Finite dimensional optimization methods
One-dimensional minimization

2021

In many descent methods it is necessary to minimize an objective function along the chosen direction, i.e., to solve the problem of one-dimensional minimization.

If we have a function of one variable and can determine that a solution of our problem lies in a particular interval $[a, b]$, then we can select a point in this interval, say c. If we can determine whether or not the solution lies in $[a, c]$ or $[c, b]$, then we can restrict the domain in which the solution lies.

In that case, we can try again: consider a new interval and get a bound on the solution.

Among such methods which do not use derivatives of functions the most famous methods are methods of a dichotomy (bisection of the interval), Golden Section and Fibonacci.

These methods are applicable to unimodal functions.

In each of these methods consistently the interval containing the minimum point is reduced.

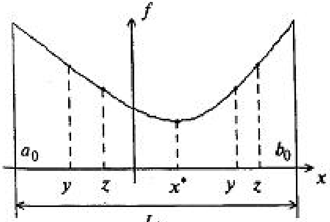
Unimodal functions.

A function $f : \mathbb{R} \to \mathbb{R}$ is called *unimodal* on an interval $[a, b]$, if there exists a point $x^* \in [a, b]$, for which the inequalities

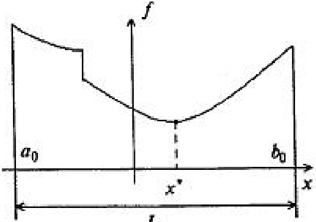
$$\begin{aligned} f(x_1) > f(x_2), &\quad \text{if } x_1 < x_2 < x^* \quad x_1, x_2 \in [a, b], \\ f(x_1) < f(x_2), &\quad \text{if } x^* < x_1 < x_2 \quad x_1, x_2 \in [a, b]. \end{aligned}$$

hold.

Unimodality is an important functional property for optimization.



a



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An unimodal function f on $[a, b]$ has the only local minimum.
It may not be differentiable and even discontinuous.
From the definition, the unimodal function f implies that if its value is calculated at four points a, x, y, b, of the interval $[a, b]$, then always there exists a subinterval which does not contain a minimizer and it can be removed.

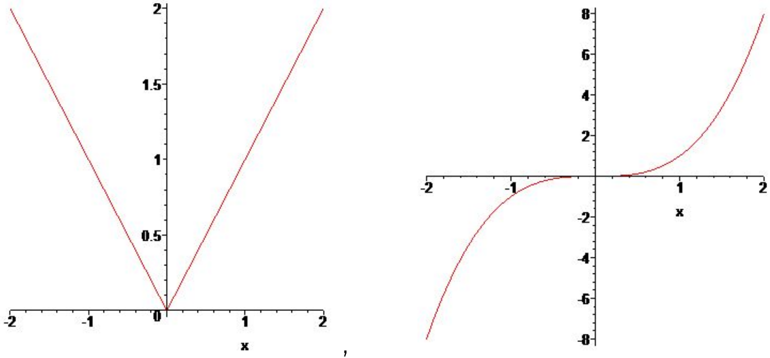

Fig. 1. Unimodal functions

Lemma 1. Suppose f is strictly unimodal on the interval $[a, b]$, points

$$x, y \in (a, b),\ x < y.$$

Let x^* be a single minimum point of f on this interval. Then

1) If $f(x) \leq f(y)$, then $x^* \leq y$.

2) If $f(x) \geq f(y)$, then $x^* \geq x$.

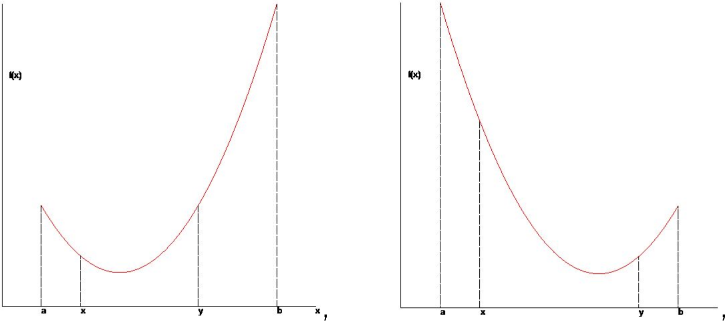

Fig. 2.

Several one-dimensional optimization approaches will be considered:

1) Dichotomous search;

2) Fibonacci search;

3) Colden section search;

4) Quadratic interpolation method.

