Lecture notes on Optimization for MDI210

Robert M. Gower

October 9, 2018

Abstract

Theses are my notes for my lectures for the MDI210 Optimization and Numerical Analysis course. Theses notes are a work in progress, and will probably contain several mistakes (let me know?). If you are following my lectures you may find them useful to recall what we covered in class. Otherwise, I recommend you read the excellent book [2] for the optimization part. Indeed, this book [2] contains all the subjects covered in these notes, and is a much better reference than these notes.

Contents

1	Linear Programming		2
	1.1	A first example	2
	1.2	Notation and definitions	4
	1.3	The simplex algorithm	6
	1.4	Degeneracy and Cycling	7
	1.5	Initialization using a first phase problem	7
	1.6	Duality	g
2	Nonlinear programming without constraints		
	2.1	The gradient, Hessian and the Taylor expansion	11
	2.2	Level sets and geometry	13
	2.3	Optimality conditions	15
	2.4	Convex functions	16
	2.5	Gradient method	18
	2.6	Newton's method	19
3	Nonlinear programming with constraints		20
	3.1	Feasible directions	22
	3.2	Characterizing the constraint qualification	24
	3.3	Lagrange's condition	26
	3.4	Karush, Kuhn and Tuckers condition	27

1 Linear Programming

Consider the problem

$$\max_{x} z \stackrel{\text{def}}{=} c^{\top} x$$
 subject to $Ax \leq b$,
$$x \geq 0,$$
 (LP)

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$. We assume that $m \leq n$, otherwise the feasible set might be trivial. For instance if $n \leq m$ and full rank, then there exists only one feasible point or no feasible points.

Before developing a method for solving the above, we will establish a standard representation of linear programs. The standard form is given in (LP). Not all LPs fit the format (LP), but all LPs can be re-written in the form (LP). A few of the standard tricks we use to re-write an LP in the standard form are listed as here

1. (**Equality**) Replace $\sum_{j=1}^{n} a_{ij} x_j = b_i$ by

$$\sum_{j=1}^{n} a_{ij} x_j \le b_i,$$

and

$$-\sum_{j=1}^{n} a_{ij} x_j \le -b_i.$$

2. (Box constraints) Replace

$$\alpha \leq x_i \leq \beta$$
,

by

$$y = x - \alpha,$$

$$y \le \beta - \alpha$$

and

$$y \ge 0$$
.

3. (Unconstrained) If x has no positivity constraint, then replace $x = x^+ - x^-$ and add the constraints $x^+ \ge 0$ and $x^- \ge 0$.

1.1 A first example

First we start with a simple 2D graphic example. We want to maximize the production of products x and y. Each unit of product x and y gives us 400 and 200 profit, respectively. To produce one unit of product x we need 30 minutes on machine 1 and 40 minutes on machine 2. To produce

one unit of product y we need 20 minutes on machine 1 and 10 minutes on machine 2. Thus our problem is to maximize 400x + 200y subject to.

$$30x + 20y \le 6000$$

 $40x + 10y \le 4000$

This graphical example leads us to believe that is the solution is attainable, then it is always at a vertex. Indeed, this is the case.

Theorem 1 (Fundamental Theorem of Linear Programming) Let $P = \{x \mid Ax = b, x \geq 0\}$. One of the three circumstances must hold

- 1. $P = \{\emptyset\}$
- 2. $P \neq \{\emptyset\}$ and there exists a vertex v of P such that $v \in \arg\min_{x \in P} c^{\top} x$
- 3. There exists $x, d \in \mathbb{R}^n$ such that $x + td \in P$ for all $t \geq 0$ and $\lim_{t \to \infty} c^{\top}(x + td) = \infty$.

This theorem suggests how we should develop an algorithm to solve the LP. First we should take care of finding a feasible point and assuring that the domain is non-empty. This is called **initialization phase** or **phase 1**. After determining a feasible point, we should traverse the vertices of P searching for the optimal point. If we find one, we say that the solution is **attainable**. If we find a direction in which $c^{T}x \to \infty$, we say that there is an **unbounded** solution.

Let us transform this insight into a method for solving. First we transform a problem given in the standard form

$$\begin{array}{rcl}
\max & 4x_1 + 2x_2 \\
& 3x_1 + 2x_2 & \leq 600 \\
& 4x_1 + 1x_2 & \leq 400 \\
& x_1 \geq 0, x_2 \geq 0.
\end{array} \tag{1}$$

into a maximization over linear constraints with non-negativity constraints

$$\max 4x_1 + 2x_2$$

$$x_3 = 600 - 3x_1 - 2x_2$$

$$x_4 = 400 - 4x_1 - x_2.$$
(2)

We arrived at the above (1) by simply adding x_3 and x_4 on the 1st and 2nd rows to fill in the *slack* of the inequality. Accordingly, the variables x_3 and x_4 are referred to as the slack variables. It is not hard to show that (1) and (2) are equivalent.

Exercise 2 Show that if (x_1^*, x_2^*) is a solution to (1) then there exists x_3^* and x_4^* such that $(x_1^*, x_2^*, x_3^*, x_4^*)$ is a solution to (2). Furthermore, if $(x_1^*, x_2^*, x_3^*, x_4^*)$ is a solution to (1).

Proof: Straightforward.

Next we re-write (2) in the *Dictionary* format

The non-negativity constraints are non longer explicitly included, so we must take care so as to ensure they hold. Note that the above has a convenient feasible point, that is, the point $(x_1^*, x_2^*, x_3^*, x_4^*) = (0, 0, 600, 400)$ satisfies the above equality constraints. The feasible point corresponds to the (0,0) point in our original 2D constraint space. We will now try to move from this vertex to a neighbouring vertex that has a larger objective value.

Note that the *cost coefficient* of x_1 in the objective function is positive, which shows that increasing x_1 will increase the objective function. But increasing x_1 decreases x_3 and x_4 . Indeed we have

$$x_3 \ge 0 \implies 600 - 3x_1 \ge 0 \implies x_1 \le 200,$$

 $x_4 \ge 0 \implies 400 - 4x_1 \ge 0 \implies x_1 \le 100.$

Thus $x_1 \leq 100$ otherwise x_4 will become negative. We will now perform row operations on (3) so that x_1 appears isolated on the left-hand side taking x_4 's position. This gives

Now we are at the vertex $(x_1^*, x_2^*) = (100, 0)$. We refer to this last operation as x_4 leaving the basis and x_1 entering the basis. Next we see that increasing x_2 increases the objective value but

$$x_3 \ge 0 \Rightarrow 240 \ge x_2,$$

 $x_1 \ge 0 \Rightarrow 400 \ge x_4.$

Consequently we can increase x_2 upto 240 while respecting the positivity constraints of x_3 . Thus x_3 will leave the basis and x_2 will enter the basis. Performing a row elimination again, we have that

Now increasing x_4 or x_3 will decrease the objective value, thus we can make no further improvement. The final optimal vertex is given by $(x_1^*, x_2^*) = (40, 240)$ and the optimal objective value is $z^* = 640$.

1.2 Notation and definitions

We will now formalize the definitions we introduced in the examples.

• The objective is to maximize the linear objective function $z = \sum_{j=1}^{n} c_j x_j$

• There are m inequality constraints in the standard form given by

$$\sum_{j=1}^{n} a_{ij} x_j \le b_i, \text{ for } i \in \{1, \dots, m\}.$$

- There are n positivity constraints given by $x_j \ge 0$, for $j \in \{1, ..., n\}$.
- We call $(x_1^*, \dots, x_n^*) \in \mathbb{R}^n$ a feasible solution if it satisfies the inequality and positivity constraints.

When passing from the standard form to the dictionary form, we had to introduce some additional notation

- We call the additionally introduced variable $(x_{n+1}, \ldots, x_{n+m}) \in \mathbb{R}^m$ the slack variables ("variables d'écart")
- We refer to

$$x_{n+1} = b_1 - \sum_{j=1}^{n} a_{1j} x_j$$

$$\vdots$$

$$x_{n+i} = b_i - \sum_{j=1}^{n} a_{ij} x_j$$

$$\vdots$$

$$x_{n+m} = b_m - \sum_{j=1}^{n} a_{mj} x_j$$

$$z = \sum_{j=1}^{n} c_j x_j,$$

as the initial dictionary.

- We say that the system of equations with non-negativity constraints forms a valid dictionary if m of the variables (x_1, \ldots, x_{n+m}) can be expressed as an explicit function of the remaining n variables.
- We refer to the *m* variables isolated on the left-hand side as the basic variable (variable de base) and the remaining *n* variables as non-basic (variable hors-base) or outside the basis.

After writing the problem in the dictionary format, we then performed several row elimination operations to change the basic variables. These row operations altered the coefficients of the constraints a_{ij} and the cost vector c_j . We introduce notation to accommodate for these changing coefficients.

- Let $I \subset \{1, ..., n+m\}$ be the set of indices of the basic variables and let $J = \{1, ..., n+m\} \setminus I$ be the non-basic variables.
- For a given basis determined by I there is a corresponding dictionary

$$\frac{x_i = b'_i + \sum_{j \in J} a'_{ij} x_j, \text{ for } i \in I}{z = z^* + \sum_{j \in J} c'_j x_j,}$$

where $a'_{ij}, b'_i, z^* \in \mathbb{R}$ are coefficients resulting from the row operations. For this to be a feasible dictionary we require that $b'_i \geq 0$.

