

Optimization

Màster de Fonaments de Ciència de Dades

Gerard Gómez

Lecture V. Constrained optimization

Equality constrained extrema

Consider the problem of finding the minimum (or maximum) of a real-valued function f with domain of definition $\mathcal{C} \subset \mathbb{R}^n$

$$f : \mathcal{C} \longrightarrow \mathbb{R},$$

subject to the **equality constraints**

$$h_i(\mathbf{x}) = 0, \quad i = 1, \dots, m, \quad m < n, \quad (1)$$

where each of the h_i is a real-valued function defined on \mathcal{C} . This is, the problem is to find an extremum of f in the region determined by the equations (1).

Example. Find the area of the largest rectangle that can be inscribed in the ellipse

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1.$$

This is, find the maximum of

$$f(x, y) = 4xy$$

subject to the constraint

$$h(x, y) = \frac{x^2}{a^2} + \frac{y^2}{b^2} - 1 = 0.$$

Lagrange's method

As we have already seen, **Lagrange's method** consists of transforming an equality constrained extremum problem into a problem of finding a stationary point $(\mathbf{x}^*, \boldsymbol{\lambda}^*)$ of the **Lagrangian** function

$$L(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) - \sum_{i=1}^m \lambda_i h_i(\mathbf{x}), \quad \text{in the example} \quad L(x, y, \lambda) = 4xy - \lambda \left(\frac{x^2}{a^2} + \frac{y^2}{b^2} - 1 \right)$$

Theorem (Necessary conditions)

Suppose that

$$f : \mathcal{C} \longrightarrow \mathbb{R}, \quad \text{and} \quad h_i : \mathcal{C} \longrightarrow \mathbb{R}, \quad i = 1, \dots, m,$$

are real-valued functions that satisfy:

- ▶ They are all continuously differentiable on a neighborhood $N_\epsilon(\mathbf{x}^*) \subset \mathcal{C}$.
- ▶ \mathbf{x}^* is a local minimum (or maximum) of f in $N_\epsilon(\mathbf{x}^*)$.
- ▶ If $\mathbf{x} \in N_\epsilon(\mathbf{x}^*)$, then

$$h_i(\mathbf{x}) = 0, \quad i = 1, \dots, m.$$

- ▶ The Jacobian matrix $(\partial h_i(\mathbf{x}^*)/\partial x_j)$ has rank m .

Then, there exists a vector of multipliers $\boldsymbol{\lambda}^* = (\lambda_1^*, \dots, \lambda_m^*)^T$ such that

$$\nabla L(\mathbf{x}^*, \boldsymbol{\lambda}^*) = 0.$$

Lagrange's method

There are two ways to interpret the necessary condition given by equation

$$\nabla L(\mathbf{x}^*, \boldsymbol{\lambda}^*) = 0 \quad \Leftrightarrow \quad \nabla f(\mathbf{x}^*) = \sum_{i=1}^m \lambda_i^* \nabla h_i(\mathbf{x}^*)$$

1. The gradient of the cost function $\nabla f(\mathbf{x}^*)$ belongs to the subspace spanned by the gradients of the constraints at \mathbf{x}^* , $\nabla h_i(\mathbf{x}^*)$.
2. Define the subspace of **first order feasible variations at \mathbf{x}^*** , $\Delta \mathbf{x}$, by:

$$V(\mathbf{x}^*) = \{\Delta \mathbf{x} \mid \nabla h_i(\mathbf{x}^*)^T \Delta \mathbf{x} = \Delta \mathbf{x}^T \nabla h_i(\mathbf{x}^*) = 0, i = 1, \dots, m\}.$$

Note that $V(\mathbf{x}^*)$ is the subspace of variations $\Delta \mathbf{x}$ for which *the point $\mathbf{x}^* + \Delta \mathbf{x}$ satisfies the constraint $h = 0$ up to the first order:*

$$h(\mathbf{x}^* + \Delta \mathbf{x}) = h(\mathbf{x}^*) + \nabla h(\mathbf{x}^*)^T \Delta \mathbf{x} = \nabla h(\mathbf{x}^*)^T \Delta \mathbf{x} = 0.$$

Then, the necessary condition implies that the cost gradient $\nabla f(\mathbf{x}^*)$ is orthogonal to the subspace of first order feasible variations at \mathbf{x}^* , since

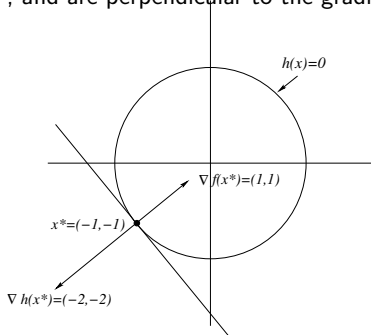
$$\nabla f(\mathbf{x}^*)^T \Delta \mathbf{x} = \sum_{i=1}^m \lambda_i \nabla h_i(\mathbf{x}^*)^T \Delta \mathbf{x} = 0.$$

Lagrange necessary conditions

Example

$$\begin{aligned} &\text{minimize} && f(x, y) = x + y, \\ &\text{subject to:} && h(x, y) = 2 - x^2 - y^2 = 0. \end{aligned}$$

At the local minimum $\mathbf{x}^* = (-1, -1)^T$, the first order feasible variations, $\nabla h_i(\mathbf{x}^*)^T \Delta \mathbf{x} = \Delta \mathbf{x}^T \nabla h_i(\mathbf{x}^*) = 0$, are the displacements, $\Delta \mathbf{x}$, tangent to the constraint circle at \mathbf{x}^* , and are perpendicular to the gradient of the cost function $\nabla f(\mathbf{x}^*)$.



In this example, the gradient of the cost function is also collinear with the gradient of the constraint $\nabla h(\mathbf{x}^*) = (-2, -2)^T$

$$\nabla f(\mathbf{x}^*) = (1/2)\nabla h(\mathbf{x}^*),$$

and the Lagrange multiplier is $\lambda = 1/2$.

Feasible variations

A point \mathbf{x} for which $h_1(\mathbf{x}) = 0, \dots, h_m(\mathbf{x}) = 0$ (feasible point) and such that the gradients $\nabla h_1(\mathbf{x}), \dots, \nabla h_m(\mathbf{x})$ **are linearly independent** is called **regular**.

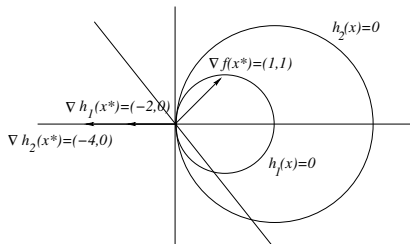
For a local minimum that is not regular there may not exist Lagrange multipliers.

Example. Consider the problem of minimizing

$$f(\mathbf{x}) = x + y$$

subject to

$$h_1(\mathbf{x}) = (x - 1)^2 + y^2 - 1 = 0, \quad h_2(\mathbf{x}) = (x - 2)^2 + y^2 - 4 = 0.$$



Note that in this example we have $m = n$ instead of $m < n$, but this is not relevant for what follows.

Example (cont.)

- Clearly, at the local minimum of f , $\mathbf{x}^* = (0, 0)^T$ (the only feasible solution), the cost gradient $\nabla f(\mathbf{x}^*) = (1, 1)^T$ cannot be expressed as a linear combination of the constraints gradients $\nabla h_1(\mathbf{x}^*) = (-2, 0)^T$ and $\nabla h_2(\mathbf{x}^*) = (-4, 0)^T$.

Thus, the Lagrange multiplier condition

$$\nabla f(\mathbf{x}^*) - \lambda_1^* \nabla h_1(\mathbf{x}^*) - \lambda_2^* \nabla h_2(\mathbf{x}^*) = 0,$$

cannot hold for any λ_1^* and λ_2^* .

- The difficulty here is that **the subspace of first order feasible variations**

$$V(\mathbf{x}^*) = \{\Delta \mathbf{x} \mid \nabla h_1(\mathbf{x}^*)^T \Delta \mathbf{x} = 0, \nabla h_2(\mathbf{x}^*)^T \Delta \mathbf{x} = 0\},$$

which is $\{\Delta \mathbf{x} = (0, y)^T\}$, **has larger dimension than the true set of feasible variations** $\{\Delta \mathbf{x} = (0, 0)^T\}$.

Lagrange's method

Theorem (Sufficient conditions).

*Let f, h_1, \dots, h_m be twice continuously differentiable real-valued functions in \mathbb{R}^n .
If there exist vectors $\mathbf{x}^* \in \mathbb{R}^n, \boldsymbol{\lambda}^* \in \mathbb{R}^m$ such that*

$$\nabla L(\mathbf{x}^*, \boldsymbol{\lambda}^*) = 0,$$

and for every $\mathbf{z} \in \mathbb{R}^n, \mathbf{z} \neq 0$ satisfying

$$(\nabla h_i(\mathbf{x}^*))^T \mathbf{z} = \mathbf{z}^T \nabla h_i(\mathbf{x}^*) = 0, \quad i = 1, \dots, m,$$

(\mathbf{z} is a feasible first order variation) it follows that

$$\mathbf{z}^T \nabla_{\mathbf{xx}}^2 L(\mathbf{x}^*, \boldsymbol{\lambda}^*) \mathbf{z} > 0,$$

then, f has a strict local minimum at \mathbf{x}^ subject to $h_i(\mathbf{x}) = 0, i = 1, \dots, m$
(similar for a maximum).*

We will see the proof of both theorems (necessary and sufficient conditions) later, when we also consider inequality constraints.