All described methods find a segment on which there is a minimizer x^*.

This segment is called a segment of uncertainty.

Thus, if the approximate value of x^* is taken in the middle of this segment, then the error of the method is half of the length of the interval of uncertainty.

For finding the minimum point of the function of one variable in general it is necessary to specify the initial interval $[a, b]$, which contains a minimizer.
In search methods, an interval $[x_p, y_p]$ containing x^* is established and then repeatedly is reduced on the basis of function evaluations until as an obtained bracket $[x_{p,k}, y_{p,k}]$ is sufficiently small.
The minimizer can be assumed to be the midpoint of the interval $[x_{p,k}, y_{p,k}]$.
These methods can be applied to any function and differentiability of f is not essential.

The dichotomy method

This method is numerically an analogue of the dichotomy method (bisection of the interval) for solving an equation

$$f(x) = 0.$$

The function f should be a strongly unimodal on the interval [a,b]. On every step the dichotomy method allows to reduce almost half the length of the interval containing the minimum point. In this method the values of f are calculated at two specific points on each iteration.

Algorithm

Step 0. Choose an initial interval $[a, b]$, which comprises a local minimum, a tolerance $\varepsilon > 0$ and a sufficiently small $\delta > 0$.
Let $a_0 = a;\ b_0 = b$.
Step 1. Calculate the internal points

$$x_1 = \frac{a+b}{2} - \delta$$

and

$$y_1 = \frac{a+b}{2} + \delta,$$

located at the distance of 2δ from the middle of the segment $[a, b]$. (midpoint)

Calculate the function f at the points x_1 and y_1 $(f(x_1),\ f(y_1))$
If $f(x_1) \leq f(y_1)$, then put $a_1 = a,\ b_1 = y_1$.
If $f(x_1) \geq f(y_1)$, then put $a_1 = x_1,\ b_1 = b$.
The length of the received segment $[a_1, b_1]$ is equal to

$$\Delta_1 = \frac{b_1 - a_1}{2} + \delta = \frac{b - a}{2} + \delta.$$

The point $x^* \in [a_1, b_1]$ can be taken as a local minimizer.
Of course, at each step, it is necessary to check the length of the resulting segment.
It must be greater than 2δ, because the distance between the points x_1 and y_1 is equal 2δ.

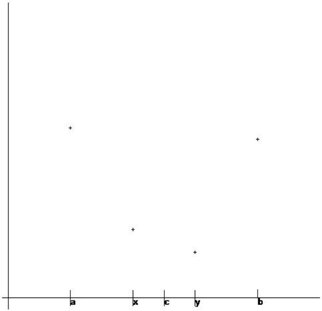

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Fig. 3.

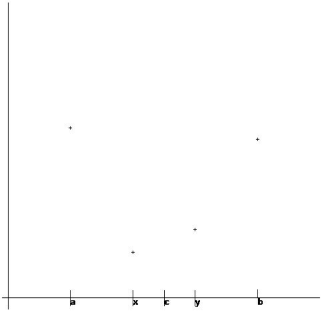

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Fig.4

Step 2. The second pair of computation is also carried out at the points spaced at a distance of δ from the midpoint of the interval $[a_1, b_1]$.

On the interval $[a_1, b_1]$ we calculate the values of f at the points $x_2,\ y_2$, spaced on either side of the midpoint at the distance of δ, and using the rule described above find the new segment $[a_2, b_2]$ the length of which is equal to

$$\Delta_2 = \Delta_1 + \delta = \frac{1}{2}\left(\frac{b-a}{2} + \delta\right) = \frac{b-a}{4} + \frac{3\delta}{2}.$$

The point $x^* \in [a_3, b_3]$.

Step 3. After the third step, we obtain the points x_3, y_3 and the segment $[a_3, b_3]$ the length of which is equal to

$$\Delta_3 = \Delta_2 + \delta = \frac{b-a}{8} + \frac{7\delta}{4}.$$

The point $x^* \in [a_3, b_3]$.

Step k. For a fixed δ after k computationals the length of the interval $[a_k, b_k]$, containing the minimum point is equal to

$$\Delta_k = \frac{b-a}{2^k} + \frac{2^k - 1}{2^{k-1}}\delta.$$

Thus, by choosing the constant δ the length of the interval can be made arbitrarily close to 0.

