Overview and Applications of the KKT Conditions And Duality

Fundamentals For Nonlinear Constrained Optimization

Luca Solbiati

Machine Learning Engineer At ZURU Tech

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Abstract

In the field of constrained nonlinear optimization the KKT conditions and the theory of duality have played a central role in the analysis and development of algorithms and modeling techniques.
While even a naive understanding of these concepts is very useful and practical, a deep knowledge of these results can aid significantly in the proper application of algorithms and models, delivering meaningful insights into the field of optimization and operation reasearch in general.
The purpose of this presentation is to give an extensive and rigorous overview of these results, together with examples, intuitions, and applications that motivate their study.

Contents

Introduction

The Nonlinear Optimization Problem

We shall consider the constrained optimization problem:

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0 & i \in \mathcal{E} \\ c_i(x) \geq 0 & i \in \mathcal{I} \end{cases} \tag{1}$$

- $f : \mathbb{R}^n \to \mathbb{R}$ is called objective function
- $x \in \mathbb{R}^n$ are called variables
- $c_i : \mathbb{R}^n \to R$ are called constraints. They are inequality constraints if $i \in \mathcal{I}$, equality constraints if $i \in \mathcal{E}$

Geometric Formulation Of The Optimization Problem

By defining the feasible set Ω as the set of points that satisfy all the constraints:

$$\Omega := \{x \in \mathbb{R}^n \mid c_i(x) = 0 \; \forall \; i \in \mathcal{E} \quad c_i(x) \geq 0 \; \forall \; i \in \mathcal{I}\} \tag{2}$$

We can rewrite problem (1) as:

$$\min_{x \in \Omega} f(x) \tag{3}$$

which is known as the geometric formulation of the problem. We may observe that the geometric formulation is unique, while the algebraic formulation (1) in general is not.

Goal Of This Presentation

The goal of this presentation is to discuss the necessary conditions that must be satisfied by solutions of problem (1). These necessary conditions are not only used to check if a given point is a (local) optimizer, but are also used to aid in the development of optimization algorithms and in the modelling of optimization problems, through the study of sensitivity and dual formulations.

Local Solutions

For many nonlinear optimization problems there is little hope to find the actual minimum of (1), also known as global solution. What one could reasonably hope for is instead to find a local solution of the problem, that we define as follows:

Definition 1

A vector $x^* \in \Omega$ is a local solution of problem (1) if there is a neighborhood $\mathcal{N}$ of x^* such that $f(x) \geq f(x^*)$ for all $x^* \neq x \in \mathcal{N} \cap \Omega$. If such inequality is strict we shall say that x^* is a strict local solution.

Smoothness of the problem

In order to characterize local solutions we shall find a set of necessary conditions that they need to satisfy. These conditions, known as KKT conditions, will rely on the smoothness of the objective function and of the constraints, in particular we assume throughout this presentation that they are $\mathcal{C}^1$ functions.

Smoothness is also required by many optimization algorithms, as it ensures that the objective function and the constraints all behave in a reasonably predictable way, therefore allowing for algorithms to make good choices for search directions.

Smoothness $\not\Rightarrow$ Smooth Geometry

We may observe that smoothness in the constraints does not necessarily produce a smooth feasible region (in the sense of manifolds). For example, even simple linear constraints can produce a diamond-shaped feasible region with sharp edges.

This also suggests that we can transform apparently nonsmooth optimization problems into smooth optimization problems by rewriting their algebraic formulations

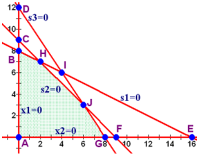


Figure: Linear constraints producing a nonsmooth feasible region

Transforming Nonsmooth Problems Into Smooth Ones

For example consider the nonsmooth constraint:

$$|x_1| + |x_2| \leq 1$$

This can be rewritten into a smooth constraint as:

$$x_1 + x_2 \leq 1, \quad x_1 - x_2 \leq 1, \quad -x_1 + x_2 \leq 1, \quad -x_1 - x_2 \leq 1$$

Similarly, nonsmooth optimization problems can sometimes be reformulated as smooth constrained problems by introducing slack variables. Consider for example:

$$\min_{x \in \mathbb{R}} f(x) = \max(x^2, x)$$

By adding an artificial variable t we can rewrite this problem as:

$$\min_{t \in \mathbb{R}} t \quad \text{s.t} \quad t \geq x, \quad t \geq x^2$$

These reformulation techniques are often used in cases where f is the maximum of a collection of functions or f is a 1-norm or ∞-norm of a vector function.

KKT Conditions

The Active Set

We may notice that, by smoothness of the constraint functions, if an inequality constraint c_i is such that $c_i(x^*) > 0$ then that constraint is actually not playing any part in the characterization of the local minimum. Indeed, by continuity we can always find a neighbourhood of x^* such that any x in that neighbourhood has $c_i(x) > 0$. In this sense the constraint is *inactive*, because whether or not it was present x^* would still be a local minimum.
For this reason we define the following set:

Definition 2

The active set $\mathcal{A}(x)$ at any feasible point $x \in \Omega$ is the set of indices of active constraints at x, i.e. :

$$\mathcal{A}(x) := \mathcal{E} \cup \{i \in \mathcal{I} \mid c_i(x) = 0\} \tag{4}$$

Example 1: Single equality constraint (1/4)

Consider the simple optimization problem:

$$\min x_1 + x_2 \quad \text{s.t} \quad x_1^2 + x_2^2 - 2 = 0$$

We can easily see that the feasible set for this problem is the circle of radius $\sqrt{2}$ and that the optimal solution is $x^* = (-1, -1)$.
Indeed, from any other point it's easy to decrease f while staying feasible. This is clearly not possible for x^*, and it is worth to discuss why in an informal way, by using first-order Taylor approximations.

