

## Numerical Algorithms (MU4IN910)

Tutorial-Practical 2 - Introduction to optimization

## 1. Tutorial

**Exercise 1** (Coercive functions and extrema). A function  $f : \mathbb{R}^n \to \mathbb{R}$  is said to be *coercive* if

$$\lim_{\|x\|\to+\infty}f(x)=+\infty.$$

Show that if f is continuous and coercive then f admits at least one minimum on  $\mathbb{R}^n$ .

**Exercise 2** (Necessary condition). Let f be a differentiable numerical function on an open set U of  $\mathbb{R}^n$ . Show that if  $a \in U$  is a local minimum of f then  $\nabla f(a) = 0$ .

**Exercise 3** (Convex functions and extrema). Let f be a numerical convex function on a convex open set U of  $\mathbb{R}^n$ . If f is differentiable in  $a \in U$  and if  $\nabla f(a) = 0$ , show that f admits a global minima in a on U. We now suppose that f is strictly convex. Show that the minimum is unique.

*Hint*: we can use the fact that f (differentiable) is convex on C if for all  $x, y \in C$ ,  $f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle$ .

**Exercise 4** (Calculation of extrema). Consider the function  $f: \mathbb{R}^2 \to \mathbb{R}$  defined by

$$f(x, y) = 3x^2 + 2y^2 + 2xy + x + y + 10.$$

- 1. Is this function convex? Justify.
- **2.** We consider the optimization problem  $\inf_{(x,y)\in\mathbb{R}^2} f(x,y)$ . What can we say about this problem?
- 3. Solve it.

**Exercise 5** (Unimodal function). A function  $f : \mathbb{R} \to \mathbb{R}$  is said to be unimodal on the interval [a, b] if it has a unique local minimum on [a, b]. Show that a continuous unimodal function is strictly decreasing until the minimum and strictly increasing after the minimum.

**Exercise 6** (Characterization of convexity). Let C be a non empty open convex subset of  $\mathbb{R}^n$  and  $f : \mathbb{R}^n \to \mathbb{R}$  a differentiable function on C. Show that the following propositions are equivalent:

- **1.** *f* is convex on *C*;
- **2.** for all  $x, y \in C$ ,  $f(y) \ge f(x) + \langle \nabla f(x), y x \rangle$ ;
- **3.** the application  $\nabla f$  is monotone on C, that is

$$\forall x, y \in C$$
,  $\langle \nabla f(y) - \nabla f(x), y - x \rangle \ge 0$ .

Show that if, in addition, f is twice differentiable on  $\mathbb{R}^n$ , then

*f* is convex on  $\mathbb{R}^n \iff \forall x \in \mathbb{R}^n, \quad \nabla^2 f(x)$  is positive semidefinite.

**Exercise** 7 (Quadratic function). Let  $f : \mathbb{R}^n \to \mathbb{R}$  be defined by  $f(x) = \frac{1}{2}\langle Ax, x \rangle - \langle b, x \rangle$  where A is a symmetric matrix of size  $n \times n$  and  $b \in \mathbb{R}^n$ .

- **1.** Show that  $\nabla f(x) = Ax b$ .
- **2.** Deduce the Hessian matrix  $H_f(x)$ .
- 3. Propose an optimization algorithm to solve a linear system Ax = b when A is symmetric positive definite.

**Exercise 8** (Optimization). Let  $n \ge 2$  be a natural number. Consider the application  $f : \mathbb{R}^n \to \mathbb{R}$  defined by

$$f(x_1, x_2,...,x_n) = \sum_{k=1}^n x_k^2 + \left(\sum_{k=1}^n x_k\right)^2 - \sum_{k=1}^n x_k.$$

- **1.** Justify that f is of class  $C^2$  on  $\mathbb{R}^n$  and calculate the gradient  $\nabla f$  as well as the Hessian matrix  $H_f$ .
- **2.** Determine the only critical point  $\overline{x} = (\overline{x}_1, \overline{x}_2, \dots, \overline{x}_n)$  of f on  $\mathbb{R}^n$ .
- **3.** We wish to prove that  $\overline{x}$  is a local minimum of f.
  - **a.** Check that the Hessian matrix  $H_f(\overline{x})$  can be written as  $H_f(\overline{x}) = 2(I_n + J_n)$  where  $I_n$  is the identity matrix of size n and  $J_n$  is the matrix of size n whose coefficients are equal to 1.
  - **b.** Determine the rank of  $J_n$ . Deduce that 0 is an eigenvalue of  $J_n$ . Determine the dimension of the associated eigenspace.
  - **c.** Calculate the product of  $J_n$  by the vector  $(1, ..., 1)^T$ . Deduce another eigenvalue of  $J_n$ .
  - **d.** Deduce the eigenvalues of  $H_f(\overline{x})$  and conclude about the nature of the point  $\overline{x}$ .