Iterations continue until the stopping criterion is satisfied. The search is complete, if $\Delta_k < \varepsilon$. And as the minimizer we can take a point

$$x^* = \frac{x_k + y_k}{2}.$$

The algorithm for finding a local maximum is analogous to the method described above.

The dichotomy method is not the best in the class of unimodal functions. There are more effective methods.

The Fibonacci method.

The Fibonacci method and the golden section search method are a technique for finding the extremum (minimum or maximum) of a strictly unimodal function by narrowing the range of values inside which the extremum is known to exist.

Now we describe methods for minimizing of a strictly unimodal function on an interval, allowing to solve the problem with the required accuracy when fewer quantity of computationals of function values.

The Fibonacci sequence is defined by recurrence conditions

$$F_0 = F_1 = 1, \quad F_{i+1} = F_i + F_{i-1}, \quad i = 1, 2, \ldots$$

Thus, the Fibonacci numbers are elements of the numerical sequence

$$1,\ 1,\ 2,\ 3,\ 5,\ 8,\ 13,\ 21,\ 34,\ 55,\ 89,\ 144, \ldots,$$

in which each subsequent number is the sum of the previous two. The name given to them is the name of the medieval mathematician Leonardo of Pisa (known as Fibonacci)(1170-1250).

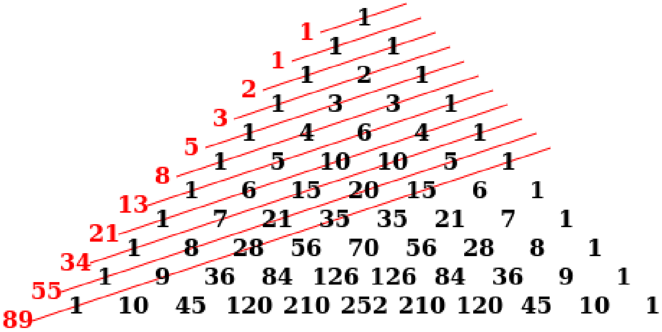

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Fig. 5. The Fibonacci numbers are the sums of the "shallow" diagonals (shown in red) of Pascal's triangle.

For the Fibonacci numbers, Binet's formula

$$F_n = \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2} \right)^n - \left(\frac{1-\sqrt{5}}{2} \right)^n \right].$$

is valid.

Sometimes the Fibonacci numbers are considered for negative numbers n as a two-way infinite sequence satisfying the same recurrence relation. In this case terms with negative indexes can be easily obtained by using the equivalent formula "back":

$$F_{-n} = (-1)^{n+1} F_n.$$

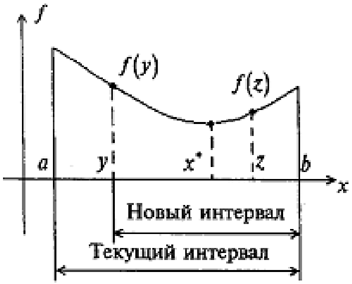
The most important feature of the Fibonacci method is that it allows for a given number of iterations to construct the optimal procedure for finding a minimum of a unimodal function.
The idea of this method is to calculate the values of the function f in N points selected so that the result obtained for each new point, allowed to delete (possibly the greatest) subinterval of the initial segment.

Suppose that we are given an initial interval $[a_1, b_1]$ and two intermediate points x_1 and y_1 are within this interval. We also have values of f at the points a_1, b_1.

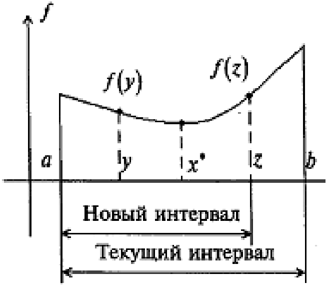
Then, by using a unimodal property of f, it is possible to delete one subinterval, $[a_1, x_1]$ or $[y_1, b_1]$. Let $\Delta_1 = b_1 - a_1$ be the length of the initial interval.

If we remove the segment $[y_1, b_1]$, it will be an interval of the length $y_1 - a_1$.