Sufficient conditions

Example.

Consider the problem:

$$\begin{array}{ll}\text{minimize} & f(\mathbf{x}) = -(x_1x_2 + x_2x_3 + x_1x_3), \\ \text{subject to:} & h(\mathbf{x}) = x_1 + x_2 + x_3 = 3.\end{array}$$

If x_1 , x_2 and x_3 represent the length, width and height of a rectangular parallelepiped P , respectively, the problem can be interpreted as maximizing the surface area of P subject to the sum of the edge lengths of P being equal to 3.

Since

$$L(\mathbf{x}, \lambda) = -(x_1x_2 + x_2x_3 + x_1x_3) - \lambda(x_1 + x_2 + x_3 - 3),$$

the first order necessary conditions ($\nabla L(\mathbf{x}^*, \lambda^*) = 0$) are

$$\begin{aligned}-x_2^* - x_3^* - \lambda^* &= 0, \\ -x_1^* - x_3^* - \lambda^* &= 0, \\ -x_1^* - x_2^* - \lambda^* &= 0, \\ x_1^* + x_2^* + x_3^* - 3 &= 0,\end{aligned}$$

which have the unique solution $x_1^* = x_2^* = x_3^* = 1$, $\lambda^* = -2$.

Sufficient conditions. Example (cont.)

The subspace of first order feasible variations V is

$$V = \{\mathbf{z} \mid \mathbf{z}^T \nabla h(\mathbf{x}^*) = 0\} = \left\{ \mathbf{z} \mid (z_1, z_2, z_3) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = 0 \right\} = \{\mathbf{z} \mid z_1 + z_2 + z_3 = 0\}$$

The Hessian of the Lagrangian is

$$\nabla_{\mathbf{xx}}^2 L(\mathbf{x}^*, \lambda^*) = \nabla_{\mathbf{xx}}^2 L\left((1, 1, 1)^T, -2\right) = \begin{pmatrix} 0 & -1 & -1 \\ -1 & 0 & -1 \\ -1 & -1 & 0 \end{pmatrix}.$$

We have for all $\mathbf{z} \in V$ with $\mathbf{z} \neq 0$, that

$$\mathbf{z}^T \nabla_{\mathbf{xx}}^2 L(\mathbf{x}^*, \lambda^*) \mathbf{z} = -z_1(z_2 + z_3) - z_2(z_1 + z_3) - z_3(z_1 + z_2) = z_1^2 + z_2^2 + z_3^2 > 0,$$

hence, the sufficient conditions for a strict local minimum

$$\mathbf{z}^T \nabla_{\mathbf{xx}}^2 L(\mathbf{x}^*, \lambda^*) \mathbf{z} > 0,$$

are satisfied.

First-order necessary conditions for inequality constrained extrema

We begin deriving **first-order** (involving only first derivatives) necessary conditions for **inequality and equality constrained extremum problems**.

- ▶ Consider the **general problem (P)** defined by

$$\begin{aligned} \min \quad & f(x_1, \dots, x_n) \\ \text{subject to:} \quad & g_i(x_1, \dots, x_n) \geq 0, \quad i = 1, \dots, p, \\ & h_j(x_1, \dots, x_n) = 0, \quad j = 1, \dots, m. \end{aligned} \quad (2)$$

The functions f , g_i , h_j are assumed to be defined and continuously differentiable on some open set $D \subset \mathbb{R}^n$.

- ▶ Let $X \subset D$ denote the **feasible set for problem (P)** this is, the set of all points $x \in D$ satisfying the constraints defined by (2). If $x \in X$, we say that x is a **feasible point**
- ▶ A point $x^* \in X$ is said to be a **local minimum of problem (P)**, if there exist $\delta > 0$ such that

$$f(x) \geq f(x^*), \quad \forall x \in X \cap N_\delta(x^*).$$

- ▶ If this condition holds for all $x \in X$

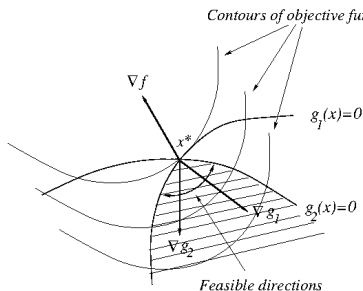
$$f(x) \geq f(x^*), \quad \forall x \in X$$

then x^* is said to be a **global minimum** of problem (P).

Feasible directions

- Note that every point $x \in N_\delta(x^*)$ can be written as $x^* + z$, where $z \neq 0$, if and only if $x \neq x^*$.
- A vector $z \neq 0$ is called a **feasible direction** from x^* if there exist $\delta_1 > 0$ such that

$$x^* + \theta z \in X \cap N_{\delta_1}(x^*) \quad \text{for all} \quad 0 \leq \theta < \delta_1 / \|z\|.$$



- Feasible directions are important in optimization algorithms. For the moment, we are interested in them for the simple reason that:

If x^ is a local minimum of problem (P), and if z is a feasible direction for x^* , then $f(x^* + \theta z) \geq f(x^*)$, if $\theta > 0$ is small enough.*

Feasible directions characterization

Recall that one set of constraints is given by $g_i(\mathbf{x}) \geq 0$, for $i = 1, \dots, p$.

Define the set of index $I(\mathbf{x}^*)$ as:

$$I(\mathbf{x}^*) = \{i \mid g_i(\mathbf{x}^*) = 0\}.$$

Lemma

If \mathbf{z} is a certain feasible direction, we must have

$$\mathbf{z}^T \nabla g_i(\mathbf{x}^*) \geq 0 \quad \text{for all } i \in I(\mathbf{x}^*)$$

Proof: Assume that for a certain $k \in I(\mathbf{x}^*)$ and a for a certain feasible direction \mathbf{z} from \mathbf{x}^* , that:

$$\mathbf{z}^T \nabla g_k(\mathbf{x}^*) < 0 \quad (\text{the angle is greater than } 90^\circ \text{ and less than } 270^\circ).$$

Then, since $k \in I(\mathbf{x}^*)$, we can write

$$g_k(\mathbf{x}^* + \theta \mathbf{z}) = g_k(\mathbf{x}^*) + \theta \mathbf{z}^T \nabla g_k(\mathbf{x}^*) + \theta \epsilon_k(\theta) = \theta \mathbf{z}^T \nabla g_k(\mathbf{x}^*) + \theta \epsilon_k(\theta),$$

with $\theta > 0$, and where $\epsilon_k(\theta)$ tends to zero as $\theta \rightarrow 0$.

If θ is small enough then, by hypothesis, $\mathbf{z}^T \nabla g_k(\mathbf{x}^*) + \epsilon_k(\theta) < 0$, so $g_k(\mathbf{x}^* + \theta \mathbf{z}) < 0$ for all $\theta > 0$ small enough, **contradicting the fact that \mathbf{z} is a feasible direction** vector from \mathbf{x}^* ($\mathbf{x}^* + \theta \mathbf{z} \in X \cap N_{\delta_1}(\mathbf{x}^*)$). So the claim is true.

Feasible directions characterization

For the equality constraints defined by $h_j(\mathbf{x}) = 0$, for $j = 1, \dots, m$, we have:

Lemma

If \mathbf{z} is a certain feasible direction, then

$$\mathbf{z}^T \nabla h_j(\mathbf{x}^*) = 0 \quad \text{for } j = 1, \dots, m.$$

The proof is similar to the reasoning of the previous lemma.

Feasible directions characterization

- Define

$$Z^1(\mathbf{x}^*) = \left\{ \mathbf{z} \mid \mathbf{z}^T \nabla g_i(\mathbf{x}^*) \geq 0, i \in I(\mathbf{x}^*) ; \mathbf{z}^T \nabla h_j(\mathbf{x}^*) = 0, j = 1, \dots, m \right\}.$$

According to what it has been said, if \mathbf{z} is a feasible direction for \mathbf{x}^* , then $\mathbf{z} \in Z^1(\mathbf{x}^*)$, but it may happen that $\mathbf{z} \in Z^1(\mathbf{x}^*)$ without being a feasible direction.

