Unconstrained optimization
Zero-Order optimization algorithms
Lecture 3

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Introduction

In this section we consider some numerical methods for solving unconstrained minimization problems, i.e. it is necessary to solve the problem

$$\inf_{x \in \mathbb{R}^n} f(x). \tag{1}$$

A point $x^* \in \mathbb{R}^n$ is called a global minimum point or a global minimizer of problem (1), if

$$f(x^*) \leq f(x) \quad \forall x \in \mathbb{R}^n.$$

A point $x^* \in \mathbb{R}^n$ is called a local minimum point or a local minimizer of problem (1), if there exists $\varepsilon > 0$, that

$$f(x^*) \leq f(x) \quad \forall x \in S(x^*, \varepsilon).$$

A point $x^* \in \mathbb{R}^n$ is called a strict local minimum point of problem (1), if there exists $\varepsilon > 0$ that

$$f(x^*) < f(x) \quad \forall x \in S(x^*, \varepsilon),\ x \neq x^*.$$

Finding global minimum is the goal of mathematical optimization. We say that a method globally converges if for any chosen initial point $x_0 \in \mathbb{R}^n$ a sequence $\{x_k\}$, generated by this method, converges to a point satisfying the necessary conditions for optimality.

If a method constructs a sequence $\{x_k\}$ for which the inequality

$$f(x_{k+1}) < f(x_k) \quad \forall k,$$

then such sequence is called relaxation, and the method is called the descent method.

Necessary and sufficient conditions for a minimum of a continuously differentiable function on $\mathbb{R}^n$

Let $f : \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable on $\mathbb{R}^n$.

Theorem 1 (Fermat). (First - order necessary condition for optimality)

For the point $x^* \in \mathbb{R}^n$ to be a minimum point of f on $\mathbb{R}^n$ it is necessary that

$$f'(x^*) = 0_n. \tag{2}$$

P r o o f. Let x^* be a minimum point of f on $\mathbb{R}^n$. Assume the opposite. Let $f'(x^*) \neq 0_n$. From the definition of the derivative we have that

$$f(x^* - \alpha f'(x^*)) = f(x^*) - \alpha \langle f'(x^*), f'(x^*) \rangle + o(\alpha) =$$

$$= f(x^*) - \alpha \left[||f'(x^*)||^2 - \frac{o(\alpha)}{\alpha} \right], \ \alpha > 0,$$

where

$$\frac{o(\alpha)}{\alpha} \xrightarrow[\alpha \to 0]{} 0.$$

Since $||f'(x^*)|| \neq 0$, then there exists a sufficiently small $\bar{\alpha} > 0$, that the inequality

$$||f'(x^*)||^2 - \frac{o(\alpha)}{\alpha} > 0 \quad \forall \alpha \in (0, \bar{\alpha}].$$

holds. Hence

$$f(x^* - \alpha f'(x^*)) < f(x^*).$$

It is a contradiction which proves the theorem.

Points satisfying equation (2), are called stationary points of the function f. The stationary points are not required to be a minimum point of f. They can be either a local minimum, either a local maximum or be neither one nor the other.

Theorem 2. (Second - order optimality conditions)

Let x^* be a stationary point of a twice continuously differentiable function f. For the point x^* to be a local minimum point of f on $\mathbb{R}^n$ it is necessary that the Hessian matrix $f''(x^*)$ is positive semi-definite at this point, and sufficient if it is positive definite.

P r o o f. (Necessity.) Let x^* be a minimum point of f on $\mathbb{R}^n$, $g \in \mathbb{R}^n$. We make use of the second-order Taylor series expansion. Since

$$f'(x^*) = 0_n,$$

then

$$0 \leq f(x^* + \alpha g) - f(x^*) = \frac{\alpha^2}{2}\langle f''(x^*)g, g\rangle + o(\alpha^2),$$

where

$$\frac{o(\alpha^2)}{\alpha^2} \xrightarrow[\alpha \to 0]{} 0.$$

Consequently,

$$\langle f''(x^*)g, g\rangle + \frac{2o(\alpha^2)}{\alpha^2} \geq 0 \quad \forall \alpha \neq 0.$$

Passing in this inequality to the limit under $\alpha \to 0$, r we obtain

$$\langle f''(x^*)g, g\rangle \geq 0 \quad \forall g \in \mathbb{R}^n.$$

The necessity is proved.

Sufficiency. (From the opposite.) Let the matrix $f''(x^*)$ be positive definite, but the stationary point x^* be not a local minimum point. Therefore there exists a such sequence of points $\{x_k\}$

$$\{x_k\} \to x^*, \; x_k \neq 0,$$

that the inuaquality

$$f(x_k) < f(x^*)$$

holds.