Example 1: Single equality constraint (2/4)

When moving from a feasible point x with a small step s, to retain feasibility we require:

$$0 = c_1(x+s) \approx c_1(x) + \nabla c_1(x)^T s = \nabla c_1(x)^T s$$

Hence, in a first order sense, we must impose:

$$\nabla c_1(x)^T s = 0 \tag{5}$$

Similarly, if we want s to produce a decrease in f we ask that:

$$0 > f(x+s) - f(x) \approx \nabla f(x)^T s$$

That in a first order sense translates into:

$$\nabla f(x)^T s < 0 \tag{6}$$

Example 1: Single equality constraint (3/4)

But for x^* it is easy to see that:

$$\nabla f(x^*) = \lambda_1^* \nabla c_1(x^*) \quad \text{for} \quad \lambda_1^* = -1/2 \tag{7}$$

and so satisfying both conditions (5) and (6) is impossible for any s ! Viceversa, we can see that the only way for those conditions to not be satisfied by any s is for $\nabla f(x)$ and $\nabla c_1(x)$ to be parallel. In fact, if they are not parallel we can set:

$$\bar{s} := -const \cdot \left(Id - \frac{\nabla c_1(x) \nabla c_1(x)^T}{||\nabla c_1(x)||^2} \right) \nabla f(x)$$

to obtain a first order feasible decrease

Example 1: Single equality constraint (4/4)

We can rewrite the parallel condition (7) by introducing the Lagrangian:

$$\mathcal{L}(x, \lambda_1) = f(x) - \lambda_1 c_1(x)$$

and stating:

$$\nabla_x \mathcal{L}(x^*, \lambda_1^*) = 0$$

This suggests that we can search for solutions of the equality constrained problem by seeking stationary points of the Lagrangian function. The scalar quantity λ_1 is called a Lagrange multiplier for c_1.

Example 2: Single inequality constraint (1/3)

We consider a simple variant of the first example, by transforming the equality constraint into an inequality constraint:

$$\min x_1 + x_2 \quad \text{s.t} \quad 2 - x_1^2 - x_2^2 \geq 0$$

For this example the feasible region is given by the centered ball of radius $\sqrt{2}$. As before, it's easy to check that the optimal solution is given by $x^* = (-1, -1)$. However, the first order analysis is slightly different. By computations similar to the first example we get that a small step s remains feasible if:

$$c_1(x) + \nabla c_1(x)^T s \geq 0 \tag{8}$$

Example 2: Single inequality constraint (2/3)

For inequality constraints we may distinguish between two cases:

1. c_1 **is inactive**: in this case any step small enough satisfies (8), and so for $\alpha > 0$ small enough we can obtain a decrease by setting $s := -\alpha \nabla f(x)$ whenever $\nabla f(x) \neq 0$
2. c_1 **is active**: in this case the step condition can be rewritten as:

$$\nabla f(x)^T s < 0, \quad \nabla c_1(x)^T s \geq 0 \tag{9}$$

These two condition define two half-planes. It can be easily proven that the intersection of these two regions is empty only when $\nabla f(x)$ and $\nabla c_1(x)$ point in the same direction, i.e.:

$$\nabla f(x) = \lambda_1 \nabla c_1(x), \quad \text{for some} \ \ \lambda_1 \geq 0$$

Unlike the case of equality constraints, the sign of the multiplier is relevant for the first order optimality condition.

Example 2: Single inequality constraint (3/3)

By defining the Lagrangian:

$$\mathcal{L}(x, \lambda_1) := f(x) - \lambda_1 c_1(x)$$

we can reformulate the first order necessary conditions as:

$$\nabla_x \mathcal{L}(x^*, \lambda_1^*) = 0 \quad \text{for some} \quad \lambda_1^* \geq 0$$

$$\lambda_1^* c_1(x^*) = 0$$

The second condition, used to include both the active and inactive case, is known as *complementarity condition*.

The Lagrangian Function

As seen in the previous examples, the Lagrangian plays a fundamental role in the definition of first order necessary conditions for optimality.

Definition 3

The Lagrangian function associated to the optimization problem (1) is defined as:

$$\mathcal{L}(x,\lambda) := f(x) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i c_i(x) \tag{10}$$

The Lagrangian can be also used to restate the optimization problem (1) as:

$$\inf_{x \in \mathbb{R}^n} \sup_{\lambda_i \geq 0 \ \forall i \in \mathcal{I}} \mathcal{L}(x,\lambda) \tag{11}$$

Indeed, when constraints are not respected we get an infinite penalization of the function: $\sup_{\lambda \geq 0} \mathcal{L}(x,\lambda) = +\infty$, and when they are respected we get $\sup_{\lambda \geq 0} \mathcal{L}(x,\lambda) = f(x)$.

The KKT Conditions

In light of the previous examples we state the first-order conditions necessary for a point to be a local minimum. These conditions, also known as Karush-Kuhn-Tucker (KKT) conditions, can be considered an extension of the theory of Lagrange multipliers.
For this result to hold we also require a set of conditions known as constraint qualifications (LICQ) that we will explain later.

