A Constrained Minimization Approach

Kenny Erleben

Contents

Chapter 1

First Order Optimality Conditions

We will start with the "mother" problem of all other problems, the constrained minimization problem.

Definition 1.1 *Given a continuously differentiable objective function,* $f(x) : \mathbb{R}^n \mapsto \mathbb{R}$ *and a continuously differentiable constraint function,* $c(x) : \mathbb{R}^n \mapsto \mathbb{R}^m$ *then the problem*

$$\min_x f(x) \tag{1.1}$$

subject to

$$c_i(x) = 0 \quad \forall i \in \mathcal{E} \tag{1.2a}$$

$$c_i(x) \geq 0 \quad \forall i \in \mathcal{I} \tag{1.2b}$$

is called a constrained minimization problem.

We call f the objective function while c_i, $i \in \mathcal{E}$ are equality constraints and c_i, $i \in \mathcal{I}$ are inequality constaints. The constraint index sets, $\mathcal{E}$ and $\mathcal{I}$, are proper subsets,

$$\mathcal{E} \subset \{1, \ldots, m\} \tag{1.3a}$$

$$\mathcal{I} \subset \{1, \ldots, m\} \tag{1.3b}$$

where

$$\mathcal{E} \cap \mathcal{I} = \emptyset \tag{1.4a}$$

$$\mathcal{E} \cup \mathcal{I} = \{1, \ldots, m\} \tag{1.4b}$$

A special index set called the active set is often used, and it includes the indexes of all constraints where equality currently holds. Thus the active set is depedent on the value of x.

Definition 1.2 *The active set, $\mathcal{A}$, at x is defined as*

$$\mathcal{A}(x) = \mathcal{E} \cup \{i \in \mathcal{I} | c_i(x) = 0\} \tag{1.5}$$

A point, x is said to be feasible if the point fulfills the constraints of the problem,

$$c_i(x) = 0 \quad \forall i \in \mathcal{E}, \tag{1.6a}$$
$$c_i(x) \geq 0 \quad \forall i \in \mathcal{I}, \tag{1.6b}$$

and non-feasible otherwise. The inequality constraint $i \in \mathcal{I}$ is said to be active at a feasible point x if $c_i(x) = 0$, and in-active if strict inequality holds, $c_i(x) > 0$. The set of all feasible points is called the feasible region and is defined as shown below.

Definition 1.3 *The feasible region is defined as*

$$\Omega = \{x | c_i(x) = 0 \quad \forall i \in \mathcal{E} \quad \wedge \quad c_i(x) \geq 0 \quad \forall i \in \mathcal{I}\} \tag{1.7}$$

The set of non-feasible points is called the non-feasible region. We can define different types of solutions, x^*, for the mimimization problem as follows

- A point, x^*, is a gobal minimizer if $f(x^*) \leq f(x)$ for all $x \in \Omega$.
- A point, x^*, is a local minimizer if there is a neighborhood $\mathcal{N}$ of x^* such that $f(x^*) \leq f(x)$ for all $x \in \mathcal{N} \cap \Omega$.
- A point, x^*, is a strict local minimizer if there is a neighborhood $\mathcal{N}$ of x^* such that $f(x^*) < f(x)$ for all $x \in \mathcal{N} \cap \Omega$ with $x \neq x^*$.

The necessary conditions for a first order optimal solution are often used as a building block for methods that solve the minimization problem or as a tool for verifying if a given solution is truly a solution to first order optimality. In the following we will simply define the first order optimality conditions with-out proof.

Definition 1.4 *Given a local solution x^* for the minimization problem in Definition 1.1 then there is a Lagrange multiplier vector, λ^*, such that the following conditions are satisfied at (x^*, λ^*),*

$$\nabla f(x^*) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i \nabla c_i(x^*) = 0 \tag{1.8a}$$
$$c_i(x^*) = 0 \quad \forall i \in \mathcal{E} \tag{1.8b}$$
$$c_i(x^*) \geq 0 \quad \forall i \in \mathcal{I} \tag{1.8c}$$
$$\lambda_i^* \geq 0 \quad \forall i \in \mathcal{I} \tag{1.8d}$$
$$\lambda_i^* c_i(x^*) = 0 \quad \forall i \in \mathcal{E} \cup \mathcal{I} \tag{1.8e}$$

Remark The conditions (1.8e) are known as the complementarity conditions. They state that either the constraint $c_i(x^*)$ is active or $\lambda_i^* = 0$ or possible both. These conditions act as a kind of switch by only turning on the constraints that have influence at x^*, corresponding to $\lambda_i^* \neq 0$. All other constraints are turned off, corresponding to $\lambda_i^* = 0$. We will provide more intuition for this later on.

Strict complementarity means we have exactly one of λ_i^* and $c_i(x^*)$ is zero for each $i \in \mathcal{I}$. We can define this formally as follows.

Definition 1.5 *Given a local solution x^* and a vector λ^* satisfying Definition 1.4 then we have strict complementarity if*

$$\lambda_i > 0 \quad \forall i \in \mathcal{I} \cap \mathcal{A}(x^*) \tag{1.9}$$

The Lagrangian function is sometimes usefull for compact notation among other things.

Definition 1.6 *The Lagrangian function is defined as*

$$\mathcal{L}(x, \lambda) = f(x) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i c(x) \tag{1.10}$$

Using the Lagrangian function we observe that

$$\nabla_x \mathcal{L}(x, \lambda) = \nabla f(x) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i \nabla c_i(x) \tag{1.11}$$

Thus this shorthand notation is often used for writting the first condition (1.8a) for first order optimality as

$$\nabla_x \mathcal{L}(x^*, \lambda^*) = 0 \tag{1.12}$$

Remark One may write the first order optimality conditions in a more compact form using matrix-vector notation,

$$\nabla f(x^*) - \nabla c(x^*)^T \lambda^* = 0 \tag{1.13a}$$

$$c(x^*) \geq 0 \tag{1.13b}$$

$$\lambda^* \geq 0 \tag{1.13c}$$

$$(\lambda^*)^T c(x^*) = 0 \tag{1.13d}$$

Here we choose $\mathcal{E} = \emptyset$, also all inequalities are to taken component-wise.

Remark The first order optimality conditions may not look very intuitive at first sight. In the following we will try to present some intuition behind the conditions. For now we will only consider that case of a single equality constraint, $c(x)$.

We have a feasible point x and want to verify if the point is a local minimizer. We do this by determining if we can take a small step Δx and add the step to

x such that the new point $x + \Delta x$ is feasible and has a lower function value than x. If no such Δx step can be found then x must be a local minimizer. By Taylors Theorem,

$$c(x + \Delta x) = c(x) + \nabla c(x)^T \Delta x + \mathbf{o}\left(\|\Delta x\|^2\right) \tag{1.14a}$$

$$f(x + \Delta x) = f(x) + \nabla f(x)^T \Delta x + \mathbf{o}\left(\|\Delta x\|^2\right) \tag{1.14b}$$

Giving us the first-order approximations

$$c(x + \Delta x) = c(x) + \nabla c(x)^T \Delta x \tag{1.15a}$$

$$f(x + \Delta x) = f(x) + \nabla f(x)^T \Delta x \tag{1.15b}$$

If we have an equality constraint then $c(x) = 0$ and we want Δx to be such that the constraint is not violated meaning that $c(x + \Delta x) = 0$. Inserting into the first order approximation yields

$$0 = \nabla c(x)^T \Delta x \tag{1.16}$$

If $x + \Delta x$ should have a lower function value than x then $f(x + \Delta x) < f(x)$. By our approximation

$$f(x + \Delta x) = f(x) + \nabla f(x)^T \Delta x \tag{1.17a}$$

$$f(x + \Delta x) - f(x) = \nabla f(x)^T \Delta x \tag{1.17b}$$

$$0 < \nabla f(x)^T \Delta x \tag{1.17c}$$

We now have two conditions for Δx that must be fulfilled

$$0 = \nabla c(x)^T \Delta x \tag{1.18a}$$

$$0 < \nabla f(x)^T \Delta x \tag{1.18b}$$

If such Δx exist then $x + \Delta x$ would be a feasible point with a lower function value than x. Meaning that x can not be a feasible local minimizer. The only way to make sure no such Δx can be found is that if $\nabla c(x)$ and $\nabla f(x)$ is parallel. That is if

$$\nabla f(x) = \lambda \nabla c(x) \tag{1.19}$$

for some λ-multiplier.