1.3 The simplex algorithm

Let us now formalize the operations of the simplex algorithm. First, we choose a variable x_{j_0} that has a positive cost c'_{j_0} to enter the basis, see Algorithm 1. Otherwise if all costs are negative, we have found the optimal. Next we must choose a variable x_{i_0} that will leave the basis. We determine i_0 as the first variable whose value equals zero as we increase $x_{j_0}^*$. That is, since $x_{j_0}^*$ will be the only non-zero non-basic variable, we have

$$x_i^* = b_i' + \sum_{i \in J} a_{ij}' x_j^* = b_i' + a_{ij_0}' x_{j_0}^*.$$

Since we require $x_i^* \geq 0$ this imposes that $b_i' + a_{ij_0}' x_{j_0}^* \geq 0$. In other words

$$x_{j_0}^* \le -\frac{b_i'}{a_{ij_0}'}$$
 if $a_{ij_0}' < 0$, for $i \in I$, (3)

$$x_{j_0}^* \ge -\frac{b_i'}{a_{ij_0}'}$$
 if $a_{ij_0}' \ge 0$, for $i \in I$. (4)

Since we are only interested in increasing the value of $x_{j_0}^*$, the case (4) where $a'_{ij_0} \geq 0$ does not restrict $x_{j_0}^*$ from increasing (since $b'_i \geq 0$). Thus we only need concern ourself with the case (3). With the preceding definitions, we can now state the Simplex method in Algorithm 1. In particular, the pivoting step in Algorithm 1 can be stated using elementwise operations as

$$\begin{array}{l} \mathbf{for} \ j \in J \ \mathbf{do} \\ \mathbf{for} \ i \in I \setminus \{i_0\} \ \mathbf{do} \\ a'_{ij} \leftarrow a'_{ij} - \frac{a'_{ij_0}}{a'_{i_0j_0}} a'_{i_0j} & \# \ \mathrm{Row \ elimination \ on \ pivot} \ (i_0,j_0). \\ c_j \leftarrow c_j - \frac{c'_{j_0}}{a'_{i_0j_0}} a'_{i_0j} & \end{array}$$

$$\mathbf{for}\ j \in J\ \mathbf{do} \\ a_{i_0j} \leftarrow -\frac{a_{i_0j}}{a'_{i_0j_0}}$$

$$a'_{i_0j_0} = 1/a'_{i_0j_0}$$

What was left unclear is how do we choose j_0 to enter the basis. There are four common choices.

- 1. The mad hatter rule: Choose the first one you see.
- 2. Dantzig's 1st rule: $j_0 = \arg \max_{i \in J} c_i$.
- 3. Dantzig's 2nd rule: Choose $j_0 \in \{j \in J : c_j > 0\}$ that results in the largest increase in the objective value. Let $t = \min_{i \in I, a_{ij_0} < 0} \left\{ -\frac{b_i}{a_{ij_0}} \right\}$. The variable entering the basis will have value $x_{j_0}^* = t$. Consequently the objective value increases by tc_{j_0} . Choosing j_0 that maximizes this increase is equivalent to choosing via

$$j_0 = \arg\max_{j \in J} \left\{ c_j \min_{i \in I, a_{ij} < 0} \left\{ -\frac{b_i}{a_{ij}} \right\} \right\}.$$

This effective but computationally expensive.

Algorithm 1 One Simplex iteration

Input: A basic index set $I \subset \{1, ..., n+m\}$, $J = I \setminus \{1, ..., n+m\}$, constraint coefficients $a'_{ij} \in \mathbb{R}$, $b'_i \geq 0$ and $c'_i \in \mathbb{R}$.

if $c_i \leq 0$ for all $i \in J$ then

STOP; # Optimal point found.

Choose a variable j_0 to **enter the basis** from the set $j_0 \in \{j \in J : c'_j > 0\}$.

if $a'_{ij_0} \geq 0$ for all $i \in I$ then

STOP; # The problem is unbounded.

Choose a variable i_0 to leave the basis from the set $i_0 \in \arg\min_{i \in I, a'_{ij_0} < 0} \left\{ -\frac{b'_i}{a'_{ij_0}} \right\}$.

 $aux \leftarrow a'_{i_0j_0}$

for $i \in I \setminus \{i_0\}$ do

 $a'_{i:} \leftarrow a'_{i:} - a'_{ij_0} \ a'_{i_0:} / a_{i_0j_0}$ # Row elimination on pivot (i_0, j_0) .

 $c' \leftarrow c' - c'_{j_0} \ a'_{i_0:} / \ a_{i_0j_0} \qquad \quad \# \ \text{Update the cost coefficients}.$

 $a'_{i_0:} \leftarrow - \, a'_{i_0:} / \, a'_{i_0j_0} \qquad \# \text{ Row normalization }.$

 $a_{i_0 j_0} \leftarrow 1/aux$

 $I \leftarrow (I \setminus \{i_0\}) \cup \{j_0\}.$ # Update basic variables set

 $J \leftarrow (J \setminus \{j_0\}) \cup \{i_0\}.$ # Update non-basic variable set

Output: I, a'_{ij}, b'_j, c'_j .

4. Bland's rule: Choose the smallest indices j_0 and i_0 . That is, choose

$$j_0 = \arg\min\{j \in J : c_j > 0\}.$$

If the set $\arg\min_{i\in I, a_{ij_0}<0} \left\{\frac{b_i}{a_{ij_0}}\right\}$ has more than one element, choose the smallest

$$i_0 = \min \left\{ \arg \min_{i \in I, a_{ij_0} < 0} \left\{ -\frac{b_i}{a_{ij_0}} \right\} \right\}.$$

Dantzig's rules were designed to maximize the objective function in a greedy manner. While Bland's rule, though apparently mundane, was designed to avoid *cycling*.

1.4 Degeneracy and Cycling

If any of the basic variables have zero value, we say that it is a *degenerate* basis. Degenerate basis require extra care because they may lead to the simplex algorithm cycling. See example on board and your alternative french notes.

1.5 Initialization using a first phase problem

Not always will we have that $b_i \geq 0$ for i = 1, ..., m. Simply including slack variables will not lead to a feasible basic solution. To find a feasible solution we will use the simplex method on an auxiliary *first phase* problem.

First assume we are given a problem

$$\max_{x} z \stackrel{\text{def}}{=} c^{\top} x$$
 subject to $Ax \leq b$,
$$x \geq 0,$$
 (5)

where at least one $b_i < 0$ where $i \in \{1, ..., m\}$. Consequently $x^* = 0$ is not a feasible solution. To remedy this we add an additional variable x_0 and **change the objective**

$$\max_{x} -x_{0}$$
 subject to $Ax \leq b + Ix_{0}$,
$$x \geq 0, x_{0} \geq 0.$$
 (LP-1st)

There now exists x_0 for which there is a feasible solution, for instance choosing $x_0^* = \max_{i=1,\dots,m} |b_i|$ and $x_i^* = 0$ for $i = 1, \dots n$. The problem (LP-1st) is known as the 1st phase simplex method. We can use the simplex method to solve (LP-1st). If the solution to (LP-1st) is such that $x_0^* \neq 0$, then we know that the original problem (5) is infeasible. If the solution to (LP-1st) is such that $x_0^* = 0$, then we can use the remaining variables $x_i^* \neq 0$ as a starting basis.

To do this, first we setup a dictionary with slack variables as the basis, even though they do not form a feasible basis.

$$x_{n+1} = b_1 - \sum_{j=1}^{n} a_{1j} x_j + x_0$$

$$\vdots$$

$$x_{n+m} = b_m - \sum_{j=1}^{n} a_{mj} x_j + x_0$$

$$z = -x_0$$
(6)

Next, different from our previous examples, we will make x_0 enter the basis even though it has a negative cost. Suppose w.l.o.g that x_{n+1} leaves the basis as x_0 enters. Thus the next dictionary would be

$$x_{0} = -b_{1} + \sum_{j=1}^{n} a_{1j}x_{j} + x_{n+1}$$

$$\vdots$$

$$x_{n+m} = b_{m} - b_{1} - \sum_{j=1}^{n} (a_{mj} - a_{1j})x_{j} + x_{n+1}$$

$$z = b_{1} - \sum_{j=1}^{n} a_{1j}x_{j} - x_{n+1}$$

$$(7)$$

Now, so long as there are positive elements in $(a_{1j})_j$, we can proceed with the simplex method as usual. Note that this indicates we should have chosen an element i_0 to leave basis such that $(a_{i_0j})_j$. has many positive coefficients. If we continue to iterate and x_0 leaves the basis, then we have found a feasible basis point and we can drop the x_0 variable.

1.6 Duality

Consider again the LP in standard form

$$\max_{x} z \stackrel{\text{def}}{=} c^{\top} x$$
 subject to $Ax \leq b$,
$$x \geq 0,$$
 (LP)

Though we now have a technique for solving (LP), at any given moment we do not know how far we are from the solution. Will we need another few minutes of computing resources or days of computing resources? This is a troublesome question. For this, and other reasons, we will now develop an alternative and equivalent formulation of (LP) that will help determine if we are near the solution, among other insights. This equivalent formulation is known as the *dual* formulation. We can first derive the dual problem as a means of finding an upper bound to the solution of (LP).