- Note that $0 \in Z^1(\mathbf{x}^*)$, so $Z^1(\mathbf{x}^*) \neq \emptyset$.
- A set $K \subset \mathbb{R}^n$ is called a **cone** if $\mathbf{x} \in K \Rightarrow \alpha \mathbf{x} \in K$ for all $\alpha \geq 0$.
- The set $Z^1(\mathbf{x}^*)$ is clearly a cone, and is also called the **linearizing cone of** the feasible set X at \mathbf{x}^* , since it is generated by linearizing the constraint functions at \mathbf{x}^* .
- Define

$$Z^2(\mathbf{x}^*) = \left\{ \mathbf{z} \mid \mathbf{z}^T \nabla f(\mathbf{x}^*) < 0 \right\}.$$

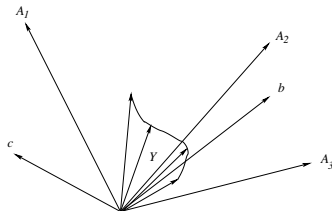
If $\mathbf{z} \in Z^2(\mathbf{x}^*)$, using Taylor's formula, it can be easily shown, using Taylor's formula, that there exist a point $\mathbf{x} = \mathbf{x}^* + \theta \mathbf{z}$, sufficiently close to \mathbf{x}^* , such that $f(\mathbf{x}^*) > f(\mathbf{x})$, this is, $Z^2(\mathbf{x}^*)$ is formed by the **directions along which the function f decreases**.

Farkas Lemma

Lemma

Let A be a given $m \times n$ real matrix and $\mathbf{b} \in \mathbb{R}^n$ a given vector. The inequality $\mathbf{b}^T \mathbf{y} \geq 0$ holds for all vectors $\mathbf{y} \in \mathbb{R}^n$ satisfying $A\mathbf{y} \geq \mathbf{0}$ if and only if there exists a vector $\boldsymbol{\rho} \in \mathbb{R}^m$, $\boldsymbol{\rho} \geq \mathbf{0}$, such that $A^T \boldsymbol{\rho} = \mathbf{b}$.

Interpretation: Let A be a 3×2 matrix and $A_1, A_2, A_3 \in \mathbb{R}^2$ the rows of A .



The set $Y = \{\mathbf{y} \mid A\mathbf{y} \geq \mathbf{0}\}$ consists of all the vectors $\mathbf{y} \in \mathbb{R}^2$ that make an acute angle with every row of A .

The Lemma states that \mathbf{b} makes an acute angle with every $\mathbf{y} \in Y$ if and only if \mathbf{b} can be expressed as a nonnegative linear combination of the rows of A .

In the figure, \mathbf{b} satisfies these conditions and \mathbf{c} does not.

Constrained optimization. Summary

- Consider the constrained optimization problem defined by

$$\begin{array}{ll}\min & f(x_1, \dots, x_n) \\ \text{subject to:} & h_i(x_1, \dots, x_n) = 0, \quad i = 1, \dots, m, \quad m < n\end{array}$$

- Lagrange's method consists of transforming an equality constrained extremum problem into a problem of finding a stationary point (x^*, λ^*) of the Lagrangian function

$$L(x, \lambda) = f(x) - \sum_{i=1}^m \lambda_i h_i(x)$$

- The necessary condition for the existence of a local minimum x^* of f in $N_\epsilon(x^*)$ is the existence of a vector of multipliers $\lambda^* = (\lambda_1^*, \dots, \lambda_m^*)^T$ such that

$$\nabla L(x^*, \lambda^*) = 0 \quad \Leftrightarrow \quad \nabla f(x^*) = \sum_{i=1}^m \lambda_i^* \nabla h_i(x^*)$$

Constrained optimization. Summary

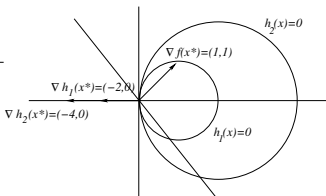
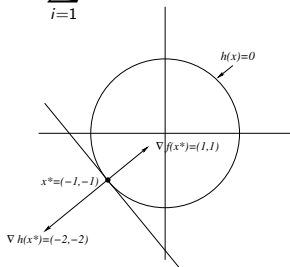
- The **first order feasible variations** at \mathbf{x}^* , $\Delta \mathbf{x}$ are defined as

$$V(\mathbf{x}^*) = \{\Delta \mathbf{x} \mid \nabla h_i(\mathbf{x}^*)^T \Delta \mathbf{x} = \Delta \mathbf{x}^T \nabla h_i(\mathbf{x}^*) = 0, i = 1, \dots, m\}$$

and satisfy the constraint in the linear approximation: $h(\mathbf{x}^* + \Delta \mathbf{x}) \approx 0$

- The necessary condition implies that **the gradient of the cost function** $\nabla f(\mathbf{x}^*)$ **is orthogonal to** $V(\mathbf{x}^*)$, since

$$\nabla f(\mathbf{x}^*) = \sum_{i=1}^m \lambda_i^* \nabla h_i(\mathbf{x}^*) \quad \Rightarrow \quad \nabla f(\mathbf{x}^*)^T \Delta \mathbf{x} = \sum_{i=1}^m \lambda_i \nabla h_i(\mathbf{x}^*)^T \Delta \mathbf{x} = 0.$$



In the second example $\nabla h_1(\mathbf{x}^*)$ and $\nabla h_2(\mathbf{x}^*)$ are not independent and λ^* does not exist

Constrained optimization. Summary

Theorem (Sufficient conditions).

Let f, h_1, \dots, h_m be twice continuously differentiable real-valued functions in \mathbb{R}^n .

If there exist vectors $\mathbf{x}^* \in \mathbb{R}^n$, $\boldsymbol{\lambda}^* \in \mathbb{R}^m$ such that for every **feasible first order variation** $\mathbf{z} \in \mathbb{R}^n$, $\mathbf{z} \neq 0$

$$\nabla L(\mathbf{x}^*, \boldsymbol{\lambda}^*) = 0, \quad (\nabla h_i(\mathbf{x}^*))^T \mathbf{z} = \mathbf{z}^T \nabla h_i(\mathbf{x}^*) = 0, \quad i = 1, \dots, m,$$

it follows that

$$\mathbf{z}^T \nabla_{\mathbf{xx}}^2 L(\mathbf{x}^*, \boldsymbol{\lambda}^*) \mathbf{z} > 0,$$

then, f has a strict local minimum at \mathbf{x}^* subject to $h_i(\mathbf{x}) = 0$, $i = 1, \dots, m$

Constrained optimization. Summary

The **general constrained optimization problem** (P) is defined by

$$\begin{array}{ll} \min & f(x_1, \dots, x_n) \\ \text{subject to:} & g_i(x_1, \dots, x_n) \geq 0, \quad i = 1, \dots, p \\ & h_j(x_1, \dots, x_n) = 0, \quad j = 1, \dots, m \end{array}$$

We look for a **feasible directions characterization** of this problem

Constrained optimization. Summary

Feasible directions characterization

- ▶ Given \mathbf{x}^* (not necessarily the solution of problem (P)), define the following sets

$$I(\mathbf{x}^*) = \{i \mid g_i(\mathbf{x}^*) = 0\}$$

$$Z^1(\mathbf{x}^*) = \left\{ \mathbf{z} \mid \mathbf{z}^T \nabla g_i(\mathbf{x}^*) \geq 0, i \in I(\mathbf{x}^*); \mathbf{z}^T \nabla h_j(\mathbf{x}^*) = 0, j = 1, \dots, m \right\} \neq \emptyset$$

$$Z^2(\mathbf{x}^*) = \left\{ \mathbf{z} \mid \mathbf{z}^T \nabla f(\mathbf{x}^*) < 0 \right\}$$

- ▶ If \mathbf{z} is a certain feasible direction, we have

$$\mathbf{z}^T \nabla g_i(\mathbf{x}^*) \geq 0, \quad i \in I(\mathbf{x}^*) \quad \text{and} \quad \mathbf{z}^T \nabla h_j(\mathbf{x}^*) = 0, \quad j = 1, \dots, m$$

- ▶ If \mathbf{z} is a feasible direction for \mathbf{x}^* , then $\mathbf{z} \in Z^1(\mathbf{x}^*)$, but it may happen that $\mathbf{z} \in Z^1(\mathbf{x}^*)$ without being a feasible direction
- ▶ If $\mathbf{z} \in Z^2(\mathbf{x}^*)$ it can be shown that there exist a point $\mathbf{x} = \mathbf{x}^* + \theta \mathbf{z}$, sufficiently close to \mathbf{x}^* , such that $f(\mathbf{x}^*) > f(\mathbf{x})$, this is, $Z^2(\mathbf{x}^*)$ is formed by the directions along which the function f decreases

Necessary conditions “candidates”

Define the Lagrangian associated with problem (P) as

$$L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\mathbf{x}) - \sum_{i=1}^p \lambda_i g_i(\mathbf{x}) - \sum_{j=1}^m \mu_j h_j(\mathbf{x}).$$

The following Theorem gives a candidate conditions to become the necessary conditions for \mathbf{x}^0 to be the solution of problem (P)