Exercise Try to substitute (1.19) into (1.18a) and (1.18b) and show that no feasible $x + \Delta x$ exist with a lower function value than x.

Answer Inserting $\nabla f(x) = \lambda \nabla c(x)$ into the first requirement yields

$$0 = \nabla c(x)^T \Delta x \tag{1.20a}$$

$$0 = \frac{1}{\lambda} \nabla f(x)^T \Delta x \tag{1.20b}$$

$$0 = \nabla f(x)^T \Delta x \tag{1.20c}$$

Clearly the second requirement $0 < \nabla f(x)^T \Delta x$ can not be fulfilled. Inserting $\nabla f(x) = \lambda \nabla c(x)$ into the second requirement yields

$$0 < \nabla f(x)^T \Delta x \tag{1.21a}$$

$$0 < \lambda \nabla c(x)^T \Delta x \tag{1.21b}$$

$$0 < \nabla c(x)^T \Delta x \tag{1.21c}$$

Clearly the first requirement $0 = \nabla c(x)^T \Delta x$ can not be fulfilled.

Remark To gain more intuition about the first-order optimality condition we will now consider the case of a single inequality constraint. We will use the same approach as the one we used for the equality case. The first order approximation to the inequality constraint yields

$$0 \leq c(x + \Delta x) \approx c(x) + \nabla c(x)^T \Delta x \tag{1.22}$$

First order feasibility means

$$0 \leq c(x) + \nabla c(x)^T \Delta x \tag{1.23}$$

Two cases exist depending on the point x. Either $c(x) = 0$ or $c(x) > 0$. We will examine both cases in turn. In the first case we have $c(x) = 0$ and the first order feasibility condition reduces to

$$0 \leq \nabla c(x)^T \Delta x \tag{1.24}$$

As in the case of the equality constraint the first order approximation to $f(x)$ and using $f(x + \Delta x) < f(x)$ lead to

$$0 < \nabla f(x)^T \Delta x. \tag{1.25}$$

Here we have assumed that $\nabla f(x) \neq 0$. The only case where we can not find a Δx fulfilling both conditions is when $\nabla f(x)$ and $\nabla c(x)$ points in opposite directions,

$$\nabla f(x) = \lambda c(x) \quad \text{and} \quad \lambda > 0 \tag{1.26}$$

In the second case $c(x) > 0$ means that we can find a sufficiently small neighborhood $\mathcal{N}$ at x such that any $\Delta x \in \mathcal{N}$ fulfill (1.23). Thus whenever $\nabla f(x) \neq 0$ we can find a step

$$\Delta x = -\alpha \nabla f(x) \tag{1.27}$$

where α is a sufficiently small positive number such that $\Delta x \in \mathcal{N}$. This step will result in $f(x + \Delta x) < f(x)$. Thus the only possibility for x to be a local minimizer is that $\nabla f(x) = 0$. In summary we have discovered

$$c(x) = 0 \Rightarrow \nabla f(x) = \lambda c(x) \quad \text{and} \quad \lambda > 0 \tag{1.28a}$$

$$c(x) > 0 \Rightarrow \nabla f(x) = 0 \tag{1.28b}$$

Which is equivalent to

$$
\begin{aligned}
\nabla f(x) - \lambda \nabla c(x) &= 0 && (1.29a)\\
\lambda &\geq 0 && (1.29b)\\
c(x) &\geq 0 && (1.29c)\\
\lambda c(x) &= 0 && (1.29d)
\end{aligned}
$$

Exercise Proove that for the case $c(x) > 0$ the choice

$$\Delta x = -\alpha \nabla f(x) \tag{1.30}$$

leads to $f(x + \Delta x) < f(x)$.

Answer The first order approximation of the object function is

$$f(x + \Delta x) = f(x) + \nabla f(x)^T \Delta x \tag{1.31}$$

Substituting $\Delta x = -\alpha \nabla f(x)$ yields

$$
\begin{aligned}
f(x + \Delta x) - f(x) &= -\alpha \nabla f(x)^T \nabla f(x)^T && (1.32a)\\
&= -\alpha \|\nabla f(x)\| < 0 && (1.32b)
\end{aligned}
$$

where equality does not hold due to $\nabla f(x) \neq 0$ and $\alpha > 0$. Thus we have $f(x + \Delta x) - f(x) < 0$ or equivalently

$$f(x + \Delta x) < f(x) \tag{1.33}$$

as we wanted to show.

Exercise Proove that $\nabla f(x) = \lambda c(x)$ for $\lambda > 0$ is the only case where there are no solutions for

$$
\begin{aligned}
0 &\leq \nabla c(x)^T \Delta x && (1.34a)\\
0 &< \nabla f(x)^T \Delta x && (1.34b)
\end{aligned}
$$

Answer The condition $0 \leq \nabla c(x)^T \Delta x$ defines a closed half-space whereas $0 < \nabla f(x)^T \Delta x$ defines an open half-space. The only case where the two half-spaces (try drawing this) do not intersect is when $\nabla f(x)$ and $\nabla c(x)$ are opposite.

Exercise Proove that (1.29) is equivalent to (1.28).

Answer We are given

$$
\begin{aligned}
\nabla f(x) - \lambda \nabla c(x) &= 0 && (1.35a)\\
\lambda &\geq 0 && (1.35b)\\
c(x) &\geq 0 && (1.35c)\\
\lambda c(x) &= 0 && (1.35d)
\end{aligned}
$$

Consider the case $c(x) > 0$. By the fourth and second condition we must have $\lambda = 0$. This indicates that the first line reduces to $\nabla f(x) = 0$ as wanted. Next consider the case $c(x) = 0$. Two possibilities exist, either $\lambda = 0$ or $\lambda > 0$. In either case the last three conditions are fulfilled. If $\lambda = 0$ the first equation results in $\nabla f(x) = 0$. However, if $\lambda > 0$ then the first equation states that $\nabla f(x)$ and $\lambda \nabla c(x)$ are opposite as wanted.

The intuition provided so far is not a rigourous proof. However, the intuition given serve our purpose of building up some familarity with the first order optimiality conditions.

Remark We have omitted one important detail in our presentation of the first order optimality conditions. We have not mentioned anything about constraint qualifications. In most of the cases in physics based modeling and simulation one would use linear bounds or constant bounds on x. This means that all $c_i(x)$ implicitly can be represented by a linear function and as such we allwas fulfill one type of constraint qualifications. Therefore, we will usually omit saying anything about constraint qualifications unless it is needed.

Constraint qualifications are assumptions that guarentee a similarity of the geometry of the feasible region with the linearized approximations of the contraints in a neighborhood of x^*. Basically when looking at a point x^* we need to make sure that the algebraic linearized aproximations, the constraint gradients of the active constraints, can be used as a true representive of the feasible region in that neighborhood.

First we need a tool to describe the geometry of the feasible region in a neighborhood of a point x without considering any algebraic representation. For this we need the definition of a tangent vector.