Say we wish to upper bound our objective $z=c^{\top}x$ and we want to do this by combining rows of the constraints $Ax \leq b$. That is, let $y \geq 0 \in \mathbb{R}^m$. If we could determine such a y so that $y^{\top}A \approx c^{\top}$ then we would have that

$$c^{\top}x \approx (y^{\top}A)x \le y^{\top}b,$$

thus $y^{\top}b$ is an approximate upper bound of $c^{\top}x$. What is more, $y^{\top}b$ does not depend on x, ergo this bound holds for all x, including the optimal solution. But just being approximate upper bound is no good. Instead, assume we have $0 \le y \in \mathbb{R}^m$ such that $y^{\top}A \ge c^{\top}$ or equivalently $A^{\top}y \ge c$. Then indeed the upper bound holds since

$$c^{\top}x \le (y^{\top}A)x \le y^{\top}b.$$

Now say we want the upper bound to be as tight as possible. We can do this by choosing $y \ge 0$ so that $y^{\top}b$ is small as possible. That is, we need to the following dual linear program.

$$\max_{x} \ w \stackrel{\text{def}}{=} y^{\top} b$$
 subject to $A^{\top} y \geq c$,
$$y \geq 0. \tag{DP}$$

By construction, the following lemma holds

Lemma 3 (Weak Duality) If $x \in \mathbb{R}^n$ is a feasible point for (LP) and $y \in \mathbb{R}^m$ is a feasible point for (DP) then

$$c^{\top}x \le y^{\top}Ax \le y^{\top}b. \tag{8}$$

Consequently

• If (LP) has an unbounded solution, that is $c^{\top}x \to \infty$, then there exists no feasible point y for (DP)

- If (DP) has an unbounded solution, that is $y^{\top}b \to -\infty$, then there exists no feasible point x for (LP)
- If x and y are primal and dual feasible, respectively, and $c^{\top}x = y^{\top}b$, then x and y are the primal and dual optimal points, respectively.

What is even more remarkable is that, not only does (DP) provide an upper bound for (LP), but they are equivalent problems, in the following sense

Theorem 4 (Strong Duality) If (LP) or (DP) is feasible, then $z^* = w^*$. Moreover, if c' is the cost vector of the optimal dictionary of the primal problem, that is, if

$$z = z^* + \sum_{i=1}^{n+m} c_i' x_i, \tag{9}$$

then $y_i^* = -c'_{n+i}$ for i = 1, ..., m.

Proof: First note that $c_i' \leq 0$ for i = 1, ..., m+n otherwise the dictionary would not be optimal. Consequently $y_i^* = -c_{n+i}' \geq 0$ for i = 1, ..., m. Furthermore, by the definition of the slack variables we have that

$$x_{n+i} = b_i - \sum_{j=1}^n a_{ij} x_j, \quad \text{for } i = 1, \dots, m.$$
 (10)

Consequently, setting $y_i^* = -c'_{n+i}$, we have that

$$z \stackrel{(9)}{=} z^* + \sum_{j=1}^n c'_j x_j + \sum_{i=n+1}^{n+m} c'_i x_i$$

$$\stackrel{(10)}{=} z^* + \sum_{j=1}^n c'_j x_j - \sum_{i=1}^m y_i^* (b_i - \sum_{j=1}^n a_{ij} x_j)$$

$$= z^* - \sum_{i=1}^m y_i^* b_i + \sum_{j=1}^n \left(c'_j + \sum_{i=1}^m y_i^* a_{ij} \right) x_j$$

$$= \sum_{j=1}^n c_j x_j, \quad \forall x_1, \dots, x_n.$$

$$(11)$$

where the last line followed by definition of the objective function $z = \sum_{j=1}^{n} c_j x_j$. Since the above holds for all $x \in \mathbb{R}^n$, we can match the coefficients to obtain

$$z^* = \sum_{i=1}^{m} y_i^* b_i (12)$$

$$c_j = c'_j + \sum_{i=1}^m y_i^* a_{ij}, \quad \text{for } j = 1, \dots, n.$$
 (13)

Since $c'_j \leq 0$ for j = 1, ..., n, the above is equivalent to

$$z^* = \sum_{i=1}^{m} y_i^* b_i \tag{14}$$

$$\sum_{i=1}^{m} y_i^* a_{ij} \leq c_j, \quad \text{for } j = 1, \dots, n.$$
 (15)

The inequalities (15) prove that y_i^* 's satisfies the constraints in (DP), and thus is feasible. The equality (14) shows that $z^* = \sum_{i=1}^m y_i^* b_i = w$, ans consequently by week duality the y_i^* 's are dual optimal. Calculating the dual optimal variables y^* using Theorem 4 requires knowing the cost vector c' of the optimal tableau. But it turns out that we do not need c' to calculate y^* . We can instead recover the y^* by only knowing x^* , and the complementary slackness theorem shows (see notes).

2 Nonlinear programming without constraints

For this section is largely based on Chapter 1 in [1].

We now move onto nonlinear optimization, that is, we wish to minimize a possibly nonlinear differentiable function $f: x \in \mathbb{R}^n \mapsto f(x) \in \mathbb{R}$. First we will consider the unconstrained optimization problem

$$x^* = \arg\min_{x \in \mathbb{R}^n} f(x). \tag{16}$$

All the methods we develop are iterative, in that they produce a sequence of iterates x^1, \ldots, x^k, \ldots , such that

$$\lim_{k \to \infty} x^k = x^*.$$

Furthermore, we will focus on descent methods where the iterates are calculated via

$$x^{k+1} = x^k + s_k d^k, (17)$$

where $s_k > 0$ is a step size and $d^k \in \mathbb{R}^n$ is search direction. The search direction and step size will satisfy the descent condition given by

$$f(x^k) < f(x^{k+1}). (18)$$

This in turn guarantees that, little by little, we get closer to the solution of (16).

The key tool in ensuring that the descent condition holds is the gradient.

2.1 The gradient, Hessian and the Taylor expansion

For a differentiable function $f: x \in \mathbb{R}^n \mapsto f(x) \in \mathbb{R}$, we refer to $\nabla f(x)$ as the gradient evaluated at x defined by

$$\nabla f(x) = \left[\frac{\partial f(x)}{\partial x_1}, \dots, \frac{\partial f(x)}{\partial x_n}\right]^{\top}.$$

Note that $\nabla f(x)$ is a column-vector.

For any vector valued function $F: x \in \mathbb{R}^n \to F(x) = [f_1(x), \dots, f_n(x)]^\top \in \mathbb{R}^n$ we define the Jacobian matrix by

$$\nabla F(x) \stackrel{\text{def}}{=} \begin{bmatrix} \frac{\partial f_1(z)}{\partial x_1} & \frac{\partial f_2(z)}{\partial x_1} & \frac{\partial f_3(z)}{\partial x_1} & \dots & \frac{\partial f_n(z)}{\partial x_1} \\ \frac{\partial f_2(z)}{\partial x_1} & \frac{\partial f_2(z)}{\partial x_2} & \frac{\partial f_3(z)}{\partial x_2} & \dots & \frac{\partial f_n(z)}{\partial x_2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_1(z)}{\partial x_n} & \frac{\partial f_2(z)}{\partial x_n} & \frac{\partial f_3(z)}{\partial x_n} & \dots & \frac{\partial f_n(z)}{\partial x_n} \end{bmatrix} = \left[\nabla f_1(x), \nabla f_2(x), \nabla f_3(x), \dots, \nabla f_2(x) \right].$$

The gradient is useful because we can use it to build a linear approximation of f(x) using the 1st order Taylor expansion

$$f(x^{0} + d) = f(x^{0}) + \nabla f(x^{0})^{\top} d + \epsilon(d) \|d\|_{2},$$
(19)

where $\epsilon(d)$ is a real valued such that

$$\lim_{d \to 0} \epsilon(d) = 0. \tag{20}$$

We will use the expansion (19) to motivate and understand the steepest descent method later.

If f(x) is twice differentiable, we refer to $\nabla^2 f(x)$ as the Hessian matrix:

$$\nabla^2 f(x) \stackrel{\text{def}}{=} \begin{bmatrix} \frac{\partial^2 f(z)}{\partial x_1 \partial x_1} & \frac{\partial^2 f(z)}{\partial x_1 \partial x_2} & \frac{\partial^2 f(z)}{\partial x_1 \partial x_3} & \cdots & \frac{\partial^2 f(z)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(z)}{\partial x_1 \partial x_2} & \frac{\partial^2 f(z)}{\partial x_2 \partial x_2} & \frac{\partial^2 f(z)}{\partial x_2 \partial x_3} & \cdots & \frac{\partial^2 f(z)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(z)}{\partial x_n \partial x_1} & \frac{\partial^2 f(z)}{\partial x_n \partial x_2} & \frac{\partial^2 f(z)}{\partial x_n \partial x_3} & \cdots & \frac{\partial^2 f(z)}{\partial x_n \partial x_n} \end{bmatrix}$$

If $f \in \mathbb{C}^2$ (twice continuously differentiable) then

$$\frac{\partial^2 f(z)}{\partial x_i \partial x_j} = \frac{\partial^2 f(z)}{\partial x_j \partial x_i}, \quad \forall i, j \in \{1, \dots, n\},$$

consequently the Hessian matrix is symmetric, that is, $\nabla^2 f(x) = \nabla^2 f(x)^{\top}$.