Let

$$g_k = \frac{x_k - x^*}{||x_k - x^*||}.$$

Without loss of generality, we can assume that the sequence points $\{g_k\}$ is convergent, i.e.,

$$g_k \to g^*, \quad ||g^*|| = 1,$$

$$0 > f(x^* + \alpha g^*) - f(x^*) = \frac{\alpha^2}{2}\langle f''(x^*)g^*, g^*\rangle + o(\alpha^2),$$

where

$$\frac{o(\alpha^2)}{\alpha^2} \xrightarrow[\alpha \to 0]{} 0.$$

Hence

$$\langle f''(x^*)g^*, g^*\rangle + \frac{2o(\alpha^2)}{\alpha^2} < 0.$$

Passing in this inequality to the limit under $\alpha \to 0$, we obtain

$$\langle f''(x^*)g^*, g^*\rangle \leq 0.$$

The last inequality contradicts the positive definiteness of the Hessian matrix.

Sufficiency is proved.

Zero-Order optimization algorithms

Minimization methods based on using only values of the objective function to be minimized is called zero-order methods or direct search methods.

One of such methods is the coordinate-wise descent method and the Nelder-Mead method (method of flexible polyhedron or simplex method). They are both based on intuitive (not strictly justified) considerations, not involving the use of linear or quadratic approximation of the objective function in the neighborhood of the point of calculations.

Direct search methods are characterized by a large number of settings, and the success of the methods are determined by how well managed to pick up the values of these parameters.
They can be used in situations where the use of more advanced methods is impossible or impractical.
Both methods are easy to implement and often used in practice.
The methods are used when the function is not differentiable or if a calculation of the derivatives involves a large amount of computations.

The cyclic coordinate-wise descent method.

It is the easiest of the presented methods of direct search. Recall that such methods which do not use information about the gradient of a function or of its Hessian.

This method has consistently pursued a one-dimensional optimization for each coordinate function.

Thus, if the function $f = f(x, y)$ then at each step of the method at the beginning this function is minimized in the direction of the axis x and then in the direction of the axis y. Finding the minimum is determined by the recurrence relation.

Note that the algorithm is effective in the cases when the objective function is separable, i.e., it can be represented as a sum of functions depending only on one coordinate.
As the direction of descent is chosen one vector of the canonical basis - the vector with only one coordinate is equal to 1, the other coordinates are equal to 0, i.e.,

$$e_i = (0, \ldots, 1, \ldots, 0).$$

Each cycle consists of n iterations. The step size during the cycle of the method remains constant.

K-cycle consists in calculating points

$$x_k, x_{k+1}, x_{k+2}, \ldots, x_{k+n-1} \in \mathbb{R}^n.$$

Assume that in a previous step we obtain $\alpha = \alpha_{k-1}$.
Consider $(i+1)$ iteration of the cycle $(0 \leq i \leq n-1)$. If

$$f(x_{k+i} - \alpha e_{i+1}) < f(x_{k+i}), \tag{3}$$

then put

$$x_{k+i+1} = x_{k+i} - \alpha e_{i+1},$$

and go to the next iteration. If

$$f(x_{k+i} - \alpha e_{i+1}) \geq f(x_{k+i}), \tag{4}$$

then calculate $f(x_{k+i} + \alpha e_{i+1})$.

If

$$f(x_{k+i} + \alpha e_{i+1}) < f(x_{k+i}),$$

then put

$$x_{k+i+1} = x_{k+i} + \alpha e_{i+1}$$

and go to the next iteration. If

$$f(x_{k+i} + \alpha e_{i+1}) \geq f(x_{k+i}), \tag{5}$$

then put

$$x_{k+i+1} = x_{k+i}$$

and go to the next iteration.

In the case where inequalities (4), (5) hold for all

$$0 \leq i \leq (n-1),$$

then the step is decreased, for example, take

$$\alpha = \frac{\alpha_{k-1}}{2}$$

and go to the next cycle, i.e., repeat all the steps, but with a smaller α.

An initial point and a step size of the method is chosen arbitrarily. Selecting of step may also be carried out by an one-dimensional minimization.