Definition 1.7 *The vector d is said to be a tangent vector of the feasible region, Ω, at a feasible point x if there is a seqeunce of feasible points $\{z_k\}$ converging to x and a sequence of positive scalars, $\{t_k\}$ with $\lim_{k\to\infty} t_k = 0$ such that*

$$\lim_{k\to\infty} \frac{z_k - x}{t_k} = d \tag{1.36}$$

Next we define the set of all tangent vectors.

Definition 1.8 *The set of all tangent vectors of Ω at x is called the tangent cone and is denoted by $\mathcal{T}_\Omega(x)$.*

Exercise Verify that $\mathcal{T}_\Omega(d)$ is a cone.

Answer By the property that defines a cone we have to show that if $d \in \mathcal{T}_\Omega(x)$ then for any scalar $\alpha > 0$ we have $\alpha d \in \mathcal{T}_\Omega(x)$. Using the definition of the tangent vector we replace t_k with $\frac{t_k}{\alpha}$ then from the definition we have $\alpha d \in \mathcal{T}_\Omega(x)$.

Remark The tangent cone is also pointed, meaning that $0 \in \mathcal{T}_\Omega x$. This is shown by choosing the sequence of feasible points as $z_k = x$ in the definition of a tangent vector.

Exercise Given a constrained minimizatinon problem with $\mathcal{E} = \emptyset$ and an interior feasible point, that is a point where $c_i(x) > 0$ for all $i \in \mathcal{I}$, what is $\mathcal{T}_\Omega(x)$?

Answer Since x is an interior point any tangent direction from $\mathbb{R}^n$ will be in the tangent cone. Thus $\mathcal{T}_\Omega(x) = \mathbb{R}^n$.

Unlike the tangent cone the set of linearized feasible directions is based completely on the algebaric representation of the constraint functions. The definition of the set is as follows.

Definition 1.9 *Given a feasible point x and the active constraint set, $\mathcal{A}(x)$, the set of linearized feasible directions, $\mathcal{F}(x)$, is*

$$\mathcal{F}(x) = \left\{ \quad d \quad \middle| \quad \begin{array}{ll} d^T \nabla c_i(x) = 0 & \forall i \in \mathcal{E} \\ d^T \nabla c_i(x) \geq 0 & \forall i \in \mathcal{A}(x) \cap \mathcal{I} \end{array} \right\} \tag{1.37}$$

Exercise Proove that $\mathcal{F}(x)$ is a pointed cone.

Answer If $d \in \mathcal{F}(x)$ then for $\alpha > 0$ we have $\alpha d \in \mathcal{F}(x)$ and clearly $0 \in \mathcal{F}(x)$ thus the set of feasible directions is a pointed cone.

Remark Observe that the definition of $\mathcal{F}(x)$ is based on the algebraic representation of $\nabla c_i(x)$ for all $i \in \mathcal{A}(x)$. This means that if we write the same constraint in a different algebraic from then set of feasible directions may look different eventhough it is the same problem we are trying to solve.

Exercise Find the set of feasible directions for the equality constrained problem

$$\min_x f(x) \quad s.t. \quad x_1^2 + x_2^2 - 2 = 0 \tag{1.38}$$

at the feasible point $x = \begin{bmatrix} -\sqrt{2} & 0 \end{bmatrix}^T$.

Answer Given

$$c(x) = x_1^2 + x_2^2 - 2 = 0 \tag{1.39}$$

We compute

$$\nabla c = \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} \tag{1.40}$$

At $\begin{bmatrix} -\sqrt{2} & 0 \end{bmatrix}^T$ the set of feasible directions are

$$0 = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}^T \begin{bmatrix} -2\sqrt{2} \\ 0 \end{bmatrix} = -2\sqrt{2} d_1 \tag{1.41}$$

where $d = \begin{bmatrix} d_1 & d_2 \end{bmatrix}^T$. Thus

$$\mathcal{F}(x) = \left\{ \begin{bmatrix} 0 & d2 \end{bmatrix}^T | d_2 \in \mathbb{R} \right\} \tag{1.42}$$

Exercise Find the set of feasible directions for the equality constrained problem

$$\min_{x} f(x) \quad s.t. \quad \left(x_1^2 + x_2^2 - 2\right)^2 = 0 \tag{1.43}$$

at the feasible point $x = \begin{bmatrix}-\sqrt{2} & 0\end{bmatrix}^T$.

Answer Given

$$c(x) = \left(x_1^2 + x_2^2 - 2\right)^2 = 0 \tag{1.44}$$

We compute

$$\nabla c = \begin{bmatrix} 4\left(x_1^2 + x_2^2 - 2\right) x_1 \\ 4\left(x_1^2 + x_2^2 - 2\right) x_2 \end{bmatrix} \tag{1.45}$$

At $\begin{bmatrix}-\sqrt{2} & 0\end{bmatrix}^T$ the set of feasible directions are

$$0 = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}^T \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{1.46}$$

where $d = \begin{bmatrix}d_1 & d_2\end{bmatrix}^T$. Thus

$$\mathcal{F}(x) = \mathbb{R}^2 \tag{1.47}$$

Constraint qualifications are assumptions such that $\mathcal{F}(x)$ is similar to $\mathcal{T}_\Omega(x)$ in a neighborhood of x. For many constraint qualifications the sets are identifical, $\mathcal{F}(x) = \mathcal{T}_\Omega(x)$. Two such constraint qualifications are given below without proof.

Definition 1.10 *If $x^* \in \Omega$ and all active constraint functions $c_i(x^*)$ for $i \in \mathcal{A}(x^*)$ are linear functions then $\mathcal{F}(x^*) = \mathcal{T}_\Omega(x^*)$*

Definition 1.11 Linear independence constraint qualification (LICQ): *If $x^* \in \Omega$ and the gradients of all active constraint functions, $\nabla c_i(x^*)$ for $i \in \mathcal{A}(x^*)$ are linear independent then $\mathcal{F}(x^*) = \mathcal{T}_\Omega(x^*)$*

Exercise Find the first order optimality conditions of the problem

$$\min f(x_1, x_2) \qquad \text{s.t.} \qquad c(x_1, x_2) \geq 0 \tag{1.48}$$

Where

$$f(x_1, x_2) = (x_2 + 100)^2 + 0.01 x_1^2 \tag{1.49a}$$
$$c(x_1, x_2) = x_2 - \cos x_1 \tag{1.49b}$$

and verify if the linear independence constraint qualification holds.

Answer The function and constraint gradients are

$$\nabla f(x_1, x_2) = \begin{bmatrix} 0.02x_1 \\ 2x_2 + 200 \end{bmatrix} \tag{1.50a}$$

$$\nabla c(x_1, x_2) = \begin{bmatrix} \sin x_1 \\ 1 \end{bmatrix} \tag{1.50b}$$

Observe we always have $\nabla c \neq 0$, thus the LICQ holds at any solution x^*. The first order optimality conditions are

$$\nabla_x \mathcal{L} = \begin{bmatrix} 0.02x_1 \\ 2x_2 + 200 \end{bmatrix} - \lambda \begin{bmatrix} \sin x_1 \\ 1 \end{bmatrix} = 0 \tag{1.51a}$$

$$c(x_1, x_2) \geq 0 \tag{1.51b}$$

$$\lambda \geq 0 \tag{1.51c}$$

$$\lambda c(x_1, x_2) = 0 \tag{1.51d}$$

Exercise Verify if LICQ holds for the constraint set defined by

$$c_1(x) = 1 - x_1^2 - (x_2 - 1)^2 \geq 0 \tag{1.52a}$$

$$c_2(x) = -x_2 \geq 0 \tag{1.52b}$$

at $x^* = (0, 0)^T$.