With the Hessian matrix we can build a quadratic approximation to our function using the 2nd order Taylor expansion.

$$f(x^{0} + d) = f(x^{0}) + \nabla f(x^{0})^{\top} d + \frac{1}{2} d^{\top} \nabla^{2} f(x^{0}) d + \epsilon(d) ||d||_{2}^{2}.$$
(21)

We will use this expansion to motivate the Newton method later on.

In calculating the gradient and the Hessian, the following techniques will be handy

• For any function $F(x): \mathbb{R}^n \to \mathbb{R}^n$ and matrix $A \in \mathbb{R}^{n \times n}$ we have

$$\nabla (F(x)^{\top} A) = \nabla F(x)^{\top} A. \tag{22}$$

• For any two vector valued functions F_1 and F_2 we have that

$$\nabla(F_1(x)^{\top} F_2(x)) = \nabla F_1(x) F_2(x) + \nabla F_2(x) F_1(x). \tag{23}$$

Exercise 5 Let $f(x) = \frac{1}{2}x^{\top}Ax + x^{\top}b + c$, where $A \in \mathbb{R}^{n \times n}$ is a symmetric positive definite matrix, $b \in \mathbb{R}^n$ and $c \in \mathbb{R}$. Calculate the gradient and Hessian of f(x).

Proof: Taking the gradient we have

$$\nabla f(x) = \frac{1}{2}\nabla(x^{\top}Ax) + \nabla(x^{\top}b) + \nabla(c)$$

$$\stackrel{(22)}{=} \frac{1}{2}\nabla(x^{\top}Ax) + b$$

$$\stackrel{(23)}{=} \frac{1}{2}\nabla(x^{\top})Ax + \frac{1}{2}\nabla(Ax)x + b$$

$$= \frac{1}{2}Ax + \frac{1}{2}\nabla(Ax)x + b.$$

Finally, from the definition of Jacobian matrix we have that

$$[\nabla(Ax)]_{:j} = A_{j:},$$

consequently $\nabla(Ax) = A^{\top} = A$, from which we have

$$\nabla f(x) = Ax + b.$$

Differentiating again to get the Hessian we have

$$\nabla^2 f(x) = \nabla(Ax) + \nabla(b) = A^{\top} = A.$$

2.2 Level sets and geometry

For a fixed constant $C \in \mathbb{R}$ we the following surface

$$\{x \in \mathbb{R}^n \mid f(x) = C\},\tag{24}$$

a level set of f(x). The level sets implicitly define a surface where f(x) has the same value.

Exercise 6 Draw the level sets

$$4 = f(x_1, x_2),$$

$$9 = f(x_1, x_2),$$

where $f(x_1, x_2,) = x_1^2 + x_2^2$.

The gradient direction is intimately linked to the geometry of the levels sets. Indeed, the gradient points orthogonal to the level sets and thus describes the tangent lines to the levels sets.

Lemma 7 The tangent directions to a point on the level set of f(x) are orthogonal to the gradient at that point. That is, for every

$$v \in T_f(x^0) = \left\{ v \in \mathbb{R}^n : v = \lim_{\substack{y \to x^0, \\ f(y) = f(x^0)}} \frac{y - x^0}{\|y - x^0\|_2} \right\},$$
 (25)

we have that $v^{\top} \nabla f(x^0) = 0$.

Proof: Let $y \in \mathbb{R}^n$ be such that $f(x^0) = f(y)$, consequently using (19) we have that

$$f(y) = f(x^0) + \nabla f(x^0)^\top (y - x^0) + \epsilon (y - x^0) \|y - x^0\|_2 = f(x^0).$$

Thus $\nabla f(x^0)^{\top}(y-x^0) + \epsilon(y-x^0)\|y-x^0\|_2 = 0$. Dividing by $\|y-x^0\|_2$ and taking the limit $y \to x^0$, gives that

$$0 = \lim_{y \to x^0} \left(\nabla f(x^0)^\top \frac{y - x^0}{\|y - x^0\|_2} + \epsilon(y - x^0) \right) \stackrel{(25) + (20)}{=} \nabla f(x^0)^\top v. \quad \blacksquare$$

Another way of phrasing the above result is that $y = f(x^0) + \nabla f(x^0)^{\top} d$ is the tangent line of f(x) at $(x^0, f(x^0))$.

The gradient is also the direction that maximizes the local change in the objective function, while the negative gradient is the direction that minimizes the local change. This is the reason why gradient methods are often referred to as steepest descent methods.

Lemma 8 The normalized gradient $d = \nabla f(x^0) / ||\nabla f(x^0)||_2$ is the direction that maximizes the local change around x^0 :

$$\Delta(d) = \lim_{s \to 0^+} \frac{f(x^0 + sd) - f(x^0)}{s},\tag{26}$$

where $d \in \mathbb{R}^n$ with $||d||_2 = 1$. Furthermore the negative normalized gradient minimizes the local change.

Proof: Using (19) we have that

$$f(x^0 + sd) - f(x^0) = s\nabla f(x^0)^{\top} d + \epsilon(sd)s.$$

Dividing by s and taking the limit $s \to 0$ we have

$$\Delta(d) = \lim_{s \to 0^+} \frac{f(x^0 + sd) - f(x^0)}{s} = \nabla f(x^0)^\top d + \lim_{s \to 0^+} \epsilon(sd) = \nabla f(x^0)^\top d.$$

Now using that $||d||_2 = 1$ together with the Cauchy inequality

$$-\|\nabla f(x^0)\|_2 \le \Delta(d) = \nabla f(x^0)^{\top} d \le \|\nabla f(x^0)\|_2.$$
 (27)

The upper and lower bound is achieved when $d = \nabla f(x^0) / \|\nabla f(x^0)\|_2$ and $d = -\nabla f(x^0) / \|\nabla f(x^0)\|_2$, respectively.

As a corollary, we have that the search direction is a descent direction if it has an obtuse angle with the gradient

Corollary 9 If $d^{\top}\nabla f(x_0) < 0$ then there exists s > 0 such that

$$f(x_0 + sd) < f(x_0).$$

Proof: From (27) we have that $\Delta(d) = \nabla f(x^0)^{\top} d < 0$. Let $a = -\nabla f(x^0)^{\top} d > 0$. Let s > 0 be such that $\epsilon(sd) < \frac{a}{2}$. Consequently from (19) we have that

$$\frac{f(x^0 + sd) - f(x^0)}{s} = \nabla f(x^0)^{\top} d + \epsilon(sd) \le -\frac{a}{2} < 0.$$

2.3 Optimality conditions

Let $f \in \mathbb{C}^2$ be twice continuously differentiable throughout this section.

In most cases it is impossible to solve a general optimization problem such as (16). A much more modest, and often attainable, objective is to find a local minima instead.

Definition 10 The point $x^* \in \mathbb{R}^n$ is a local minima of f(x) is there exists r > 0 such that

$$f(x^*) \le f(x), \quad \forall ||x - x^*||_2 < r.$$
 (28)

Thus a local minima point x^* is one where all neighbouring points are worst. This is often good enough for most applications (though not *all* applications). Finding local minima is made possible through the following necessary and sufficient conditions.

Theorem 11 (Necessary optimality conditions) If x^* is a local minima of f(x) then

1.
$$\nabla f(x^*) = 0$$

2.
$$d^{\top} \nabla^2 f(x^*) d \ge 0$$
, $\forall d \in \mathbb{R}^n$.

Proof: The fact that $\nabla f(x^*) = 0$ follows from Corollary 9.

Now suppose there exists $d \in \mathbb{R}^n$ such that $d^\top \nabla^2 f(x^*) d < 0$. Suppose w.l.o.g that $||d||_2 = 1$. Using the second order Taylor expansion we have that

$$f(x^* + sd) = f(x^*) + \frac{s^2}{2}d^{\top}\nabla^2 f(x^*)d + \epsilon(sd)s^2.$$

Let $\bar{s} > 0$ be such that for $s \leq \bar{s}$ we have that $\epsilon(sd) < |d^{\top}\nabla^2 f(x^*)d|/4$. Dividing the above by s^2 , for $s \leq \bar{s}$ we have that

$$\frac{f(x^* + sd)}{s^2} = \frac{f(x^*)}{s^2} + \frac{1}{2}d^{\top}\nabla^2 f(x^*)d + \epsilon(sd)$$

$$< \frac{f(x^*)}{s^2} + \frac{1}{4}d^{\top}\nabla^2 f(x^*)d,$$

thus $f(x^* + sd) < f(x^*)$ for all $s \leq \bar{s}$ which contradicts the definition of local minima.

Not only are the conditions in Theorem 11 necessary, with a slight modification, they are also sufficient.

Theorem 12 (Sufficient Local Optimality conditions) If $x^* \in \mathbb{R}^n$ is such that

1.
$$\nabla f(x^*) = 0$$

2.
$$d^{\top} \nabla^2 f(x^*) d > 0$$
, $\forall d \in \mathbb{R}^n \text{ with } d \neq 0$,

then x^* is a local optima.

