Chapter 2.

Minimization of functions with several variables

2.1. Introduction

Numerical methods of several variables function minimization can be divided into three classes:

- simple searching methods e.g. Hook-Jeeves method, Rosenbrock method;
- methods of directional improvement:
  - — non-gradient methods; a value of the objective function has to be known in one point $f(\boldsymbol{x})$ e.g. Gauss-Seidel method or Powell method;
  - — gradient methods; in the minimization process the objective function $f(\boldsymbol{x})$ values as well as its gradient $\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})$ is used e.g. methods of steepest descent and conjugate gradient methods;
  - — Newton methods; in the minimization process the objective function $f(\boldsymbol{x})$ values as well as its gradient $\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})$ and hessian $\boldsymbol{\nabla}_{\boldsymbol{x}} \left[\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})\right]^T$ are used e.g. Newton-Raphson method or quasi-newton Davidon-Fletcher-Powell method.

In each method the same scheme of iteration is used. Minimum is searched step by step along improved directions of n-th dimensional space. These directions can be constant in succeeding iterations or may change according to objective function, its gradient or hessian. The following common phases can be distinguished in all methods:

- Choice of an initial point $\boldsymbol{x}_0$.
- Determination of the next point $\hat{\boldsymbol{x}}^{k+1}$ being an approximation of minimal point $\hat{\boldsymbol{x}}$. A new point is calculated along a chosen direction. The direction as well as the length of the step depends on the method.
- Test of convergence condition (a criterion of minimal point achievement).

2.2. Non-gradient methods

Two methods are described below: one of the simplest – Gauss-Seidel method with constant directions and Powell method with directions changing in every iteration.

2.2.1. Gauss-Seidel method

Gauss-Seidel method is effective if the objective function can be approximated around the minimum with a strictly convex quadratic function. The minimization is realized sequentially with respect to one of the decision variables $x_1, \ldots, x_n$. This means that improvement directions are constant, orthogonal and respect to axes of coordinate systems. Length of a step in a direction is determined to achieve minimum of the objective function in this direction.

Single minimization along $x_1, \ldots, x_n$ constitutes an iteration. The searching directions $\boldsymbol{e}_j$ are orthogonal unity vectors i.e.

$$\boldsymbol{e}_j^T = \left[\underbrace{0 \quad \ldots \quad 0}_{j-1 \text{ elements}} \quad 1 \quad 0 \quad \ldots \quad 0\right], \tag{2.1}$$

$$\boldsymbol{e}_j^T \boldsymbol{e}_k = \begin{cases} 0 & \text{for } k \neq j; \\ 1 & \text{for } k = j. \end{cases} \tag{2.2}$$

If after $j-1$ steps of the optimization a point $\hat{\boldsymbol{x}}^{j-1}$ is reached then the next step of the algorithm is the minimization along a line determined by the point $\hat{\boldsymbol{x}}^{j-1}$ and the vector $\boldsymbol{e}_j$ i.e. finding an optimal $\hat{\alpha_j}$ that

$$\hat{\alpha_j} : \min_{\alpha_j} f(\hat{\boldsymbol{x}}^{j-1} + \alpha_j \boldsymbol{e}_j) \tag{2.3}$$

or solving an optimization problem for one-variable (α_j) function.

Non-convergence may happen in Gauss-Seidel method due to constant improvement directions. Generally, this method is slow but its advantage is simplicity.

2.2.2. Powell method

Powell method is non-gradient improvement method where specially chosen improvement directions are determined in R^n space creating *basis* of this space. In every iteration minimization in n directions is realized (n is the number of decision variables). In the end of iteration the additional (n+1)'th direction is determined and minimization is realized. Improvement directions are not constant in Powell method: in the initial iteration directions are usually equal to axes of coordinate system.

The first step of the method is determination of n linearly independent vectors $\boldsymbol{d_1}$, ..., $\boldsymbol{d_n}$ being initial basis. In the end of **initial phase** minimization along the *last* of the initial directions is done beginning from the initial point $\boldsymbol{x}^0$ and reaching $\boldsymbol{x}^{1,0}$ – an initial point for the first iteration of the main algorithm.

Powell method consists of four stages (notation concerns the k'th iteration):

1. Beginning from the point $\boldsymbol{x}^{k,0}$ n succeeding minimizations are realized along directions: $\boldsymbol{d}_1^k, \ldots, \boldsymbol{d}_n^k$. As the result of minimization new points are determined: $\boldsymbol{x}^{k,1}, \boldsymbol{x}^{k,2}, \ldots, \boldsymbol{x}^{k,n}$.