Theorem 4 (KKT Conditions)

Suppose that x^* *is a local minimum of problem* (1) *and that the functions* f *and* c_i *are* $\mathcal{C}^1$. *If the LICQ holds at* x^*, *then there exists a Lagrange multiplier vector* λ^* *such that the following conditions are satisfied:*

$$\nabla_x \mathcal{L}(x^*, \lambda^*) = 0 \qquad \textit{(stationarity)} \tag{12a}$$

$$c_i(x^*) = 0 \qquad \forall i \in \mathcal{E} \qquad \textit{(primal feasibility)} \tag{12b}$$

$$c_i(x^*) \geq 0 \qquad \forall i \in \mathcal{I} \qquad \textit{(primal feasibility)} \tag{12c}$$

$$\lambda_i^* \geq 0 \qquad \forall i \in \mathcal{I} \qquad \textit{(dual feasibility)} \tag{12d}$$

$$\lambda_i^* c_i(x^*) = 0 \qquad \forall i \in \mathcal{E} \cup \mathcal{I} \qquad \textit{(complementary slackness)} \tag{12e}$$

KKT Conditions Proof Outline

What are Constraint Qualifications

For the examples' informal first order analysis to hold, smoothness is not sufficient. We also require that the first order description of the constraints accurately reflects the geometry of the feasible set. This will translate into a set of conditions known as constraint qualifications.

The Tangent Cone

Definition 5

Given a feasible point $x \in \Omega$ we call $\{z_k\}_k$ a feasible sequence approaching x if $z_k \in \Omega$ and $z_k \to x$ as $k \to \infty$.

Definition 6

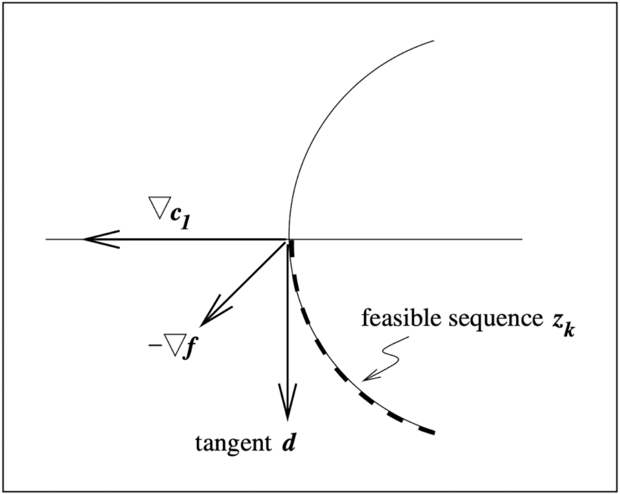
We say that $d \in \mathbb{R}^n$ is tangent to Ω at x if there exists a feasible sequence $\{z_k\}_k$ approaching x and a sequence of scalars $t_k \to 0$ such that:

$$d = \lim_{k \to \infty} \frac{z_k - x}{t_k} \tag{13}$$

The tangent cone $T_\Omega(x^*)$ is the set of all tangents to Ω at x. It's easy to verify that the tangent cone is indeed a cone.

The tangent cone is a geometric way to determine the directions tangent to Ω at x, and it will play an important role in the construction of the necessary optimality conditions.

The Tangent Cone



Linearized Feasible Directions

Definition 7

Given a feasible point $x \in \Omega$ the set of linearized feasible directions $\mathcal{F}(x)$ is:

$$\mathcal{F}(x) := \left\{ d \in \mathbb{R}^n \mid \begin{array}{ll} d^T \nabla c_i(x) = 0 & \forall i \in \mathcal{E} \\ d^T \nabla c_i(x) \geq 0 & \forall i \in \mathcal{I} \cap \mathcal{A}(x) \end{array} \right\} \tag{14}$$

It's easy to verify that $\mathcal{F}(x)$ is also a cone. Observe that inactive constraints don't play any role in determining the first order tangent directions. We also note that changing the algebraic formulation of the constraints may change $\mathcal{F}(x)$. For example $c_1(x) := x_1^2 + x_2^2 - 2 = 0$ is equivalent to $\bar{c}_1(x) := (x_1^2 + x_2^2 - 2)^2 = 0$ but produces different linearized feasible directions.

Constraint Qualifications: LICQ

Constraint qualifications will ensure that the first order description $\mathcal{F}(x)$ of the feasible set is equal to the tangent cone $T_\Omega(x)$, so that we can translate the tangent cone optimality conditions into first order (algebraic) conditions. The most used constraint qualification is the following:

Definition 8

Given a feasible point $x \in \Omega$ we say that the linear independence constraint qualification (LICQ) holds if the set of active constraint gradients $\{\nabla c_i(x) \mid i \in \mathcal{A}(x)\}$ is linearly independent.

Relationship between $\mathcal{F}(x)$ and $T_\Omega(x)$

The following result states that the set of linearized feasible directions $\mathcal{F}(x)$ is in general bigger than $T_\Omega(x)$, however, thanks to the LICQ, we can guarantee that they are equal.

Lemma 9

Let $x^* \in \Omega$ be a feasible point, then:

1. $T_\Omega(x^*) \subseteq \mathcal{F}(x^*)$;
2. *If the LICQ holds at x^* then $\mathcal{F}(x^*) = T_\Omega(x^*)$*

Relationship between $\mathcal{F}(x)$ and $T_\Omega(x)$ (Proof Sketch)

For any $d \in T_\Omega(x^*)$ we have that:

$$z_k = x^* + t_k d + o(t_k) \tag{15}$$

For equality constraints $i \in \mathcal{E}$ this implies:

$$\begin{aligned} 0 &= \frac{1}{t_k} c_i(z_k) = \frac{1}{t_k}\left[c_i(x^*) + t_k \nabla c_i(x^*)^T d + o(t_k)\right] \\ &= \nabla c_i(x^*)^T d + \frac{o(t_k)}{t_k} \end{aligned}$$

hence for $k \to +\infty$ we get $\nabla c_i(x^*)^T d = 0$, as required. We conclude in a similar way for inequality constraints that $\nabla c_i(x^*)^T d \geq 0$ and so $d \in \mathcal{F}(x^*)$.
The second statement is more complicated, and exploits the LICQ to use the implicit function theorem to build an approaching sequence whose tangent direction is $d \in \mathcal{F}$.