Answer From the geometry of the feasible region it is clear the x^* is the only possible feasible solution. This is because it is the only single feasible point shared by both constraints. By straightforward computation we have

$$\nabla c_1(x^*) = \begin{bmatrix} -2x_1 \\ -2(x_2 - 1) \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \end{bmatrix} \tag{1.53a}$$

$$\nabla c_2(x^*) = \begin{bmatrix} 0 \\ -1 \end{bmatrix} \tag{1.53b}$$

It is clear that the LICQ does not hold, since the constraint gradients are a multiple of each other.

Exercise Consider the feasible region $\Omega \in \mathbb{R}^2$ defined by

$$c_1(x) = x_2 \geq 0 \tag{1.54a}$$

$$c_2(x) = x_1^2 - x_2 \geq 0, \tag{1.54b}$$

That is the set closed set lying above the x_1-axis and below the parabolla x_1^2.

(a) For $x^* = (0, 0)^T$, write down $\mathcal{F}(x^*)$ and $\mathcal{T}_\Omega(x^*)$.

(b) Is LICQ satisfied at x^*?

(c) If the objective function is $f(x) = -x_2$, verify that the first order optimality conditions are satisfied at x^*.

(d) Find a feasible sequence $\{z_k\}$ approacing x^* with $f(z_k) < f(x^*)$ for all k

Answer By straightforward differentiation we have

$$\nabla c_1(x) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{1.55a}$$

$$\nabla c_2(x) = \begin{bmatrix} 2x_1 \\ -1 \end{bmatrix} \tag{1.55b}$$

$$\nabla f = \begin{bmatrix} 0 \\ -1 \end{bmatrix} \tag{1.55c}$$

Now we can proceed,

(a) At x^* we have

$$\nabla c_1(x^*) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{1.56a}$$

$$\nabla c_2(x^*) = \begin{bmatrix} 0 \\ -1 \end{bmatrix} \tag{1.56b}$$

By definition

$$\mathcal{F}(x^*) = \{w | \nabla c_i(x^*)^T w \geq 0 \quad i \in \mathcal{A} \cap \mathcal{I}\} \tag{1.57}$$

For any $w = (\alpha, 0)^T$ with $\alpha \in \mathbb{R}$ we have $\nabla c_i(x^*)^T w \geq 0$, Thus

$$\mathcal{F}(x^*) = \{w | w = (\alpha, 0)^T \quad \text{and} \quad \alpha \in \mathbb{R}\} \tag{1.58}$$

From the geometry of Ω is is clear that we have $\mathcal{T}_\Omega(x*) = \mathcal{F}(x^*)$, since x^* is "sandwiched" by c_1 and c_2 and both constraints have a horizontal tangent at x^*.

(b) Obvioiusly the LICQ do not hold since ∇c_1 is a multiplum of ∇c_2.

(c) Let us start by the gradient of the Lagrangian

$$\nabla \mathcal{L}(x^*) = \nabla f(x^*) - \lambda_1 \nabla c_1(x^*) - \lambda_2 \nabla c_2(x^*) = 0 \tag{1.59}$$

From this we get

$$\begin{bmatrix} 0 \\ -1 \end{bmatrix} - \lambda_1 \begin{bmatrix} 0 \\ 1 \end{bmatrix} - \lambda_2 \begin{bmatrix} 0 \\ -1 \end{bmatrix} = 0 \tag{1.60}$$

From the bottom-most row we have $\lambda_2 = \lambda_1 + 1$. Notice that multiple solutions of the λ's exist since no constraint qualification hold at x^*. However, let us choice $\lambda_1 = 0$, then we can easily verify that

$$c(x^*) \geq 0 \tag{1.61a}$$

$$\lambda \geq 0 \tag{1.61b}$$

$$\lambda^T c(x^*) = 0 \tag{1.61c}$$

Thus the first order conditions hold at x^* (but not the constraint qualification).

(d) Since it is required that $f(z_k) < f(x^*)$ it seems like a good idea to follow points on the parabolla down towards the point x^*. Therefore

$$z_k = \begin{bmatrix} \frac{1}{k+1} \\ \frac{1}{(k+1)^2} \end{bmatrix} \tag{1.62}$$

For all k

Exercise Show that for the feasible region defined by

$$c_1(x) = 2 - (x_1 - 1)^2 - (x_2 - 1)^2 \geq 0 \tag{1.63a}$$
$$c_2(x) = 2 - (x_1 - 1)^2 - (x_2 + 1)^2 \geq 0 \tag{1.63b}$$
$$c_3(x) = x_1 \geq 0 \tag{1.63c}$$

the LICQ is not satisfied.

Answer First we compute the constraint gradients

$$\nabla c_1(x^*) = \begin{bmatrix} -2(x_1 - 1) \\ -2(x_2 - 1) \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \end{bmatrix} \tag{1.64a}$$
$$\nabla c_2(x^*) = \begin{bmatrix} -2(x_1 - 1) \\ -2(x_2 + 1) \end{bmatrix} = \begin{bmatrix} 2 \\ -2 \end{bmatrix} \tag{1.64b}$$
$$\nabla c_3(x^*) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{1.64c}$$

LICQ can not be satisfied since 3 vectors in $\mathbb{R}^2$ must be lineary dependent.

Exercise We are given the problem

$$\min_{x,y} f(x, y) = (x - 1)^2 + (y - 2)^2 \tag{1.65}$$

subject to

$$c(x, y) = (x - 1)^2 - 5y = 0 \tag{1.66}$$

Now

(a) Find all the first order optimality points for this problem. Is the LICQ satisfied?

(b) Which of these points are solutions?

(c) By directly substituting the constraint into the objective function and eliminating the variable x, we obtain an unconstrained optimization problem. Show that the solutions of this problem cannot be solutions of the original problem.

Answer Before we start let us compute all the gradients

$$\nabla f(x,y) = \begin{bmatrix} 2(x-1) \\ 2(y-2) \end{bmatrix} \tag{1.67a}$$

$$\nabla c(x,y) = \begin{bmatrix} 2(x-1) \\ -5 \end{bmatrix} \tag{1.67b}$$

Now

(a) From $\nabla \mathcal{L}(x^*, y^*) = 0$ we have

$$\begin{bmatrix} 2(x^*-1) \\ 2(y^*-2) \end{bmatrix} - \lambda^* \begin{bmatrix} 2(x^*-1) \\ -5 \end{bmatrix} = 0 \tag{1.68}$$

From the top-row we derive

$$2(x^*-1) - \lambda^* 2(x^*-1) = 0 \tag{1.69a}$$

$$\lambda^* = 1 \tag{1.69b}$$

when $x^* \neq 1$, substituting $\lambda^* = 1$ into the second row we obtain

$$2(y^*-2) - \lambda^*(-5) = 0 \tag{1.70a}$$

$$y^* = -\frac{1}{2} \tag{1.70b}$$

Thus we have $x^* \neq 1$, $y^* = -\frac{1}{2}$, and $\lambda^* = 1$. However observe what happens if we substitute into $c(x,y)$

$$c(x^*, y^*) = \underbrace{(x-1)^2}_{>0} + \frac{5}{2} > 0 \tag{1.71}$$

Hence since this solution do not fulfill the constraint it can not be a solution to our problem. Assume now that $x^* = 1$ then from $c(1,y) = 0$ we find

$$c(1,y) = (1-1)^2 - 5y = 0 \tag{1.72a}$$

$$y = 0 \tag{1.72b}$$

Substituting into the second row yields

$$2(0-2) - \lambda^*(-5) = 0 \tag{1.73a}$$

$$\lambda^* = \frac{4}{5} \tag{1.73b}$$

Thus we have $x = 1$, $y = 0$, and $\lambda = \frac{4}{5}$. This is in fact a solution since $c(1,0) = 0$, $\lambda > 0$ and the LICQ is also satisfied,

$$\nabla c(1,0) = \begin{bmatrix} 0 \\ -5 \end{bmatrix} \neq 0 \tag{1.74}$$

(b) From (a) it is clear that only one first order optimality point exist and it is the solution.

