$ evaluations.

$$\begin{aligned}
 (1) \quad g(x) &= f(x^{(R(1))}) + \alpha(x^{(R(1))} - x), -\infty < x \leq x^{(R(1))}, \\
 &= f(x^{(R(i))}) + (x - x^{(R(i))}) \frac{f(x^{(R(i+1))}) - f(x^{(R(i))})}{x^{(R(i+1))} - x^{(R(i))}}, x^{(R(i))} < x \leq x^{(R(i+1))}, \\
 &\hspace{25em} i = 1, 2, \dots, n-2; \\
 &= f(x^{(R(n-1))}) - (x - x^{(R(n-1))}) \frac{\Delta A}{x^{(*)} - x^{(R(n-1))}}, x^{(R(n-1))} < x \leq x^{(*)}; \\
 &= (f(x^{(R(n-1))}) - \Delta A) + \alpha(x - x^{(*)}), x^{(*)} < x < \infty,
 \end{aligned}$$

where $\alpha > 0$, $x^{(*)} > B$ is the global minimum of $g(x)$ with value $(f(x^{(R(n-1))}) - \Delta A)$.

The function $g(x)$ satisfies the assumptions. The choice of the first point for evaluation for $g(x)$ is also $x^{(1)}$. Subsequently, all $n-1$ points chosen would be the same, since $f(x^{(i)}) = g(x^{(i)})$, $i = 1, 2, \dots, n-1$. The method cannot conclude correctly after n evaluations for $g(x)$, since $x^{(*)}$ is not in any interval as $[x^{(R(s))}, x^{(R(t))}]$, $s, t \in \{1, 2, \dots, n\}$. Hence the method either fails for $g(x)$ or requires more function evaluations than n . Thus, a correct method requiring bounded number of function evaluations for all functions cannot exist. This completes the proof. \square

Remark 2.1. From the above proposition, also, there cannot exist any method, satisfying the assumptions, with which the global minimum point can be located for any strongly unimodal function, with a bounded number of function evaluations. This is because, if a method finds the global minimum x^* , in next two iterations points as $(x^* + \Delta x)$ and $(x^* - \Delta x)$, with a pre-fixed

$\Delta x > 0$, can be evaluated redundantly and a bracketing interval as $[x^* + \Delta x, x^* - \Delta x]$ can be given.

2.1.4. An Example of a Method

Here we give an example of a method which satisfies the assumptions. Also, $f(x)$ is a strongly unimodal function.

i. Select $x_0, \Delta x > 0, \alpha > 1$.

Take $x^{(1)} = x_0; x^{(2)} = x_0 + \alpha \Delta x; x^{(3)} = x_0 - \alpha \Delta x$.

If $f(x^{(2)}) \geq f(x^{(1)}) \geq f(x^{(3)})$, $\Delta x = -\Delta x$; $i = 3, j = 1$ and go to step iii; (minimum lies on the left);

If $f(x^{(3)}) \geq f(x^{(1)}) \geq f(x^{(2)})$, $\Delta x = \Delta x$; $i = 2, j = 1$ and go to step iii; (minimum lies on the right);

If $f(x^{(2)}) \geq f(x^{(1)}), f(x^{(3)}) \geq f(x^{(1)})$, output bracketing interval as $[x^{(2)}, x^{(3)}]$ and stop.

ii. If $f(x^{(i)}) \geq f(x^{(j)})$, give bracketing interval as $[x^{(i)}, x^{(k)}]$ and stop. Else, go to step iii.

iii. $k = j; j = i$; if $i = 2, i = 4$, else, $i = i + 1$; $\Delta x = \alpha \Delta x; x^{(i)} = x_0 + \alpha \Delta x$;

Go to step ii.

Above method is commonly referred to as “Acceleration Method” for bracketing and is often used in practice. It may be an acceptable method in the practical sense, but does not have the required theoretical properties, as explained next.