**Exercise 9** (Least Squares). Given n points  $(x_i, y_i)$  of  $\mathbb{R}^2$  with  $x_i$  not all equal to each other, show that there are unique numbers  $\lambda$  and  $\mu$ , which minimize the sum

$$\sum_{i=1}^n (\lambda x_i + \mu - y_i)^2.$$

**Exercise 10** (Hadamard's inequality). We provide the space  $E = \mathbb{R}^n$  with the usual scalar product. We denote by  $f(v_1, \dots, v_n)$  the determinant of the matrix  $n \times n$  of column vectors  $v_1, \dots, v_n \in E$ .

**1.** Show that the maximum of *f* on the set *X* defined by

$$\|v_1\| = \cdots = \|v_n\| = 1$$

is reached and is strictly positive.

- **2.** Show using Lagrange multiplier that if the maximum is reached in  $(v_1, \ldots, v_n)$ , then the  $v_i$  form an orthonormal basis of E.
- 3. Prove that Hadamard's inequality:

$$|\det(v_1,\ldots,v_n)| \leq ||v_1|\cdots||v_n|,$$

for any vector  $v_1, \ldots, v_n$ . When do we have equality?

**Exercise 11** (Choleski decomposition). Let A be a symmetric positive definite matrix of size n. Let  $A = LL^T$  be its Choleski decomposition (L being lower triangular).

**1.** For n = 3, write  $a_{ij}$  for i, j = 1, 2, 3 as a function of the coefficients of L.

- **2.** Note that if we calculate column by column, we can then calculate in order  $l_{11}$ ,  $l_{21}$ ,  $l_{31}$ ,  $l_{22}$ ,  $l_{32}$  and  $l_{33}$ . Write a MATLAB function calculating the Choleski decomposition for any value of n.
- 3. Compute the Choleski decomposition of the matrix

$$A = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 5 & 1 \\ 1 & 1 & 3 \end{pmatrix}.$$

## 2. Practical

Exercise 12 (Golden section search).

- 1. Write a MATLAB program implementing the Golden section search. Your program must take a function and an interval as parameters. The search should continue until the desired accuracy but should not exceed 100 iterations.
- 2. Write a MATLAB program implementing Newton's method.
- **3.** Test your algorithms on the following examples. You will compare your results with those given by the fminbnd function of MATLAB.
  - **a)**  $f(x) = \sin(x)$  on  $[0, \pi/2]$
  - **b**)  $f(x) = (\arctan x)^2$  on [-1, 1]
  - c)  $f(x) = |\ln(x)| \text{ on } [1/2, 4]$
  - **d)** f(x) = |x| on [-1, 1]

**Exercise 13** (Rosenbrock's function and Newton's method). The Rosenbrock function is a non-convex function of two variables used as a test for mathematical optimization problems. It was introduced by Rosenbrock in 1960. It is defined by

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2.$$

- **1.** Compute the gradient g(x) and the Hessian H(x) of the function f (we will use the Symbolic Math Toolbox).
- **2.** Check that  $x^* = [1,1]^T$  is a local minimum of f.
- 3. Compute the first 5 iterates of Newton's method for minimizing f starting with  $x_0 = [-1, -2]^T$ . Draw the level lines of the function f using ezcontour in the domain [-1.5;2;-3;3]. Display the iterates on the same graph.
- **4.** Compute the norm of the error  $||x x^*||$  at each iteration and determine if the convergence rate is quadratic.

**Exercise 14** (Optimal step gradient method and Wolfe's method). Let  $f : \mathbb{R}^n \to \mathbb{R}$  be a real valued function of n variables. The constant step gradient method consists in computing the iterations

$$x_{k+1} = x_k - \alpha \nabla f(x_k)$$

where  $\alpha$  is a constant.

