Tutorial 1: Basics of optimization

Optimization for data science, M2 MIAGE ID/ID Apprentissage

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Exercise 1: Linear least squares

We consider a dataset $\{(\boldsymbol{x}_i,y_i)\}_{i=1}^n$, wherein $\boldsymbol{x}_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$ for every $i=1,\ldots,n$. We seek a linear model that best fits the data, which we formulate as the following optimization problem:

$$\underset{\boldsymbol{w} \in \mathbb{R}^d}{\operatorname{minimize}} f(\boldsymbol{w}) := \frac{1}{2n} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2 = \frac{1}{2n} \sum_{i=1}^n (\boldsymbol{x}_i^{\mathrm{T}} \boldsymbol{w} - y_i)^2, \tag{1}$$

where $oldsymbol{X} \in \mathbb{R}^{n imes d}$ and $oldsymbol{y} \in \mathbb{R}^n$ are given by

$$m{X} = \left[egin{array}{c} m{x}_1^{
m T} \ dots \ m{x}_n^{
m T} \end{array}
ight], \quad m{y} = \left[egin{array}{c} y_1 \ dots \ y_n \end{array}
ight].$$

This problem is among the most classical in data analysis. Its objective function is C^2 , and the problem (1) always has at least one solution.

- a) Let $w^* \in \mathbb{R}^d$ satisfy $Xw^* = y$ (hence w^* is a solution of the linear system Xw = y). Justify then that w^* is a global minimum of the objective function.
- b) The gradient of f at any $w \in \mathbb{R}^d$ is given by $\nabla f(w) = \frac{1}{n} X^T (Xw y)$. If w^* satisfies $Xw^* = y$ as in question a), what is the value of $\nabla f(w^*)$?
- c) The Hessian matrix of f at $\boldsymbol{w} \in \mathbb{R}^d$ is given by $\nabla^2 f(\boldsymbol{w}) = \frac{1}{n} \boldsymbol{X}^T \boldsymbol{X}$. Note that it is constant with respect to \boldsymbol{w} , and that it only depends on the data matrix \boldsymbol{X} .
 - i) By construction, we have $\frac{1}{n}X^{T}X \succeq 0$. What property on f does this imply?
 - ii) Suppose that $\frac{1}{n}X^TX \succeq \mu I_d$ with $\mu > 0$. Given $w \in \mathbb{R}^d$, what can we say about $\nabla^2 f(w)$ in that case? What information does this provide about the set of solutions of problem (1)?

Exercise 2: Convex function

Let $q: \mathbb{R}^d \to \mathbb{R}$ be defined as $q(w) = \frac{1}{4} ||w||^4$. This function is \mathcal{C}^2 , and for every $w \in \mathbb{R}^d$, we have

$$abla q(\boldsymbol{w}) = \|\boldsymbol{w}\|^2 \boldsymbol{w}, \qquad
abla^2 q(\boldsymbol{w}) = 2 \boldsymbol{w} \boldsymbol{w}^{\mathrm{T}} + \|\boldsymbol{w}\|^2 \boldsymbol{I}_d.$$

- a) Using the expression of the Hessian matrix of q, show that the function q is convex. What does it imply on its local minima?
- b) Show that the zero vector $\mathbf{0}_{\mathbb{R}^d}$ is a local minimum of q. Does it satisfy the second-order sufficient condition?
- c) Given the answer to the previous question, can the function q be strongly convex?
- d) Justify that the function has a single global minimum.

Exercise 3: Quasiconvex functions

A function $f: \mathbb{R}^d \to \mathbb{R}$ is called **quasiconvex** if

$$\forall \boldsymbol{w}, \boldsymbol{v} \in \mathbb{R}^d, \ \forall t \in [0, 1], \quad f(t\boldsymbol{w} + (1 - t)\boldsymbol{v}) \le \max\{f(\boldsymbol{w}), f(\boldsymbol{v})\}. \tag{2}$$

Any convex function is quasiconvex, but the converse is not true.