A particular choice of x_0, α and Δx defines one method, for the application of the Proposition 2.1. In this method, the points selected for function evaluations are dependent only on the choice of x_0 and other parameters, which is arbitrary. If the minimum point is in $[x_0 - \alpha \Delta x, x_0 + \alpha \Delta x]$, it is bracketed with 3 function evaluations with the method. If it is in $[x_0 + \alpha^{m-2} \Delta x, x_0 + \alpha^m \Delta x]$ or $[x_0 + \alpha^m \Delta x, x_0 + \alpha^{m-2} \Delta x]$, the method will require $m+2$ ($m \geq 2$) function evaluations to do so. Thus, no bound can exist on the number of function evaluations, for any choice of the parameters. A similar method for bracketing is discussed in Rardin 1998.

2.2. Bracketing for Multimodal Functions

In actuality, the concerned function may not be unimodal or it may not be known whether it is unimodal or not. Next we consider a problem of, perhaps, greater practical relevance- the problem of bracketing the global minimum for the case of single variable multimodal function. We have an analogous result, which holds even if the function is defined over a bounded domain.

2.2.1. Assumption about the Function

i) Let $f(x): [a, b] \rightarrow R$, where $a, b \in R$, $-\infty < a < b < \infty$, $b - a > 1/K$, where K is a fixed positive integer. The numbers a, b may depend on the function. The function is finite ($-\infty < f(x) < \infty$, $b \leq x \leq a$) and continuous in $[a, b]$. There is a unique global minimum x^* of $f(x)$ in $[a, b]$, such that, $f(x) > f(x^*)$, $x \neq x^*$, $x, x^* \in [a, b]$.

2.2.2. Assumptions about the Method

The method is required to find a finite interval, dependant on the function given, as $[x_1, x_2] (a \leq x_1 < x_2 \leq b, x_2 - x_1 < b - a)$ which includes the global minimum point, $x_1 \leq x^* \leq x_2$. We make the following assumptions about the method.

i) The selection of the point for first evaluation is the same for any two functions, having the same domain interval $[a, b]$.

Other assumptions are as in Assumptions (i), (iii) and (iv) in 2.1.2.

2.2.3. Result on Bracketing for Multimodal Functions

We give the following proposition for this case.

Proposition 2.2: *There cannot exist a single method, satisfying the assumptions (2.2.2), with which an interval as $[x_1, x_2] (a \leq x_1 < x_2 \leq b, x_2 - x_1 < b - a)$, containing the global minimum point $(x_1 \leq x^* \leq x_2)$ can be determined with a number of function evaluations that is bounded, for every function satisfying the assumptions (2.2.1).*

Proof. The proof is in the same line as in Proposition 2.1, using the same notation.

Suppose, there exists such a method which determines an interval as required with maximum N function evaluations, where N is known and independent of the function.

Note that, there must be at least two function evaluations. Consider a function $f(x)$ for which n ($N \geq n \geq 2$) function evaluations are required in the method to give a correct bracketing interval. After n evaluations, arrange the points in increasing order, $x^{(R(1))} < x^{(R(2))} < \dots < x^{(R(n))}$, where $s, R(s) \subset \{1, 2, \dots, n\}$, $R(s) \neq R(t)$, if $s \neq t$. Let it be correctly concluded for $f(x)$ that, $x^{(R(i))} \leq x^* \leq x^{(R(j))}$, for some $i, j \subset \{1, 2, \dots, n\}$, $i < j$.

Construct another function $g(x)$ in the following way.

