

MATH60005/70005: Optimization (Autumn 23-24)

Week 4: Exercises

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1. Find the exact linesearch stepsize when $f(\mathbf{x})$ is a quadratic function $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A} \mathbf{x} + 2\mathbf{b}^\top \mathbf{x} + \mathbf{c}$ where \mathbf{A} is an $n \times n$ positive definite matrix, $\mathbf{b} \in \mathbb{R}^n$ and $\mathbf{c} \in \mathbb{R}$.
2. Let \mathbf{A} be a symmetric $n \times n$ matrix, $\mathbf{b} \in \mathbb{R}^n$ and $c \in \mathbb{R}$. Then the function $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A} \mathbf{x} + 2\mathbf{b}^\top \mathbf{x} + \mathbf{c}$ is a $C^{1,1}$ function. The smallest Lipschitz constant of f is $2\|\mathbf{A}\|_2$.
3. Show that $f(x) = \sqrt{1+x^2} \in C_L^{1,1}$.
4. Give an example of a function $f \in C_L^{1,1}(\mathbb{R})$ and a starting point $x_0 \in \mathbb{R}$ such that the problem $\min f(x)$ has an optimal solution and the gradient method with constant stepsize $t = \frac{2}{L}$ diverges.
5. Consider the localization problem where we are given m locations of sensors $\mathcal{A} := \{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_m\}$, with each sensor in \mathbb{R}^n , and approximate distances between the sensors and an unknown source located at $\mathbf{x} \in \mathbb{R}^n$: $d_i \approx \|\mathbf{x} - \mathbf{a}_i\|$. We try to find the source location \mathbf{x} given the sensor locations \mathcal{A} and the approximate distances d_1, d_2, \dots, d_m . For this, we write the optimization problem:

$$\min_{\mathbf{x}} \left\{ f(\mathbf{x}) \equiv \sum_{i=1}^m (\|\mathbf{x} - \mathbf{a}_i\| - d_i)^2 \right\}.$$

- a) State the first-order optimality condition for this problem, and show that for $\mathbf{x} \notin \mathcal{A}$ it is equivalent to

$$\mathbf{x} = \frac{1}{m} \left\{ \sum_{i=1}^m \mathbf{a}_i + \sum_{i=1}^m d_i \frac{\mathbf{x} - \mathbf{a}_i}{\|\mathbf{x} - \mathbf{a}_i\|} \right\}$$

- b) Show that the iteration:

$$\mathbf{x}^{k+1} = \frac{1}{m} \left\{ \sum_{i=1}^m \mathbf{a}_i + \sum_{i=1}^m d_i \frac{\mathbf{x}^k - \mathbf{a}_i}{\|\mathbf{x}^k - \mathbf{a}_i\|} \right\}$$

is a gradient method, assuming that $\mathbf{x}^k \notin \mathcal{A}$ for all $k \geq 0$. What is the stepsize?



c) Write an explicit Gauss-Newton iteration of the form

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \mathbf{d}^k,$$

giving an expression for \mathbf{d}^k in terms of the Jacobian and vectorized cost for this problem, without computing the inverse.

6. Consider the quadratic function $f : \mathbb{R}^2 \rightarrow \mathbb{R}$

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^\top Q \mathbf{x}$$

where Q is a symmetric matrix of size 2×2 with eigenvalues $0 < \lambda_{\min} < \lambda_{\max}$. Suppose we apply the gradient descent method to the problem of minimizing f , with exact line search and initial point

$$\mathbf{x}_0 = \frac{1}{\lambda_{\min}} \mathbf{u}_{\min} + \frac{1}{\lambda_{\max}} \mathbf{u}_{\max}$$

where \mathbf{u}_{\min} and \mathbf{u}_{\max} are the norm one eigenvectors associated with λ_{\min} and λ_{\max} , respectively.