Let f be a quasiconvex, C^2 function. We consider:

- a) Write the first- and second-order optimality conditions for problem (3).
- b) Since f is quasiconvex, it can be shown that

$$\forall \boldsymbol{w} \in \mathbb{R}^d, \ \forall \boldsymbol{v} \in \mathbb{R}^d, \quad \boldsymbol{v}^{\mathrm{T}} \nabla f(\boldsymbol{w}) = 0 \Rightarrow \boldsymbol{v}^{\mathrm{T}} \nabla^2 f(\boldsymbol{w}) \boldsymbol{v} \ge 0.$$
 (4)

Let w^* be a first-order stationary point. Justify that w^* is also a second-order stationary point.

Solutions

Solutions for Exercise 1

a) If $\boldsymbol{X}\boldsymbol{w}^*=\boldsymbol{y}$, then

$$f(w^*) = \frac{1}{2n} ||Xw^* - y||^2 = \frac{1}{2n} ||\mathbf{0}||^2 = 0.$$

Since f is always nonnegative (definition of a norm), we also have

$$\forall \boldsymbol{w} \in \mathbb{R}^d, f(\boldsymbol{w}) \geq 0 = f(\boldsymbol{w}^*).$$

The latter property corresponds to the definition of a global minimum for f, from which we conclude that w^* is a global minimum of f or, equivalently, a solution of the unconstrained problem (1).

b) The function f is continuously differentiable (\mathcal{C}^2 , so \mathcal{C}^1). If $X w^* = y$, then

$$\nabla f(\boldsymbol{w}^*) = \frac{1}{n} \boldsymbol{X}^{\mathrm{T}} (\boldsymbol{X} \, \boldsymbol{w}^* - \boldsymbol{y}) = \frac{1}{n} \boldsymbol{X}^{\mathrm{T}} (\boldsymbol{y} - \boldsymbol{y}) = \boldsymbol{0},$$

confirming the first-order optimality condition.

c)

- i) If $\frac{1}{n}X^{\mathrm{T}}X\succeq \mathbf{0}$, then $\nabla^2 f(w)\succeq \mathbf{0}$ for any $w\in\mathbb{R}^d$ This property is a characterization of convexity for a \mathcal{C}^2 function, from which we conclude that f is a convex function.
- ii) Similarly to the previous question, the fact that $\frac{1}{n}X^TX \succeq \mu I_d$ means that $\nabla^2 f(w) \succeq \mu I_d$ for any $w \in \mathbb{R}^d$. This is again a characterization of strong convexity for \mathcal{C}^2 functions, and therefore f is μ -strongly convex. As a result, there exists a unique solution for the optimization problem (or equivalently, f has a unique global minimum).

Solutions for Exercise 2

a) For any $w \in \mathbb{R}^d$ and any $v \in \mathbb{R}^d$, the linearity of both scalar products and matrix-vector products gives:

$$\mathbf{v}^{\mathrm{T}}\nabla^{2}q(\mathbf{w})\mathbf{v} = \mathbf{v}^{\mathrm{T}}(2\mathbf{w}\mathbf{w}^{\mathrm{T}} + \|\mathbf{w}\|^{2}\mathbf{I}_{d})\mathbf{v}$$

$$= \mathbf{v}^{\mathrm{T}}(2\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{v} + \|\mathbf{w}\|^{2}\mathbf{v})$$

$$= 2\mathbf{v}^{\mathrm{T}}\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{v} + \|\mathbf{w}\|^{2}\mathbf{v}^{\mathrm{T}}\mathbf{v}$$

$$= 2(\mathbf{w}^{\mathrm{T}}\mathbf{v})^{2} + \|\mathbf{w}\|^{2}\mathbf{v}^{\mathrm{T}}\mathbf{v}$$

$$= 2(\mathbf{w}^{\mathrm{T}}\mathbf{v})^{2} + \|\mathbf{w}\|^{2}\|\mathbf{v}\|^{2}$$

$$\geq 0.$$

Thus, for any $w \in \mathbb{R}^d$, the Hessian matrix $\nabla^2 q(w)$ is positive semidefinite, i.e. $\nabla^2 q(w) \succeq \mathbf{0}$. Consequently, the (\mathcal{C}^2) function q is convex, and all its local minima are global.

