

Intro to optimization

Data Science 2: AC 209b

Javier Zazo

Pavlos Protopapas

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Abstract

We present the basic concepts of unconstrained and constrained optimization. This will allow you to understand the derivations to obtain the dual problem of the optimal transport formulation.

1 Intro to optimization

We say an optimization problem is unconstrained when we minimize in the whole Euclidean space, i.e., $x \in \mathbb{R}^n$:

$$\min_{x \in \mathbb{R}^n} f(x). \quad (1)$$

We have a constrained optimization problem when the minimization is with respect to $X \subset \mathbb{R}^n$:

$$\min_{x \in X} f(x). \quad (2)$$

A set $X \subseteq \mathbb{R}^n$ is convex if every point between two points belonging to the set, also belongs to the same set. Examples of convex sets include the whole Euclidean space, half-spaces (subspaces divided by hyperplanes), hyperplanes, polytopes (the intersection of multiple halfspaces), etc. See also Figure 1.

A function $f(x)$ is convex in an open set X , if for every two points x_1 and $x_2 \in X$, the points connecting $f(x_1)$ and $f(x_2)$ are greater than or equal to the function f evaluated at those points. If the function $f(x)$ is doubly differentiable, the function is convex if its Hessian is positive semidefinite on every point $x \in X$. An example is given in Figure 2.

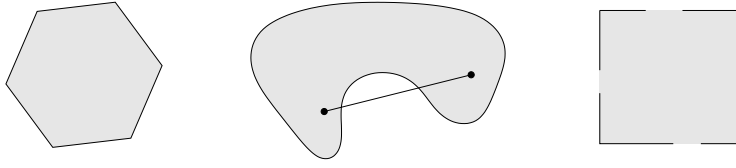


Figure 1: Three sets. The hexagon on the left is convex, the kidney shaped set is non-convex, the squared set excluding part of the boundary is also non-convex.

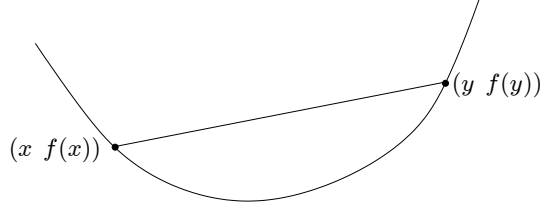


Figure 2: Example of a convex function.

2 Unconstrained optimization

We want to solve problem (1). If the function is differentiable, a necessary condition for optimality on point x^* is that its gradient is null evaluated on that point, i.e.,

$$\nabla_x f(x^*) = 0. \quad (3)$$

If $f(x)$ is additionally a convex function, then the condition is both necessary and sufficient.

An example is to minimize the convex parabola $f_1(x) = ax^2 + bx + c$ with $a > 0$. Its derivate is $\frac{d}{dx}f(x) = 2ax + b$, and its minimum becomes $x^* = \frac{-b}{2a}$. We can generalize to the multivariate case:

$$f_2(x) = x^T A x + 2b^T x + c, \quad (4)$$

with A being a symmetric positive definite matrix. The gradient is

$$\nabla_x f_2(x) = 2Ax + 2b, \quad (5)$$

and finding its root we obtain $x^* = -A^{-1}b$.

3 Constrained optimization

We want to solve problem (2). We can assume that X is represented in analytical with equality and inequality equations as follows:

$$X = \{x \in \mathbb{R}^n \mid g_i(x) \leq 0 \wedge h_j(x) = 0, \quad i \in \{1, \dots, m\}, j \in \{1, \dots, p\}\}. \quad (6)$$

This allows us to rewrite (2) in standard form:

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ \text{s.t.} \quad & g_i(x) \leq 0 \quad i \in \{1, \dots, m\} \\ & h_j(x) = 0 \quad j \in \{1, \dots, p\}. \end{aligned} \tag{7}$$

We say that problem (7) is convex if $f(x)$ is convex, every $g_i(x)$ is convex, and every $h_j(x)$ are affine functions. Otherwise, the problem is non-convex. The SVM problem that we introduced in the course is convex.

If we have a constrained convex problem, and it satisfies a special constraint qualification, then we can use duality theory to solve it. The motivation to derive the dual is threefold: it allows to check specific conditions for optimality; it introduces other optimization tools to solve the original problem, hopefully more efficient; it may give some theoretical insights about the problem, such as pricing of a certain resource in an economic model.

Regarding the constraint qualification we mentioned, we need to verify if the problem satisfies Slater's condition:

$$\exists \hat{x} \mid g_i(\hat{x}) < 0 \quad \forall i \text{ and } h_j(\hat{x}) = 0 \quad \forall j. \tag{8}$$

The previous expression can be relaxed to a simple feasibility requirement as $g_i(\hat{x}) \leq 0$, if g_i is an affine expression.

We call (7) the primal problem, because we optimize in the primal variable x . We will derive now the dual problem. First we form the Lagrangian:

$$L(x, \lambda, \nu) = f(x) + \sum_i \lambda_i g_i(x) + \sum_j \nu_j h_j(x). \tag{9}$$

The dual function is the minimum of the Lagrangian over variable x , and it is a function over λ_i and ν_j :

$$q(\lambda, \nu) = \min_x L(x, \lambda, \nu). \tag{10}$$

And finally, the dual problem consists on the maximization of the dual function over $\lambda_i \geq 0$:

$$\begin{aligned} \max_{\lambda \in \mathbb{R}^m, \nu \in \mathbb{R}^p} \quad & q(\lambda, \nu) \\ \text{s.t.} \quad & \lambda_i \geq 0 \quad \forall i. \end{aligned} \tag{11}$$

The motivation behind using duality theory to solve problem (7) is that sometimes it is easy to solve the minimum over x in the Lagrangian, and the dual problem has an amenable form. Notice that the minimization over x of the Lagrangian is an unconstrained problem, and therefore it is necessary that

$$\nabla_x L(x^*, \lambda, \nu) = 0 \tag{12}$$

for any candidate solution x^* . This is the first necessary condition of the Karush-Kuhn-Tucker (KKT) conditions. The rest of them refer to feasibility:

$$g_i(x^*) \leq 0 \quad \forall i \quad (13a)$$

$$h_j(x^*) = 0 \quad \forall j \quad (13b)$$

$$\lambda_i^* \geq 0 \quad \forall i \quad (13c)$$

$$\nu_j^* \in \mathbb{R} \quad \forall j, \quad (13d)$$

and complementarity slackness:

$$\sum_i \lambda_i^* g_i(x^*) = 0 \quad (14a)$$

$$\sum_j \nu_j^* h_j(x^*) = 0. \quad (14b)$$

The reason of imposing (14) is to have the following relation:

$$\begin{aligned} \max_{\lambda, \nu} \min_x \quad & L(x, \lambda, \nu) \\ = \quad & f(x^*) + \sum_i \underbrace{\lambda_i^* g_i(x^*)}_{=0} + \sum_j \underbrace{\nu_j^* h_j(x^*)}_{=0} = f(x^*). \end{aligned}$$

We see then that when the KKT conditions are satisfied for points x^* , λ_i^* , ν_j^* , and the problem is convex, then we achieve optimality of the primal problem. The KKT conditions (provided that Slater condition holds) are then necessary and sufficient.

References

- [1] Stephen Boyd and Lieven Vandenberghe. *Convex Optimization*. Cambridge University Press, 2003.

Acknowledgments

Figures 1 and 2 are borrowed from [1].