a) Show that after 1 iteration

$$\mathbf{x}_1 = \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right) \left(\frac{1}{\lambda_{\min}} \mathbf{u}_{\min} - \frac{1}{\lambda_{\max}} \mathbf{u}_{\max} \right).$$

b) Assuming that

$$\mathbf{x}_k = \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right)^k \left(\frac{1}{\lambda_{\min}} \mathbf{u}_{\min} + \frac{(-1)^k}{\lambda_{\max}} \mathbf{u}_{\max} \right) \quad \text{for } k = 0, 1, \dots,$$

show that

$$\frac{f(\mathbf{x}_{k+1})}{f(\mathbf{x}_k)} = \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right)^2.$$

Using this, what can be said about the convergence of this method based on the ratio $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}}$?

Quadratic Optimization Benchmark

Consider the quadratic minimization problem

$$\min_{\mathbf{x}} \{ \mathbf{x}^\top \mathbf{A} \mathbf{x} : \mathbf{x} \in \mathbb{R}^5 \}$$

where \mathbf{A} is the 5×5 Hilbert matrix defined by

$$\mathbf{A}_{i,j} = \frac{1}{i+j-1}, \quad i, j = 1, 2, 3, 4, 5$$

The matrix can be constructed via the MATLAB command `A=hilb(5)`. Run the following methods and compare the number of iterations required by each of the methods when the initial vector is $\mathbf{x}^0 = (1, 2, 3, 4, 5)^\top$ to obtain a solution \mathbf{x}^* with $\|\nabla f(\mathbf{x})\| \leq 10^{-4}$:



- Gradient method with backtracking stepsize rule and parameters $\alpha = 0.5, \beta = 0.5, s = 1$
- Gradient method with backtracking stepsize rule and parameters $\alpha = 0.1, \beta = 0.5, s = 1$
- Diagonally scaled gradient method with diagonal elements $D_{i,i} = \frac{1}{A_{i,i}}, i = 1,2,3,4,5$ and exact line search;
- Diagonally scaled gradient method with diagonal elements $D_{i,i} = \frac{1}{A_{i,i}}, i = 1,2,3,4,5$ and backtracking line search with parameters $\alpha = 0.1, \beta = 0.5 s = 1$.

Solutions

1) For the quadratic function $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A} \mathbf{x} + 2\mathbf{b}^\top \mathbf{x} + \mathbf{c}$, the gradient reads $\nabla f(\mathbf{x}) = 2(\mathbf{A} \mathbf{x} + \mathbf{b})$, and the gradient descend iteration is

$$\mathbf{x}^{k+1} = \mathbf{x}^k - t^k \nabla f(\mathbf{x}^k),$$

where we tune the stepsize t^k using linesearch. This amounts to solve

$$\min_{t \geq 0} \{g(t) := f(\mathbf{y} + t\mathbf{d})\}, \quad \text{with } \mathbf{d} = -\nabla f(\mathbf{x}^k), \quad \mathbf{y} = \mathbf{x}^k.$$

Substituting the definition of $f(\cdot)$ and $\nabla f(\cdot)$ into $g(t)$, we obtain

$$\begin{aligned} g(t) &= (\mathbf{y} + t\mathbf{d})^\top \mathbf{A}(\mathbf{y} + t\mathbf{d}) + 2\mathbf{b}^\top (\mathbf{y} + t\mathbf{d}) + \mathbf{c} \\ &= t^2 (\mathbf{d}^\top \mathbf{A} \mathbf{d}) + 2(\mathbf{d}^\top \mathbf{A} \mathbf{y} + \mathbf{d}^\top \mathbf{b})t + \mathbf{x}^\top \mathbf{A} \mathbf{y} + 2\mathbf{b}^\top \mathbf{y} + \mathbf{c} \\ &= t^2 (\mathbf{d}^\top \mathbf{A} \mathbf{d}) + 2(\mathbf{d}^\top \mathbf{A} \mathbf{y} + \mathbf{d}^\top \mathbf{b})t + f(\mathbf{y}). \end{aligned}$$