A Necessary Optimality Condition For The Tangent Cone

As we have previously discussed, the relationship between the linearized feasible directions $\mathcal{F}(x)$ and the tangent cone $T_\Omega(x^*)$ is important because through the tangent cone we are able to get a simple necessary condition of optimality. This condition is stated in the following theorem:

Theorem 10

If x^* is a local solution of (1)*, then we have:*

$$\nabla f(x^*)^T d \geq 0 \quad \forall\, d \in T_\Omega(x^*) \tag{16}$$

Proof.

We proceed by contradiction. Suppose that there exists $d \in T_\Omega(x^*)$ such that $\nabla f(x^*)^T d < 0$ that is defined by the sequences $\{z_k\}$ and $\{t_k\}$. Using Taylor and definition (13) we get:

$$\begin{aligned} f(z_k) &= f(x^*) + (z_k - x^*)^T \nabla f(x^*) + o(||z_k - x^*||) \\ &= f(x^*) + t_k d^T \nabla f(x^*) + o(t_k) \end{aligned}$$

For t_k small enough $t_k d^T \nabla f(x^*)$ dominates $o(t_k)$ and, since $d^T \nabla f(x^*) < 0$ we can write:

$$f(z_k) < f(x^*) + \frac{1}{2} t_k d^T \nabla f(x^*) \quad \forall\, k \text{ big enough}$$

which leads to a contradiction, since x^* is a local minimum. $\square$

Farkas' Lemma

In order to prove the main result we will need a classical theorem of the alternative known as Farkas' lemma.
Consider two matrices $B \in \mathbb{R}^{n\times m}$ and $C \in \mathbb{R}^{n\times p}$. We define the cone K as:

$$K := \{By + Cw \mid w \in \mathbb{R}^p, \quad y \in \mathbb{R}^m, \quad y \geq 0\} \tag{17}$$

Given a vector $g \in \mathbb{R}^n$ Farkas' lemma states that either $g \in K$ or else there is a vector $d \in \mathbb{R}^n$ such that:

$$g^t d < 0, \quad B^T d \geq 0, \quad C^T d = 0 \tag{18}$$

In other terms, either g is in the cone K or there exists a "particular" separating hyperplane between K and g.

Theorem 11 (Farkas' lemma)

Let K be defined as in (17). *Given $g \in \mathbb{R}^n$ we have either that $g \in K$ or that there exists $d \in \mathbb{R}^n$ satisfying* (18), *but not both.*

Proof.

It's easy to prove that both cannot hold at the same time. If such were the case then $g = By + Cw$ and there would be a vector $d \in \mathbb{R}^n$ such that:

$$0 > d^T g = d^T By + d^t Cw \overset{(18)}{\geq} 0$$

We show now that one of the alternatives must hold, in particular we show that if $g \notin K$ then we can construct d that satisfies (18).
Let $\hat{s}$ be the euclidean projection of g on K. We claim that the vector $d := \hat{s} - g$ satisfies (18).
By properties of projection it's easy to see that for any $s \in K$:

$$\hat{s}^T(\hat{s} - g) = 0 \tag{19}$$

$$s^T(\hat{s} - g) \geq 0 \tag{20}$$

So we have that:

$$d^T g = d^T(\hat{s} - d) = (\hat{s} - g)^T \hat{s} - d^T d \overset{(19)}{=} -||d||^2 < 0$$

and for each $y \geq 0$, w we have $s = By + Cw \in K$ so by (20):

$$d^T(By + Cw) \geq 0$$

For $y = 0$ this implies $(C^T d)^T w \geq 0$ for every w, hence $C^T d = 0$. Similarly, for $w = 0$ we have $(B^T d)^T y \geq 0$ for all $y \geq 0$, which implies $B^T d \geq 0$, therefore concluding the proof. □

Farkas' Lemma Corollary

Farkas' lemma can be applied to limit the possibilities on the objective function and constraint gradients configurations:

Corollary 12

Given a feasible point $x^* \in \Omega$, one and only one of the following holds:

1. *There exists λ^* such that:*

$$\nabla f(x^*) = \sum_{i \in \mathcal{A}(x^*)} \lambda_i \nabla c_i(x^*) \quad \textit{with} \;\; \lambda_i \geq 0 \textit{ for } i \in \mathcal{I} \cap \mathcal{A}(x^*) \tag{21}$$

2. *There exists $d \in \mathcal{F}(x^*)$ such that $d^T \nabla f(x^*) < 0$.*

Proof.

It follow directly from Farkas' lemma by setting $g := \nabla f(x^*)$ and:

$$K := \left\{ \sum_{i \in \mathcal{A}(x^*)} \lambda_i \nabla c_i(x^*) \mid \lambda_i \geq 0 \; \forall i \in \mathcal{I} \cap \mathcal{A}(x^*) \right\}$$

□

KKT Conditions Proof

We are now ready to state and prove the KKT conditions that we restate for the proof's sake:

$$
\begin{aligned}
\nabla_x \mathcal{L}(x^*, \lambda^*) &= 0 & & \text{(stationarity)} \\
c_i(x^*) &= 0 & \forall i \in \mathcal{E} & \quad \text{(primal feasibility)} \\
c_i(x^*) &\geq 0 & \forall i \in \mathcal{I} & \quad \text{(primal feasibility)} \\
\lambda_i^* &\geq 0 & \forall i \in \mathcal{I} & \quad \text{(dual feasibility)} \\
\lambda_i^* c_i(x^*) &= 0 & \forall i \in \mathcal{E} \cup \mathcal{I} & \quad \text{(complementary slackness)}
\end{aligned}
$$

Proof.

