Optimization and Computational Linear Algebra for Data Science Lecture 10: Optimality conditions

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Warning: This material is not meant to be lecture notes. It only gathers the main concepts and results from the lecture, without any additional explanation, motivation, examples, figures...

1 Local and global minimizers

We aim at minimizing a function $f: \mathbb{R}^n \to \mathbb{R}$. We say that $x^* \in \mathbb{R}^n$ is

- a global minimizer of f if for all $x \in \mathbb{R}^n$, $f(x^*) \leq f(x)$.
- a local minimizer of f if there exists $\delta > 0$ such that for all $x \in B(x^*, \delta), f(x^*) \leq f(x)$.

Of course, a global minimizer if also a local minimizer but the converse is not true.

Proposition 1.1

Let $x \in \mathbb{R}^n$ be a point at which f is differentiable. Then $x \text{ is a local minimizer of } f \implies \nabla f(x) = 0.$

If f is convex then the converse is true:

Proposition 1.2

Assume that f is convex. Let $x \in \mathbb{R}^n$ be a point at which f is differentiable. Then

$$\nabla f(x) = 0 \implies x \text{ is a global minimizer of } f.$$

2 Constrained optimization

We would now like to investigate constrained optimization problems:

minimize
$$f(x)$$

subject to $g_i(x) \le 0$, $i = 1, ..., m$
 $h_i(x) = 0$, $i = 1, ..., p$, (1)

with variable $x \in \mathbb{R}^n$. Here we have m inequality constraints $g_1(x) \leq 0, \ldots, g_m(x) \leq 0$ and p equality constraints $h_1(x) = 0, \ldots, h_p(x) = 0$ to satisfy.

Definition 2.1 (Feasible point)

A point $x \in \mathbb{R}^n$ is feasible if it satisfies all the constraints: $g_1(x) \leq 0, \ldots, g_m(x) \leq 0$ and $h_1(x) = 0, \ldots, h_p(x) = 0$. We will denote by F the set of feasible points.

We would now get for the problem (1) the analog of Proposition 1.1. Since an equality constraint $h_i(x) = 0$ can be equivalently written in two inequality constraints $h_i(x) \leq 0$ and

 $-h_i(x) \le 0$, we can assume to have only inequality constraints. For simplicity, we first assume to have only one inequality constraint $g(x) \le 0$ so that (1) reduces to

minimize
$$f(x)$$
 subject to $g(x) \le 0$. (2)

Let x be a solution of (2), i.e. $g(x) \le 0$ and $f(x) \le f(x')$ for all x' such that $g(x') \le 0$ We distinguish two cases:

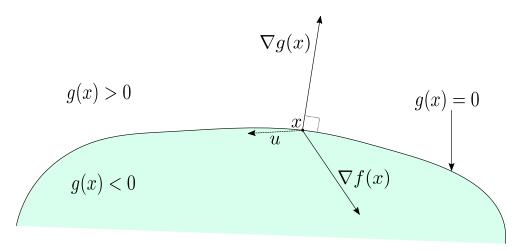
Case 1: x is "strictly feasible" g(x) < 0. In that case x is in the interior of F: one can find $\delta > 0$ such that $B(x, \delta) \subset F$. Since x is a solution of (2) we have for all $x' \in B(0, \delta)$, $f(x) \leq f(x')$. One can therefore apply Proposition 1.1 to get that $\nabla f(x) = 0$.

We conclude that in the case where the constraint is not active, the constraint does not play any role and one gets the same optimality condition as in the unconstrained setting.

Case 2: the constraint is active in x, g(x) = 0. In that case, there exists $\lambda \ge 0$ such that

$$\nabla f(x) = -\lambda \nabla g(x). \tag{3}$$

To see that, assume that (3) does not hold. Then we are in the following situation:



As we can see on the figure, we can find a vector u such that

$$\langle u, \nabla g(x) \rangle < 0$$
 and $\langle u, \nabla f(x) \rangle < 0$.

Starting from x and following the direction u one remains in the feasible set because for small $\delta > 0$

$$g(x + \delta u) \simeq g(x) + \delta \langle u, \nabla g(x) \rangle \le 0.$$

Moreover, f decreases locally on the direction u:

$$f(x + \delta u) \simeq f(x) + \delta \langle u, \nabla f(x) \rangle < f(x).$$

This means that one can find $\delta > 0$ such that $x + \delta u$ is feasible and such that $f(x + \delta u) < f(x)$. This contradicts the assumption that x is solution of (2). We conclude that (3) holds, i.e. that there exists $\lambda \geq 0$ such that

$$\nabla f(x) + \lambda \nabla g(x) = 0.$$

We will only cover the case where the equality constraints are linear, i.e. $h_i(x) = \langle a_i, x \rangle + b_i$ for from $a_i \in \mathbb{R}^n$ and $b_i \in \mathbb{R}$.