2. A new direction is determined:

$$\boldsymbol{d}_{n+1}^k = \boldsymbol{x}^{k,n} - \boldsymbol{x}^{k,0}, \tag{2.4}$$

and directional minimization is realized giving the point $\boldsymbol{x}^{k,n+1}$.

3. The stop criterion checked:

$$\left\|\boldsymbol{x}^{k,n+1} - \boldsymbol{x}^{k,0}\right\| \leq \epsilon, \tag{2.5}$$

where ϵ is assumed accuracy. If the criterion is satisfied the calculations are terminated and the point $\boldsymbol{x}^{k,n+1}$ is accepted as the optimal point $\hat{\boldsymbol{x}}$.

4. Searching directions for the next iteration are redefined

$$\begin{array}{rcl} \boldsymbol{d}_1^{k+1} & \leftarrow & \boldsymbol{d}_2^k, \\ \boldsymbol{d}_2^{k+1} & \leftarrow & \boldsymbol{d}_3^k, \\ \vdots & \vdots & \vdots \\ \boldsymbol{d}_n^{k+1} & \leftarrow & \boldsymbol{d}_{n+1}^k. \end{array} \tag{2.6}$$

Theoretical justification of Powell method

Conjugate directions: Directions $\boldsymbol{d_1}$, $\boldsymbol{d_2}$, ..., $\boldsymbol{d_r}$, $\boldsymbol{d_i} \neq 0$ are called reciprocally conjugate towards positive definite **symmetrical** matrix $\boldsymbol{A}$ of $n \times n$ dimension if the following holds:

$$\bigwedge_{\substack{i,j=1,\ldots,n \\ i \neq j}} \boldsymbol{d}_i^T \boldsymbol{A} \boldsymbol{d}_j = 0. \tag{2.7}$$

Note: 1. $\boldsymbol{A}$-conjugate directions are linearly independent.

2. Relation of $\boldsymbol{A}$-conjugations is not transitive i.e. from $\boldsymbol{d}_i^T \boldsymbol{A} \boldsymbol{d}_j = 0$ and $\boldsymbol{d}_j^T \boldsymbol{A} \boldsymbol{d}_k = 0$ does not follow that $\boldsymbol{d}_i^T \boldsymbol{A} \boldsymbol{d}_k = 0$.

Linear manifold: r-dimensional linear manifold in n-dimensional space is the set:

$$\boldsymbol{x} \in R^n : \boldsymbol{x} = \boldsymbol{x}^0 + \sum_{i=1}^{r} \alpha_i \boldsymbol{d}_i, \tag{2.8}$$

where
$\alpha_i \in (-\infty, \infty), \quad i = 1, \ldots, r,$
$\boldsymbol{d}_i \in R^n$ – direction in n-dimensional space of searching,
$\boldsymbol{d}_i, \quad i = 1, \ldots, r$ – linearly independent directions,
$\boldsymbol{x}^0 \in R^n$ – any point in n-dimensional searching space.

Theorem 1

If $\boldsymbol{d_1}$, ..., $\boldsymbol{d_n}$ are $\boldsymbol{A}$-conjugate directions then minimum of the quadratic function of n variables

$$f(\boldsymbol{x}) = c + \boldsymbol{b}^T \boldsymbol{x} + \frac{1}{2} \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \tag{2.9}$$

in the linear manifold determined by these directions and any point $\boldsymbol{x^0}$ can be calculated in n steps by single minimization of the function $f(\boldsymbol{x})$ in every direction.

Theorem 2

If $\boldsymbol{x}^0$ is minimum of quadratic function of n variables $f(\boldsymbol{x})$ in a linear manifold containing direction $\boldsymbol{d}$ and $\boldsymbol{x}^n$ is minimum of the function $f(\boldsymbol{x})$ in other linear manifold containing also direction $\boldsymbol{d}$ (assumed $\boldsymbol{x}^0 \neq \boldsymbol{x}^n$) then direction $\boldsymbol{x}^n - \boldsymbol{x}^0$ is conjugate with

the direction $\boldsymbol{d}$ towards the matrix $\boldsymbol{A}$.