Since x^* is a feasible point, primal feasibility must obviously be satisfied. By corollary 12 we either have that:

1. There exists λ^* such that:

$$\nabla f(x^*) = \sum_{i \in \mathcal{A}(x^*)} \lambda_i \nabla c_i(x^*) \quad \text{with} \quad \lambda_i \geq 0 \text{ for } i \in \mathcal{I} \cap \mathcal{A}(x^*) \tag{23}$$

2. There exists $d \in \mathcal{F}(x^*)$ such that $d^T \nabla f(x^*) < 0$.

Since by theorem 10 it cannot happen that there exists a $d \in T_\Omega(x^*) \overset{\text{lemma 9}}{=} \mathcal{F}(x^*)$ with $d^T \nabla f(x^*) < 0$, then the first option must hold, hence there exists a λ^* that respects stationarity. In particular, by corollary 12, we can pick $\lambda_i = 0$ for the inactive constraints i, and $\lambda_i \geq 0$ for the active inequality constraints, hence dual feasibility and complementary slackness are satisfied. □

Comments On KKT Conditions

Other Constraint Qualifications

We have stated the KKT Conditions under the assumption that the LICQ held at x^*. It is important to note that while the LICQ is the most widely used assumption in constrained optimization, there are other constraint qualifications that can be considered.
An important example is the one of linear constraints:

$$c_i(x) = a_i^T x + b_i \tag{24}$$

for these kind of constraints it's not difficult to prove a version of lemma 9:

Lemma 13

Suppose that at some $x^* \in \Omega$ all active constraints are linear. Then $\mathcal{F}(x^*) = T_\Omega(x^*)$

Since the LICQ is only used in the KKT proof to have $\mathcal{F}(x^*) = T_\Omega(x^*)$ we can immediately conclude that for linear constraints the KKT-theorem holds.

Another useful constraint qualification is the Mangasarian-Fromovitz constraint qualification (MFCQ):

Definition 14

We say that the Mangasarian-Fromovitz constraint qualification (MFCQ) holds at x^* if there exists a vector $w \in \mathbb{R}^n$ such that:

$$\nabla c_i(x^*)^T w > 0 \qquad \forall i \in \mathcal{I} \cap \mathcal{A}(x^*) \tag{25a}$$

$$\nabla c_i(x^*)^T w = 0 \qquad \forall i \in \mathcal{E} \tag{25b}$$

This set of conditions is weaker than LICQ, since by linear independence of the constraint gradients we can easily find such a w as a solution to a linear system. A version of the KKT conditions can be proven under MFCQ, but these results are out of the scope of this presentation.

Intuitive Explanation Of Lagrange Multipliers And Sensitivity

While the importance of the Lagrangian and of its multipliers in optimality theory is clear, their intuitive significance may be lost when studying them only through a rigorous treatment. We will argue that Lagrange multipliers say something about the sensitivity of the optimal objective value $f(x^*)$ to the presence of the constraint c_i, i.e. how much perturbations (or noise) to the constraint may influence the solution.
This kind of information can be useful when modeling a problem, as it is usually undesirable for a model to be too sensitive to variations of the data.

Let us assume that the constraint $i \in \mathcal{I}$ is active and let us relax the constraint by perturbing its r.h.s., asking that:

$$c_i(x) \geq -\epsilon||\nabla c_i(x^*)||$$

Let $x^*(\epsilon)$ be the new solution to this perturbed problem, and assume that for ϵ small enough the Lagrange multipliers don't change much (in particular i is still active). Then:

$$-\epsilon||\nabla c_i(x^*)|| = c_i(x^*(\epsilon)) - c_i(x^*) \approx \nabla c_i(x^*)^T(x^*(\epsilon) - x^*)$$

$$0 = c_j(x^*(\epsilon)) - c_j(x^*) \approx \nabla c_j(x^*)^T(x^*(\epsilon) - x^*) \quad \forall i \neq j \in \mathcal{A}(x^*)$$

By the KKT Condition (22a) and previous computations we get:

$$f(x^*(\epsilon)) - f(x^*) \approx \nabla f(x^*)^T(x^*(\epsilon) - x^*) = \sum_{j \in \mathcal{A}(x^*)} \lambda_j^* \nabla c_j(x^*)^T(x^*(\epsilon) - x^*) \approx$$

$$\approx -\epsilon||\nabla c_i(x^*)||\lambda_i^*$$

So by taking limits of the above we can conclude that:

$$\frac{df(x^*(\epsilon))}{d\epsilon} = -\lambda_i^*||\nabla c_i(x^*)|| \tag{26}$$

So the larger $\lambda_i^*||\nabla c_i(x^*)||$ is, the more the optimal value is sensitive to the placement of the i-th constraint.

Physical Interpretation Of Lagrange Multipliers

Another interesting way to look at the Lagrange multipliers is through the lens of physics.

We can imagine f as the potential energy of a force. The force associated to this potential energy is $-\nabla f(x)$, and it tends to push the "particle" x towards lower values of f.
When we have reached a minimum x^*, we have either that the force is null, or that it is pushing against the constraint. For the system to stay still, the reaction from the constraints must be equal to the force. The reaction of each constraint can only be orthogonal to the constraint itself, i.e. it must be parallel to $\nabla c_i(x^*)$.