b) Since the function q is convex, every local minimum is global. Moreover, we have

$$q(\boldsymbol{w}) = \frac{1}{4} \|\boldsymbol{w}\|^4 \ge 0 = q(\boldsymbol{0}_{\mathbb{R}^d})$$

for any $\boldsymbol{w} \in \mathbb{R}^d$. The zero vector $\mathbf{0}_{\mathbb{R}^d}$ is thus a global minimum of q. If the zero vector were to satisfy the second-order sufficient optimality conditions, we would have $\nabla^2 q(\mathbf{0}_{\mathbb{R}^d}) \succ \mathbf{0}$. However, the expression for $\nabla^2 q$ gives

$$\nabla^2 q(\mathbf{0}_{\mathbb{R}^d}) = \mathbf{0},$$

and the zero matrix is only positive semidefinite (instead of positive definite). As a result, the zero vector does not satisfy the second-order sufficient optimality conditions. *Note: This does not contradict the fact that this vector is a global minimum, as the condition is sufficient but not necessary.*

- c) If the function were strongly convex, there would exist $\mu > 0$ such that $\nabla^2 q(w) \succeq \mu I_d \succ 0$ for any w, including the zero vector. Since the Hessian is zero at the zero vector, this cannot be true, from which we conclude that q is not strongly convex.
- d) For every $\boldsymbol{w} \in \mathbb{R}^d$, we have $q(\boldsymbol{w}) \geq q(\mathbf{0}_{\mathbb{R}^d}) = 0$, hence the zero vector is a global minimum. Moreover, $q(\boldsymbol{w}) = 0$ if and only if $\boldsymbol{w} = \mathbf{0}_{\mathbb{R}^d}$, and thus the zero vector is the only global minimum of q.

Note: Classical argument in this last question, typical first question of an exam.

Solutions for Exercise 3

a) The result is expected to be known. The first-order necessary optimality conditions can be stated as follows. If a vector $\boldsymbol{w}^* \in \mathbb{R}^d$ is a local minimum of a \mathcal{C}^1 function f, then $\nabla f(\boldsymbol{w}^*) = \boldsymbol{0}$. The second-order necessary optimality conditions are a stronger characterization. If $\boldsymbol{w}^* \in \mathbb{R}^d$ is a local minimum of f, then

$$\nabla f(\boldsymbol{w}^*) = \mathbf{0}$$
 and $\nabla^2 f(\boldsymbol{w}^*) \succeq \mathbf{0}$.

b) Since ${m w}^*$ is a first-order stationary point, it satisfies the first-order necessary conditions, hence $\nabla f({m w}^*) = {m 0}$ and

$$\forall \boldsymbol{v} \in \mathbb{R}^d, \quad \boldsymbol{v}^{\mathrm{T}} \nabla f(\boldsymbol{w}^*) = \boldsymbol{v}^{\mathrm{T}} \mathbf{0} = 0.$$

The left-hand side of the implication (4) thus holds for w^* and any vector v. Thus the right-hand also holds, i.e.

$$\boldsymbol{v}^{\mathrm{T}} \nabla^2 f(\boldsymbol{w}^*) \boldsymbol{v} > 0 \ \forall \boldsymbol{v} \in \mathbb{R}^d$$

which is equivalent to $\nabla^2 f(w^*) \succeq \mathbf{0}$. Therefore, the vector w^* satisfies the second-order necessary optimality conditions, and it is a second-order stationary point.