Proof: Let $d \in \mathbb{R}^n$ such that $||d||_2 = 1$. Because $\nabla^2 f(x^*)$ is positive definite, the smallest non-zero eigenvalue must also be strictly positive. Consequently

$$\lambda_{\min}(\nabla^2 f(x^*)) \le d^{\top} \nabla^2 f(x^*) d, \quad \forall ||d||_2 = 1.$$

Using the second-order Taylor expansion, we have that

$$f(y) = f(x^*) + \frac{1}{2} (y - x^*)^{\top} \nabla^2 f(x^*) (y - x^*) + \epsilon (y - x^*) \|y - x^*\|_2^2$$

$$\geq \frac{\|y - x^*\|_2^2}{2} \lambda_{\min}(\nabla^2 f(x^*)) + \epsilon (y - x^*) \|y - x^*\|_2^2.$$

Let r > 0 be such that every y with $||y - x^*|| \le r$ we have that

$$|\epsilon(y - x^*)| < \lambda_{\min}(\nabla^2 f(x^*))/4.$$

Thus for $||y - x^*|| \le r$ we have

$$f(y) \geq f(x^*) + \frac{\|y - x^*\|_2^2}{2} \lambda_{\min}(\nabla^2 f(x^*)) + \epsilon(y - x^*) \|y - x^*\|_2^2$$

$$\geq f(x^*) + \frac{\|y - x^*\|_2^2}{4} \lambda_{\min}(\nabla^2 f(x^*)) \geq f(x^*). \quad \blacksquare$$

Exercise 13 Let $f(x) = \frac{1}{2}x^{T}Ax + x^{T}b + c$, with A symmetric positive definite. How many local/global minimas can f(x) have? Find a formula for the minima using only the data A and b.

2.4 Convex functions

In some cases, original problem of finding the global minima (16) can be solved. Indeed, for the convex functions, there exists a unique global minima. We say a function is convex if

$$f(tx + (1-t)y) \le tf(x) + (1-t)f(y), \quad \forall x, y \in \mathbb{R}^d, t \in [0, 1].$$
(29)

Theorem 14 If f is a convex function, then every local minima of f is also a global minima.

Proof: Let x^* be a local minima and suppose there exists $\bar{x} \in \mathbb{R}^n$ such that $f(\bar{x}) < f(x^*)$. Now consider the line segment $z = t\bar{x} + (1-t)x^*$ for $t \in [0, 1]$. By the definition of convexity we have that

$$f(z) = f(t\bar{x} + (1-t)x^*) \le tf(\bar{x}) + (1-t)f(x^*) < tf(x^*) + (1-t)f(x^*) = f(x^*).$$
 (30)

This shows that x^* cannot be a local minima. Indeed, since $z = t\bar{x} + (1-t)x^*$, for any radius r > 0 by choosing $t \le r/\|\bar{x} + x^*\|_2$ we have that

$$||z - x^*||_2 = t||\bar{x} + x^*||_2 \le r.$$

Yet from (30) we have that $f(z) < f(x^*)$. A contraction. Thus there exists no \bar{x} with $f(\bar{x}) < f(x^*)$.

When f is twice differentiable, there are three equivalent ways of defining convexity.

Theorem 15 If f is twice continuously differentiable, then the following three statements are equivalent

$$f(tx + (1-t)y) \le tf(x) + (1-t)f(y), \quad \forall x, y \in \mathbb{R}^d, t \in [0, 1].$$
 (31)

$$f(y) \ge f(x) + \nabla f(x)^{\top} (y - x), \quad \forall x, y \in \mathbb{R}^d.$$
 (32)

$$0 \le d^{\top} \nabla^2 f(x) d, \quad \forall x, d \in \mathbb{R}^d. \tag{33}$$

Proof: We only prove that $(31) \Rightarrow (32) \Rightarrow (33)$. The remaining proof of $(33) \Rightarrow (32) \Rightarrow (31)$ is left as an exercise.

 $((31)\Rightarrow(32))$ We can deduce (32) from (31) by dividing by t and re-arranging

$$\frac{f(y+t(x-y))-f(y)}{t} \le f(x)-f(y).$$

Now taking the limit $t \to 0$ gives

$$\langle \nabla f(y), x - y \rangle \le f(x) - f(y).$$

 $((32)\Rightarrow(33))$ First we prove this holds for 1-dimensional functions $f:\mathbb{R}\to\mathbb{R}$. From (32) we have that

$$f(y) \ge f(x) + f'(x)(y - x),$$

$$f(x) \ge f(y) + f'(y)(x - y).$$

Combining the above two we have that

$$f'(x)(y-x) \le f(y) - f(x) \le f'(y)(y-x).$$

Dividing by $(y-x)^2$ we have

$$\frac{f'(y) - f'(x)}{y - x} \ge 0, \quad \forall x, y, x \ne y.$$

It remains to take the limit. To then extend to any n-dimensional function, use that

$$\left. \frac{d^2 f(x+tv)}{dv^2} \right|_{t=0} = v^\top \nabla^2 f(x) v \ge 0, \forall v \ne 0.$$

We also say that f(x) is strictly convex when $d^{\top}\nabla^2 f(x)d > 0$, $\forall d \in \mathbb{R}^d$ with $d \neq 0$.

Exercise 16 (Homework) Prove Theorem (15) for quadratic functions $f(x) = \frac{1}{2}x^{\top}Ax + x^{\top}b + c$. What can we say about A when f is convex or strictly convex?

2.5 Gradient method

Since the negative gradient is the direction that minimizes the local change, it is only natural to use the negative gradient as a descent direction. This suggests the following method

$$x^{k+1} = x^k - s^k \nabla f(x^k).$$

But the question still remains how to choose s^k the stepsize? One natural strategy is to choose s^k that results in the maximum descent. That is,

$$s^k = \arg\min_{s>0} f(x^k + sd^k). \tag{34}$$

Finally, we also need a criteria to determine when we should stop iterating. Typically the user will choose a tolerance to error $\epsilon > 0$, and then stop the algorithm either when we are at an approximate stationary point

$$\|\nabla f(x^k)\|_2 \le \epsilon \tag{35}$$

or when the rate in decrease is small

$$f(x^{k+1}) - f(x^k) \le \epsilon. \tag{36}$$

This gives the steepest descent method in Algorithm (2).

Algorithm 2 Steepest Descent

- 1: Choose $x^0 \in \mathbb{R}^n$.
- 2: while $\|\nabla f(x^k)\|_2 > 0\epsilon$ or $f(x^{k+1}) f(x^k) \le \epsilon$ do
- 3: Calculate $d^k = -\nabla f(x^k)$
- 4: Calculate $s^k = \arg\min_{s>0} f(x^k + sd^k)$
- 5: Update $x^{k+1} = x^k + s^k \overline{d}^k$.

The rate of convergence in (38) may be slow. Indeed, it depends on how far the smallest and largest singular are from each other. Perhaps the issue is that we used a fixed stepsize instead of the "best" stepsize (34)? It turns out that also this greedy strategy of choosing the best step size in (34) can also lead slow convergence. This is partly due to a phenomenon called *zig-zagging*. When using the optimal stepsize (34), sequential gradients are orthogonal to one another, that is

$$\nabla f(x^{k+1})^{\top} \nabla f(x^{k+1}) = 0. \tag{37}$$

To prove this, note that by the definition of s^k in (34) we have that

$$\frac{d}{ds} f(x^k - s\nabla f(x^k))\Big|_{s=s^k} = 0.$$

Using the chain-rule we have that

$$\frac{d}{ds} f(x^k - s\nabla f(x^k))\Big|_{s=s^k} = -s^k \nabla f(x^k - s\nabla f(x^k))^\top \nabla f(x^k) = 0.$$

Thus so long as $s^k \neq 0$, then (37) holds. This zigzagging can make the global convergence of steepest descent painfully slow. One way to fix this zigzagging is to use a constant stepsize.

We now prove that Algorithm 2 converges for a constant stepsize and quadratic functions

Theorem 17 Let $f(x) = \frac{1}{2}x^{\top}Ax - x^{\top}b + c$. If we choose a fixed stepsize of $s^k = 1/\sigma_{\max}(A)$ then the iterates of Algorithm 2 converge according to

$$\|\nabla f(x^{k+1})\|_2 \le \left(1 - \frac{\sigma_{\min}(A)}{\sigma_{\max}(A)}\right)^k \|\nabla f(x^0)\|.$$
 (38)

Proof:

$$\nabla f(x^{k+1}) = Ax^{k+1} - b
= A(x^k - s\nabla f(x^k)) - b
= A(x^k - s(Ax^k - b)) - b
= Ax^k - b - sA(Ax^k - b)
= (I - sA)\nabla f(x^k).$$

Taking norms

$$\|\nabla f(x^{k+1})\|_2 \le \|I - sA\|_2 \|\nabla f(x^k)\|.$$

By choosing $s = 1/\sigma_{\text{max}}(A)$ we have that I - sA is symmetric positive definite and

$$||I - sA||_2 = 1 - s\sigma_{\min}(A) = 1 - \frac{\sigma_{\min}(A)}{\sigma_{\max}(A)} < 1.$$

Robert: Homework: Prove this last step!

Thus finally

$$\|\nabla f(x^{k+1})\|_{2} \le \left(1 - \frac{\sigma_{\min}(A)}{\sigma_{\max}(A)}\right) \|\nabla f(x^{k})\| \le \left(1 - \frac{\sigma_{\min}(A)}{\sigma_{\max}(A)}\right)^{k} \|\nabla f(x^{0})\|.$$

Algorithm 2 also converges for all *smooth* functions, that is when there exists L>0 such that

$$\|\nabla f(x) - \nabla f(y)\|_2 \le L\|x - y\|_2, \quad \forall x, y \in \mathbb{R}^n.$$
(39)

See the notes here http://users.ece.utexas.edu/~cmcaram/EE381V_2012F/Lecture_4_Scribe_Notes.final.pdf for a similar proof for all smooth functions.