Conclusions: In every iteration of Powell method applied to quadratic function number of $\boldsymbol{A}$-conjugate directions increases by 1 in a set of n directions. Thus minimum of the quadratic function is obtained in not more then n iterations.

Justification of the conclusion

1. It follows from the second theorem that after first iteration directions $\boldsymbol{d_n^1}$ and $\boldsymbol{d_{n-1}^1}$ are $\boldsymbol{A}$-conjugate. Linear manifold is a line in this case.

2. Assume that at the beginning of the k-th iteration in the set of n searching directions $\boldsymbol{d}_i^k (i=1,\ldots,n)$, directions $\boldsymbol{d}_{n-k+1}^k$, $\boldsymbol{d}_{n-k+2}^k$, ..., $\boldsymbol{d}_n^k$ are $\boldsymbol{A}$-conjugate. At the end of the k-th iteration minimization is realized along k $\boldsymbol{A}$-conjugate directions. It follows from the first theorem that the point $\boldsymbol{x^{k,n}}$ is the minimum of the function $f(\boldsymbol{x})$ in linear manifold spanned on directions $\boldsymbol{d}_{n-k+1}^k$, ..., $\boldsymbol{d}_n^k$.

   The same directions conjugated in the $(k-1)$'th iteration have been denoted by $\boldsymbol{d_{n-k+2}^{k-1}}$, ..., $\boldsymbol{d_{n+1}^{k-1}}$. Thus in the last $k-1$ minimization of the first stage of the $(k-1)$'th iteration and in the second stage of this iteration the minimum of the function $f(\boldsymbol{x})$ is reached in k-dimensional linear manifold spanned on the same conjugate vectors as for k last minimization of the first stage of the k'th iteration. This minimum is located in the point $\boldsymbol{x}^{k,0} = \boldsymbol{x}^{k-1,n+1}$.

It follows from the second theorem that the direction $\boldsymbol{x}^{k,n} - \boldsymbol{x}^{k,0}$ is $\boldsymbol{A}$-conjugate with *each* directions $\boldsymbol{d_{n-k+1}^k}$, ..., $\boldsymbol{d_n^k}$. Thus in the end of k'th iteration after directions redefining there are $k+1$ $\boldsymbol{A}$-conjugate directions in the set of n directions.

The theory of Powell method concerns quadratic functions. However, this method can be applied to other objective functions. Clearly, a number of iterations is greater than n.

It follows from the first theorem and the conclusion that for an objective function of the type (2.9) (if $\boldsymbol{A}$ is symmetrical and positive definite) it is ,,worthy to search a minimum along the $\boldsymbol{A}$-conjugate improvement directions". Thus if one can approximate the objective function with (2.9) and it is possible to determine or evaluate matrix $\boldsymbol{A}$ then it becomes efficient to determine $\boldsymbol{A}$-conjugate directions using definition (2.7) and minimize the objective function along them. The first theorem proves that doing so one can find the minimum of quadratic function (2.9) not longer then after *one* iteration. This can not be achieved using axes of coordinate system as searching directions as in Gauss-Seidel method. This approach (so called method of searching along $\boldsymbol{A}$-conjugate directions) should be used if matrix$\boldsymbol{A}$ is known and the objective function can be approximated with (2.9).

2.3. Gradient methods

Gradient methods use values of the objective function as well as its gradient. Below two methods are described: steepest descent method and conjugate gradient method.

2.3.1. Steepest descent method

One of the simplest gradient method is steepest descent method. A searching direction is opposite to the objective function gradient Assuming that the objective function can be

enough accurately approximated by the first (linear) element of Taylor series expansion the objective function can be expressed around the point $\hat{\boldsymbol{x}}^{j-1}$ as follows:

$$f(\boldsymbol{x}^j) \approx f(\hat{\boldsymbol{x}}^{j-1}) + \left(\boldsymbol{x}^j - \hat{\boldsymbol{x}}^{j-1}\right)^T \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{j-1}}. \tag{2.10}$$

It is clear from the above that negative increase of the objective function is the greatest if the next point in the optimization process is determined opposite to the objective function gradient i.e.

$$\boldsymbol{x}^j = \hat{\boldsymbol{x}}^{j-1} - \alpha_j \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{j-1}}. \tag{2.11}$$

In the steepest descent method the next point $\hat{\boldsymbol{x}}^j$ is determined by minimization of the objective function along the above direction i.e.

$$\hat{\boldsymbol{x}}^j = \hat{\boldsymbol{x}}^{j-1} - \hat{\alpha_j} \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{j-1}}, \tag{2.12}$$

where:

$$\hat{\alpha_j} : \min_{\alpha_j} f\left(\hat{\boldsymbol{x}}^{j-1} - \hat{\alpha_j} \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{j-1}}\right). \tag{2.13}$$

This method is specially efficient if the initial point is far from the optimum. In the region close to minimum where gradient is small the efficiency of the method is poor.