1. Implement the gradient method with  $\alpha = 1$ . Test your program on the function  $f(x) = x_1^2 + 2x_2^2$  starting from  $x_0 = (-1, -1)$ . Test for several steps of descent: for example  $\alpha = 0.1$ ,  $\alpha = 0.1$ ,  $\alpha = 0.5$  and  $\alpha = 1$ . Comment on this.

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- **2.** Do the same with the Rosenbrock function starting for example in  $x_0 = (-1, 1.2)$  and  $\alpha = 0.001$ .
- **3.** In the optimal step gradient method, we look for  $\alpha_k$  such that

$$\min_{\alpha_k \ge 0} f(x_k - \alpha_k \nabla f(x_k)).$$

To find  $\alpha_k$ , we will use Wolfe's method. Let g(t) = f(x + td). where d is a direction of descent. Given  $t \in \mathbb{R}^+$ , the Wolfe's linear search method consists in narrowing a confidence interval  $[t_g, t_d]$  in which we choose a t that we test.

- Initially,  $t_g = 0$ ,  $t_d = +\infty$  and t = 1,  $m_1 = 0.1$ ,  $m_2 = 0.9$
- if  $g(t) \le g(0) + m_1 t g'(0)$  and  $g'(t) \ge m_2 g'(0)$  then stop
- if  $g(t) > g(0) + m_1 t g'(0)$  then let  $t_d = t$ ,  $t_g = t_g$  and  $t = (t_d + t_g)/2$  (if  $t_d = +\infty$  then  $t = 10t_g$ )
- if  $g(t) \le g(0) + m_1 t g'(0)$  and  $g'(t) < m_2 g'(0)$  then  $t_g = t$ ,  $t_d = t_d$  and  $t = (t_d + t_g)/2$  (if  $t_d = +\infty$  then  $t = 10t_g$ )

Implement the optimal step gradient method with Wolfe's method. Test your implementation on the Rosenbrock function.

**Exercise 15** (Nelder-Meade algorithm). The Nelder-Mead method is a nonlinear optimization algorithm that was proposed by John Nelder and Roger Mead in 1965. It is a numerical heuristic method that tries to minimize a continuous function in a multidimensional space.

- 1. Choice of N+1 points of the N-dimensional space of the unknowns, forming a simplex:  $\{x_1, x_2, \dots, x_{N+1}\}$ ,
- 2. Compute the values of the function f at these points, sort the points so as to have  $f(x_1) \le f(x_2) \le \cdots \le f(x_{N+1})$ . In fact, it is enough to know the first and the last two.
- 3. Compute  $x_0$ , center of gravity of all points except  $x_{N+1}$ .
- 4. Compute  $x_r = x_0 + (x_0 x_{N+1})$  (reflection of  $x_{N+1}$  from  $x_0$ ).
- 5. If  $f(x_r) < f(x_N)$ , compute  $x_e = x_0 + 2(x_0 x_{N+1})$  (simplex expansion). If  $f(x_e) < f(x_r)$ , replace  $x_{N+1}$  by  $x_e$ , otherwise, replace  $x_{N+1}$  by  $x_r$ . Return to step 2.
- 6. If  $f(x_N) < f(x_r)$ , compute  $x_c = x_{N+1} + 1/2(x_0 x_{N+1})$  (simplex contraction). If  $f(x_c) \le f(x_N)$ , replace  $x_{N+1}$  by  $x_c$  and return to step 2, otherwise go to step 7.
- 7. Shrink toward  $x_1$ : replace  $x_i$  by  $x_1 + 1/2(x_i x_1)$  for  $i \ge 2$ . Return to step 2.

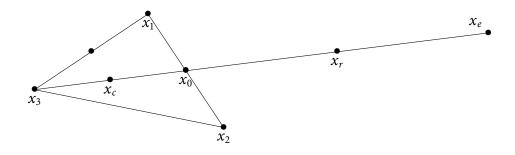


Figure 1: Nelder-Meade algorithm

- 1. Implement the Nelder-Meade algorithm.
- **2.** Test your code on the Rosenbrock function.
- 3. Compare your result with the MATLAB command fminsearch.