Theorem

Assume that $\mathbf{x}^0 \in X$, then $Z^1(\mathbf{x}^0) \cap Z^2(\mathbf{x}^0) = \emptyset$ **if and only if** there exist vectors $\boldsymbol{\lambda}^0, \boldsymbol{\mu}^0$ such that

$$\nabla_{\mathbf{x}} L(\mathbf{x}^0, \boldsymbol{\lambda}^0, \boldsymbol{\mu}^0) = \nabla f(\mathbf{x}^0) - \sum_{i=1}^p \lambda_i^0 \nabla g_i(\mathbf{x}^0) - \sum_{j=1}^m \mu_j^0 \nabla h_j(\mathbf{x}^0) = 0, \quad (3)$$

$$\lambda_i^0 g_i(\mathbf{x}^0) = 0, \quad i = 1, \dots, p \quad (4)$$

$$\lambda_i^0 \geq 0, \quad i = 1, \dots, p. \quad (5)$$

((3), (4) and (5) are called Lagrange conditions)

Remark 1: The condition $Z^1(\mathbf{x}^0) \cap Z^2(\mathbf{x}^0) = \emptyset$ implies that **there are no feasible directions along which f decreases**

Necessary conditions “candidates”*

Proof: The $Z^1(\mathbf{x}^0)$ is never empty, since $\mathbf{0} \in Z^1(\mathbf{x}^0)$. The condition $Z^1(\mathbf{x}^0) \cap Z^2(\mathbf{x}^0) = \emptyset$ holds if and only if for every \mathbf{z} satisfying

$$\mathbf{z}^T \nabla g_i(\mathbf{x}^0) \geq 0, \quad i \in I(\mathbf{x}^0), \quad (6)$$

$$\mathbf{z}^T \nabla h_j(\mathbf{x}^0) = 0, \quad j = 1, \dots, m, \quad (7)$$

we have

$$\mathbf{z}^T \nabla f(\mathbf{x}^0) \geq 0, \quad (8)$$

this is, if $\mathbf{z} \in Z^1(\mathbf{x}^0)$, then $\mathbf{z} \notin Z^2(\mathbf{x}^0)$.

We can write (7) as

$$\mathbf{z}^T \nabla h_j(\mathbf{x}^0) \geq 0, \quad j = 1, \dots, m \quad (9)$$

$$\mathbf{z}^T [-\nabla h_j(\mathbf{x}^0)] \geq 0, \quad j = 1, \dots, m \quad (10)$$

From Farkas Lemma, it follows that (8) holds for all vectors \mathbf{z} satisfying (6), (9) and (10) if and only if there exist vectors $\boldsymbol{\lambda}^0 \geq 0$, $\boldsymbol{\mu}^1 \geq 0$, $\boldsymbol{\mu}^2 \geq 0$ such that

$$\nabla f(\mathbf{x}^0) = \sum_{i \in I(\mathbf{x}^0)} \lambda_i^0 \nabla g_i(\mathbf{x}^0) + \sum_{j=1}^m (\mu_j^1 - \mu_j^2) \nabla h_j(\mathbf{x}^0).$$

Letting $\lambda_i^0 = 0$ for $i \notin I(\mathbf{x}^0)$, $\mu_j^0 = \mu_j^1 - \mu_j^2$, we conclude that $Z^1(\mathbf{x}^0) \cap Z^2(\mathbf{x}^0) = \emptyset$ if and only if (3), (4) and (5) hold. □

Some remarks

- ▶ The Lagrange conditions of the above Theorem are the natural candidates to become the necessary conditions for \mathbf{x}^0 to be the solution \mathbf{x}^* of problem (P) .
- ▶ According to them, we must guarantee that $Z^1(\mathbf{x}^*) \cap Z^2(\mathbf{x}^*) = \emptyset$ when \mathbf{x}^* is a solution of (P) . This condition (that will be characterized later) ensures that f can not decrease along any feasible direction.
- ▶ For most problems $Z^1(\mathbf{x}^*) \cap Z^2(\mathbf{x}^*) = \emptyset$, and then the Lagrange conditions (3), (4) and (5) hold at \mathbf{x}^* ; however, this is not always the case as the following example shows.
- ▶ Unfortunately, we can not state that if \mathbf{x}^0 is a solution of problem (P) and $Z^1(\mathbf{x}^0) \cap Z^2(\mathbf{x}^0) = \emptyset$, then the Lagrange conditions are satisfied, as we will see in the next example

Example

Example: Consider $\mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^2$, $f(\mathbf{x}) = -x_1$ with the following constraints:

$$g_1(\mathbf{x}) = (1 - x_1)^3 - x_2 \geq 0,$$

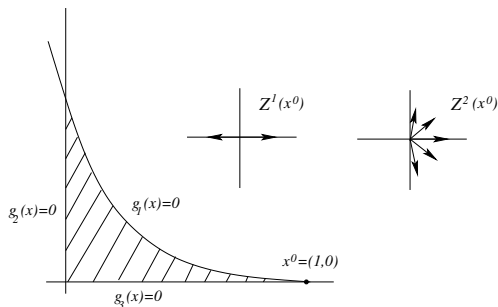
$$g_2(\mathbf{x}) = x_1 \geq 0,$$

$$g_3(\mathbf{x}) = x_2 \geq 0,$$

that define the feasible set X . The feasible point $\mathbf{x}^0 = (1, 0)^T$ is the solution of the problem

$$\max_{\mathbf{x}} x_1 = \min_{\mathbf{x}} (-x_1)$$

Let's see that $Z^1(\mathbf{x}^*) \cap Z^2(\mathbf{x}^*) \neq \emptyset$.

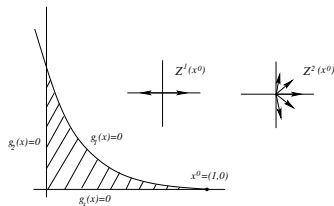


Example (cont.)

We can easily verify that

$$I(\mathbf{x}^0) = I((1, 0)^T) = \{1, 3\}, \quad \nabla g_1(\mathbf{x}^0) = (0, -1)^T, \quad \nabla g_3(\mathbf{x}^0) = (0, 1)^T$$

$$Z^1(\mathbf{x}^0) = \left\{ \mathbf{z} \in \mathbb{R}^2 \mid \mathbf{z}^T \nabla g_i(\mathbf{x}^0) \geq 0, i \in I(\mathbf{x}^0) \right\} = \left\{ \mathbf{z} = (z_1, z_2)^T \mid z_2 = 0 \right\}.$$



As we have seen, \mathbf{x}^0 is a solution of the constrained optimization problem. But at this point

$$Z^2(\mathbf{x}^0) = \left\{ \mathbf{z} \in \mathbb{R}^2 \mid \mathbf{z}^T \nabla f(\mathbf{x}^0) < 0 \right\} = \left\{ \mathbf{z} = (z_1, z_2)^T \mid z_1 > 0 \right\},$$

and

$$Z^1(\mathbf{x}^0) \cap Z^2(\mathbf{x}^0) = \left\{ \mathbf{z} \in \mathbb{R}^2 \mid z_1 > 0, z_2 = 0 \right\} \neq \emptyset,$$

hence, there exist no λ^0 satisfying Lagrange conditions (3), (4) and (5).

Weak necessary optimality conditions

It is possible to derive weak necessary conditions for optimality without requiring the set $Z^1(\mathbf{x}^*) \cap Z^2(\mathbf{x}^*)$ to be empty at the solution.

Let the **weak Lagrangian** \tilde{L} be defined by

$$\tilde{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = \lambda_0 f(\mathbf{x}) - \sum_{i=1}^p \lambda_i g_i(\mathbf{x}) - \sum_{j=1}^m \mu_j h_j(\mathbf{x}),$$

where λ_0 is an additional parameter.

To prove necessary conditions for equality and inequality constrained problems we need the following result, called “**Theorem of the Alternative**”.

Theorem

Let A be an $m \times n$ real matrix. Then, either there exists an $\mathbf{x} \in \mathbb{R}^n$ such that

$$A\mathbf{x} < \mathbf{0},$$

or there exists a nonzero vector $\mathbf{u} \in \mathbb{R}^m$, $\mathbf{u} \neq \mathbf{0}$ such that

$$\mathbf{u}^T A = \mathbf{0}, \quad \mathbf{u} \geq \mathbf{0},$$

but never both.

Theorem*

Proof: Assume that there exist \mathbf{x} and \mathbf{u} such that both

$$\mathbf{Ax} < 0, \quad \text{and} \quad \mathbf{u}^T \mathbf{A} = 0, \quad \mathbf{u} \geq 0$$

are satisfied. Then we have $\mathbf{u}^T \mathbf{Ax} < 0$, and $\mathbf{u}^T \mathbf{Ax} = 0$, simultaneously, which is a contradiction.

Assume now that there exist no \mathbf{x} satisfying the first condition ($\mathbf{Ax} < 0$), and let us see that we can find \mathbf{u} that satisfies the second condition of the Theorem. The assumption means that we cannot find a negative number $w < 0$ satisfying

$$(\mathbf{Ax})_i = A_i \mathbf{x} = \sum_{j=1}^n a_{ij} x_j \leq w, \quad i = 1, \dots, m,$$

for every $\mathbf{x} \in \mathbb{R}^n$, where A_i is the i th-row of A . This is, if for $i = 1, \dots, m$, and $\forall \mathbf{x} \in \mathbb{R}^n$

$$A_i \mathbf{x} \leq w \quad \Leftrightarrow \quad w - A_i \mathbf{x} \geq 0, \quad \text{then } w \geq 0.$$

Take $\mathbf{y} = (w, \mathbf{x})^T$, $\mathbf{b} = (1, 0, \dots, 0)^T \in \mathbb{R}^{n+1}$, $\mathbf{e} = (1, \dots, 1)^T \in \mathbb{R}^m$, and $\tilde{A} = (\mathbf{e} \mid -A)$.