(c) The reformulated unconstrained minimzation problem is

$$\min_y f(y) = fy + (y-2)^2 = y^2 + y + 4 \tag{1.75}$$

We find the unconstrained minimizer by computing $\nabla f(y) = 0$,

$$2y + 1 = 0 \tag{1.76a}$$

$$y = -\frac{1}{2} \tag{1.76b}$$

recall from (a) that $c(x, -\frac{1}{2}) > 0$. Hence, the constraint is not fulfilled, and the unconstrained minimizer is not a solution for the original problem.

Exercise Consider the problem

$$\min_x f(x) = -2x_1 + x_2 \tag{1.77}$$

subject to

$$c_1(x) = (1 - x_1)^3 - x_2 \geq 0 \tag{1.78a}$$

$$c_2(x) = x_2 + \frac{1}{4}x_1^2 - 1 \geq 0 \tag{1.78b}$$

The optimal solution is at $x^* = (0, 1)^T$, where both constraints are active.

(a) Do the LICQ hold at this point?

(b) Are the first order optimality conditions satisfied?

(c) Write down the sets $\mathcal{F}(x^*)$

Answer First we compute the gradients

$$\nabla f(x^*) = \begin{bmatrix} -2 \\ 1 \end{bmatrix} \tag{1.79a}$$

$$\nabla c_1(x^*) = \begin{bmatrix} -3(1 - x_1^*)^2 \\ -1 \end{bmatrix} = \begin{bmatrix} -3 \\ -1 \end{bmatrix} \tag{1.79b}$$

$$\nabla c_2(x^*) = \begin{bmatrix} \frac{1}{2}x_1^* \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{1.79c}$$

(a) Yes LICQ holds since $(0, 1)^T$ and $(-3, -1)^T$ are not a multiplum of each other. Thus the constraint gradients are linear independent.

(b) From the "gradient" equation we have

$$\begin{bmatrix} -2 \\ 1 \end{bmatrix} - \lambda_1^* \begin{bmatrix} -3 \\ -1 \end{bmatrix} - \lambda_2^* \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0 \tag{1.80}$$

From this we have

$$\lambda_1^* = \frac{2}{3} \geq 0 \tag{1.81a}$$

$$\lambda_2^* = \frac{5}{3} \geq 0 \tag{1.81b}$$

and $c_1(x^*) = c_2(x^*) = 0$. Thus the first order optimality conditions are satisfied.

(c) By definition of $\mathcal{F}$ we seek $w = (w_1, w_2)^T$ such that

$$\begin{bmatrix} -3 & -1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = -3w_1 - w_2 \geq 0 \tag{1.82}$$

and

$$\begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = w_2 \geq 0 \tag{1.83}$$

From the first condition we have $-3w_1 \leq w_2$ (everything below the line with slope -3 and crossing 0) and the second condition $w_2 \geq 0$ implies that we must be above the w_1-axis thus have

$$\mathcal{F}(x^*) = \{w | w_2 \geq 0 \quad \text{and} \quad w_2 \leq -3w_1\} \tag{1.84}$$

Chapter 2

Constrained Optimization and Problem Reformulations

In physics based modeling and simulation one often need to solve for constraint forces or contact forces or other types of motion constraints. From the basic principle of physics, the principle of least action, we can derive problem formulations which solutions yield the results we want. The principle of least action is a minimization problem of an action integral. Therefore most problems start out as being formulated as a constrained minimization problem.

In this chapter we will study the “mother” of all problems: the constrained minimization problem. We will show how this archetype problem can be reformulated into other well-known problem types, which again can be reformulated to other problem types.

We hope the chapter will offer the reader valuable insight in how to manipulate one problem formulation into another problem formulation. Thereby allowing the reader to pick and use the problem formulation that is most profitable for a given modeling or simulation problem.

This chapter is no substitute for a textbook on these matters. The chapter seek only to present the wisdom and experience gained by the authors from working with these topics.

We will start with the “mother” problem of all other problems, the constrained minimization problem.

Definition 2.1 *Given $f(x) : \mathbb{R}^n \mapsto \mathbb{R}$ and $c(x) : \mathbb{R}^n \mapsto \mathbb{R}^m$ then the problem*

$$\min_x f(x) \quad \textit{subject to} \quad c(x) \geq 0 \tag{2.1}$$

is a constrained minimization problem.

The necessary conditions for a first order optimal solution are often used as a building block for methods that solve the minimization problem or as a tool for verifying if a given solution is truly a solution to first order optimality. In the following we will simply define the first order optimality conditions with-out proof and for our specific case.

Definition 2.2 *The first order optimality conditions for the minimization problem in Definition 2.1 are*

$$\nabla f(x^*) - \nabla c(x^*)^T \lambda = 0 \tag{2.2a}$$
$$c(x^*) \geq 0 \tag{2.2b}$$
$$\lambda^* \geq 0 \tag{2.2c}$$
$$(\lambda^*)^T c(x^*) = 0 \tag{2.2d}$$

where x^* is a feasible minimizer of the problem and λ^* is the corresponding Lagrange multiplier.

The last three equations are known collectively as a complementarity condition. We name the first equation as the zero-gradient equation to ease reference for it later on.

Let us assume that the real-function f and the vector constraint function c have properties that allow us to re-write the first equation, the zero-gradient equation, of the first-order optimality conditions as,

$$\nabla f(x^*) - \nabla c(x^*)^T \lambda^* = 0 \qquad \Leftrightarrow \qquad x^* = g(\lambda^*). \tag{2.3}$$

If this is the case then we can make a substitution into the constraint function, $c(x^*) = c(g(\lambda^*)) = h(\lambda^*)$. The first order optimality conditions now reduces to the complementarity conditions

$$h(\lambda^*) \geq 0 \tag{2.4a}$$
$$\lambda^* \geq 0 \tag{2.4b}$$
$$(\lambda^*)^T h(\lambda^*) = 0 \tag{2.4c}$$

This problem type is called a non-linear complementarity problem.

Definition 2.3 *Given $h(\lambda) : \mathbb{R}^n \mapsto \mathbb{R}^n$ then the equations*

$$h(\lambda) \geq 0 \tag{2.5a}$$
$$\lambda \geq 0 \tag{2.5b}$$
$$\lambda^T h(\lambda) = 0 \tag{2.5c}$$

is collectively known as a non-linear complementarity problem.

Remark We have just shown how a constrained minimization problem can be recast into a complementarity problem.

Remark Observe that one can obtain the first-order optimality solution of the constrained minimization problem by solving the complementarity problem for λ^* and then use $g(\lambda^*)$ to find x^*.

Remark In physics based modeling and simulation $h(\lambda)$ is in many cases an affine function,

$$h(\lambda) = A\lambda + b, \tag{2.6}$$

where A is a symmetric positive semi-definite matrix that is extremely sparse. In this particular case one will have a linear complementarity problem.

Definition 2.4 *Given $A \in \mathbb{R}^{n\times n}$ and $\lambda, b \in \mathbb{R}^n$ then*

$$A\lambda + b \geq 0 \tag{2.7a}$$
$$\lambda \geq 0 \tag{2.7b}$$
$$\lambda^T (A\lambda + b) = 0 \tag{2.7c}$$

is named the linear complementarity problem.