2.6 Newton's method

Using the second order Taylor expansion we can motivate the Newton method. At each iteration, the *Newton Method* minimizes the local quadratic approximation

$$q_k(x) = f(x^k) + \nabla f(x^k)^{\top} (x - x^k) + \frac{1}{2} (x - x^k)^{\top} \nabla^2 f(x^k) (x - x^k), \tag{40}$$

as a proxy for minimizing f(x). Assuming f(x) is strictly convex, the stationary point x^{k+1} characterized by $\nabla_x q_k(x) = 0$ of (40) is given by

$$\nabla_x q_k(x) = \nabla f(x^k) + \nabla^2 f(x^k)(x^{k+1} - x^k) = 0.$$

Isolating x^{k+1} we have

$$x^{k+1} = x^k - \nabla^2 f(x^k)^{-1} \nabla f(x^k).$$

The advantage that Newton's method has over the steepest descent is that it converges quadratically when x is close to the minimum.

Theorem 18 Let f(x) be a μ -strongly convex function, that is, we have a global lower bound on the Hessian given by

$$\nabla^2 f(x) \succeq \mu I, \quad \forall x \in \mathbb{R}^n. \tag{41}$$

Furthermore, if the Hessian is also Lipschitz

$$\|\nabla^2 f(x) - \nabla^2 f(y)\|_2 \le L\|x - y\|_2 \tag{42}$$

then Newton's method converges locally and quadratically fast according to

$$||x^{k+1} - x^*||_2 \le \frac{L}{2\mu} ||x^* - x^k||_2^2.$$
(43)

In particular if $||x^0 - x^*||_2 \le \frac{\mu}{2L}$, then

$$||x^{k+1} - x^*||_2 \le \frac{1}{2^{2^k}} \frac{L}{2\mu}.$$

Proof:

$$x^{k+1} - x^* = x^k - x^* - \nabla^2 f(x^k)^{-1} \left(\nabla f(x^k) - \nabla f(x^*) \right)$$

$$= x^k - x^* - \nabla^2 f(x^k)^{-1} \int_{s=0}^1 \nabla^2 f(x^k + s(x^* - x^k))(x^k - x^*) ds \quad \text{(Mean value theorem)}$$

$$= \nabla^2 f(x^k)^{-1} \int_{s=0}^1 \left(\nabla^2 f(x^k) - \nabla^2 f(x^k + s(x^* - x^k)) \right) (x^k - x^*) ds$$

Taking norms we have that

$$\begin{aligned} \|x^{k+1} - x^*\|_2 & \leq & \|\nabla^2 f(x^k)^{-1}\|_2 \int_{s=0}^1 \|\nabla^2 f(x^k) - \nabla^2 f(x^k + s(x^* - x^k))\|_2 \|x^k - x^*\|_2 ds \\ & \leq & \frac{L}{\mu} \int_{s=0}^1 s \|x^* - x^k\|_2^2 ds \\ & = & \frac{L}{2\mu} \|x^* - x^k\|_2^2. \quad \blacksquare \end{aligned}$$

The assumptions on for this proof can be relaxed, since we only require the Hessian is Lipschitz and lower bounded in a $\frac{\mu}{L}$ -ball around x^* .

3 Nonlinear programming with constraints

For this section, I highly recommend reading Chapter 12 in [2].

Let f, g_i and h_j be C^1 continuous functions, for i = 1, ..., m and j = 1, ..., p. Consider the constrained optimization problem

$$\min_{x \in \mathbb{R}^n} \qquad f(x)$$
 subject to
$$g_i(x) \le 0, \quad \text{for } i \in I.$$

$$h_j(x) \le 0, \quad \text{for } j \in J,$$
 (44)

where $I = \{1, ..., m\}$, $J = \{1, ..., p\}$, $g_i(x) \leq 0$ are the inequality constraints and $h_j(x) = 0$ are the equality constraint. If a point $x \in \mathbb{R}^n$ satisfies all the inequality and equality constraints we say that x is a feasible point. We refer to the set of all feasible points as the feasible set which we denote by

$$X \stackrel{\text{def}}{=} \{ x \in \mathbb{R}^n : g_i(x) \le 0, h_j(x) = 0, \text{ for } i = 1, \dots, m, \text{ and } j = 1, \dots, p. \}.$$

If x is such that $g_i(x) = 0$, we say that the ith inequality constraint is saturated or active at x.

Adding constraints can make the problem easier to solve as compared to the unconstrained problem (16), since now we do not need to search the whole of \mathbb{R}^n for a solution, but rather only a subset X. Indeed, if $X = \{x_0\}$ then clearly the solution is x_0 . But constraints can add many difficulties. Indeed, even with smooth differentiable functions g_i and h_j , the frontier of X may be non-smooth (linear constraints define a polyhedron!). Often the difficulty of dealing with constraints is guaranteeing feasibility and descent directions that are feasible. That is why we focus next on characterizing feasible descent directions. See the examples in the beginning of Chapter 12 in [2] for examples on the difficulties that constraints introduce.

Theorem 19 (Existence) If the feasible set X is bounded and non-empty, then there exists a solution to (44).

Proof: Given that the sets \mathbb{R}_+ and $\{0\}$ are closed, by the continuity of g_i and h_j we have that X is closed. By assumption X is bounded, thus it is compact. By the continuity of f we have that f(X) is also compact (The Extreme value theorem.) Consequently there exists a minimum in f(X).

Definition 20 We say that $f: \mathbb{R}^n \to \mathbb{R}$ is coercive is $\lim_{\|x\| \to \infty} f(x) = \infty$.

Theorem 21 If X is non-empty and f is coercive, then there exists a solution to (44)

Proof: Let $x' \in X$. Let $B_r(x) = \{x : ||x|| \le r\}$. Since f is coercive, there exists r such that for each x with $||x|| \ge r$ we have that $f(x) \ge f(x')$. Thus clearly the minimum of f is in $B_r(x)$. Since $B_r(x)$ is bounded and closed, we have that $B_r(x) \cap X$ is bounded and closed. Again by the extreme value theorem, f(x) attains its minimum in $B_r(x) \cap X$, which is also the minimum in X.

3.1 Feasible directions

The following definition is enough for most cases

Definition 22 We say that d is a feasible or an admissible direction at $x_0 \in X$ if there exists $\epsilon > 0$ such that $x_0 + td \in X$ for all $0 \le t \le \epsilon$. We denote by $A(x_0)$ the set of feasible directions at x_0 .

Sometimes we will need the more robust definition

Definition 23 We say that d is a feasible or an admissible direction at $x_0 \in X$ if there exists a C^1 differentiable curve $\phi : \mathbb{R}_+ \to \mathbb{R}^n$ such that

- 1. $\phi(0) = x_0$
- 2. $\phi'(0) = d$
- 3. There exists $\epsilon > 0$ such that $t \leq \epsilon$ we have $\phi(t) \in X$

We denote by $A(x_0)$ the set of feasible directions at x_0 .

The reason we can use a straight line segment $x_0 + td$ in Definition 22 in all proofs as opposed to the complex Definition 3.1 is because, applying the 1st order Taylor expansion of $\phi(t)$ around t = 0 we have that

$$\phi(t) = x_0 + td + t\epsilon(t).$$

Thus $\phi(t)$ can be replaced by a line segment up to terms that go to zero faster than t.

Let $I_0(x_0) = \{i : g_i(x_0) = 0, i \in I\}$ be the indexes of saturated inequalities.

A necessary condition on a direction being feasible is given in the following.

Proposition 24 If $d \in A(x_0)$ is a feasible direction then

- 1. For every $i \in I(x_0)$ we have that $d^{\top} \nabla g_i(x^0) \leq 0$.
- 2. For every $j \in J$ we have that $d^{\top} \nabla h_j(x^0) = 0$.

Let $B(x_0)$ be the set of directions that satisfy the above two conditions. Thus $A(x_0) \subset B(x_0)$.

Proof: 1. Let $i \in I$ and let $d_1 = d/\|d\|$. If $g_i(x_0) = 0$ Consider the 1st order Taylor expansion of g_i around x_0 in the d_1 direction which is

$$g_i(x_0 + td_1) = td^{\mathsf{T}} \nabla g_i(x^0) + t\epsilon(t) \le 0, \tag{45}$$

where we used $g_i(x_0 + td_1) \leq 0$ for t sufficiently small. Thus from (45) we have that

$$d^{\top} \nabla g_i(x^0) + \epsilon(t) \le 0.$$

Letting $t \to 0$ we have that $d^{\top} \nabla g_i(x^0) \leq 0$.

2. Using the first order Taylor expansion of h_i around x_0 we have that

$$h_j(x_0 + td_1) = td^{\mathsf{T}} \nabla h_j(x^0) + t\epsilon(t) = 0.$$
 (46)

Dividing by t and then taking the limit as $t \to 0$ gives $d^{\top} \nabla h_i(x^0) = 0$.