To find the minimizer of $g(t)$, we impose the first order optimality condition for

$$g'(t) := 2t(\mathbf{d}^\top \mathbf{A} \mathbf{d}) + 2(\mathbf{d}^\top \mathbf{A} \mathbf{y} + \mathbf{d}^\top \mathbf{b}),$$

i.e. we are looking for $t \geq 0$ such that $g'(t) = 0$. This leads to

$$t = -\frac{\mathbf{d}^\top 2(\mathbf{A} \mathbf{y} + \mathbf{b})}{2(\mathbf{d}^\top \mathbf{A} \mathbf{d})} = -\frac{\mathbf{d}^\top (\nabla f(\mathbf{y}))}{2(\mathbf{d}^\top \mathbf{A} \mathbf{d})}$$

and substituting back $\mathbf{d} = -\nabla f(\mathbf{x}^k), \mathbf{y} = \mathbf{x}^k$, we have

$$t^k = +\frac{\|\nabla f(\mathbf{x}^k)\|^2}{2\nabla f(\mathbf{x}^k)^\top \mathbf{A} \nabla f(\mathbf{x}^k)}.$$

To conclude, we need check whether the computed stepsize is positive. Under the assumption $\nabla f(\mathbf{x}^k) \neq 0$, we have that both the numerator and the denominator (remember that $\mathbf{A} > 0$) are strictly positive, hence $t^k > 0$, and finally

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \frac{\|\nabla f(\mathbf{x}^k)\|^2}{2\nabla f(\mathbf{x}^k)^\top \mathbf{A} \nabla f(\mathbf{x}^k)} \nabla f(\mathbf{x}^k).$$



2) We want to show that – for f and ∇f as before – we have

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\|, \quad \text{for } L = 2\|\mathbf{A}\|_2.$$

Substituting the expression of the gradient on the left-hand side, we have

$$\|2(\mathbf{A}\mathbf{x} + b) - 2(\mathbf{A}\mathbf{y} + b)\| = 2\|\mathbf{A}(\mathbf{x} - \mathbf{y})\|$$

for which the Lipschitz condition becomes

$$\|\mathbf{A}(\mathbf{x} - \mathbf{y})\| \leq \|\mathbf{A}\|_2\|\mathbf{x} - \mathbf{y}\|.$$

Thus, we aim at showing $\|\mathbf{A}(\mathbf{z})\| \leq \|\mathbf{A}\|_2\|\mathbf{z}\|$ by using the definition of norm

$$\|\mathbf{A}\|_2 = \|\mathbf{A}\|_{2,2} = \max_{\|\mathbf{z}\|_2 \leq 1} \|\mathbf{A}\mathbf{z}\|.$$

We proceed by contradiction: assume that $\|\mathbf{A}\mathbf{z}\| > \|\mathbf{A}\|_2\|\mathbf{z}\|$. Dividing both sides by $\|\mathbf{z}\|$, we obtain

$$\left\| \mathbf{A} \frac{\mathbf{z}}{\|\mathbf{z}\|} \right\| > \|\mathbf{A}\|_2,$$

which is equivalent to $\|\mathbf{A}\mathbf{v}\| > \|\mathbf{A}\|_2$ for all $\|\mathbf{v}\| = 1$. In particular, this holds for the maximum

$$\max_{\|\mathbf{v}\| \leq 1} \|\mathbf{A}\mathbf{v}\| > \|\mathbf{A}\|_2$$

which contradicts the definition of norm. Thus, we have the required inequality

$$\|\mathbf{A}\mathbf{z}\| \leq \|\mathbf{A}\|_2\|\mathbf{z}\|,$$

for $\mathbf{z} = \mathbf{x} - \mathbf{y}$.