If we remove the segment $[a_1, x_1]$, it will be an interval of the length $b_1 - x_1$.


f
f(y)
f(z)
a
y
x*
z
b
x
Новый интервал
Текущий интервал

а


f
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The length of the obtained interval is independent from the result and a test (and thus of the function) must be satisfied the following equality

$$y_1 - a_1 = b_1 - x_1 = \Delta_2,$$

i.e., the points x_1 and y_1 must be symmetrical about the midpoint of the interval.
To continue the calculation with the new segment, for example, $[a_1, y_1]$, it is necessary to calculate the value of the additional point x_2, and this point is symmetric to point x_1 relative to the midpoint of the interval $[a_1, y_1]$.

Then, from

$$b_1 - a_1 = (y_1 - a_1) + (b_1 - y_1) = (y_1 - a_1) + (x_1 - a_1),$$

we obtain

$$\Delta_1 = \Delta_2 + \Delta_3.$$

Summarizing the above reasoning, it is easy to prove the equality

$$\Delta_k = \Delta_{k+1} + \Delta_{k+2} \quad \forall k \geq 0,$$

where Δ_k is the length of the interval considering at the k-step.

In addition, if the relation

$$\frac{\Delta_1}{\Delta_2} = \frac{F_{N-1}}{F_{N-2}},$$

is valid, where F_{N-1} X F_{N-2} are two consecutive terms of the Fibonacci sequence, then after computing the length of the resulting segment containing the minimum point will be equal to $\dfrac{b-a}{F_N}$.

It should be noted that, in this method, the location of the first point depends on the number N.

Thus, at each subsequent step (a subsequent iteration), the point of the next calculation is chosen symmetrically remaining points. On the first iteration two calculations of the function f are performed, at each subsequent, only one calculation is performed. Therefore, $N-1$ steps (iterations) will be calculated for a given N.

Example.

Let $N = 11$. Then

$$F_{11} = 114, \ F_{10} = 89, \ F_9 = 55, \ \Delta_1 = 1,$$

and

$$\Delta_2 = \frac{55}{89}\Delta_1 \approx 0,62\Delta_1, \ \Delta_3 = \Delta_1 - \Delta_2 \approx 0.38\Delta_1.$$

In 10 steps, the length of the considering interval will be equal $\dfrac{1}{114}$.

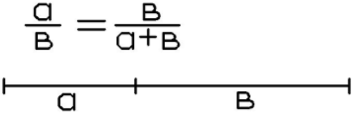
The Golden Section Search method

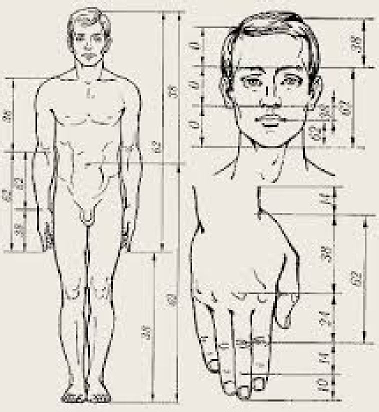
The golden section is a technique to find the extremum (minimum or maximum) of a strictly unimodal function by narrowing the range of values inside of the interval in which the extremum is known to exist. The technique derives its name from the fact that the algorithm maintains the function values for triples of points whose distances form the golden ratio. The algorithm is the limit of the Fibonacci search for a large number of function evaluations.

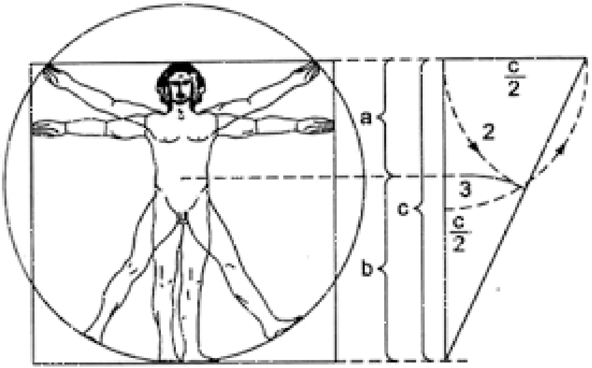
The golden section search method has been known since ancient times and is closely related to geometry. However, this ratio has been found in a number of fractions arising from a purely arithmetical sequence. This connection between geometry and arithmetic was found by Fibonacci

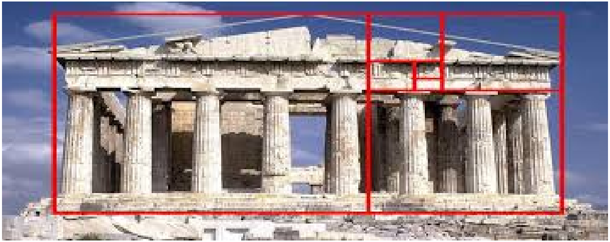
If we do not know in advance the number of calculations to be performed, it is possible to use the method of the golden section search. The golden section (golden proportion, the division in extreme and mean ratios) is the division of the interval into two parts by a triple of points. The ratio of the length of most part to the length of the whole segment is equal to the ratio of the length of the lower part to the length of the most part. The ratio of the larger part to the smaller this ratio is expressed in a quadratic irrationality. The golden section search method is almost as effective as the Fibonacci method but it does not depend on N.