2.3.2. Conjugate gradient methods

The conjugate gradient method uses gradient of the objective function as well as non-gradient searching based on conjugate improvement direction. The method is iterative. Every iteration consists of two phases. The first improvement direction is opposite to gradient of the objective function:

$$\boldsymbol{d}^1 = -\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\boldsymbol{x}^0}. \tag{2.14}$$

A new direction is determined according to the following:

$$\boldsymbol{d}^{k+1} = -\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^k} + \beta^k \boldsymbol{d}^k. \tag{2.15}$$

The factor β^k is chosen so the direction $\boldsymbol{d}^{k+1}$ is $\boldsymbol{A}$-conjugate with the previous direction $\boldsymbol{d}^k$ towards quadratic approximation of the objective function $f(\boldsymbol{x})$. The choice of β^k can be as follows

$$\beta^k = \frac{\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^k}{}^T \left(\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^k} - \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{k-1}}\right)}{\left\| \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{k-1}} \right\|^2} \tag{2.16}$$

(Polak-Ribiére algorithm).

For a quadratic function of n variables the algorithm should find a global minimum in not more then n iterations (see 2.2.). In conjugate gradient method after n iterations or if a new direction is not an improvement direction so called direction renewal is provided: the actual direction is replaced with the last best i.e. direction used previously for which an optimum has been obtained.

The calculations are terminated if the norm of the objective function gradient is smaller then assumed accuracy.

2.4. Newton and quasi-newton methods

In newton methods values of the objective function as well as objective function gradient and its hessian are used to determine an optimum. The gradient and hessian are calculated in vicinity of the last approximation in an iterative procedure. As the example Newton-Raphson method is described. In quasi-newton methods an approximation of the hessian is used. As an example Davidon-Fletcher-Powell method is presented.

2.4.1. Newton-Raphson method

Similarly to steepest descent method in Newton-Raphson method Taylor series expansion is used to approximate the objective function in a vicinity of the last obtained approximation of the optimum. The first elements of the expansion are used (up to quadratic):

$$f(\boldsymbol{x}^j) \approx f(\hat{\boldsymbol{x}}^{j-1}) + \left(\boldsymbol{x}^j - \hat{\boldsymbol{x}}^{j-1}\right)^T \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{j-1}} + \frac{1}{2}\left(\boldsymbol{x}^j - \hat{\boldsymbol{x}}^{j-1}\right)^T \boldsymbol{\nabla}_{\boldsymbol{x}} \left[\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})\right]^T\Big|_{\hat{\boldsymbol{x}}^{j-1}} \left(\boldsymbol{x}^j - \hat{\boldsymbol{x}}^{j-1}\right). \tag{2.17}$$

The necessary condition to obtain an optimum is:

$$\frac{\partial f(\boldsymbol{x}^j)}{\partial \boldsymbol{x}^j} = \boldsymbol{0}, \tag{2.18}$$

or

$$\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{j-1}} + \boldsymbol{\nabla}_{\boldsymbol{x}} \left[\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})\right]^T\Big|_{\hat{\boldsymbol{x}}^{j-1}} \left(\boldsymbol{x}^j - \hat{\boldsymbol{x}}^{j-1}\right) = \boldsymbol{0}. \tag{2.19}$$

The above condition allows to determine the next approximation of the optimum:

$$\hat{\boldsymbol{x}}^j = \hat{\boldsymbol{x}}^{j-1} - \left(\boldsymbol{\nabla}_{\boldsymbol{x}} \left[\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})\right]^T\Big|_{\hat{\boldsymbol{x}}^{j-1}}\right)^{-1} \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{j-1}}. \tag{2.20}$$

A direction determined using previous point $\boldsymbol{x}^{j-1}$. New $\boldsymbol{x}^j$ is a direction of steepest descent $\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{j-1}}$ of the objective function modified by hessian $\boldsymbol{\nabla}_{\boldsymbol{x}} \left[\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})\right]^T\Big|_{\hat{\boldsymbol{x}}^{j-1}}$.