Proof (cont.)*

Using this notation, what we have established is that: if for any $\mathbf{y} = (w, \mathbf{x})^T$ the following inequality is fulfilled

$$w - A_i \mathbf{x} = (\tilde{A} \mathbf{y})_i \geq 0, \quad i = 1, \dots, m, \quad \Leftrightarrow \quad \tilde{A} \mathbf{y} \geq 0,$$

then

$$w = \mathbf{b}^T \mathbf{y} \geq 0.$$

According to Farkas lemma, there exists a m -vector $\mathbf{u} \geq 0$, such that

$$\tilde{A}^T \mathbf{u} = \begin{pmatrix} 1 & \dots & 1 \\ & -A^T & \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_m \end{pmatrix} = \mathbf{b} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

so

$$\sum_{i=1}^m u_i = 1, \quad \sum_{i=1}^m u_i a_{ij} = 0, \quad j = 1, \dots, n,$$

hence, we have found \mathbf{u} that satisfies the second condition of the Theorem of the Alternative.



Weak necessary optimality conditions

We consider problem (P) when there are no equality constraints $h_i(\mathbf{x}) = 0$, $i = 1, \dots, m$, this is:

$$\min \quad f(x_1, \dots, x_n) \quad (P)$$

$$\text{subject to: } g_i(x_1, \dots, x_n) \geq 0, \quad i = 1, \dots, p,$$

Remark: The equality constraints become inequality constraints according to:

$$\begin{aligned} h_j(\mathbf{x}) &= g_{p+j}(\mathbf{x}) \geq 0, \quad j = 1, \dots, m, \\ -h_j(\mathbf{x}) &= g_{p+m+j}(\mathbf{x}) \geq 0, \quad j = 1, \dots, m. \end{aligned}$$

Theorem

Let f, g_1, \dots, g_m be real continuously differentiable functions on an open set containing X . If \mathbf{x}^* is a solution of problem (P), then there exist $\lambda^* = (\lambda_0^*, \lambda_1^*, \dots, \lambda_p^*)^T$ such that

$$\nabla_{\mathbf{x}} \tilde{L}(\mathbf{x}^*, \lambda^*) = \lambda_0^* \nabla f(\mathbf{x}^*) - \sum_{i=1}^p \lambda_i^* \nabla g_i(\mathbf{x}^*) = 0, \quad (11)$$

$$\lambda_i^* g_i(\mathbf{x}^*) = 0, \quad i = 1, \dots, p, \quad (12)$$

$$\lambda^* \neq 0, \quad \lambda^* \geq 0. \quad (13)$$

Theorem*

Proof: We must prove that the necessary conditions for \mathbf{x}^* to be the solution of problem (P), is the existence of a vector $\boldsymbol{\lambda}^*$ satisfying (11), (12) and (13).

If $g_i(\mathbf{x}^*) > 0$ for all i (the point \mathbf{x}^* is in the interior of the feasible set X), then $I(\mathbf{x}^*) = \{i \mid g_i(\mathbf{x}^*) = 0\} = \emptyset$. Choose $\lambda_0^* = 1$, $\lambda_1^* = \lambda_2^* = \dots = \lambda_p^* = 0$ and the conditions (11), (12) and (13) hold since $\nabla f(\mathbf{x}^*) = 0$.

Suppose now that $I(\mathbf{x}^*) \neq \emptyset$. Then, for every \mathbf{z} satisfying

$$\mathbf{z}^T \nabla g_i(\mathbf{x}^*) > 0, \quad i \in I(\mathbf{x}^*), \quad (14)$$

we **cannot** have

$$\mathbf{z}^T \nabla f(\mathbf{x}^*) < 0. \quad (15)$$

This follows from the following: According to Taylor's formula, we can see that if there exists \mathbf{z} satisfying (14), then we can find a sufficiently small δ such that if $0 < \theta < \delta$, then $\mathbf{x} = \mathbf{x}^* + \theta \mathbf{z}$ satisfies

$$g_i(\mathbf{x}) = g_i(\mathbf{x}^*) + \theta \mathbf{z}^T \nabla g_i(\mathbf{x}^*) + O_2,$$

and, since $g_i(\mathbf{x}^*) = 0$ we get

$$g_i(\mathbf{x}) > 0, \quad \text{if } i \in I(\mathbf{x}^*),$$

for all $0 < \theta < \delta$, that is, \mathbf{x} is a feasible point.

Proof (cont.)*

Now, if (15) also holds, then

$$f(\mathbf{x}) = f(\mathbf{x}^*) + \theta \mathbf{z}^T \nabla f(\mathbf{x}^*) + O_2 < f(\mathbf{x}^*),$$

contradicting that \mathbf{x}^* is a minimum.

Thus, the system of inequalities (14) and (15), that can also be written as

$$\begin{aligned} \mathbf{z}^T \nabla f(\mathbf{x}^*) &< 0, \\ \mathbf{z}^T [-\nabla g_i(\mathbf{x}^*)] &< 0, \quad i \in I(\mathbf{x}^*), \end{aligned}$$

has no solution. Using the matrix A with rows equal to $\nabla f(\mathbf{x}^*)$ and $-\nabla g_i(\mathbf{x}^*)$:

$$A = \begin{pmatrix} \nabla f(\mathbf{x}^*) \\ -\nabla g_{i_1}(\mathbf{x}^*) \\ \vdots \\ -\nabla g_{i_r}(\mathbf{x}^*) \end{pmatrix},$$

the above system of inequalities, which has no solution, can be written as $A\mathbf{z} < 0$. According to the Theorem of the Alternative, we get that there exists a nonzero vector $\boldsymbol{\lambda}^* \geq 0$, such that

$$(\boldsymbol{\lambda}^*)^T A = A^T \boldsymbol{\lambda}^* = \lambda_0^* \nabla f(\mathbf{x}^*) + \sum_{i \in I(\mathbf{x}^*)} \lambda_i^* [-\nabla g_i(\mathbf{x}^*)] = 0.$$

Proof (cont.)*

Letting $\lambda_i^* = 0$ for $i \notin I(\mathbf{x}^*)$, we can write this last equation as

$$\lambda_0^* \nabla f(\mathbf{x}^*) - \sum_{i=1}^p \lambda_i^* \nabla g_i(\mathbf{x}^*) = 0,$$

and clearly

$$\lambda_i^* g_i(\mathbf{x}^*) = 0, \quad i = 1, \dots, p.$$



Weak necessary optimality conditions

If we don't want to transform the equality constraints into inequalities, the following theorem also holds.

Theorem

Let f, h_1, \dots, h_m and g_1, \dots, g_p be real continuously differentiable functions on an open set containing X .

If \mathbf{x}^* is a solution of problem (P), then there exist $\boldsymbol{\lambda}^* = (\lambda_0^*, \lambda_1^*, \dots, \lambda_p^*)^T$ and $\boldsymbol{\mu}^* = (\mu_1^*, \dots, \mu_m^*)^T$ such that:

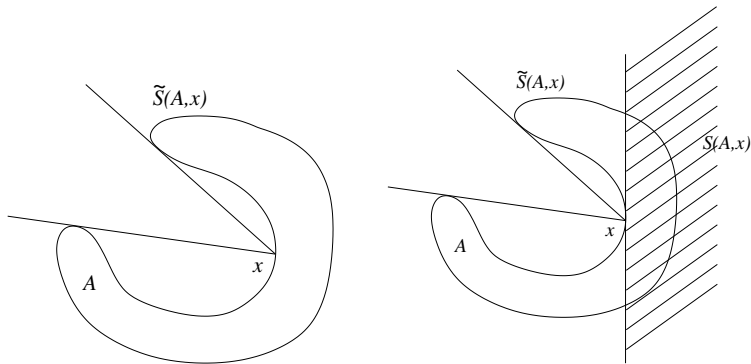
$$\begin{aligned}\nabla_{\mathbf{x}} \tilde{L}(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) &= \lambda_0^* \nabla f(\mathbf{x}^*) - \sum_{i=1}^p \lambda_i^* \nabla g_i(\mathbf{x}^*) - \sum_{j=1}^m \mu_j^* \nabla h_j(\mathbf{x}^*) = 0, \\ \lambda_i^* g_i(\mathbf{x}^*) &= 0, \quad i = 1, \dots, p, \\ (\boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) &\neq 0, \quad \lambda^* \geq 0.\end{aligned}$$

The closed cone of tangents

Let $\mathbf{x} \in A \subset \mathbb{R}^n$, where A is a nonempty set.