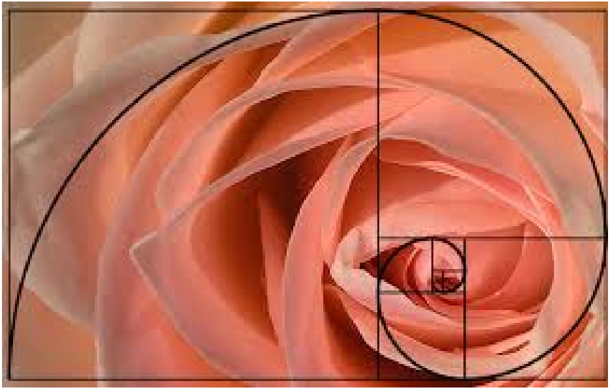
The search algorithm on the Golden section method is defined the same rule of symmetry as the Fibonacci algorithm.
As in the Fibonacci method at the first iteration two points situated symmetrically relative to the middle of the original segment are chosen and at each subsequent iteration one point is only chosen.
The difference rests in the selection of points.


$\frac{a}{B} = \frac{B}{a+B}$
a
B




a
b
c
$\frac{c}{2}$
2
3
$\frac{c}{2}$





Following the same principle as in the Fibonacci method (excepting subintervals calculated for each new point), in the golden section search method, the lengths of consecutive intervals are taken at a fixed ratio, and namely:

$$\frac{\Delta_1}{\Delta_2} = \frac{\Delta_2}{\Delta_3} = ... = \frac{\sqrt{5}+1}{2}.$$

The number $\Phi = \dfrac{\sqrt{5}+1}{2} \simeq 1,618$ is a root of the quadratic equation

$$x^2 - x - 1 = 0.$$

Moreover the following statement

$$\lim_{N\to\infty} \frac{F_N}{F_{N-1}} = \frac{\sqrt{5}+1}{2} = \Phi.$$

holds.

Formulate the algorithm of the golden section search method.

Step 1. Choose an initial interval $[a, b]$, which comprises a local minimum x^*, a tolerance $\varepsilon > 0$

Step 2. Calculate

$$\Delta_0 = b_0 - a_0,\ \Delta_1 = \frac{\sqrt{5}-1}{2}\Delta_0,\ \Delta_2 = \Delta_0 - \Delta_1,$$

$$x_0 = a_0 + \Delta_2,\ y_0 = b_0 - \Delta_2,\ f(x_0),\ f_(y_0),$$

and let $k = 1$.

Step 3. Calculate $\Delta_{k+2} = \Delta_k - \Delta_{k+1}$.

1) If $f(x_{k-1}) \leq f(y_{k-1})$, then

$$a_k = a_{k-1},\ b_k = y_{k-1},\ y_k = x_{k-1},\ x_k = a_k + \Delta_{k+1},\ f(y_k) = f(x_{k-1}).$$

If $x_k < y_k$, then calculate $f(x_k)$ and go to step 4.

2) If $f(x_{k-1}) > f(y_{k-1})$, then

$$a_k = x_{k-1},\ b_k = b_{k-1},\ x_k = y_{k-1},\ y_k = b_k - \Delta_{k+1},\ f(x_k) = f(y_{k-1}).$$

If $x_k < y_k$, then calculate $f(y_k)$ and go to step 4.

Step 4. If $\Delta_k > \varepsilon$, then go to step 3.

If $\Delta_k \leq \varepsilon$, then the search is over

and the point

$$x^* = \frac{x_k + y_k}{2}.$$

can be taken as a minimizer.

Remark 1. It should be noted that at each step the choice of the next point, symmetrical the previously constructed point, leads to the rapid accumulation of computational errors.