This generalize to the case (1) where we have multiple constraints:

Definition 2.2

We say that the constraints are qualified at $x \in F$ if there exists a vector $v \in \mathbb{R}^n$ such that $\langle v, \nabla h_i \rangle = 0$ for all i = 1, ..., p and such that for all i = 1, ..., m we have either

- $\langle v, \nabla g_i \rangle < 0$
- or $\langle v, \nabla g_i \rangle \leq 0$, and g_i is affine.

Theorem 2.1 (Karush-Kuhn-Tucker conditions)

Assume that the functions f, g_1, \ldots, g_m are differentiable and that h_1, \ldots, h_p are linear. If x is solution of (1) and if the constraints are qualified at x then there exists $\lambda_1, \ldots, \lambda_m \geq 0$ and $\nu_1, \ldots, \nu_p \in \mathbb{R}$ such that:

$$\nabla f(x) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x) + \sum_{i=1}^{p} \nu_i \nabla h_i(x) = 0.$$

$$\tag{4}$$

Moreover $\lambda_i = 0$ if $g_i(x) < 0$.

The scalars λ_i , ν_i are often called Lagrange multipliers.

3 The Lagrangian and the dual problem

We define the Lagrange dual function L associated with the problem (1) by

$$L(x, \lambda, \nu) = f(x) + \sum_{i=1}^{m} \lambda_i g_i(x) + \sum_{i=1}^{p} \nu_i h_i(x),$$
 (5)

where $x \in \mathbb{R}^n$, $\lambda \in \mathbb{R}^m_{\geq 0}$ and $\nu \in \mathbb{R}^p$. We define the Lagrange dual function by

$$\ell(\lambda, \nu) = \inf_{x \in \mathbb{R}^n} L(x, \lambda, \nu).$$

Notice that for all feasible point x,

$$L(x, \lambda, \nu) = f(x) + \sum_{i=1}^{m} \lambda_i g_i(x) \le f(x)$$

because $h_i(x) = 0$ and $\lambda_i g_i(x) \leq 0$. By taking the infimum in x on both sides of the inequality we get a lower bound on the value of the optimization problem (1):

Proposition 3.1

Let p^* be the optimal value of the problem (1). For all $\lambda_1, \ldots, \lambda_m \geq 0$ and all $\nu_1, \ldots, \nu_p \in \mathbb{R}$ we have:

$$\ell(\lambda, \nu) \le p^*. \tag{6}$$

3.1 Dual problem

We would like to make the lower bound (6) as tight as possible: one would like therefore to solve the so-called *dual problem*:

maximize
$$\ell(\lambda, \nu)$$

subject to $\lambda_i \ge 0, \quad i = 1, \dots, m$
 $\nu_i \in \mathbb{R}, \quad i = 1, \dots, p.$ (7)

Notice that the Lagrange dual function is always concave, as an infimum of linear functions. Hence, the dual problem might be easier to solve than the original problem.

From (6) we deduce that the optimal value of the primal problem is greater or equal than the one of the dual problem:

$$\sup_{\lambda > 0, \nu} \ell(\lambda, \nu) \le p^*. \tag{8}$$

This is known as weak duality.

Notice that $p^* = \inf_{x \in \mathbb{R}^n} F(x)$ where

$$F(x) \stackrel{\text{def}}{=} \sup_{\lambda \ge 0, \nu} L(x, \lambda, \nu) = \begin{cases} f(x) & \text{if } x \text{ is feasible,} \\ +\infty & \text{otherwise.} \end{cases}$$

Hence, the weak duality inequality can be rewritten as:

$$\sup_{\lambda > 0, \nu} \inf_{x \in \mathbb{R}^n} L(x, \lambda, \nu) \le \inf_{x \in \mathbb{R}^n} \sup_{\lambda > 0, \nu} L(x, \lambda, \nu). \tag{9}$$

When there is equality in (8) (or equivalently in (9)) we say that there is *strong duality*. We will see in the next section that strong duality holds for convex problems under mild assumptions.