Define $\tilde{S}(A, \mathbf{x})$ as the intersection of all closed cones containing the set $\{\mathbf{a} - \mathbf{x} \mid \mathbf{a} \in A\}$, this is

$$\tilde{S}(A, \mathbf{x}) = \{\alpha(\mathbf{a} - \mathbf{x}) \mid \alpha \geq 0, \mathbf{a} \in A\}.$$

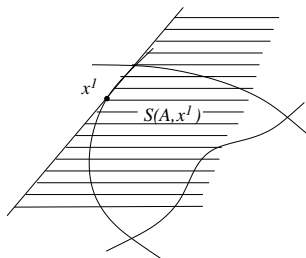
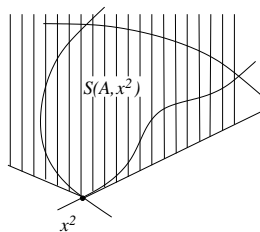


The closed cone of tangents

The **closed cone of tangents** of the set A at $x \in A$, $S(A, x)$, is defined as

$$S(A, x) = \bigcap_{k=1}^{\infty} \tilde{S}(A \cap N_{1/k}(x), x),$$

where $N_{1/k}(x)$ is a spherical neighborhood of x with radius $1/k$, $k \in \mathbb{N}$.



The following lemma characterizes $S(A, x)$.

The closed cone of tangents. Characterization

Lemma

A vector \mathbf{z} belongs to $S(A, \mathbf{x})$ if and only if there exists a sequence of vectors $\{\mathbf{x}^k\} \subset A$ converging to \mathbf{x} , and a sequence of nonnegative numbers $\{\alpha^k\}$ such that the sequence $\{\alpha^k(\mathbf{x}^k - \mathbf{x})\}$ converges to \mathbf{z} .

Proof: Assume that $\mathbf{z} \in S(A, \mathbf{x})$. Then $\mathbf{z} \in \tilde{S}(A \cap N_{1/k}(\mathbf{x}), \mathbf{x})$ for $k = 1, 2, \dots$, and, by definition:

$$\tilde{S}(A \cap N_{1/k}(\mathbf{x}), \mathbf{x}) = \text{cl}\{\alpha(\mathbf{y} - \mathbf{x}) \mid \alpha \geq 0, \mathbf{y} \in A \cap N_{1/k}(\mathbf{x})\}, \quad k = 1, 2, \dots, \quad (16)$$

where cl denotes the closure operation of sets in \mathbb{R}^n .

Choose any sequence of positive numbers $\{\epsilon^k\} \rightarrow 0$, and consider the vectors $\mathbf{z}(\epsilon^k) \in \{\alpha(\mathbf{y} - \mathbf{x}) \mid \alpha \geq 0, \mathbf{y} \in A \cap N_{1/k}(\mathbf{x})\}$ such that

$$\|\mathbf{z}(\epsilon^k) - \mathbf{z}\| \leq \epsilon^k. \quad (17)$$

Due to the condition (16), the points $\mathbf{z}(\epsilon^k)$ can be written as

$$\mathbf{z}(\epsilon^k) = \alpha(\epsilon^k)(\mathbf{y}(\epsilon^k) - \mathbf{x}), \quad \alpha(\epsilon^k) \geq 0, \quad \mathbf{y}(\epsilon^k) \in A \cap N_{1/k}(\mathbf{x}). \quad (18)$$

The closed cone of tangents. Characterization (cont.)*

Letting $k = 1, 2, \dots$ we generate a sequence of vectors $y(\epsilon^1), y(\epsilon^2), \dots$ that is contained in A and converges to x , and a sequence of nonnegative numbers $\alpha(\epsilon^1), \alpha(\epsilon^2), \dots$ such that, according to (17) and (18), the sequence $\{\alpha(\epsilon^k)(y(\epsilon^k) - x)\}$ converges to z .

Conversely, suppose that there exist a sequence of vectors $\{x^k\} \subset A$ converging to x and a sequence of nonnegative numbers $\{\alpha^k\}$ such that $\{\alpha^k(x^k - x)\}$ converges to z . Let p be any natural number. Then, there exists a natural number K such that $k \geq K$ implies $x^k \in A \cap N_{1/p}(x)$, so

$$\alpha^k(x^k - x) \in \tilde{S}(A \cap N_{1/p}(x)), \quad k \geq K,$$

and, since \tilde{S} is closed

$$z \in \tilde{S}(A \cap N_{1/p}(x)).$$

Since this last expression holds for any natural number p , it follows that

$$z \in \bigcap_{p \geq 1} \tilde{S}(A \cap N_{1/p}(x)) = S(A, x).$$



The closed cone of tangents

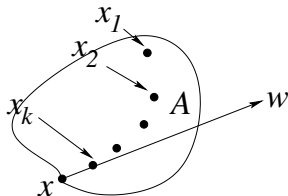
With the aid of this lemma, it is possible to give alternative descriptions of $S(A, x)$.

- First observe that the vector $w = 0$ is always in $S(A, x)$ for every A and x .
- Let w be a unit vector, and suppose that there exists a sequence of points $\{x^k\} \subset A$ such that: $x^k \rightarrow x$, $x^k \neq x$ and

$$\lim_{k \rightarrow \infty} \frac{x^k - x}{\|x^k - x\|} = w.$$

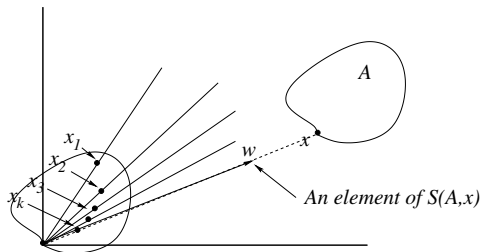
This is, a sequence of vectors $\{x^k\}$ converging to x in the direction of w .

- The cone of tangents of the set A at x contains all the vectors that are nonnegative multiples of the w obtained by this method.



The closed cone of tangents (second description)

- ▶ Translate the set A to the origin by subtracting x from each of its elements.
- ▶ Let $\{x^k\}$ be a sequence of the translated set, $x^k \neq \mathbf{0}$, converging to the origin.
- ▶ Construct a sequence of half-lines from the origin and passing through x^k .
- ▶ These half-lines tend to a half-line that will be a member of $S(A, x)$.
- ▶ The union of all the half-lines formed by taking all such sequences will then be the cone of tangents of A at x .



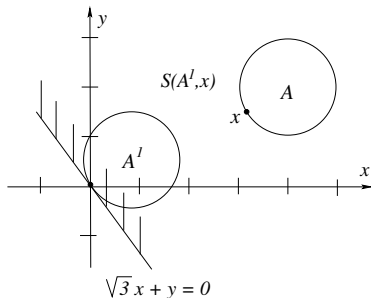
The closed cone of tangents. Example

Example: Consider the closed ball A with center at $(4, 2)$ and radius 1:

$$A = \{(x_1, x_2) \mid (x_1 - 4)^2 + (x_2 - 2)^2 \leq 1\}.$$

Let us find the cone of tangents of A at the boundary point

$$x = (4 - \sqrt{3}/2, 3/2)^T$$



First we translate A to the origin, obtaining the ball

$$A^1 = \{(x_1, x_2) \mid (x_1 - \sqrt{3}/2)^2 + (x_2 - 1/2)^2 \leq 1\}.$$

Taking sequences of points $\{x^k\}$ on the boundary of A^1 converging to the origin we generate sequences of half-lines converging to a line that is actually the tangent line to the circle A^1 at the origin.

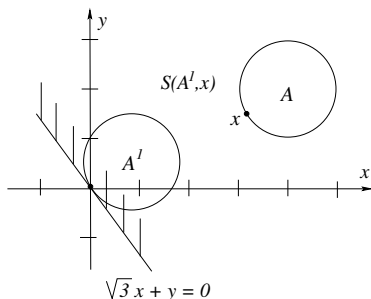
The closed cone of tangents. Example

The tangent line to the circle at the origin satisfies

$$\sqrt{3}x_1 + x_2 = 0.$$

Repeating this process for all sequences in the interior of A^1 converging to the origin, we get the cone of tangents of A^1 at 0 as

$$S(A^1, x) = \{(x_1, x_2) \mid \sqrt{3}x_1 + x_2 \geq 0\}.$$

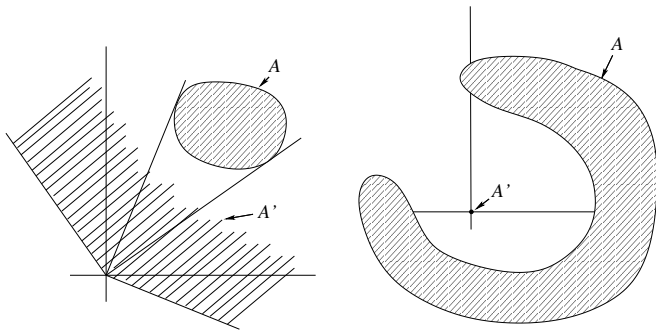


Positively normal cones

The next notion is the **positively normal cone** to a set $A \subset \mathbb{R}^n$, that will be denoted by A' , and is defined by

$$A' = \{x \in \mathbb{R}^n \mid x^T y \geq 0, \forall y \in A\},$$

This is, A' consists of **all vectors** $x \in \mathbb{R}^n$ **that make an angle less or equal to 90° with all $y \in A$.**



An important property of normal cones is the following: given two sets $A_1 \subset \mathbb{R}^n$, $A_2 \subset \mathbb{R}^n$, then

$$A_1 \subset A_2 \implies A_2' \subset A_1'.$$

Cones of tangents and positively normal cones

Cones of tangents and positively normal cones play a central role in establishing strong optimality conditions.