Remark 2. The Fibonacci method and the golden section search method are based on a single the same algorithm for finding the next point and are differed only way to select the first point.

The quadratic interpolation method

If the objective function is not only unimodal, but convex, then this information can be used to speed up the search for an extremum. The simplest zero-order method for convex functions is the method of parabolas. Let f be a convex function and we determine the triple of points on the plane

$$(x_1, f(x_1)),\ (x_1, f(x_1)),\ (x_1, f(x_1)),$$

which do not lie on one line, and moreover,

$$x_1 < x_2 < x_3, \quad f(x_2) \le f(x_1),\ f(x_2) \le f(x_3).$$

Then through these three points we can be made the parabola

$$y = ax^2 + bx + c.$$

This equation contains three unknown coefficients a, b, c. The minimizer

$$x^* = -\frac{b}{2a}$$

can be taken as an approximate extremum value. The coefficients a and b are determined by solving the system of equations

$$\begin{cases} ax_1^2 + bx_1 + c = y_1, \\ ax_2^2 + bx_2 + c = y_2, \\ ax_3^2 + bx_3 + c = y_3. \end{cases} \tag{1}$$

Write the determinant of the system (1):

$$\Delta = \begin{vmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{vmatrix}.$$

The determinant of this kind is called *the Vandermonde determinant*. It is different from zero for all different x_1, x_2, x_3.

Thus, the solution of the problem (1) exists and is unique. Then, using the Cramer rule, we have

$$a = \frac{\begin{vmatrix} y_1 & x_1 & 1 \\ y_2 & x_2 & 1 \\ y_3 & x_3 & 1 \end{vmatrix}}{\Delta}, \quad b = \frac{\begin{vmatrix} x_1^2 & y_1 & 1 \\ x_2^2 & y_2 & 1 \\ x_3^2 & y_3 & 1 \end{vmatrix}}{\Delta}, \quad c = \frac{\begin{vmatrix} x_1^2 & x_1 & y_1 \\ x_2^2 & x_2 & y_2 \\ x_3^2 & x_3 & y_3 \end{vmatrix}}{\Delta}.$$

The minimizer of this parabola can be found by the formula

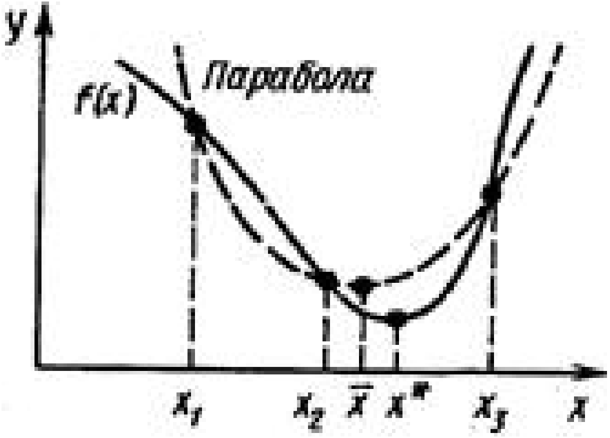
$$x^* = -\frac{1}{2}\frac{\begin{vmatrix} x_1^2 & y_1 & 1 \\ x_2^2 & y_2 & 1 \\ x_3^2 & y_3 & 1 \end{vmatrix}}{\begin{vmatrix} y_1 & x_1 & 1 \\ y_2 & x_2 & 1 \\ y_3 & x_3 & 1 \end{vmatrix}}.$$

It is easy to verify that

$$x_1 \le x^* \le x_3, \ y(x^*) \le y_2.$$

If it turns out that $x^* < x_2$, then for the next convex triples we take the points (x_1, x^*, x_2), otherwise (x_2, x^*, x_3). Such methods are widespread in the practice.

They provide good results under minimizing of sufficiently smooth unimodal functions.


y
Парабола
f(x)
x_1
x_2
$\bar{x}$
x^*
x_3
x

Example.

Consider three points

$$(-0.15; 2.00),\ (0.30; 3.00),\ (0.40; 5.00).$$

The system (1) has the form

$$\begin{cases} 0.0225\,a - 0.15\,b + c = 2.00, \\ 0.09\,a + 0.30\,b + c = 3.00, \\ 0.16\,a + 0.40\,b + c = 5.00. \end{cases}$$

Solving this system, we find

$$a = 32.32,\ b = -2.62,\ c = 0.87,\ x^* = 0.08.$$