3) We start by dealing with the one-dimensional case. If we define the function f and its derivative as

$$f(x) = \sqrt{1+x^2}, \quad f'(x) = \frac{x}{\sqrt{1+x^2}},$$

the Lipschitz condition reads

$$\left\| \frac{x}{\sqrt{1+x^2}} - \frac{y}{\sqrt{1+y^2}} \right\| \leq L\|x - y\|.$$

Since the above inequality is difficult to prove, we rely on the link between Lipschitz continuity and the norm of the Hessian: for f convex and twice differentiable (as in this case), we have

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\| \iff \|\nabla^2 f(\mathbf{x})\| \leq L.$$

Since we are considering $f : \mathbb{R} \rightarrow \mathbb{R}$, we want to bound the absolute value of the second derivative

$$f''(x) = \frac{\sqrt{1+x^2} - \frac{\sqrt{1+x^2}}{x^2}}{1+x^2} = \frac{1}{(1+x^2)^{\frac{3}{2}}}, \quad \|f''(x)\| \leq 1 \iff f \in C_1^{1,1}.$$



Moving to the multi-dimensional case, we consider

$$f(\mathbf{x}) = \sqrt{1 + \|\mathbf{x}\|^2}, \quad \nabla f(\mathbf{x}) = \frac{\mathbf{x}}{\sqrt{1 + \|\mathbf{x}\|^2}}, \quad \mathbf{x} = [x_1, \dots, x_n]^\top \in \mathbb{R}^n$$

for which the partial derivatives read

$$\frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j} = \frac{\delta_{i,j}}{\sqrt{1 + \|\mathbf{x}\|^2}} - \frac{x_i x_j}{(1 + \|\mathbf{x}\|^2)^{\frac{3}{2}}}, \quad i, j = 1, \dots, n$$

where $\delta_{i,j}$ are the Dirac deltas defined as $\delta_{i,j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$.

Moreover, we obtain the Hessian

$$\mathcal{H} := \nabla^2 f(\mathbf{x}) = a \mathbb{1} - a^3 \mathbf{x} \mathbf{x}^\top, \quad a = \frac{1}{\sqrt{1 + \|\mathbf{x}\|^2}},$$

whose norm can be computed as

$$\|\nabla^2 f(\mathbf{x})\| = \sqrt{\lambda_{\max}(\mathcal{H}^\top \mathcal{H})} = \sqrt{\lambda_{\max}(\mathcal{H}^2)} = \sqrt{\lambda_{\max}(\mathcal{H})^2} = |\lambda_{\max}(\mathcal{H})|.$$

The Hessian \mathcal{H} has eigenvectors \mathbf{x} and \mathbf{x}^\perp , associated to eigenvalues $\lambda_1 = (a - a^3 \|\mathbf{x}\|^2)$ and $\lambda_2 = a$ respectively. We conclude by noticing that $a \geq 0$, hence $\lambda_{\max} = \lambda_2 = a$, and finally

$$a = \frac{1}{\sqrt{1 + \|\mathbf{x}\|^2}} \leq 1 \iff f \in C_1^{1,1}.$$

- 4) We consider the function $f(x) = x^2$, with first derivative $f'(x) = 2x$. Then, f is L -Lipschitz continuous with $L = 2$, since we have that

$$\|f'(x) - f'(y)\| \leq 2\|x - y\|.$$

The gradient descend iteration for f with constant stepsize $t = \frac{2}{L} = 1$ reads

$$x^{k+1} = x^k - t2x^k = x^k - 2x^k = -x^k.$$

Hence, the method diverges for every $x_0 \neq 0$, as its iterations oscillate repeatedly between x_0 and $-x_0$. It would be enough to consider $t = \frac{2}{L} - \varepsilon$, with $\varepsilon > 0$ to have convergence of the gradient method for f .

