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Optimal Search under Constraints

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Abstract In general, if we know the values a and b at which a continuous function has different signs – and the function is given as a black box – the fastest possible way to find the root x for which $f(x) = 0$ is by using bisection (also known as binary search). In some applications, however – e.g., in finding the optimal dose of a medicine – we sometimes cannot use this algorithm since, for avoid negative side effects, we can only try value which exceed the optimal dose by no more than some small value $\delta > 0$. In this paper, we show how to modify bisection to get an optimal algorithm for search under such constraint.

1 Where This Problem Came From

Need to select optimal dose of a medicine. This research started with a simple observation about how medical doctors decide on the dosage. For many chronic health conditions like high cholesterol, high blood pressure, etc., there are medicines that bring the corresponding numbers back to normal. An important question is how to select the correct dosage:

- on the one hand, if the dosage is too small, the medicine will not have the full desired effect;
- on the other hand, we do not want the dosage to be higher than needed: every medicine has negative side effects, side effects that increase with the increase in dosage, and we want to keep these side effects as small as possible.

In most such cases, there are general recommendations providing a range of possible doses depending on the patient's age, weight, etc., but a specific dosage within this

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range has to be selected individually, based on how this patient's organism reacts to this medicine.

How the first doctor selected the dose. It so happened that two people having similar conditions end up with the same daily dosage of 137 units of medicine, but interestingly, their doctors followed a different path to this value.

For the first patient, the doctor seems to have followed the usual bisection algorithm:

- this doctor started with the dose of 200 – and it worked,
- so, the doctor tried 100 – it did not work,
- the doctor tried 150 – it worked,
- the doctor tried 125 – it did not work,
- so, the doctor tried 137 – and it worked.

The doctor could have probably continued further, but the pharmacy already had trouble with maintaining the exact dose of 137, so this became the final arrangement.

This procedure indeed follows the usual bisection (= binary search) algorithm (see, e.g., [1]) – which is usually described as a way to solve the equation $f(x) = 0$ when we have an interval $[a,b]$ for which $f(a) < 0 < f(b)$. In our problem, $f(a)$ is the difference between the effect of the dose a and the desired effect:

- if the dose is not sufficient, this difference is negative, and
- if the dose is sufficient, this difference is non-negative (positive or 0).

In the bisection algorithm, at each iteration, we have a range $[\underline{x},\overline{x}]$ for which $f(\underline{x}) < 0$ and $f(\overline{x}) > 0$. In the beginning, we have $[\underline{x},\overline{x}] = [a,b]$. At each iteration, we take a midpoint $m = \dfrac{\underline{x}+\overline{x}}{2}$ and compute $f(m)$. Depending on the sign of $f(m)$, we make the following changes:

- if $f(m) < 0$, we replace $\underline{x}$ with m and thus, get a new interval $[m,\overline{x}]$;
- if $f(m) > 0$, we replace $\overline{x}$ with m and thus, get a new interval $[\underline{x},m]$.

In both cases, we decrease the width of the interval $[\underline{x},\overline{x}]$ by half. We stop when this width becomes smaller than some given value $\varepsilon > 0$; this value represents the accuracy with which we want to find the solution.

In the above example, based on the first experiment, we know that the desired dose is within the interval $[0,200]$. So:

- we try $m = 100$ and, after finding that $f(m) < 0$ (i.e., that the dose $m = 100$ is not sufficient), we come up with the narrower interval $[100,200]$;
- then, we try the new midpoint $m = 150$, and, based on the testing result, we come up with the narrower interval $[100,150]$;
- then, we try the new midpoint $m = 125$, and, based on the testing result, we come up with the narrower interval $[125,150]$;
- in the last step, we try the new midpoint $m = 137$ (strictly speaking, it should be 137.5, but, as we have mentioned, the pharmacy cannot provide such an accuracy); now we know that the desired value is within the narrower interval $[125,137]$.

Out of all possible values from the interval $[125, 137]$, the only value about which we know that this value is sufficient is the value 137, so this value has been prescribed to the first patient.

The second doctor selected the same dose differently. Interestingly, for the second patient, the process was completely different:

- the doctor started with 25 units;
- then – since this dose was not sufficient – the dose was increased to 50 units;
- then the dose was increased to 75, 100, 125 units, and, finally, to 150 units.

The 150 units dose turned out to be sufficient, so the doctor knew that the optimal dose is between 125 and 150. Thus, this doctor tried 137, and it worked.

Comment. Interestingly, in contrast to the first doctor, this doctor could not convince the pharmacy to produce a 137 units dose. So this doctor's prescription of this dose consists of taking 125 units and 150 units in turn.

Why the difference? Why did the two doctors use different procedures?

Clearly, the second doctor needed more steps – and longer time – to come up with the same optimal dose: this doctor used 7 steps (25, 50, 75, 100, 125, 150, 137) instead of only 5 steps used by the first doctor (200, 100, 150, 125, 137). Why did this doctor not use a faster bisection procedure?

At first glance, it may seem that the second doctor was not familiar with bisection – but clearly this doctor *was* familiar with it, since, after realizing that the optimal does is within the interval $[125, 150]$, he/she checked the midpoint dose of 137.

