TD 5 – Optimization

Mathematics of data

16/10/24

Exercise 1. Consider the least squares problem:

$$\min_{x\in\mathbb{R}^d} f(x) := \frac{1}{2}\|Ax-b\|^2,$$

where $A \in \mathbb{R}^{n\times p}$ is the data matrix and $b \in \mathbb{R}^n$ is the vector of labels, and $\|c\| := \sqrt{\sum c_i^2}$ is the Euclidean norm.

1. Assume that $n < p$ and that $AA^\top$ is invertible. We define $A^+ := A^\top(AA^\top)^{-1}$ the pseudo-inverse of A. Check that $x^* := A^+b$ is a solution of the least squares problem. What is the set of all solutions of this problem?

The aim of this exercise is to determine to which solution gradient descent converges. Note that we cannot apply the method seen in TD 4 ex 2, as here the conditioning of the problem is equal to 0.

2. Denote $x^0, x^1, \dots, x^k, \dots$ the iterates of gradient descent with step-size α, starting from $x^0 = 0$. Demonstrate that there exists $u^k \in \mathbb{R}^n$ such that $x^k = A^\top u^k$ for all $k \geq 0$. What is the recursion satisfied by u^k?
3. Assume that $\alpha \leq \frac{1}{\lambda_{\max}(AA^\top)}$. Show that $\lim_{k\to+\infty} u^k = (AA^\top)^{-1}b$.
4. What is the limit of x^k? Show that this is the vector with the smallest norm among all minimizers of f.

Exercise 2.

1. Show that the set of minimizers of a convex function is a convex set.
2. Let $y \in \mathbb{R}$ and
$$f\colon x \in \mathbb{R} \mapsto \frac{1}{2}(x-y)^2 \qquad \text{and} \qquad g\colon (a,b) \in \mathbb{R}^2 \mapsto \frac{1}{2}(ab-y)^2.$$
   (a) What is the set of minimizers of f? Of g?
   (b) If f convex, coercive? Same question for g.
3. (a) Compute the gradient and Hessian of f and g.
   (b) Assume that y is positive. Give the equation of the region where g is locally convex, and draw it.
4. Let $Y \in \mathbb{R}^{n\times n}$. Define
$$f\colon X \in \mathbb{R}^{n\times n} \mapsto \frac{1}{2}\|X-Y\|_F^2 \qquad \text{and} \qquad g\colon (A,B) \in \mathbb{R}^{n\times n}\times\mathbb{R}^{n\times n} \mapsto \frac{1}{2}\|AB-Y\|_F^2.$$
   (a) What is the set of minimizers of f? Of g? If f convex, coercive? Same question for g.
   (b) Compute the gradient of f and g (represented as matrices).

Exercise 3. Let $b \in \mathbb{R}^d$ and denote $\mathbf{1}$ the d-dimensional vector with all coordinates equal to 1. What is the solution (i.e. the minimizer) of

$$\min_{x\in\mathbb{R}} \|x\mathbf{1} - b\|$$

1. when $\|y\| := \sqrt{\sum_{i=1}^d y_i^2}$ (ℓ_2 norm)?
2. when $\|y\| := \max_{i=1}^d |y_i|$ (ℓ_∞ norm)?
3. when $\|y\| := \sum_{i=1}^d |y_i|$ (ℓ_1 norm)?

If you have finished all the exercises, you can move on to the TP5 on github.com/vcastin/teaching

Solutions

Exercise 1.

1. The set of solutions is $x^* + \ker A$. Indeed, the minimal value of f is zero, and a vector $x^* + h \in \mathbb{R}^p$ is a minimizer of f if $\|Ax^* + Ah - b\|^2 = \|Ah\|^2 = 0$, i.e., if $h \in \ker A$.

2. The iterates of gradient descent read
$$x^{k+1} = x^k - \alpha A^\top (Ax^k - b).$$
We have $x^0 = A^\top u^0$ with $u^0 = 0$. If $x^k = A^\top u^k$, then
$$x^{k+1} = A^\top (u^k - \alpha(AA^\top u^k - b))$$
so the claim is true by recursion, and
$$u^{k+1} = u^k - \alpha(AA^\top u^k - b) = (I - \alpha AA^\top)u^k + \alpha b.$$

3. The vector $(AA^\top)^{-1}b$ is a fixed point of the recursion of u, so
$$u^{k+1} - (AA^\top)^{-1}b = (I - \alpha AA^\top)(u^k - (AA^\top)^{-1}b).$$
Unfolding the recurrence gives
$$u^k = (AA^\top)^{-1}b - (I - \alpha AA^\top)^k (AA^\top)^{-1}b$$
as $u^0 = 0$. Hence
$$\left\|u^k - (AA^\top)^{-1}b\right\| \leq \left\|I - \alpha AA^\top\right\|_2^k \left\|(AA^\top)^{-1}b\right\|.$$
The operator norm $\left\|I - \alpha AA^\top\right\|_2 = \max(|1 - \alpha\lambda_{\max}(AA^\top)|, |1 - \alpha\lambda_{\min}(AA^\top)|)$ is < 1 if and only if $\alpha < 2/\lambda_{\max}$, which is the case for $\alpha \leq 1/\lambda_{\max}$. Under this assumption, $\left\|I - \alpha AA^\top\right\|_2^k$ goes to 0 when $k \to \infty$, which allows us to conclude.