We have defined the positively normal cone to a set $A \subset \mathbb{R}^n$ as

$$A' = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x}^T \mathbf{y} \geq 0, \forall \mathbf{y} \in A\},$$

so, the positively normal cone of $Z^1(\mathbf{x}^0)$ is

$$(Z^1(\mathbf{x}^0))' = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{z}^T \mathbf{x} \geq 0, \forall \mathbf{z} \in Z^1(\mathbf{x}^0)\}.$$

Lemma

Let $\mathbf{x}^0 \in X$. The set $Z^1(\mathbf{x}^0) \cap Z^2(\mathbf{x}^0)$ is empty if and only if

$$\nabla f(\mathbf{x}^0) \in (Z^1(\mathbf{x}^0))'.$$

Proof: The set $Z^1(\mathbf{x}^0) \cap Z^2(\mathbf{x}^0)$ is empty if and only if for all $\mathbf{z} \in Z^1(\mathbf{x}^0)$ we have $\mathbf{z}^T \nabla f(\mathbf{x}^0) \geq 0$. This means that $\nabla f(\mathbf{x}^0)$ is contained in the positively normal cone of $Z^1(\mathbf{x}^0)$, that is $(Z^1(\mathbf{x}^0))'$. □

Cones of tangents and positively normal cones

Lemma

Assume that \mathbf{x}^0 is a solution of problem (P). Then

$$\nabla f(\mathbf{x}^0) \in (S(X, \mathbf{x}^0))'.$$

Remark: $(S(X, \mathbf{x}^0))'$ is the positively normal cone of the closed tangent cone of the feasible set X at the point \mathbf{x}^0 .

Proof: We must show that $\mathbf{z}^T \nabla f(\mathbf{x}^0) \geq 0$ for every $\mathbf{z} \in S(X, \mathbf{x}^0)$.

Let $\mathbf{z} \in S(X, \mathbf{x}^0)$. According to the previous characterization Lemma of the tangent cone (see page 33), there exists a sequence $\{\mathbf{x}^k\} \subset X$ converging to \mathbf{x}^0 and a sequence of nonnegative numbers $\{\alpha^k\}$ such that $\{\alpha^k(\mathbf{x}^k - \mathbf{x}^0)\}$ converges to \mathbf{z} .

Since f is differentiable at \mathbf{x}^0 , we can write

$$f(\mathbf{x}^k) = f(\mathbf{x}^0) + (\mathbf{x}^k - \mathbf{x}^0)^T \nabla f(\mathbf{x}^0) + \epsilon \|\mathbf{x}^k - \mathbf{x}^0\|,$$

where ϵ tends to zero as $k \rightarrow \infty$. Hence

$$\alpha^k(f(\mathbf{x}^k) - f(\mathbf{x}^0)) = (\alpha^k(\mathbf{x}^k - \mathbf{x}^0))^T \nabla f(\mathbf{x}^0) + \epsilon \|\alpha^k(\mathbf{x}^k - \mathbf{x}^0)\|.$$

Cones of tangents and positively normal cones (cont.)*

Since $\mathbf{x}^k \in X$, and \mathbf{x}^0 is a local minimum ($f(\mathbf{x}^k) - f(\mathbf{x}^0) \geq 0$ if k is large enough), it follows that, by letting $k \rightarrow \infty$, the term $\epsilon \|\alpha^k(\mathbf{x}^k - \mathbf{x}^0)\|$ in the above equation

$$\alpha^k(f(\mathbf{x}^k) - f(\mathbf{x}^0)) = (\alpha^k(\mathbf{x}^k - \mathbf{x}^0))^T \nabla f(\mathbf{x}^0) + \epsilon \|\alpha^k(\mathbf{x}^k - \mathbf{x}^0)\|,$$

goes to 0, and $\alpha^k(f(\mathbf{x}^k) - f(\mathbf{x}^0))$ converges to a non-negative limit. Thus

$$\lim_{k \rightarrow \infty} (\alpha^k(\mathbf{x}^k - \mathbf{x}^0))^T \nabla f(\mathbf{x}^0) = \mathbf{z}^T \nabla f(\mathbf{x}^0) \geq 0,$$

That is

$$\nabla f(\mathbf{x}^0) \in (S(X, \mathbf{x}^0))'.$$

□

The Kuhn-Tucker necessary optimality conditions

The (generalized) **Kuhn-Tucker necessary conditions** for optimality are given by the following theorem.

Theorem

Let \mathbf{x}^* be a solution of problem (P) and suppose that

$$(Z^1(\mathbf{x}^*))' = (S(X, \mathbf{x}^*))'. \quad (19)$$

Then, there exist $\boldsymbol{\lambda}^* = (\lambda_1^*, \dots, \lambda_p^*)^T$ and $\boldsymbol{\mu}^* = (\mu_1^*, \dots, \mu_m^*)^T$ such that

$$\nabla f(\mathbf{x}^*) - \sum_{i=1}^p \lambda_i^* \nabla g_i(\mathbf{x}^*) - \sum_{j=1}^m \mu_j^* \nabla h_j(\mathbf{x}^*) = 0, \quad (20)$$

$$\lambda_i^* g_i(\mathbf{x}^*) = 0, \quad i = 1, \dots, p, \quad (21)$$

$$\lambda^* \geq 0. \quad (22)$$

(Kuhn-Tucker conditions).

Proof: Suppose that \mathbf{x}^* is a solution of (P). According to a previous Lemma, $\nabla f(\mathbf{x}^*) \in (S(X, \mathbf{x}^*))'$. If $(Z^1(\mathbf{x}^*))' = (S(X, \mathbf{x}^*))'$, then $\nabla f(\mathbf{x}^*) \in (Z^1(\mathbf{x}^*))'$, and we have already seen that then $Z^1(\mathbf{x}^*) \cap Z^2(\mathbf{x}^*)$ is empty (see page 40).

According to the characterization theorem of the condition

$Z^1(\mathbf{x}^*) \cap Z^2(\mathbf{x}^*) = \emptyset$ (see page 18), conditions (20), (21) and (22) hold. \square

The Kuhn-Tucker necessary optimality conditions

Essentially, what the above theorem says is that the condition

$$(Z^1(\mathbf{x}^*))' = (S(X, \mathbf{x}^*))'$$

is a sufficient condition for the existence of the multipliers λ^* and μ^* satisfying conditions (20), (21) and (22).

Notice that if

$$Z^1(\mathbf{x}^*) = S(X, \mathbf{x}^*),$$

at a solution point \mathbf{x}^* of problem (P) implies the hypotheses of the last theorem.

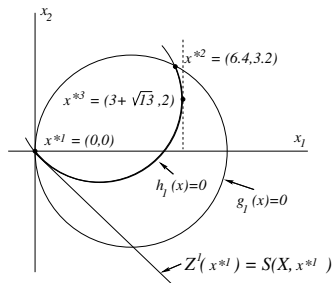
The Kuhn-Tucker necessary optimality conditions

Example: Consider the following problem

$$\min f(\mathbf{x}) = x_1,$$

subject to

$$g_1(\mathbf{x}) = 16 - (x_1 - 4)^2 - x_2^2 \geq 0, \quad h_1(\mathbf{x}) = (x_1 - 3)^2 + (x_2 - 2)^2 - 13 = 0.$$



From the figure it follows that f has local minima at $\mathbf{x}^{*1} = (0, 0)$ and $\mathbf{x}^{*2} = (32/5, 16/5)$. At both points, $l(\mathbf{x}^{*1}) = l(\mathbf{x}^{*2}) = \{1\}$. At the first point $\nabla g_1(\mathbf{x}^{*1}) = (8, 0)^T$, $\nabla h_1(\mathbf{x}^{*1}) = (-6, -4)^T$, so

$$\begin{aligned} Z^1(x^{*1}) &= \{z \mid z^T \nabla g_1(x^{*1}) \geq 0, z^T \nabla h_1(x^{*1}) = 0\} \\ &= \{(z_1, z_2) \mid z_1 \geq 0, z_2 = -(3/2)z_1\}, \end{aligned}$$

The Kuhn-Tucker necessary optimality conditions (cont.)