We will refer to $B(x_0)$ as the cone of feasible directions. Because the cone $B(x_0)$ is easy to work with, we would like to use $B(x_0)$ instead $A(x_0)$. Indeed, it only depends on linear constraints involving gradients. But sometimes $B(x_0)$ is not equivalent to $A(x_0)$ when there exists certain degeneracies. For instance, if

$$h_1(x) = (x_1^2 + x_2^2 - 2)^2 = 0,$$

then $\nabla h_1(x) = 0$ for all feasible points, and thus we cannot use $\nabla h_1(x)$ to describe feasible directions.

To exclude the possibility of such degeneracies, we impose the *Constraint qualifications*, which are the conditions that ensure we can use $B(x_0)$ instead of $A(x_0)$.

Definition 25 We say that constraint qualifications hold at x_0 if for every $d \in B(x_0)$ there exists a sequence $(d_t)_{t=1}^{\infty} \in A(x_0)$ such that $d_t \to d$.

An example where the constraint qualifications do not hold, and consequently $B(x_0) \neq A(x_0)$ is given now.

Example 26 Consider the constraints given by

$$\begin{cases} x^2 + (y-1)^2 \ge 1\\ x \le 1\\ y \ge 0. \end{cases}$$

That is, $g_1(x,y) = 1 - x^2 - (y-1)^2$, $g_2(x,y) = x-1$ and $g_3(x,y) = -y$. At the point $(x^0, y^0) = (0,0)$ it is easy to show that $B(x^0, y^0) = \{(t, 0) : \forall t \in \mathbb{R}\}$ while $A(x^0, y^0) = \{(t, 0) : \forall t \geq 0\}$. Thus the constraint qualification cannot hold, and $B(x^0, y^0)$ is a bad substitute for $A(x^0, y^0)$.

The following theorem justifies why constraint qualifications are important.

Theorem 27 Let x^* be a local minimum of (44) and suppose the constraint qualification holds at x^* . It follows that for every $d \in B(x^*)$ we have that $\nabla f(x^*)^{\top} d \geq 0$. In other words, all feasible directions are not descent directions.

Proof: Let $d_t \in A(x_*)$ be a sequence such that $d_t \to d$. Let $\phi_t(\alpha_t) = x_* + \alpha_t d_t$. Now consider the 1st order Taylor expansion of f around x_* given by

$$f(\phi_t(\alpha_t)) = f(x_*) + \alpha_t \nabla f(x_*)^{\top} d_t + \alpha_t \epsilon(\alpha_t).$$

Since x_* is a local minima, let $\tilde{\alpha}_t$ be such that for $\alpha_t \leq \tilde{\alpha}_t$ we have that $f(x_*) \leq f(\phi_t(\alpha_t))$. Consequently

$$\alpha_t \nabla f(x_*)^{\top} d_t + \alpha_t \epsilon(\alpha_t) \ge 0, \quad \text{for } \alpha_t \le \tilde{\alpha}_t.$$

Dividing by α_t and taking the limit we have

$$0 \le \lim_{t} \nabla f(x_*)^{\top} d_t + \epsilon(\alpha_t) = \nabla f(x_*)^{\top} d.$$

3.2 Characterizing the constraint qualification

First we need a sufficient characterization of feasible directions which is given in the following lemma.

Lemma 28 Suppose that h_j is an affine function for $j \in J$. Let $x^0 \in X$ and $d \in \mathbb{R}^n$ be such that

$$d^{\top} \nabla g_i(x^0) < 0, \quad for \ i \in I$$

 $d^{\top} \nabla h_j(x^0) = 0, \quad for \ j \in J.$

Then d is a feasible direction, that is $d \in A(x_0)$.

Proof: Let $\phi(t) = x^0 + td$. Since h_i is affine we have that

$$h_j(\phi(t)) = h_j(x^0) + td^{\top} \nabla h_j(x^0).$$

Furthermore, given that x^0 is feasible we have that $h_j(x^0) = 0$ and by assumption $d^{\top} \nabla h_j(x^0) = 0$, consequently $h_j(\phi(t)) = 0$. Furthermore, for $i \in I(x_0)$ we have that

$$g_i(\phi(t)) = g_i(x_0) + td^{\top} \nabla g_i(x^0) + t\epsilon(t).$$

Since $g_i(x^0) = 0$ and $d^{\top} \nabla g_i(x^0) < 0$, there exists t > 0 sufficiently small so that $g_i(\phi(t)) \leq 0$. Thus $x^0 + td \in X$ for t > 0 sufficiently small, which proves that d is a feasible direction.

We now give a sufficient condition for the constraint qualifications to hold.

Lemma 29 Suppose h_j is affine for all $j \in J$. Let $x_0 \in X$. If there exists \tilde{d} such that

$$\tilde{d}^{\top} \nabla g_i(x^0) < 0, \quad \text{for } i \in I(x^0)$$

 $\tilde{d}^{\top} \nabla h_j(x^0) = 0, \quad \text{for } j \in J,$

then the constraint qualification holds at x^0 .

Proof: Let $d \in B(x^0)$. We will now show that

$$d_t = td + (1 - t)\tilde{d},$$

for $t \in [0, 1[$ we have that $d_t \in A(x_0)$ and for $t \to 0$ we have that d_t converges to d, which in turn shows that the constraint qualifications hold. Indeed, for $i \in I(x_0)$ we have that

$$d_t^{\top} \nabla g_i(x^0) = t \underbrace{d^{\top} \nabla g_i(x^0)}_{\leq 0, \ d \in B(x^0)} + (1 - t) \tilde{d}^{\top} \nabla g_i(x^0) < 0.$$

Furthermore

$$d_t^{\top} \nabla h_i(x^0) = t d^{\top} \nabla h_i(x^0) + (1 - t) \tilde{d}^{\top} \nabla h_i(x^0) = 0.$$

Consequently, by Lemma 28, we have that for all $t \in [0, 1[$ we have shown that $d_t \in A(x_0)$. Now taking any sequence $t_n \to 1$ we have that $d_t \to d$, thus by definition the constraint qualifications hold at x_0 .

The following proposition establish sufficient conditions for the constraint qualifications hold.

Proposition 30 If g_i for $i \in I$ are convex and h_j for $j \in J$ are affine and there exists a single point $\tilde{x} \in X$ such that

$$g_i(\tilde{x}) < 0, \quad h_j(\tilde{x}) = 0 \quad \forall i \in I, j \in J,$$
 (47)

then the constraint qualification holds for all feasible points in X.

Proof: Let $x^0 \in X$ and let \tilde{x} satisfy (47). Using the 1st order Taylor expansion around \tilde{x} we have that

$$0 \stackrel{(47)}{>} g_i(\tilde{x}) \stackrel{\text{convexity}}{\geq} g_i(x^0) + \nabla g_i(x^0)^{\top} (\tilde{x} - x^0).$$

If $i \in I(x^0)$ then $g_i(x^0)$ and from the above we have that $\nabla g_i(x^0)^{\top}(\tilde{x}-x^0) < 0$. Let $\tilde{d} \stackrel{\text{def}}{=} (\tilde{x}-x^0)$. Furthermore, for the equality constraints we have that

$$h_j(\tilde{x}) \stackrel{\text{affine.}}{=} h_j(x^0) + \nabla h_j(x^0)^{\top} \tilde{d}.$$

Since $h_j(x^0) = 0$ and thus $\nabla h_j(x^0)^{\top} \tilde{d} = 0$. This shows that \tilde{d} satisfies the conditions of Lemma 29, and thus the constraint qualifications hold at x^0 .

Yet another alternative characterization of constraint qualifications is given in the following proposition.

Proposition 31 Suppose that h_j are affine functions for $j \in J$. For a given feasible point $x_0 \in X$ we have that the set

$$\{\nabla g_i(x_0): i \in I_0(x_0)\} \cup \{\nabla h_j(x_0): j \in J\},\$$

is a linearly independent set, then the constraint qualifications hold at x_0 .

Proof: Let $x^0 \in X$ and consider the following to Linear Programs

$$\max_{\lambda,\mu} z = \sum_{i \in I(x^0)} \lambda_i + \sum_{j \in J} 0 \times \mu_j.$$
subject to
$$\sum_{j \in J} \mu_j \nabla h_j(x^0) - \sum_{i \in I(x^0)} \lambda_i \nabla g_i(x^0) = 0,$$

$$\lambda_i \ge 0, \text{ for } i \in I(x^0). \tag{P}$$

and

$$\min_{d} w = 0$$
subject to $d^{\top} \nabla g_i(x^0) \le -1$, for $i \in I(x^0)$,
$$d^{\top} \nabla h_j(x^0) = 0$$
, for $j \in J$. (D)

It is not hard to show that (P) is the primal and (D) is its associated dual problem. Indeed, to see this, first we right (P) in the standard form by introducing variables $\mu^+, \mu^- \in \mathbb{R}^p$ with $\mu = \mu^+ - \mu^-$ and including the constraints $\mu^+, \mu^- \geq 0$. Then write $c = (\underbrace{1, \dots, 1}_{|I(x^0)|}, \underbrace{0, \dots, 0}_{2p}), b = 0 \in \mathbb{R}^n$, and

$$A = \left[-\nabla g_1(x^0), \dots, -\nabla g_m(x^0), \nabla h_1(x^0), \dots, \nabla h_p(x^0), -\nabla h_1(x^0), \dots, -\nabla h_p(x^0). \right]$$

From (DP) the dual constraints are given by

$$A^{\top}d \ge c \Rightarrow \begin{cases} d^{\top}\nabla h_j(x^0) \ge 0, \\ -d^{\top}\nabla h_j(x^0) \ge 0, \\ -d^{\top}\nabla g_i(x^0) \ge 1, & \text{for } i \in I(x^0), j \in J. \end{cases}$$

Which exactly the constraint of (D). The rest follows by examining (DP).