Given the complementarity problem,

$$h(\lambda) \geq 0 \tag{2.8a}$$
$$\lambda \geq 0 \tag{2.8b}$$
$$\lambda^T h(\lambda) = 0 \tag{2.8c}$$

We observe that the left-hand-side of the last equation, $\lambda^T h(\lambda)$, is always non-negative and bounded from below by zero by the properties of the first two equations. Thus we can find λ^* by finding the global minimizer of

$$\min_{\lambda} \lambda^T h(\lambda) \tag{2.9}$$

subject to

$$h(\lambda) \geq 0 \tag{2.10a}$$
$$\lambda \geq 0 \tag{2.10b}$$

It is instructive to try to derive the original complementarity problem from the minimization problem (2.9). The first-order optimality conditions read

$$h(\lambda^*) + \nabla h(\lambda^*)^T \lambda^* - \nabla h(\lambda^*)^T x^* - y^* = 0 \tag{2.11a}$$
$$\lambda^* \geq 0 \tag{2.11b}$$
$$h(\lambda^*) \geq 0 \tag{2.11c}$$
$$x^* \geq 0 \tag{2.11d}$$
$$y^* \geq 0 \tag{2.11e}$$
$$(x^*)^T h(\lambda^*) = 0 \tag{2.11f}$$
$$(y^*)^T \lambda = 0 \tag{2.11g}$$

Where x^* and y^* are the Lagrange multipliers. Making the clever choice $x^* = \lambda^*$ and $y^* = h(\lambda^*)$ the above set of equations reduces to

$$h(\lambda^*) \geq 0 \tag{2.12a}$$
$$\lambda^* \geq 0 \tag{2.12b}$$
$$(\lambda^*)^T h(\lambda^*) = 0 \tag{2.12c}$$

which is the original complementarity problem.

Remark In case of the linear complementarity problem the left-hand-side of the last equation of the complementarity condition yields

$$\lambda^T(A\lambda + b) = \lambda^T A\lambda + \lambda^T b \tag{2.13}$$

By the properties of A (symmetric and positive semi-definite) this is a convex minimization problem also known as a quadratic programming (QP) problem.

Exercise Derive the complementarity problem corresponding to the constrained minimization problem

$$\min_\lambda \frac{1}{2}\lambda^T A\lambda + \lambda^T b \tag{2.14}$$

subject to

$$\lambda \geq 0 \tag{2.15}$$

Assuming $A \in \mathbb{R}^{n\times n}$ is symmetric, and $\lambda, b \in \mathbb{R}^n$.

Answer The first order optimality conditions are

$$A\lambda^* + b - Ix^* = 0 \tag{2.16a}$$
$$x^* \geq 0 \tag{2.16b}$$
$$\lambda^* \geq 0 \tag{2.16c}$$
$$(x^*)^T(\lambda^*) = 0 \tag{2.16d}$$

From the zero-gradient equation we have $x^* = A\lambda^* + b$, substitution yields

$$A\lambda^* + b \geq 0 \tag{2.17a}$$
$$\lambda^* \geq 0 \tag{2.17b}$$
$$(\lambda^*)^T(A\lambda^* + b) = 0 \tag{2.17c}$$

which is a linear complementarity problem.

Exercise Derive the complementarity problem corresponding to the constrained minimization problem

$$\min_\lambda \frac{1}{2}\lambda^T A\lambda + \lambda^T b \tag{2.18}$$

subject to

$$\lambda \geq 0 \tag{2.19a}$$
$$B\lambda + c \geq 0 \tag{2.19b}$$

Assuming $A \in \mathbb{R}^{n\times n}$ is symmetric, $B \in \mathbb{R}^{m\times n}$, and $\lambda, b \in \mathbb{R}^n$.

Answer The first order optimality conditions are

$$A\lambda^* + b - B^T y^* - I x^* = 0 \tag{2.20a}$$
$$\lambda^* \geq 0 \tag{2.20b}$$
$$B\lambda^* + c \geq 0 \tag{2.20c}$$
$$x^* \geq 0 \tag{2.20d}$$
$$y^* \geq 0 \tag{2.20e}$$
$$(x^*)^T (\lambda^*) = 0 \tag{2.20f}$$
$$(y^*)^T (B\lambda^* + c) = 0 \tag{2.20g}$$

where x^* and y^* are the Lagrange multipliers. From the zero-gradient equation we have, $x^* = A\lambda^* + b - B^T y^*$. Substitution yields

$$\lambda^* \geq 0 \tag{2.21a}$$
$$B\lambda^* + c \geq 0 \tag{2.21b}$$
$$A\lambda^* + b - B^T y^* \geq 0 \tag{2.21c}$$
$$y^* \geq 0 \tag{2.21d}$$
$$\left(A\lambda^* + b - B^T y^*\right)^T (\lambda^*) = 0 \tag{2.21e}$$
$$(y^*)^T (B\lambda^* + c) = 0 \tag{2.21f}$$

This is two simultaneous complementarity problems. We can rewrite them into a single complementarity problem by defining,

$$M = \begin{bmatrix} A & -B^T \\ B & 0 \end{bmatrix}, q = \begin{bmatrix} b \\ c \end{bmatrix}, \quad \text{and} \quad z^* = \begin{bmatrix} \lambda^* \\ y^* \end{bmatrix} \tag{2.22}$$

and we have

$$Mz^* + q \geq 0 \tag{2.23a}$$
$$z^* \geq 0 \tag{2.23b}$$
$$(z^*)^T (Mz^* + q) = 0 \tag{2.23c}$$

This is a linear complementarity problem. Note that M is non-symmetric.

Exercise Derive the complementarity problem corresponding to the constrained minimization problem

$$\min_{\lambda} \frac{1}{2}\lambda^T A \lambda + \lambda^T b \tag{2.24}$$

subject to

$$\lambda \geq 0 \tag{2.25a}$$
$$c(\lambda) \geq 0 \tag{2.25b}$$

Assuming $A \in \mathbb{R}^{n\times n}$ is symmetric, $c(\lambda) : \mathbb{R}^n \mapsto \mathbb{R}^m$, and $\lambda, b \in \mathbb{R}^n$.

Answer The first order optimality conditions are

$$A\lambda^* + b - \nabla c(\lambda^*)^T y^* - Ix^* = 0 \tag{2.26a}$$
$$\lambda^* \geq 0 \tag{2.26b}$$
$$c(\lambda^*) \geq 0 \tag{2.26c}$$
$$x^* \geq 0 \tag{2.26d}$$
$$y^* \geq 0 \tag{2.26e}$$
$$(x^*)^T (\lambda^*) = 0 \tag{2.26f}$$
$$(y^*)^T (c(\lambda^*)) = 0 \tag{2.26g}$$

where x^* and y^* are the Lagrange multipliers. From the zero-gradient equation we have, $x^* = g(\lambda^*, y^*) = A\lambda^* + b - \nabla c(\lambda^*)^T y^*$. Substitution yields

$$g(\lambda^*, y^*) \geq 0 \tag{2.27a}$$
$$c(\lambda^*) \geq 0 \tag{2.27b}$$
$$\lambda^* \geq 0 \tag{2.27c}$$
$$y^* \geq 0 \tag{2.27d}$$
$$(\lambda^*)^T (g(\lambda^*, y^*)) = 0 \tag{2.27e}$$
$$(y^*)^T (c(\lambda^*) = 0 \tag{2.27f}$$

This is two simultaneous non-linear complementarity problems. We can rewrite them into a single non-linear complementarity problem by defining,

$$z^* = \begin{bmatrix} \lambda^* \\ y^* \end{bmatrix} \quad \text{and} \quad h(z^*) = \begin{bmatrix} g(\lambda^*, y^*) \\ c(\lambda^*) \end{bmatrix} \tag{2.28}$$

we have

$$h(z^*) \geq 0 \tag{2.29a}$$
$$z^* \geq 0 \tag{2.29b}$$
$$(z^*)^T (h(z^*)) = 0 \tag{2.29c}$$

This is a non-linear complementarity problem.

The complementarity problem may also be re-cast into a zero finding problem as we will study in the following. This is equivalent to solving an equation. First we will define what we mean by a zero finding problem.