The real explanation of why the second doctor did not use the faster procedure is that the second doctor was more cautious about possible side effects – probably, in this doctor's opinion, the second patient was vulnerable to possible side effects. Thus, this doctor decided not to increase the dose too much beyond the optimal value, to minimize possible side effects – while the first doctor, based on the overall health of the first patient, was less worried about possible side effects.

Natural general question. A natural next question is: under such restriction on possible tested values x, what is the optimal way to find the desired solution (i.e., to be more precise, the desired ε-approximation to the solution)?

It is known that if we do not have any constraints, then bisection is the optimal way to find the solution to the equation $f(x) = 0$; see, e.g., [1]. So, the question is – how to optimally modify bisection under such constraints?

2 Precise Formulation of the Problem and the Optimal Algorithm

Definition 1. *Let $f(x)$ be a function from real numbers to real numbers, and let $\delta > 0$ be a real number. We say that a number x is* δ-f-legitimate *if $x \le x_0 + \delta$ for some number x_0 for which $f(x_0) = 0$.*

Definition 2. *By* search under constraints*, we mean the following problem:*

- Given:
  - *(computable) real numbers $a < b$, $\varepsilon > 0$, and $\delta > 0$, and*
  - *an algorithm that – for some continuous function $f(x)$ for which $f(a) < 0 < f(b)$ – given a δ-f-legitimate value x, checks whether $f(x) < 0$ or $f(x) \geq 0$.*
- Find: *a value x such that $f(x) \geq 0$ and $|x - x_0| \leq \varepsilon$ for some value x_0 for which $f(x_0) = 0$.*

Comment. The corresponding algorithm can ask, given a δ-f-legitimate value x, whether $f(x) < 0$ or not. Each such call to f will be counted as one step.

Definition 3. *We say that an algorithm for solving search-under-constraints problems is (asymptotically)* optimal *if:*

- *this algorithm always produces the solution, and*
- *for each instance (a, b, f, δ) of the search under constraints problem, this algorithms uses, for all sufficiently small ε, the smallest possible number of calls to f.*

Proposition 1. *The following is the optimal algorithm for solving search-under-constraints problems:*

- *First, for the values $a_i \stackrel{\text{def}}{=} a + i \cdot \delta$ for $i = 1, 2, \ldots$, if $a_i < b$, we check whether $f(a_i) < 0$. We stop:*
  - *either when we found i for which $f(a_i) \geq 0$*
  - *or if we exhausted all i's without finding such an i, i.e., if we have $f(a_i) < 0$ and $a + (i+1) \cdot \delta \geq b$.*
- *If we have stopped because we found i for which $f(a_i) \geq 0$, then we apply bisection to the interval $[a_{i-1}, a_i]$ to find the desired solution.*
- *If we have stopped because we have reached i for which $f(a_i) < 0$ and $b < a + (i+1) \cdot \delta$, then we apply bisection to the interval $[a_i, b]$.*

Comments.

- This is exactly what the second doctor did, with $\delta = 25$.
- When δ is large enough, i.e., when $\delta \geq b - a$ and thus, $a + \delta \geq b$, this algorithm becomes the bisection – exactly what the first doctor did.

Proof of Proposition 1: main idea. Let us first show that this algorithm is legitimate, i.e., that in this algorithm, we only test whether $f(x) < 0$ for δ-f-legitimate values x. Indeed, if we know that $f(x) < 0$ for some x, then, since $f(x) < 0 < f(b)$, there exists a value $x_0 \in [x, b]$ for which $f(x_0) = 0$. So, for $x' = x + \delta$, from $x \leq x_0$, we conclude that $x' \leq x_0 + \delta$. Thus, after we found out that $f(a_i) < 0$ checking whether $f(a_{i+1}) < 0$ for $a_{i+1} = a_i + \delta$ is δ-f-legitimate.

The faster we get to some δ-f-legitimate value x for which $f(x) \geq 0$, the faster we will find the solution. Can we go faster than by increasing by δ every time? Not really. Indeed, if we take $x' > x + \delta$, then it is easy to come up with a piece-wise linear monotonic function $f(x)$ for which the only root x_0 if $x_0 = x + (x' - (x + \delta))/2$. In this case, we will have

$$x' - (x_0 + \delta) = (x' - (x + \delta)) - (x_0 - x) = (x' - (x + \delta))/2 > 0,$$

so $x' > x_0 + \delta$ and asking whether $f(x') > 0$ is not legitimate.

We cannot go faster than by increasing the value by δ, and increasing by δ is legitimate, so to find the result as fast as possible, we should increase exactly by δ every time – exactly as our algorithm does.

One can easily check that if a value x is δ-f-legitimate, then all smaller values are also δ-f-legitimate. Thus, once we have found a δ-f-legitimate value x for which $f(x) \geq 0$, we can use the optimal bisection algorithm – since all the values that we try in this algorithm will also be δ-f-legitimate.

The proposition is proven.

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References

1. Th. H. Cormen, C. E. Leiserson, R. L. Rivest, and C. Stein, *Introduction to Algorithms*, MIT Press, Cambridge, Massachusetts, 2009.