3.2 Saddle-points

Definition 3.1 (Saddle-point)

We say that $(x; \lambda, \nu) \in \mathbb{R}^n \times \mathbb{R}^m_{\geq 0} \times \mathbb{R}^p$ is a saddle-point of L if

$$\forall (\lambda', \nu') \in \mathbb{R}^m_{\geq 0} \times \mathbb{R}^p \quad L(x, \lambda', \nu') \leq L(x, \lambda, \nu) \leq L(x', \lambda, \nu) \quad \forall x' \in \mathbb{R}^n.$$
 (10)

Notice that if $(x; \lambda, \nu)$ is a saddle point of L, then x is solution of (1). Indeed, by taking the supremum in (10) we get:

$$F(x) < L(x, \lambda, \nu) < L(x', \lambda, \nu) < F(x')$$

for all $x' \in \mathbb{R}^n$. By an analog argument one also get that (λ, ν) is a solution of the dual problem (7). In fact, it is not difficult to verify the stronger statement below:

Theorem 3.1

 $(x; \lambda, \nu) \in \mathbb{R}^n \times \mathbb{R}^m_{>0} \times \mathbb{R}^p$ is a saddle-point of L if and only if

$$F(x) = \inf_{x'} \sup_{\lambda' \ge 0, \nu'} L(x', \lambda', \nu') = \sup_{\lambda' \ge 0, \nu'} \inf_{x'} L(x', \lambda', \nu') = \ell(\lambda, \nu), \tag{11}$$

i.e. if and only if x is a solution of the primal problem (1), (λ, ν) is a solution of the dual problem (7) and strong duality holds.

3.3 Solving the primal problem via the dual

Assume that strong duality holds and that we have found a solution (λ^*, ν^*) of the dual problem. By Theorem 3.1 we get that a point $x^* \in \mathbb{R}^n$ is a solution of the primal problem if and only if $(x^*; \lambda^*, \nu^*)$ is a saddle-point of L:

$$x^*$$
 is solution of the primal problem \iff
$$\begin{cases} x^* & \text{minimizes} \quad L(\cdot, \lambda^*, \nu^*), \\ (\lambda^*, \nu^*) & \text{maximizes} \quad L(x^*, \cdot, \cdot). \end{cases}$$

Notice that (λ^*, ν^*) maximizes the linear function $L(x^*, \cdot, \cdot)$ if and only x^* is feasible. We obtain:

$$x^*$$
 is solution of the primal problem \iff
$$\begin{cases} x^* & \text{minimizes} \quad L(\cdot, \lambda^*, \nu^*), \\ x^* & \text{is feasible.} \end{cases}$$

This is particularly useful, indeed the dual problem might be easier to solve than the primal one. In the case when there is strong duality, the equivalence above tells us that it suffices then to solve the **unconstrained** optimization problem $\min_{x \in \mathbb{R}^n} L(x, \lambda^*, \nu^*)$. Assume for simplicity that $x \mapsto L(x, \lambda^*, \nu^*)$ admits a unique minimizer x^* . Then if x^* is feasible then it is a solution of the problem (1). If x^* is not feasible then the minimum of (1) can not be attained.

4 Kuhn Tucker Theorem

In this section, we assume that the functions f, g_1, \ldots, g_m are convex and that h_1, \ldots, h_p are linear. We say then that the optimization problem (1) is convex.

We will see in this section that **strong duality holds for convex problems under mild assumptions**, known as "Slater's condition".

Definition 4.1 (Slater's condition)

We say that the problem (1) verifies Slater's condition if there exists a feasible point x such that $g_i(x) < 0$ for all $i \in \{1, ..., m\}$.

One can verify that is the problem (1) is convex and verifies Slater's condition, then the constraints are qualified at every feasible point.

Theorem 4.1 (Kuhn Tucker)

Assume that the functions f, g_1, \ldots, g_m are **convex**, differentiable and that h_1, \ldots, h_p are linear. Assume that (1) verifies Slater's condition. Then $x \in \mathbb{R}^n$ is solution of (1) if and only if x is feasible and there exists $\lambda \in \mathbb{R}^m_{>0}$ and $\nu \in \mathbb{R}^p$ such that

$$\begin{cases} \nabla f(x) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x) + \sum_{i=1}^{p} \nu_i \nabla h_i(x) = 0\\ \lambda_i g_i(x) = 0 \quad \text{for all} \quad i = 1, \dots, m. \end{cases}$$
 (12)

In other words, x is a solution of (1) if and only if there exists $\lambda \in \mathbb{R}^m_{\geq 0}$ and $\nu \in \mathbb{R}^p$ such that $(x; \lambda, \nu)$ is a saddle point of the Lagrangian L.

Further reading

See [2] for a very nice introduction to spectral clustering and [1] for lecture notes on spectral graph theory.



References

- [1] Daniel Spielman. Spectral graph theory. Lecture Notes, Yale University, http://www.cs.yale.edu/homes/spielman/561/2012/, 2012.
- [2] Ulrike Von Luxburg. A tutorial on spectral clustering. Statistics and computing, 17(4):395–416, 2007.