It's easy to understand that the higher λ_i is, the harder the force is pushing against the constraint, which means that in that direction there is a rapid decrease of potential energy (i.e. the optimal value is sensitive to the constraint). In particular, we may observe that inactive constraints cannot react to the force, because the particle it's not pushing against them, which explains the complementary slackness condition $\lambda_i^* = 0$.

Duality Theory

Duality Theory: Motivations

Another important concept in constrained optimization is *duality*. Duality theory builds an alternative *dual problem* related to the original optimization problem (1), that in this context is usually called *primal*.

The dual formulation is often times considered because it can deliver important insights of the primal problem, either by simplifying it, or by adding descriptive variables that aid in system modelization or in the development of optimization algorithms.

We shall consider only the special case where there are no equality constraints and $f, -c_i$ are all convex functions:

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to } c_i(x) \geq 0 \quad \forall i = 1, ..., m \tag{27}$$

The Dual Problem

The Lagrangian associated to problem (27) is given by:

$$\mathcal{L}(x, \lambda) := f(x) - \lambda^T c(x)$$

We define the *dual objective function* $q : \mathbb{R}^n \to \mathbb{R}$ as follows:

$$q(\lambda) := \inf_{x \in \mathbb{R}^n} \mathcal{L}(x, \lambda) \tag{28}$$

For some values of λ it may happen that $q(\lambda) = -\infty$. To avoid this problem we restrict q to the domain $\mathcal{D}$ where it is finite.
The dual problem is defined as follows:

$$\max_{\lambda \in \mathcal{D}} q(\lambda) \quad \text{subject to } \lambda \geq 0 \tag{29}$$

We recall that the original problem (27) can be stated in terms of its Lagrangian as:

$$\inf_{x \in \mathbb{R}^n} \sup_{\lambda \geq 0} \mathcal{L}(x, \lambda)$$

The dual problem is obtained by simply swapping the infimum with the supremum:

$$\sup_{\lambda \geq 0} \inf_{x \in \mathbb{R}^n} \mathcal{L}(x, \lambda) = \sup_{\lambda \geq 0} q(\lambda)$$

Concavity of the Dual Objective

Theorem 15

The dual objective function q is concave and its domain $\mathcal{D}$ is convex.

Proof.

For any λ^1, λ^2 and $\alpha \in [0,1]$ it trivially holds that:

$$\begin{aligned} q(\alpha\lambda^1 + (1-\alpha)\lambda^2) &= \inf_x [\alpha\mathcal{L}(x,\lambda^1) + (1-\alpha)\mathcal{L}(x,\lambda^2)] \geq \alpha \inf_x [\mathcal{L}(x,\lambda^1)] + (1-\alpha) \\ &\geq \alpha q(\lambda^1) + (1-\alpha) q(\lambda^2) \end{aligned}$$

hence q is concave. If both $\lambda^1, \lambda^2 \in \mathcal{D}$ it follows immediately that $q(\alpha\lambda^1 + (1-\alpha)\lambda^2) > -\infty$, hence $\alpha\lambda^1 + (1-\alpha)\lambda^2 \in \mathcal{D}$, which implies that $\mathcal{D}$ is convex. $\square$

Weak Duality

In general the dual has only weak connections with the primal, but under proper assumptions there are strong links between the two.

Theorem 16 (Weak duality)

For any feasible $\bar{x} \in \Omega$ *and* $\bar{\lambda} \geq 0$, *we have:*

$$q(\bar{\lambda}) \leq f(\bar{x}) \tag{30}$$

Proof.

The proof is quite straightforward:

$$q(\bar{\lambda}) = \inf_x f(x) - \bar{\lambda}^T c(x) \leq f(\bar{x}) - \bar{\lambda}^T c(\bar{x}) \leq f(\bar{x})$$

□

from primal to dual

Theorem 17 (from primal to dual)

Suppose that $\bar{x}$ is a solution of the primal problem (27) *and that $f, -c_i$ are all convex functions differentiable at $\bar{x}$. Then any $\bar{\lambda}$ for which $(\bar{x}, \bar{\lambda})$ satisfies the KKT conditions is a solution of the dual problem* (29)*.*

To prove this result we will use the KKT conditions related to the primal problem (27):

$$\nabla f(\bar{x}) - \nabla c(\bar{x})\bar{\lambda} = 0 \tag{31a}$$

$$c(\bar{x}) \geq 0 \tag{31b}$$

$$\bar{\lambda} \geq 0 \tag{31c}$$

$$\bar{\lambda}_i c_i(\bar{x}) = 0, \qquad \forall i = 1, ..., m \tag{31d}$$

Proof.