4. We have $x^k \to_{k\to\infty} A^\top(AA^\top)^{-1}b = x^*$. This is the minimizer with the smallest norm, indeed for any $z \in \ker A$ it holds
$$\left\|A^\top(AA^\top)^{-1}b + z\right\|^2 = \left\|A^\top(AA^\top)^{-1}b\right\|^2 + \|z\|^2 \geq \|x^*\|^2.$$

Exercise 2.

1. Let x, y be two minimizers of a convex function f. Let $z \in [x, y] := \{(1-t)x + ty : t \in [0,1]\}$. Then $f(z) \leq (1-t)f(x) + tf(y) = \min f$, so z is also a minimizer of f.

2. (a) We find $\operatorname{argmin} f = \{y\}$ and $\operatorname{argmin} g = \{(a,b) : ab = y\}$, which is a hyperbola if $y \neq 0$, and is the union $\{(0,b) : b \in \mathbb{R}\} \cup \{(a,0) : b \in \mathbb{R}\}$ if $y = 0$.
   (b) f is convex and coercive, whereas g is neither coercive (take $(a, 1/a)$ for $a \to +\infty$) nor convex (the set of its minimizers is not convex).

3. (a) We compute
$$f'(x) = x - y \quad \text{and} \quad f''(x) = 1,$$
and
$$\nabla g(a,b) = (ab - y)(b,a) \quad \text{and} \quad D^2 g(a,b) = \begin{pmatrix} b^2 & 2ab - y \\ 2ab - y & a^2 \end{pmatrix}.$$
   (b) The matrix $D^2 g(a,b)$ is non-negative if and only if its trace and its determinant are non-negative. Its trace is always non-negative, so the condition reduces to $a^2b^2 - (2ab - y)^2 \geq 0$, which can be factorized as $(3ab - y)(y - ab) \geq 0$. Therefore, g is locally convex between the hyperbolas given by $ab = y/3$ and $ab = y$.

4. (a) We find $\operatorname{argmin} f = \{Y\}$ and $\operatorname{argmin} g = \{A, B \in \mathbb{R}^{n\times n} : AB = Y\}$. The function f is convex and coercive, whereas g is neither coercive (take $(\lambda I, \frac{1}{\lambda}Y)$ with $\lambda \to \infty$) nor convex (the set of its minimizers is not convex).
   (b) We compute $\nabla f(X) = X - Y$ and $\nabla g(A,B) = ((AB - Y)B^\top, A^\top(AB - Y))$.

Exercise 3.

1. The mean $\frac{1}{d}\sum_{i=1}^{d} b_i$.

2. The middle point $\frac{1}{2}(\max_i b_i + \min_i b_i)$.

3. Let $k = \mathrm{card}\{b_1, \dots, b_d\}$ be the number of distinct values for the b_i. Denote $\{b_1, \dots, b_d\} = \{a_1, \dots, a_k\}$ with $a_1 < \cdots < a_k$ pairwise distinct, and denote $\nu_i = \mathrm{card}\{b_j : b_j = a_i\}$ the multiplicity of a_i in $(b_1, \dots, b_d)$. Then, the problem can be rewritten as

$$\min_{x\in\mathbb{R}} \sum_{i=1}^{k} \nu_i \left|x - a_i\right| .$$

Let $f\colon x \in \mathbb{R} \mapsto \sum_{i=1}^{k} \nu_i \left|x - a_i\right|$. If $x \in (a_{i_0}, a_{i_0+1})$, then

$$f(x) = \sum_{i=1}^{i_0} \nu_i (x - a_i) + \sum_{i=i_0+1}^{k} \nu_i (a_i - x) \quad \text{and} \quad f'(x) = \sum_{i=1}^{i_0} \nu_i - \sum_{i=i_0+1}^{k} \nu_i.$$

We see that when x grows, f' goes from being negative to being positive.

- If there exists i_0 such that $\sum_{i=1}^{i_0} \nu_i = \sum_{i=i_0+1}^{k} \nu_i$, then every $x \in [a_{i_0}, a_{i_0+1}]$ is a minimizer of f (f decreases on $(-\infty, a_{i_0}]$, then is constant, then increases on $[a_{i_0+1}, +\infty)$).
- Otherwise, let i_0 be the smallest index such that $\sum_{i=1}^{i_0} \nu_i > \sum_{i=i_0+1}^{k} \nu_i$. The unique minimizer of f is then a_{i_0} (f decreases on $(-\infty, a_{i_0}]$ and increases on $[a_{i_0}, +\infty)$).

Note that we have obtained that the minimizers of f are the medians of $(b_1, \dots, b_d)$.