- 5a) The first order optimality condition reads $\nabla f(\mathbf{x}) = 0$. Recalling that for $g(\mathbf{x}) = \|\mathbf{x}\|$ we write (for $\mathbf{x} \neq \mathbf{0}$) its gradient $\nabla g(\mathbf{x}) = \mathbf{x}/\|\mathbf{x}\|$, a direct calculation shows that

$$\nabla f(\mathbf{x}) = 2 \sum_{i=1}^m (\|\mathbf{x} - \mathbf{a}_i\| - d_i) \frac{\mathbf{x} - \mathbf{a}_i}{\|\mathbf{x} - \mathbf{a}_i\|} = 2 \left(\sum_{i=1}^m (\mathbf{x} - \mathbf{a}_i) - \sum_{i=1}^m d_i \frac{\mathbf{x} - \mathbf{a}_i}{\|\mathbf{x} - \mathbf{a}_i\|} \right).$$



Then, setting $\nabla f(\mathbf{x}) = \mathbf{0}$ leads to

$$\begin{aligned}\nabla f(\mathbf{x}) &= \mathbf{0} \\ 2 \left(\sum_{i=1}^m (\mathbf{x} - \mathbf{a}_i) - \sum_{i=1}^m d_i \frac{\mathbf{x} - \mathbf{a}_i}{\|\mathbf{x} - \mathbf{a}_i\|} \right) &= \mathbf{0} \\ \sum_{i=1}^m \mathbf{x} &= \sum_{i=1}^m \mathbf{a}_i + \sum_{i=1}^m d_i \frac{\mathbf{x} - \mathbf{a}_i}{\|\mathbf{x} - \mathbf{a}_i\|} \\ \mathbf{x} &= \frac{1}{m} \left(\sum_{i=1}^m \mathbf{a}_i + \sum_{i=1}^m d_i \frac{\mathbf{x} - \mathbf{a}_i}{\|\mathbf{x} - \mathbf{a}_i\|} \right).\end{aligned}$$

5b) If the iteration is a gradient method, it can be expressed as

$$\mathbf{x}^{k+1} = \frac{1}{m} \left\{ \sum_{i=1}^m \mathbf{a}_i + \sum_{i=1}^m d_i \frac{\mathbf{x}^k - \mathbf{a}_i}{\|\mathbf{x}^k - \mathbf{a}_i\|} \right\} = \mathbf{x}^k + t^k \mathbf{d}^k$$

From part a) we now that

$$\mathbf{x}^k - \frac{1}{m} \left\{ \sum_{i=1}^m \mathbf{a}_i + \sum_{i=1}^m d_i \frac{\mathbf{x}^k - \mathbf{a}_i}{\|\mathbf{x}^k - \mathbf{a}_i\|} \right\} = \frac{1}{2m} \nabla f(\mathbf{x}^k),$$

or rearranging

$$\mathbf{x}^k - \frac{1}{2m} \nabla f(\mathbf{x}^k) = \frac{1}{m} \left\{ \sum_{i=1}^m \mathbf{a}_i + \sum_{i=1}^m d_i \frac{\mathbf{x}^k - \mathbf{a}_i}{\|\mathbf{x}^k - \mathbf{a}_i\|} \right\},$$

that is, the iteration corresponds to gradient descent with constant stepsize $t = \frac{1}{2m}$.

5c) In the Gauss-Newton method the direction \mathbf{d}^k is given by

$$\mathbf{d}^k = (J(\mathbf{x}^k)^\top J(\mathbf{x}^k))^{-1} J(\mathbf{x}^k)^\top F(\mathbf{x}^k),$$

where $F(\mathbf{x})$ in \mathbb{R}^m corresponds to the vector function associated to the cost

$$F(\mathbf{x}) = \begin{bmatrix} \|\mathbf{x} - \mathbf{a}_1\| - d_1 \\ \vdots \\ \|\mathbf{x} - \mathbf{a}_m\| - d_m \end{bmatrix},$$

and $J(\mathbf{x})$ in $\mathbb{R}^{m \times n}$ is the Jacobian matrix given by

$$J(\mathbf{x}) = \begin{bmatrix} \frac{(\mathbf{x} - \mathbf{a}_1)^\top}{\|\mathbf{x} - \mathbf{a}_1\|} \\ \vdots \\ \frac{(\mathbf{x} - \mathbf{a}_m)^\top}{\|\mathbf{x} - \mathbf{a}_m\|} \end{bmatrix}.$$