Equation (2.20) determines a new approximation of the optimum but not a new searching direction as it is in previously described methods. This means that in Newton-Raphson method minimization is not realized along chosen directions; one calculate the objective function values, its gradient and hessian and finally a new approximation of the optimum from the equation (2.20).

It can be proven that for quadratic functions $f(\boldsymbol{x})$, Newton-Raphson method assures achievement of the global minimum in one step independently on initial point.

2.4.2. Davidon-Fletcher-Powell method

In Davidon-Fletcher-Powell (DFP) method an approximation of inverse hessian matrix is used. The approximation is obtained using changes of the objective function gradient. In succeeding iterations of DFP method a searching direction is determined:

$$\boldsymbol{d}^k = -\boldsymbol{V}^k \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{k-1}}, \tag{2.21}$$

and directional minimization is realized. A new point $\hat{\boldsymbol{x}}^k$ is reached. If matrix $\boldsymbol{V}^k$ is equal to hessian then DPF method is identical with Newton-Raphson method.

Initial matrix $\boldsymbol{V}^1$ is usually assumed to be a unit matrix , $\boldsymbol{V}^1 = \boldsymbol{I}$; this means that in the first iteration searching direction is opposite to gradient of the objective function $\boldsymbol{d}^1 = -\boldsymbol{\nabla_x} f(\boldsymbol{x})|_{\boldsymbol{x}^0}$. In the next iterations matrix $\boldsymbol{V}^k$ is modified according to:

$$\boldsymbol{s}^k = \hat{\boldsymbol{x}}^k - \hat{\boldsymbol{x}}^{k-1}, \tag{2.22}$$

$$\boldsymbol{r}^k = \boldsymbol{\nabla_x} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^k} - \boldsymbol{\nabla_x} f(\boldsymbol{x})|_{\hat{\boldsymbol{x}}^{k-1}}, \tag{2.23}$$

$$\boldsymbol{V}^{k+1} = \boldsymbol{V}^k + \frac{\boldsymbol{s}^k (\boldsymbol{s}^k)^T}{(\boldsymbol{s}^k)^T \boldsymbol{r}^k} - \frac{\boldsymbol{V}^k \boldsymbol{r}^k (\boldsymbol{r}^k)^T \boldsymbol{V}^k}{(\boldsymbol{r}^k)^T \boldsymbol{V}^k \boldsymbol{r}^k} \tag{2.24}$$

Similarly to conjugate gradient method if the algorithm is slow convergent a renewal is provided: matrix $\boldsymbol{V}^{k+1}$ becomes unit matrix. The renewal is provided after $2n$+1 iterations of DFP method and if a new direction determined with (2.21) is not an improvement direction.

The calculations are terminated if norm of the objective function gradient is smaller then assumed accuracy.

2.5. Problems

Find extremum of one of the following function

1. $z(x,y) = sin^2(x-0.5) + artg^2(y-0.5) \qquad x \in [-1,1], \quad y \in [-1,1]$
2. $z(x,y) = (x-0.5)^2 + (y-0.5)^2 \qquad x \in [-1,1], \quad y \in [-1,1]$
3. $z(x,y) = sin^2(x-0.5) + sin^2(y-0.5) \qquad x \in [-1,1], \quad y \in [-1,1]$
4. $z(x,y) = arctg^2(x-0.5) + art^2(y-0.5) \qquad x \in [-1,1], \quad y \in [-1,1]$
5. $z(x,y) = e^{cos(x-0.5)} + e^{cos(y-0.5)} \qquad x \in [-1,1], \quad y \in [-1,1]$
6. $z(x,y) = \dfrac{y(1-x^2)}{1.2 - sin(2y)} \qquad x \in [-1,1], \quad y \in [-1,1]$
7. $z(x,y) = (2-3x^4)tg(sin(2y+1)) \qquad x \in [-1,1], \quad y \in [-1,1]$
8. $z(x,y) = (2-y^2)e^{-sin(2x-1)} \qquad x \in [-1,1], \quad y \in [-1,1]$

Choose one of the method described above. There are two tasks to be done:

1. Perform 2-3 iterations of the chosen method for the assumed starting point.
2. Write a computer program solving the problem. Run the program for the assumed accuracy. In this point a procedure of directional searching has to be used. The procedure is prepared previously on another exercise.

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