

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 ∇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 ∇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 λ and μ , 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 α 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 α_k such that

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

To find α_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.

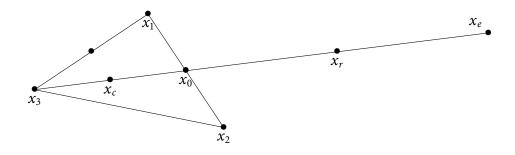


Figure 1: Nelder-Meade algorithm

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