Get $x^{(R(k))}, x^{(R(k+1))}$ such that, either, $a \leq x^{(R(k))} < x^{(R(k+1))} \leq x^{(i)}$, or, $x^{(j)} \leq x^{(R(k))} < x^{(R(k+1))} \leq b$. Such a k is possible, since this cannot be the case that, $x^{(i)} = a$ and $x^{(j)} = b$. Let, $A = \min \{ \min_{i \in \{1, 2, \dots, n\}} \{ f(x^{(i)}) \}, f(a), f(b) \}$, $\Delta A > 0$. Then,

$$\begin{aligned}
 (2) \quad g(x) &= f(a) + (x - a) \frac{f(x^{(R(1))}) - f(a)}{x^{(R(1))} - a}, a \leq x \leq x^{(R(1))}; \\
 &= f(x^{(R(s))}) + (x - x^{(R(s))}) \frac{f(x^{(R(s+1))}) - f(x^{(R(s))})}{x^{(R(s+1))} - x^{(R(s))}}, x^{(R(s))} < x \leq x^{(R(s+1))}, \\
 &\hspace{25em} s = 1, 2, \dots, k - 1; \\
 &= f(x^{(R(k))}) + (x - x^{(R(k))}) \frac{(A - \Delta A) - f(x^{(R(k))})}{x^{(*)} - x^{(R(k))}}, x^{(R(k))} < x \leq x^{(*)}; \\
 &= (A - \Delta A) + (x - x^{(*)}) \frac{f(x^{(R(k+1))}) - (A - \Delta A)}{x^{(R(k+1))} - x^{(*)}}, x^{(*)} < x \leq x^{(R(k+1))}; \\
 &= f(x^{(R(s))}) + (x - x^{(R(s))}) \frac{f(x^{(R(s+1))}) - f(x^{(R(s))})}{x^{(R(s+1))} - x^{(R(s))}}, x^{(R(s))} < x \leq x^{(R(s+1))},
 \end{aligned}$$

$$s = k + 1, k + 2, \dots, n - 1;$$

$$= f(x^{(R(n))}) + (x - x^{(R(n))}) \frac{f(b) - f(x^{(R(n))})}{b - x^{(R(n))}}, x^{(R(n))} \leq x \leq b;$$

where $x^{(*)} = (x^{(R(k))} + x^{(R(k+1))}) / 2$ is the global minimum of $g(x)$ with value $(A - \Delta A)$. The function $g(x)$ satisfies the assumptions. The first point for evaluation for $g(x)$ is also $x^{(1)}$. Subsequently, all $n-1$ points chosen would be the same, since $f(x^{(s)}) = g(x^{(s)})$, $s = 1, 2, \dots, n$, by construction. Hence, after n function evaluations, the method would conclude the same for $g(x)$ that the global minimum point is in $[x^{(R(i))}, x^{(R(j))}]$. But, this would be a wrong conclusion for $g(x)$ and so the method fails for $g(x)$.

Thus, such a method, as supposed, cannot exist, proving the proposition. \square

Remark 2.2. From the above proposition, it is also clear that, no such method, satisfying the required assumptions, can exist to bracket only the global minimum, but no other local minimum (with usual definition) being in the bracketing interval, for the said type of functions. This is simply because such an interval brackets the global minimum point also.

Remark 2.3. Further, there cannot exist any method, satisfying the required assumptions, to locate the global minimum of any such function.

3. Discussions

Finding an interval containing the global minimum point for a single variable function is an important problem in single variable optimization, which, in turn, is often used as a step in optimization of multivariable functions. We have presented results implying the impossibility of a single, universal method, following some assumptions, which may find an interval containing the minimum point for a strongly unimodal function, or a method that finds an interval containing the global minimum for multimodal functions. In the later case, the function may be defined over a

bounded domain. The methods are allowed to carry out function evaluations and calculations with such values. No information such as differentiability is used in the methods. The methods considered are, essentially, deterministic search methods, which use no or little prior information about the function.

The results given in this article highlight the theoretical difficulty inherent in the problems considered. As an alternative approach, different methods may be applied for different functions, dependant on the properties of respective functions. Randomized algorithms may be more suitable for the purpose. Efficient methods for bracketing and locating a global minima for different types of problems and different functions would indeed be very useful in various ways. Extensions of the results given in this article may be possible and also would be desired.

4. References

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