Definition 2.5 *Given $H(\lambda) : \mathbb{R}^n \mapsto \mathbb{R}^n$ and the problem of finding all, λ^*, such that*

$$H(\lambda^*) = 0 \tag{2.30}$$

Then we call this an equation solving problem or a zero finding problem and a solution λ^* is sometimes called a root of H.

One of the simplest of such re-formulations of the complementarity problem into a zero finding problem is the minimal-map reformulation

$$H(\lambda) = \min(\lambda, h(\lambda)) = 0 \tag{2.31}$$

Notice that by requiring the minimum to be zero prevents both λ and $h(\lambda)$ to become negative. Also either λ or $h(\lambda)$ or both must be zero thus the term $\lambda^T h(\lambda)$ will always be zero. Thus a solution λ^* of the zero finding problem is equivalent to finding a solution for the complementarity problem.

Definition 2.6 *The solution of the equation*

$$H(\lambda) = \min(\lambda, h(\lambda)) = 0 \tag{2.32}$$

is also a solution of the complementarity problem in Defintion 2.3.

There exist many such reformulations each with different properties. The one above is a so-called non-smooth function because it is non-differentiable. Different reformulations have different properties. We will just mention two other popular reformulations

Smooth Reformulation: Mangassarian,

$$H_i(\lambda) = \phi_{\mathrm{M}}(h_i(\lambda), \lambda_i) = (h_i(\lambda) - \lambda_i)^2 - |h_i(\lambda)|h_i(\lambda) - |\lambda_i|\lambda_i = 0 \tag{2.33}$$

Semi-Smooth Reformulation: Fischer-Burmeister,

$$H_i(\lambda) = \phi_{\mathrm{FB}}(h_i(\lambda), \lambda_i) = \sqrt{h_i(\lambda)^2 + \lambda_i^2} - h_i(\lambda_i) - \lambda_i = 0 \tag{2.34}$$

Exercise Verify that the Mangassarian reformulation corresponds to the complementarity problem (Tip: try a case by case analysis of the signs of λ_i and $h_i(\lambda)$).

Answer Let us assume that $\lambda_i < 0$ and $h_i(\lambda) < 0$ then insertion into the Mangassarian reformulation yields

$$\begin{aligned}
H_i(\lambda) &= (h_i(\lambda) - \lambda_i)^2 - |h_i(\lambda)|h_i(\lambda) - |\lambda_i|\lambda_i && \text{(2.35a)}\\
&= h_i(\lambda)^2 + \lambda_i^2 - 2h_i(\lambda)\lambda_i - (-h_i(\lambda))h_i(\lambda) - (-\lambda_i)\lambda_i && \text{(2.35b)}\\
&= h_i(\lambda)^2 + \lambda_i^2 - 2h_i(\lambda)\lambda_i + h_i(\lambda)^2 + \lambda_i^2 && \text{(2.35c)}\\
&= 2(h_i(\lambda)^2 + \lambda_i^2 - h_i(\lambda)\lambda_i) > 0 && \text{(2.35d)}
\end{aligned}$$

Computing the remaining sign-combinations yields the table below. Observe that the value zero is only obtained if input is a feasible solution for the complementarity problem.

	$\lambda_i < 0$	$\lambda_i = 0$	$\lambda_i > 0$
$h_i(\lambda) < 0$	$+$	$+$	$+$
$h_i(\lambda) = 0$	$+$	0	0
$h_i(\lambda) > 0$	$+$	0	$-$

Exercise Perform case-by-case analysis of the sign of the minimum map reformulation,

$$H_i(\lambda) = \min\left(\lambda_i, h_i(\lambda)\right) \tag{2.36}$$

Answer The case-by-case analysis of the minimum map reformulation results in

	$\lambda_i < 0$	$\lambda_i = 0$	$\lambda_i > 0$
$h_i(\lambda) < 0$	$-$	$-$	$-$
$h_i(\lambda) = 0$	$-$	0	0
$h_i(\lambda) > 0$	$-$	0	$+$

Exercise Verify that the Fischer-Burmeister reformulation corresponds to the complementarity problem (Tip: try a case by case analysis of the signs of λ_i and $h_i(\lambda)$).

Answer The sign-table should be that same as the one of the Mangassarian reformulation.

A zero finding problem can be reformulated into a fixed-point formulation. For instance, we define $F(\lambda) = \lambda - H(\lambda)$. If there exist a λ^* such that

$$F(\lambda^*) = \lambda^* \tag{2.37}$$

then λ^* is called a fixed-point for $F(\lambda)$. Furhter λ^* is a root of $H(\lambda)$, which can be seen by substitution,

$$F(\lambda^*) = \lambda^* \tag{2.38a}$$
$$\lambda^* - H(\lambda^*) = \lambda^* \tag{2.38b}$$
$$H(\lambda^*) = 0 \tag{2.38c}$$

In a similar fashion can any fixed-point formulation, $F(\lambda) = \lambda$, be reformulated into a zero finding formulation, $H(\lambda) = 0$, by defining $H(\lambda) = \lambda - F(\lambda)$.

Exercise Rewrite the minimum map reformulation into a fixed-point formulation.

Answer The minimum map reformulation is given as

$$H(\lambda) = \min(\lambda, h(\lambda)) = 0 \tag{2.39}$$

The fixed-point reformulation is then

$$F(\lambda) = \lambda - H(\lambda) \tag{2.40a}$$
$$= \lambda - \min(\lambda, h(\lambda)) \tag{2.40b}$$
$$= \lambda + \max(-\lambda, -h(\lambda)) \tag{2.40c}$$
$$= \max(0, \lambda - h(\lambda)) \tag{2.40d}$$

Given a zero finding problem

$$H(\lambda) = 0 \tag{2.41}$$

it can be re-formulated into a minimization problem. For instance by using a so-called natural merit function. A natural merit function is simply the squared norm of the vector function

$$\theta(\lambda) = \frac{1}{2} H(\lambda)^T H(\lambda) \tag{2.42}$$

The natural merit function is clearly non-negative and is bounded from below by zero. Finding a global minimizer of the merit function is equivalent to finding a root. Clearly there is a connection between zero finding problems and minimization problems.

Remark Observe the constraints are no-longer explicitly written when we reformulate a constrained optimization problem or complementarity problem as a zero finding problem or a unconstrained minimzation problem. This may be an advantage to consider when choosing a numerical method.

The lesson learned from this introduction to the different problem formulations and reformulations are

- We have introduced four main problem classes: The minimization problem, the complementarity problem, the zero finding problem, and the fixed-point problem.

- We have shown how one problem formulation can be reformulated into the other.

In the following we will study a few selected numerical methods for solving the complementarity problem.

Chapter 3

Numerical Methods for Complementarity Problems

3.1 The Splitting Methods

The types of methods we will present here is often used in interactive simulations for solving for contact forces. The methods are iterative and each iteration is computational cheap. The methods are therefore well-suited for large size problems. Due to the linear convergence rate of the methods they are not without problems when applied to problems. Technically the methods are termed splitting methods. However, the interative simulation and computer graphics communities refer to them as projection methods. In the following we will only consider the linear complementarity problem,

$$A\lambda + b \geq 0 \tag{3.1a}$$

$$\lambda \geq 0 \tag{3.1b}$$

$$\lambda^T (A\lambda + b) = 0 \tag{3.1c}$$

We introduce the splitting

$$A = M - N \tag{3.2}$$

Next we let $c^k = b - N\lambda^k$ then

$$M\lambda^{k+1} + c^k \geq 0 \tag{3.3a}$$

$$\lambda^{k+1} \geq 0 \tag{3.3b}$$

$$(\lambda^{k+1})^T (M\lambda^{k+1} + c^k) = 0 \tag{3.3c}$$

This results in a fixed-point formulation where we hope that for a suitable choice of M and N the complementarity sub-problem might be easier to solve than the original problem.