Since (P) is non-empty, since it admits the zero solution Now suppose that (P) admits a solution λ_i^*, μ^* that is not zero. In which case, we have that the gradients of the constraints must be linearly independent. This contracts our assumption, thus $(\lambda_i^*, \mu^*) = (0,0)$ is the optimal solution. Thus (P) is bounded and by weak duality Lemma 3 that (D) is feasible. Let \tilde{d} be a feasible solution to (D). Note that \tilde{d} satisfies the assumptions of Lemma 29, consequently the constraint qualification holds at x_0 .

3.3 Lagrange's condition

Consider the problem (44) but without inequality constraints, that is,

$$\min_{x \in \mathbb{R}^n} \qquad f(x)$$
 subject to
$$h_j(x) = 0, \quad \text{for } j \in J,$$
 (48)

The following theorem gives us necessary conditions for a point to be a local minima that requires only using linear algebra.

Theorem 32 Let $x^* \in X$ be a local minima and suppose that the constraint qualifications hold at x^* for (44). It follows that the gradient of the objective is a linear combination of the gradients of constraints at x^* , that is, there exists $\mu_j \in \mathbb{R}$ for $j \in J$ such that

$$\nabla f(x^*) = \sum_{j \in J} \mu_j \nabla h_j(x^*). \tag{49}$$

Proof: Let $E = \text{span}(\{\nabla h_1(x^*), \dots, \nabla h_p(x^*)\})$. Let us re-write $\nabla f(x^*) = y + z$ where $y \in E$ and $w \in E^{\perp}$. By definition

$$-z^{\top} \nabla h_j(x^*) = 0, \quad \forall j \in J.$$

Thus $-z \in B(x^*)$. Consequently by Theorem 27 we have that

$$-z^{\top} \nabla f(x^*) \ge 0.$$

Thus

$$-z^{\mathsf{T}} \nabla f(x^*) = -z^{\mathsf{T}} y - \|z\|_2^2 = -\|z\|_2^2 \ge 0.$$

Consequently z = 0 and $\nabla f(x^*) = y \in E$.

3.4 Karush, Kuhn and Tuckers condition

The extension of Lagrange's condition to allow to our general problem (44) with inequality constraints is known at the Karush, Kuhn Tuckers

Theorem 33 Let $x^* \in X$ be a local minima and suppose that the constraint qualifications hold at x^* for (48). It follows that there exists $\mu_j \in \mathbb{R}$ and $\lambda_i \in \mathbb{R}_+$ for $j \in J$ and $i \in I(x^*)$ such that

$$\nabla f(x^*) = \sum_{j \in J} \mu_j \nabla h_j(x^*) - \sum_{i \in I(x^*)} \lambda_i \nabla g_i(x^*). \tag{50}$$

Proof: From Theorem 27 we know that for every $d \in B(x^*)$ we have that $\nabla f(x^*)^{\top} d \geq 0$. That is, said more explicitly, we have that for every $d \in \mathbb{R}^n$ that satisfies

$$-d^{\top} \nabla g_i(x^*) \ge 0, \quad \text{for } i \in I(x^*)$$
$$d^{\top} \nabla h_j(x^*) = 0, \quad \text{for } j \in J,$$

we have that $d^{\top}\nabla f(x^*) \geq 0$. This statement fits perfectly the 2nd version of Farkas Theorem 35. That is, let

$$A = [-\nabla g_1(x^*), \dots - \nabla g_m(x^*)] \quad \text{and} \quad B = [\nabla h_1(x^*), \dots \nabla h_p(x^*)],$$

and $b = \nabla f(x^*)$. Thus for every

$$d \in \{d : A^{\top}d \ge 0, \quad B^{\top}d = 0\}$$

we have that $d^{\top}b \geq 0$. By Farkas Theorem 35 we have that this statement can be equivalently re-written as there exists $d \in P$ where

$$P = \{(\lambda, \mu) : A\lambda + B\mu = b, \quad \lambda \ge 0\}.$$

Through which we conclude that the set

$$P = \{ \mu \in \mathbb{R}^p, \ \lambda \in \mathbb{R}^m_+ : \sum_{j \in J} \mu_j \nabla h_j(x^*) - \sum_{i \in I(x^*)} \lambda_i \nabla g_i(x^*) = \nabla f(x^*) \},$$

is non-empty, which concludes the proof.

I will now illustrate the above theorem, on the board, with only inequality constraints. First, what is the largest sphere that fits in an ellipsoid?

Exercise 34

$$\min -x^2 - y^2$$

subject to $ax^2 + by^2 \le 1$,

where a > b > 0.

Using the KKT conditions and assuming that the constraint is not active, that is $ax^2 + by^2 < 1$, we quickly arrive at the solution (x, y) = (0, 0).

Now assuming the constraint is active, that is $ax^2 + by^2 = 1$, we have the KKT conditions

$$2x = 2a\lambda x$$

$$2y = 2b\lambda y.$$

From which we conclude that either 1) $\lambda = a^{-1}$, y = 0 and $x = \pm a^{-1}$ or 2) $\lambda = b^{-1}$, x = 0 and $y = \pm b^{-1/2}$. In the first case, we have that $f(x,y) = -x^2 - y^2 = -a^{-1}$. Alternatively in the second case we have $f(x,y) = -b^{-1}$. Since $-b^{-1} < -a^{-1} \le 0$, we have that $(x,y) = (0,\pm b^{-1/2})$ are the two minimum. What is the maximum?

Appendix

Theorem 35 (2nd Version of Farkas) Consider the set

$$P = \{(\lambda, \mu) : A\lambda + B\mu = b, \quad \lambda \ge 0\}$$

and

$$Q = \{ y : A^{\top} y \ge 0, \quad B^{\top} y = 0 \}.$$

The set P is non-empty if and only every $y \in Q$ is such that $b^{\top}y \geq 0$.

Proof: (1) If P non-empty then $y \in Q \Rightarrow b^{\top}y \geq 0$: Let $\mu = z^+ - z^-$ where $z^+, z^- \geq 0$. Then clearly P is non-empty if and only if

$$\hat{P} = \{ (\lambda, z^+, z^-) : A\lambda + Bz^+ - Bz^- = b, \quad \lambda, z^+, z^- \ge 0 \},$$

is non-empty. The dual program of \hat{P} if we consider a zero objective function (z=0) is given by

$$\min_{y} y^{\top} b$$
subject to $A^{\top} y \ge 0$, $B^{\top} y \ge 0$, $-B^{\top} y \ge 0$. (51)

see Lemma 37 for how to deduce this version of duality. The feasible region of (51) is equivalent to Q. By the weak duality Lemma 3 we have that if there exists a feasible primal point then for all feasible y, that is, all $y \in Q$ we have $b^{\top}y \geq c^{\top}(\lambda, z^+, z^-) = 0$.

(2)If $y \in Q \Rightarrow b^{\top}y \geq 0$ then P non-empty: Clearly $0 \in Q$ and thus the dual (51) is feasible. Since $y \in Q$ implies that $b^{\top}y \geq 0$, we have that (51) is feasible and bounded. This proves by duality that P is feasible.

Proof: [Using 1st Farkas Theorem] Let $\mu = z^+ - z^-$ where $z^+, z^- \ge 0$. Then clearly P is non-empty if and only if

$$\hat{P} = \{ (\lambda, z^+, z^-) : A\lambda + Bz^+ - Bz^- = b, \quad \lambda, z^+, z^- \ge 0 \},$$

is non-empty. Applying the 1st Farkas Theorem 36, we have that \hat{P} is non-empty if every $y \in \hat{Q}$ implies that $y^{\top}b \geq 0$ where

$$\hat{Q} = \{ y : A^{\top} y \ge 0, \quad B^{\top} y \ge 0, \quad -B^{\top} y \ge 0 \}.$$

Clearly $Q = \hat{Q}$ which concludes the proof.

Theorem 36 (Farkas Version 1) Consider the set

$$P = \{x : Ax = b, \quad x \ge 0\}$$

and

$$Q = \{ y : A^{\top} y \ge 0 \}.$$

The set P is non-empty if and only every $y \in Q$ is such that $b^{\top}y \geq 0$.

Proof: Any text on optimization.

Lemma 37 (Duality 2nd version) Consider the following LP with equality constraints

$$\max_{x} c^{\top} x$$

$$subject \ to \ Ax = b,$$

$$x \geq 0, \tag{LP}$$

Then the dual is given by

$$\min_{y} y^{\top} b$$
 subject to $A^{\top} y \ge c$. (DP)

Proof: First we re-write (LP) as

$$\max_{x} c^{\top} x$$
 subject to $Ax \leq b$,
$$-Ax \leq -b$$
,
$$x \geq 0$$
, (LP)

The dual program (DP) of the above is given by

$$\min \ w^{\top}b - z^{\top}b$$
 subject to $A^{\top}w - A^{\top}z \ge c,$
$$w, z \ge 0.$$

Substituting y = w - z gives the result.