By hypothesis we have that $\bar{\lambda} \geq 0$ and that $\mathcal{L}(\cdot, \bar{\lambda})$ is a convex differentiable function, hence it holds that:

$$\mathcal{L}(x, \bar{\lambda}) \geq \mathcal{L}(\bar{x}, \bar{\lambda}) + \nabla_x \mathcal{L}(\bar{x}, \bar{\lambda})^T (x - \bar{x}) \overset{\text{(31a)}}{=} \mathcal{L}(\bar{x}, \bar{\lambda})$$

Therefore, we have:

$$q(\bar{\lambda}) = \inf_x \mathcal{L}(x, \bar{\lambda}) = \mathcal{L}(\bar{x}, \bar{\lambda}) = f(\bar{x}) - \bar{\lambda}^T c(\bar{x}) \overset{\text{(31d)}}{=} f(\bar{x}) \tag{32}$$

By weak duality $q(\lambda) \leq f(\bar{x})$ for all $\lambda \geq 0$, hence $\bar{\lambda}$ is the maximum of q and a solution of the dual problem. $\square$

From Dual To Primal

Conversely, the dual problem can give information on the primal under certain conditions

Theorem 18 (From dual to primal)

Suppose that f *and* $-c_i$ *are convex and* $\mathcal{C}^1$*. Let* $\bar{x}$ *be a solution of the primal problem* (27) *at which LICQ holds. Suppose that* $\hat{\lambda}$ *solves the dual problem* (29) *with* $q(\hat{\lambda}) = \mathcal{L}(\hat{x}, \hat{\lambda})$*. If* $\mathcal{L}(\cdot, \hat{\lambda})$ *is a strictly convex function then* $\hat{x} = \bar{x}$*. That is* $\hat{x}$ *is the unique solution of the primal problem* (27) *and* $f(\hat{x}) = \mathcal{L}(\hat{x}, \hat{\lambda})$*.*

Proof.

We proceed by contradiction. Assume that $\bar{x} \neq \hat{x}$, then, by LICQ and continuous differentiability, there exists a $\bar{\lambda}$ that satisfies the KKT conditions. By equation (32) and theorem 17 then:

$$\mathcal{L}(\bar{x}, \bar{\lambda}) \overset{(32)}{=} q(\bar{\lambda}) \overset{\text{thm 17}}{=} q(\hat{\lambda}) = \mathcal{L}(\hat{x}, \hat{\lambda})$$

Since by definition $\hat{x}$ is the minimum of $\mathcal{L}(\cdot, \hat{\lambda})$ we have $\nabla_x \mathcal{L}(\hat{x}, \hat{\lambda}) = 0$. Moreover, by strict convexity of $\mathcal{L}(\cdot, \hat{\lambda})$ it follows that:

$$\mathcal{L}(\bar{x}, \hat{\lambda}) > \mathcal{L}(\hat{x}, \hat{\lambda}) + \nabla_x \mathcal{L}(\hat{x}, \hat{\lambda})^T (\bar{x} - \hat{x}) = \mathcal{L}(\hat{x}, \hat{\lambda})$$

which implies:

$$-\hat{\lambda}^T c(\bar{x}) > -\bar{\lambda}^T c(\bar{x}) \overset{(31d)}{=} 0$$

But $\hat{\lambda} \geq 0$ and $c(\bar{x}) \geq 0$, so $-\hat{\lambda}^T c(\bar{x}) > 0$ is absurd! □

Wolfe Dual

A slightly different formulation of the dual problem, that is more convenient for computations, is given by the *Wolfe dual* problem, that can be stated as follows:

$$\max_{x,\lambda} \mathcal{L}(x, \lambda) \tag{33a}$$

$$\text{subject to:} \quad \nabla_x \mathcal{L}(x, \lambda) = 0, \qquad \lambda \geq 0 \tag{33b}$$

In this formulation we don't ask to find a global minimum to define the dual objective q, but we restrict ourselves to stationary points of the Lagrangian so to satisfy the stationarity KKT condition.

From Primal To Wolfe Dual

By using convexity, this usually leads to a comparable dual problem:

Theorem 19 (From primal to Wolfe dual)

Suppose that $f, -c_i$ are convex $\mathcal{C}^1$ functions. Let $(\bar{x}, \bar{\lambda})$ be a solution pair of the primal problem at which LICQ holds. Then $(\bar{x}, \bar{\lambda})$ solves the Wolfe dual problem (33)

Proof.

By the KKT conditions of the primal, $(\bar{x}, \bar{\lambda})$ satisfy the constraints of the Wolfe dual. We just need to prove that they are the maximum of the Lagrangian. By primal feasibility we have $\mathcal{L}(\bar{x}, \bar{\lambda}) = f(\bar{x})$ and $c(\bar{x}) \geq 0$, therefore for any other (x, λ) satisfying the Wolfe dual constraints we have:

$$\mathcal{L}(\bar{x}, \bar{\lambda}) = f(\bar{x}) \geq f(\bar{x}) - \lambda^T c(\bar{x}) = \mathcal{L}(\bar{x}, \lambda) \overset{\text{(convexity)}}{\geq}$$
$$\geq \mathcal{L}(x, \lambda) + \nabla_x \mathcal{L}(x, \lambda)^T (\bar{x} - x) = \mathcal{L}(x, \lambda)$$

hence concluding the proof. □

Applications

Revised And Dual Simplex Method

The nonlinear programming theory that we have developed thus far can be used to derive quite trivially many classical results of linear programming. These results are otherwise proved with a significant amount of effort, and can be considered for the most part subcases of the optimality conditions we have found.