- 6a) For a quadratic function, one has that the stepsize when performing an exact line search at the point \mathbf{x}_k in the direction $-\mathbf{d}_k \equiv -\nabla f(\mathbf{x}_k) = -Q\mathbf{x}_k$ is

$$\alpha_k = \frac{\mathbf{d}_k^\top \mathbf{d}_k}{\mathbf{d}_k^\top Q \mathbf{d}_k}$$

Thus, we obtain

$$\begin{aligned} \mathbf{d}_0 &= Q \left(\frac{1}{\lambda_{\min}} \mathbf{u}_{\min} + \frac{1}{\lambda_{\max}} \mathbf{u}_{\max} \right) = \mathbf{u}_{\min} + \mathbf{u}_{\max} \\ \mathbf{d}_0^\top \mathbf{d}_0 &= (\mathbf{u}_{\min} + \mathbf{u}_{\max})^\top (\mathbf{u}_{\min} + \mathbf{u}_{\max}) = \|\mathbf{u}_{\min}\|^2 + \|\mathbf{u}_{\max}\|^2 = 2 \\ \mathbf{d}_0^\top Q \mathbf{d}_0 &= (\mathbf{u}_{\min} + \mathbf{u}_{\max})^\top (\lambda_{\min} \mathbf{u}_{\min} + \lambda_{\max} \mathbf{u}_{\max}) = \lambda_{\min} + \lambda_{\max} \end{aligned}$$

Therefore,

$$\alpha_0 = \frac{2}{\lambda_{\min} + \lambda_{\max}}$$

and

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{x}_0 - \alpha_0 \mathbf{d}_0 = \frac{1}{\lambda_{\min}} \mathbf{u}_{\min} + \frac{1}{\lambda_{\max}} \mathbf{u}_{\max} - \frac{2}{\lambda_{\min} + \lambda_{\max}} (\mathbf{u}_{\min} + \mathbf{u}_{\max}) \\ &= \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \left(\frac{1}{\lambda_{\min}} \mathbf{u}_{\min} - \frac{1}{\lambda_{\max}} \mathbf{u}_{\max} \right) \end{aligned}$$

- 6b) Using the expression for \mathbf{x}_k we obtain

$$\begin{aligned} \mathbf{x}_k^\top Q \mathbf{x} &= \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right)^{2k} \left(\frac{1}{\lambda_{\min}} \mathbf{u}_{\min} + \frac{(-1)^k}{\lambda_{\max}} \mathbf{u}_{\max} \right)^\top Q \left(\frac{1}{\lambda_{\min}} \mathbf{u}_{\min} + \frac{(-1)^k}{\lambda_{\max}} \mathbf{u}_{\max} \right) \\ &= \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right)^{2k} \left(\frac{1}{\lambda_{\min}} \mathbf{u}_{\min} + \frac{(-1)^k}{\lambda_{\max}} \mathbf{u}_{\max} \right)^\top (\mathbf{u}_{\min} + (-1)^k \mathbf{u}_{\max}) \\ &= \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right)^{2k} \left(\frac{1}{\lambda_{\min}} + \frac{(-1)^{2k}}{\lambda_{\max}} \right). \end{aligned}$$

The expression for $f(\mathbf{x}_{k+1})$ follows analogously evaluating at $k+1$, and noting that $(-1)^{2k} = (-1)^{2k+2}$, we conclude

$$\frac{f(\mathbf{x}_{k+1})}{f(\mathbf{x}_k)} = \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right)^2.$$

This indicates the value of the function decreases by a factor of

$$\left(\frac{\kappa - 1}{\kappa + 1} \right)^2,$$

where $\kappa > 1$. The closer κ gets to 1, the faster the method. As κ increases, the method becomes slower.