Stop condition of the iteration process is carried out after a set number of calculations of the function f, or when the condition

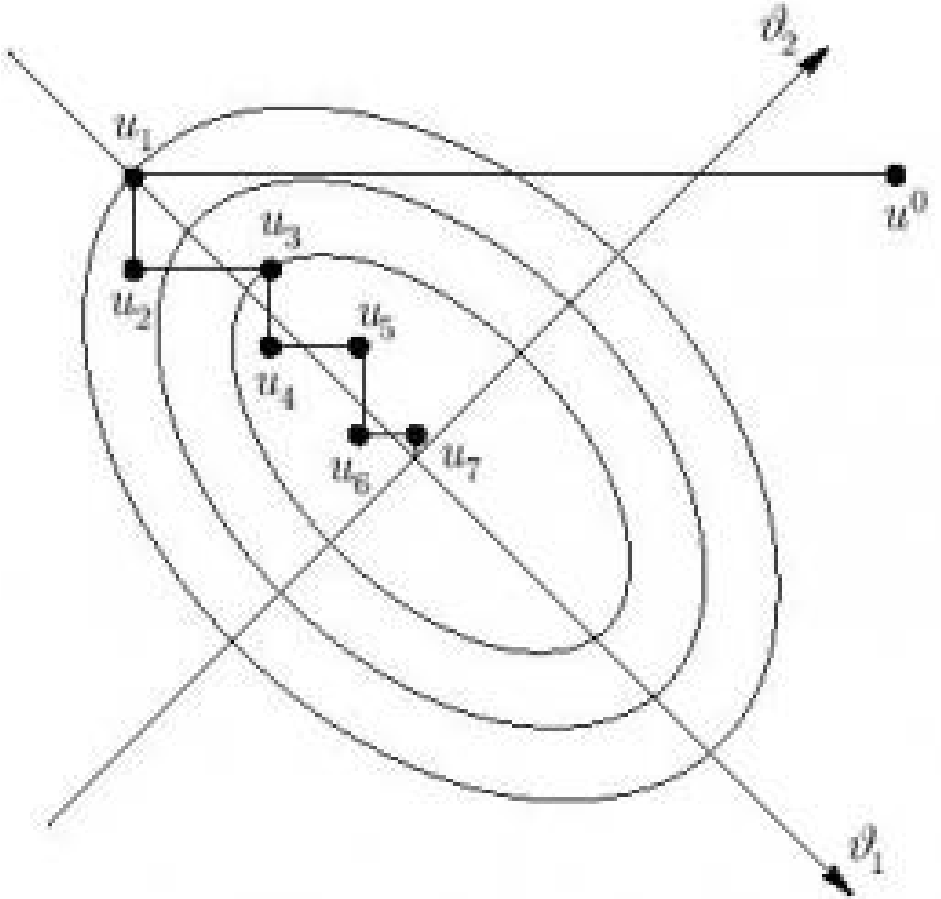
$$||x_{k+1} - x_k|| \leq \varepsilon$$

holds, where $\varepsilon > 0$ is a given accuracy.

Thus the coordinate-wise descent method reduces the problem of finding the smallest value of f towards the multiple decision-dimensional optimization problems.

For smooth functions under successfully chosen an initial approximation (in a neighborhood of a minimum), the process converges to a minimum.

The cyclic coordinate-wise descent method.



Nelder-Mead method

A simplex method for finding a local minimum of a function of several variables was devised by Nelder and Mead.
The Nelder-Mead method is also known as the method of the deformed polyhedron, a method of the unconstrained optimization of a real function of several variables. This method uses the geometric configuration, which is called a simplex.
A simplex is a convex polyhedron with a number of vertices being equal to $n + 1$ with non-empty interior, where n is the dimension of the space.
In two dimension space the regular simplex is an equilateral triangle, and in three dimensional space is a regular tetrahedron.

The idea of the method is to compare the values of the function at the vertices of the simplex and moving in the direction of the simplex optimum point using an iterative procedure.
In the simplex method proposed initially ther regular simplex is used at each step. Nelder and Mead suggested several modifications of this method, it is assumed that the polyhedrons were wrong. This method is very reliable for the direct search and it is one of the most effective when $n \leq 6$.

A search using the simplex is a search in which values of the minimizing function are calculated at the vertices of this simplex and then is chosen the worst value.
The vertex corresponding to this value is replaced by a certain rule to another, thereby forming a new simplex.
This procedure is repeated until the required accuracy will be reached.
Among the methods of deformation of the initial simplex (which occurs after rejecting the worst vertex and searching for a suitable new vertices) found:

1. **reflection vertices** (a vertex is simply reflected with respect to one of the simplex-sides);
2. **reduction** (the simplex retains its shape, but its dimensions are reduced);
3. **compression**.

Also very importantly how the vertices are numbered. Numbering is called regular if the vertex with the smaller the numbers corresponds to a smaller value of the function. In other words, the smaller the number has the smaller the value of the function.

The method consists in the sequential displacement and deformation of the simplex around the point of extreme.

Let there be a set of $n+1$ points

$$x_1, x_2, \ldots, x_{n+1},\ x_i \in \mathbb{R}^n,\ i = 1 : n+1,$$

ranked thus that for the corresponding values of the function f the inequalities

$$f(x_{n+1}) \geq f(x_n) \geq \cdots \geq f(x_2) \geq f(x_1).$$

hold.