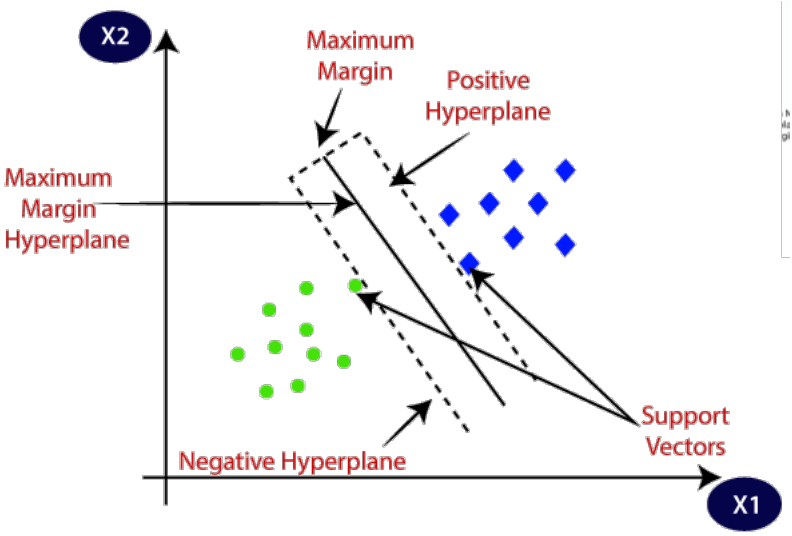
We may observe that the KKT conditions associated to a linear program are not only necessary, but also sufficient, due to the convexity of the problem. It does not come up as a surprise then, that when designing the revised and dual simplex method to solve a linear programming problem, the KKT conditions are extensively used to relate the primal and dual formulation, and the information given by the multipliers is exploited to determine each step of the algorithm.

Support Vector Machines

Support Vector Machines (SVM) are a machine learning model used for supervised and unsupervised learning.

In the case of a supervised binary classification problem, we want to classify two classes of points in $\mathbb{R}^d$, and we're given n points $x^i \in \mathbb{R}^d$ labeled by $y^i \in \{+1, -1\}$.

The main idea of SVMs is to find a hyperplane that separates almost all the points of the two classes, finding the hyperplane with maximum margin between the two.


X2
Maximum
Margin
Positive
Hyperplane
Maximum
Margin
Hyperplane
Support
Vectors
Negative Hyperplane
X1

SVMs Optimization Problem

Finding such a hyperplane leads to a quadratic optimization problem:

$$\min_{w,b,\xi_i} ||w||^2 + c\sum_i \xi_i \tag{34a}$$

$$\text{s.t. :} \quad y^i[w^T x^i + b] \geq 1 - \xi_i \tag{34b}$$

$$\xi_i \geq 0 \tag{34c}$$

where $w \in \mathbb{R}^d$, $b \in \mathbb{R}$ define the separating hyperplane, which classifies points as $+1$ or -1 based on the sign of $w^T x + b$. ξ_i are slack variables introduced to allow some misclassification errors.

SVMs Dual Problem

Due to the strict convexity of the problem, we can equivalently consider the dual formulation of the problem (simplified through the use of KKT conditions), given by:

$$\max_{\alpha \in \mathbb{R}^n} -\frac{1}{4}||\sum_{i=1}^{n} \alpha_i y^i x^i||^2 + \sum_{i=1}^{n} \alpha_i \tag{35a}$$

$$\text{s.t} \quad 0 \leq \alpha_i \leq c \tag{35b}$$

$$\sum_{i=1}^{n} \alpha_i y^i = 0 \tag{35c}$$

The solution of the dual problem α defines a separating hyperplane with the following formulas:

$$w = \frac{1}{2}\sum_{i=1}^{n} \alpha_i y^i x^i, \quad b = y^i - w^T x^i \quad \text{for any } i \text{ s.t. } \alpha_i \neq 0, c \tag{36}$$

SVMs: Interpetability of Dual Problem

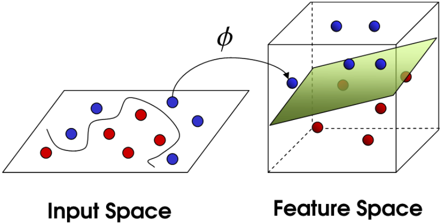
While the primal formulation is somewhat easier to tackle from an optimization point of view, the dual formulation offers the advantage of interpretability.

Indeed, the resulting separating hyperplane w is given by the linear combination of the x^i vectors for which $\alpha_i \neq 0$. These kind of vectors are known as support vectors (hence the name Support Vector Machine).

Knowing how many support vectors there are is important to qualitatively establish the robustness of the SVM, since having too many of them usually indicates that we are relying too much on the data, therefore overfitting it

SVMs: The Kernel Trick

The real power of the dual formulation though comes from the application of the *kernel trick*.
Most complex data isn't usually linearly separable, so a simple SVM would be a bad model for classification. However, by mapping the vectors x^i into a space of higher dimension, the data may become separable.



Mercer's theorem relates the computation of a kernel function $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ to the computation of the scalar product of transformed data $x \to \phi(x)$, where $\phi : \mathbb{R}^n \to \ell^2(\mathbb{R})$ is a transformation function associated to K. In particular :

$$K(x, y) =< \phi(x), \phi(y) >_{\ell^2}$$

So, if we were to use data transformed by ϕ, the resulting SVM dual formulation would be:

$$\max_{\alpha \in \mathbb{R}^n} -\frac{1}{4} \sum_{i,j=1}^{n} \alpha_i \alpha_j y^i y^j K(x^i, x^j) + \sum_{i=1}^{n} \alpha_i \tag{37a}$$

$$\text{s.t} \quad 0 \le \alpha_i \le c \tag{37b}$$

$$\sum_{i=1}^{n} \alpha_i y^i = 0 \tag{37c}$$

which is an optimization problem with the same dimensions as before. Note that this cannot be done with the primal formulation. The dual problem allows us to transform the data without explicitly computing the function ϕ, thus leading to a more tractable optimization problem. This computational trick is known as the kernel trick.

Method of Multipliers

Of course the KKT conditions and multipliers are extensively used to develop nonlinear optimization algorithms.

Such is the case for the method of multipliers, where a progressive approximation of the Lagrange multipliers improves the stability of a quadratic penalization method.

Let's see a coded example!

Thank you for your attention!