Algorithm 3.1 The Splitting Algorithm

Step 0 *Initialization, set $k = 0$ and choice arbitary nonnegative $\lambda^k \geq 0$,*

Step 1 *Given $\lambda^k \geq 0$ solve the linear complementarity problem*

$$M\lambda^{k+1} + c^k \geq 0, \tag{3.4a}$$

$$\lambda^{k+1} \geq 0, \tag{3.4b}$$

$$(\lambda^{k+1})^T(M\lambda^{k+1} + c^k) = 0, \tag{3.4c}$$

where $c^k = b - N\lambda^k$.

Step 2 *If λ^{k+1} satisify some stopping rule then stop otherwise set $k = k + 1$ and go to step 1.*

The splitting is often chosen such that M is a Q-matrix. This means that M belongs to the matrix class of matrices where the corresponding linear complimentarity problem has a solution for all right-hand side vectors c^k.

Clearly if λ^{k+1} is a solution for (3.4) and we have $\lambda^{k+1} = \lambda^k$ then by substitution into the sub-problem given by (3.4) we see that λ^{k+1} is also a solution of the original problem (3.1).

3.1.1 Solving the Sub-Problem

Next we will use the minimum map reformulation on the complementarity subproblem this is equivalent to

$$\min(\lambda^{k+1}, M\lambda^{k+1} + c^k) = 0 \tag{3.5}$$

subtract λ^{k+1}

$$\min(0, M\lambda^{k+1} + c^k - \lambda^{k+1}) = -\lambda^{k+1} \tag{3.6}$$

multiply by minus one

$$\max(0, -M\lambda^{k+1} - c^k + \lambda^{k+1}) = \lambda^{k+1} \tag{3.7}$$

Again we re-discover a fixed-point formulation. Let us perform a case-by-case analysis. If

$$(\lambda^{k+1} - M\lambda^{k+1} - c^k)_i < 0 \tag{3.8}$$

then

$$\lambda_i^{k+1} = 0 \tag{3.9}$$

Otherwise

$$(\lambda^{k+1} - M\lambda^{k+1} - c^k)_i = \lambda_i^{k+1} \tag{3.10}$$

That is

$$(M\lambda^{k+1})_i = c_i^k \tag{3.11}$$

For suitable choice of M and back-substitution of $c^k = b - N\lambda^k$ we have

$$(M^{-1}N\lambda^k - b)_i = \lambda_i^{k+1} \tag{3.12}$$

Combining it all we have derived the solution for the complementarity subproblem

$$\max(0, (M^{-1}N\lambda^k - b)) = \lambda^{k+1} \tag{3.13}$$

Iterative schemes like these are often also termed projection methods. The reason for this is that if we introduce the vector $z^k = M^{-1}N\lambda^k - b$ then

$$\lambda^{k+1} = \max(0, z^k) \tag{3.14}$$

that is the $k+1$ iterate is obtained by projecting the vector z^k onto the positive octant.

One would want to use a clever splitting such that the inversion of M is computationally cheap. Three popular choices are

The Projected Jacobi Method:

$$M = D \tag{3.15a}$$
$$N = L + D \tag{3.15b}$$

The Projected Gauss Seidel (PGS) Method:

$$M = (L + D) \tag{3.16a}$$
$$N = U \tag{3.16b}$$

The Projected Successive Over Relaxation (PSOR) Method:

$$M = (D + \omega L) \tag{3.17a}$$
$$N = ((1 - \omega)\, D - \omega U) \tag{3.17b}$$

3.1.2 Convergence

To study the convergence of the splitting algorithm we will use the quadratic programming problem reformulation of the linear complementarity problem,

$$\min_{\lambda} f(\lambda) \quad \text{subject to} \quad \lambda \geq 0 \tag{3.18}$$

where

$$f(\lambda) = \frac{1}{2}\lambda^T A\lambda + \lambda^T b \tag{3.19}$$

Assuming that A is symmetric we can write the difference in the function value between two succeding iterates λ^{k+1} and λ^k as

$$f(\lambda^k) - f(\lambda^{k+1}) = (\lambda^k - \lambda^{k+1})^T b + \frac{1}{2}\left(\lambda^k\right)^T A\lambda^k - \frac{1}{2}\left(\lambda^{k+1}\right)^T A\lambda^{k+1} \tag{3.20a}$$

$$= \left(\lambda^k - \lambda^{k+1}\right)^T \left(b + A\lambda^{k+1}\right) + \frac{1}{2}\left(\lambda^k - \lambda^{k+1}\right)^T A\left(\lambda^k - \lambda^{k+1}\right) \tag{3.20b}$$

Using the splitting $A = M - N$ and rewritting slightly we have

$$f(\lambda^k) - f(\lambda^{k+1}) = \left(\lambda^k - \lambda^{k+1}\right)^T \left(b - N\lambda^k + M\lambda^{k+1}\right) + \frac{1}{2}\left(\lambda^k - \lambda^{k+1}\right)^T (M+N)\left(\lambda^k - \lambda^{k+1}\right) \tag{3.21}$$

Recall that λ^{k+1} is the solution of the complementarity problem given by (3.4) and that $\lambda^k \geq 0$ from this we conclude that $\left(\lambda^k - \lambda^{k+1}\right)^T \left(b - N\lambda^k + M\lambda^{k+1}\right) \geq 0$ and thus

$$f(\lambda^k) - f(\lambda^{k+1}) \geq \frac{1}{2}\left(\lambda^k - \lambda^{k+1}\right)^T (M+N)\left(\lambda^k - \lambda^{k+1}\right) \tag{3.22}$$

We will assume that $\lambda^k \neq \lambda^{k+1}$ otherwise we would have a solution. If we can say someting about the properties of the matrix $(M+N)$ then the quadratic form can be very usefull. We will make use of the following definition

Definition 3.1 A (Weakly) Regular Splitting: *The splitting $A = M - N$ is said to be a weakly regular splitting if $(M+N)$ is positive semi-definite, and regular if $(M+N)$ is positive definite.*

Using the definition of weakly regular and regular splittings together with (3.22) results in the following theorem.

Theorem 3.1.1 *Let A be a symmetric matrix with the weakly regular Q-splitting, $A = M - N$, then*

$$f(\lambda^k) - f(\lambda^{k+1}) \geq \frac{1}{2}\left(\lambda^k - \lambda^{k+1}\right)^T (M+N)\left(\lambda^k - \lambda^{k+1}\right) \geq 0 \tag{3.23}$$

If the splitting is regular then $f(\lambda^k) = f(\lambda^{k+1})$ if an only if $\lambda^k = \lambda^{k+1}$.

With this theorem in place we can now make a statement about the behaviour of the splitting algorithm under the assumption that there exist a sub-sequence which converges to an accumulation point.

Theorem 3.1.2 *Let $A = M - N$ be a regular Q-splitting of the symmetric matrix A. Then any accumulation point of the sequence $\left\{\lambda^k\right\}$ produced be the splitting algorithm is a solution of the linear complementarity problem*

Proof Let λ^* be an accumulation point of the sequence $\left\{\lambda^k\right\}$ and suppose the sub-sequence $\left\{\lambda^{k_i}\right\}$ converges to λ^* then $f(\lambda^{k_i})$ converges to $f(\lambda^*)$.

From (3.23) the sequence $\left\{f(\lambda^k)\right\}$ is nonincreasing and because the sub-sequence $\left\{f(\lambda^{k_i})\right\}$ converges it must mean that $f(\cdot)$ is bounded below.

That must mean that the sequence $\left\{f(\lambda^k)\right\}$ converges.

Since the splitting is regular then (3.23) implies that $\lambda^k - \lambda^{k+1} \to 0$ as $k \to \infty$. Therefore?