These points can be interpreted as the vertices of the polyhedron from n - dimensional space.

At each iteration, the current polyhedron is replaced by a new polyhedron: the point with the highest value of the function (point x_{n+1}) is rejected and instead of it the "more suitable"point is entered into the set.

Let m be a centroid of n the best vertices

$$m = \frac{1}{n}\sum_{i=1}^{n} x_i.$$

$$x_k = m + \alpha(m - x_{n+1}),$$

where $\alpha > 0$. Calculate $f(x_k)$.

They say that the point x_k obtained by the reflection the point x_{n+1} and the number of $\alpha > 0$ is called the coefficient of reflection.

May be variants

1. If

$$f(x_1) \leq f(x_k) \leq f(x_n)$$

(the point x_k is not the worst and not the best), then x_{n+1} is replaced by x_k, whereupon the next iteration is executed.

2. If

$$f(x_k) \leq f(x_1),$$

then x_k is the best point and along this direction doing an attempt to stretch the polyhedron. For this the point

$$x_p = m + \beta(x_k - m),\ \beta > 0,$$

is calculated, where β is the expansion coefficient.

If $f(x_p) < f(x_k)$, then x_{n+1} is replaced on x_p. in the opposite case x_{n+1} is replaced on x_k.

3. If $f(x_k) > f(x_n)$, then the polyhedron is too large and it is necessary to compress. Introduce the point

$$x_m = \begin{cases} m + \gamma(x_{n+1} - m), & \text{если } f(x_k) \geq f(x_{n+1}), \\ m + \gamma(x_k - m), & \text{если } f(x_k) < f(x_{n+1}), \end{cases} \qquad 0 < \gamma < 1,$$

where γ $(0 < \gamma < 1)$ is the compression coefficient.

If

$$f(x_m) < \min\{f(x_k), f(x_{n+1})\},$$

then the goal of compression is achieved and the point x_{n+1} is replaced with x_m. Otherwise, another step of compression is performed and etc.

The coefficient of reflection α is used for projecting on the vertex with the most value of the objective function f through the centroid.

The coefficient of compression γ is used for decreasing of the vectors of the search, if the operation of reflection does not lead to the vertex with the value of objective function f, smaller than the second largest value of f, received before the reflection.
It is proposed to use the following values of the coefficients:

$$\alpha = 1, \quad 2.8 \leq \beta \leq 3, \quad 0.4 \leq \gamma \leq 0.6.$$

In addition to the operations of reflection, expansion and compression, it is periodically necessary to carry out the recovery operation - replace the received polyhedron on the regular one.

As the length of the sides of a regular polyhedron is taken the value $||x_1 - x_{n+1}||$, as well as its center is taken the point x_1. If after $2n$ iterations this point is unsurpassed it is considered as solution.

The end condition of calculating is the next condition:

$$\sqrt{\frac{1}{n+1}\sum_{i=1}^{n+1}[f(x_i) - f(x_m)]^2} \leq \varepsilon,$$

where $\varepsilon > 0$ is the given error.

Here is the formula for finding the vertices of a regular polyhedron with edge length l.

Let $x^0 = (x_1, x_2, \ldots, x_n)$ be an initial value at the minimizer then as a regular simplex you can choose a polyhedron with vertices at the points

$$
\begin{aligned}
x^0 &= (x_1, x_2, x_3, \ldots, x_n), \\
x^1 &= (x_1 + r, x_2 + s, x_3 + s \ldots, x_n + s), \\
x^2 &= (x_1 + s, x_2 + r, x_3 + s \ldots, x_n + s), \\
x^3 &= (x_1 + s, x_2 + s, x_3 + r \ldots, x_n + s) \\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
x^n &= (x_1 + s, x_2 + s, x_3 + s \ldots, x_n + r),
\end{aligned}
$$

where

$$r = \frac{l\left(\sqrt{n+1}-1+n\right)}{\sqrt{2}n}, \quad s = \frac{l\left(\sqrt{n+1}-1\right)}{\sqrt{2}n},$$

The method finds a local extremum and can "get stuck" in one of them.

If you still want to find a global extremum you can try to choose a different initial simplex.

The main features of the algorithm are the following:

The Nelder-Mead method does not impose restrictions on the smoothness of the function.

This method is efficient at low speed of calculating values of the function which to be minimized.

As a rule at each iteration values of the function is calculated not more than at 3 points.

There is no theory of convergence.

In addition one of the main advantages of this method is that it does not use the gradient of the objective function which allows to use it for nonsmooth functions.