It can be verified that the set $Z^1(\mathbf{x}^{*1})$ is also $S(X, \mathbf{x}^{*1})$. Now

$$Z^2(\mathbf{x}^{*1}) = \{\mathbf{z} \mid \mathbf{z}^T \nabla f(\mathbf{x}^{*1}) < 0\} = \{(z_1, z_2) \mid z_1 < 0\},$$

hence $Z^1(\mathbf{x}^{*1}) \cap Z^2(\mathbf{x}^{*1}) = \emptyset$. The Kuhn-Tucker conditions (20), (21) and (22) are satisfied for $\lambda_1^* = 1/8$ and $\mu_1^* = 0$.

At the second point

$$Z^1(\mathbf{x}^{*2}) = \{(z_1, z_2) \mid z_1 \geq 0, z_2 = -(17/6)z_1\},$$

$$Z^2(\mathbf{x}^{*2}) = \{(z_1, z_2) \mid z_1 < 0\},$$

and again $Z^1(\mathbf{x}^{*2}) \cap Z^2(\mathbf{x}^{*2}) = \emptyset$. At this point $\lambda_1^* = 3/40$ and $\mu_1^* = 1/5$.

It turns out that at $\mathbf{x}^{*3} = (3 + \sqrt{13}, 2)$ the Kuhn-Tucker necessary conditions also hold. At this point $Z^1(\mathbf{x}^{*3}) \cap Z^2(\mathbf{x}^{*3}) = \emptyset$ and the corresponding multipliers are $\lambda_1^* = 0$ and $\mu_1^* = \sqrt{13}/26$.

From the above figure is clear that \mathbf{x}^{*3} is not a solution of our problem but is a solution of

$$\max f(\mathbf{x}) = x_1,$$

with the same constraints.

Second-order optimality conditions

Let us see optimality conditions for problem (P) that involve second derivatives.

We begin with the second-order necessary conditions that complement the above Kuhn–Tucker conditions; later we will give the sufficient conditions for optimality.

In what follows all the functions $f, g_1, \dots, g_p, h_1, \dots, h_m$ will be twice continuously differentiable.

Let $\mathbf{x} \in X$, we define the following modification of the set $Z^1(\mathbf{x})$:

$$\hat{Z}^1(\mathbf{x}) = \{\mathbf{z} \mid \mathbf{z}^T \nabla g_i(\mathbf{x}) = 0, i \in I(\mathbf{x}), \mathbf{z}^T \nabla h_j(\mathbf{x}) = 0, j = 1, \dots, m\}.$$

Recall that $Z^1(\mathbf{x})$ is

$$Z^1(\mathbf{x}) = \{\mathbf{z} \mid \mathbf{z}^T \nabla g_i(\mathbf{x}) \geq 0, i \in I(\mathbf{x}), \mathbf{z}^T \nabla h_j(\mathbf{x}) = 0, j = 1, \dots, m\}.$$

Second-order optimality conditions

Definition: The **second-order constraint qualification** is said to hold at $\mathbf{x}^0 \in X$ if for each $\mathbf{z} \in \hat{Z}^1(\mathbf{x}^0)$ there is a twice differentiable function

$$\alpha : [0, \epsilon] \subset \mathbb{R} \longrightarrow \mathbb{R}^n,$$

such that

$$\begin{aligned}\alpha(0) &= \mathbf{x}^0, \\ g_i(\alpha(t)) &= 0, \quad i \in I(\mathbf{x}^0), \\ h_j(\alpha(t)) &= 0, \quad j = 1, \dots, m,\end{aligned}$$

for $0 \leq t \leq \epsilon$ ($\alpha(t) \in X$) and

$$\frac{d\alpha(0)}{dt} = \lambda \mathbf{z},$$

for some positive $\lambda > 0$.

Since $\hat{Z}^1(\mathbf{x}^*)$ is a cone, we can always assume that $\lambda = 1$.

The above conditions mean that **every $\mathbf{z} \in \hat{Z}^1(\mathbf{x}^0)$, $\mathbf{z} \neq 0$, is tangent to a twice differentiable arc, α , contained in the boundary of X**

It can be shown that if $\nabla g_i(\mathbf{x})$, $i \in I(\mathbf{x})$, $\nabla h_j(\mathbf{x})$, $j = 1, \dots, p$, are linearly independent, then the *second-order constraint qualification* hold at $\mathbf{x} \in X$.

Second-order optimality conditions theorem

Theorem

Let \mathbf{x}^* be feasible for problem (P) that holds the second-order constraint qualification.

- ▶ If there exist $\boldsymbol{\lambda}^* = (\lambda_1^*, \dots, \lambda_p^*)^T$ and $\boldsymbol{\mu}^* = (\mu_1^*, \dots, \mu_m^*)^T$ satisfying the Kuhn–Tucker conditions (20), (21) and (22):

$$\begin{aligned}\nabla f(\mathbf{x}^*) - \sum_{i=1}^p \lambda_i^* \nabla g_i(\mathbf{x}^*) - \sum_{j=1}^m \mu_j^* \nabla h_j(\mathbf{x}^*) &= 0, \\ \lambda_i^* g_i(\mathbf{x}^*) &= 0, \quad i = 1, \dots, p, \\ \lambda^* &\geq 0,\end{aligned}$$

and

- ▶ If for every $\mathbf{z} \neq 0$ such that $\mathbf{z} \in \hat{Z}^1(\mathbf{x}^*)$, it follows that

$$\mathbf{z}^T \left[\nabla^2 f(\mathbf{x}^*) - \sum_{i=1}^p \lambda_i^* \nabla^2 g_i(\mathbf{x}^*) - \sum_{j=1}^m \mu_j^* \nabla^2 h_j(\mathbf{x}^*) \right] \mathbf{z} > 0, \quad (23)$$

then \mathbf{x}^* is a strict local minimum of problem (P).

Second-order optimality conditions theorem*

Proof: Let $\mathbf{z} \neq 0$ such that $\mathbf{z} \in \hat{Z}^1(\mathbf{x}^*)$ and $\alpha(t)$ the function that appears in the second order constraint qualification; that is

$$\alpha(0) = \mathbf{x}^*, \quad d\alpha(0)/dt = \mathbf{z}.$$

Let $d^2\alpha(0)/dt^2 = \mathbf{w}$. From the second order conditions and the chain rule it follows that for $i \in I(\mathbf{x}^*)$

$$\begin{aligned} \frac{dg_i(\alpha(0))}{dt} &= \mathbf{z}^T \nabla g_i(\mathbf{x}^*) \Rightarrow \\ \frac{d^2 g_i(\alpha(0))}{dt^2} &= \mathbf{z}^T \nabla^2 g_i(\mathbf{x}^*) \mathbf{z} + \mathbf{w}^T \nabla g_i(\mathbf{x}^*) = 0, \quad i \in I(\mathbf{x}^*), \end{aligned} \quad (24)$$

$$\begin{aligned} \frac{dh_j(\alpha(0))}{dt} &= \mathbf{z}^T \nabla h_j(\mathbf{x}^*) \Rightarrow \\ \frac{d^2 h_j(\alpha(0))}{dt^2} &= \mathbf{z}^T \nabla^2 h_j(\mathbf{x}^*) \mathbf{z} + \mathbf{w}^T \nabla h_j(\mathbf{x}^*) = 0, \quad j = 1, \dots, p. \end{aligned} \quad (25)$$

From condition (20), $\nabla_x L(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) = 0$, and the definition of $\hat{Z}^1(\mathbf{x}^*)$, we have

$$\frac{df(\alpha(0))}{dt} = \mathbf{z}^T \nabla f(\mathbf{x}^*) = \mathbf{z}^T \left[\sum_{i=1}^m \lambda_i^* \nabla g_i(\mathbf{x}^*) + \sum_{j=1}^p \mu_j^* \nabla h_j(\mathbf{x}^*) \right] = 0.$$

Second-order optimality conditions theorem (cont.)*

Since \mathbf{x}^* is a local minimum, and $df(\alpha(0))/dt = 0$, it follows that $d^2f(\alpha(0))/dt^2 \geq 0$, this is

$$\frac{d^2f(\alpha(0))}{dt^2} = \mathbf{z}^T \nabla^2 f(\mathbf{x}^*) \mathbf{z} + \mathbf{w}^T \nabla f(\mathbf{x}^*) \geq 0. \quad (26)$$

Multiplying (24) and (25) by the corresponding multipliers, subtracting from (26) and using the Kuhn–Tucker conditions (20), we get the desired inequality (23). □

Sufficient optimality conditions

Denote by $\bar{I}(\mathbf{x}^*)$ the set of indices i for which $g_i(\mathbf{x}^*) = 0$ and the Kuhn–Tucker conditions (20), (21) and (22) are satisfied by $\lambda_i^* > 0$.

Clearly $\bar{I}(\mathbf{x}^*) \subset I(\mathbf{x}^*)$. Let

$$\begin{aligned}\bar{Z}^1(\mathbf{x}^*) = \{ \mathbf{z} \mid & \mathbf{z}^T \nabla g_i(\mathbf{x}^*) = 0, i \in \bar{I}(\mathbf{x}^*), \\ & \mathbf{z}^T \nabla g_i(\mathbf{x}^*) \geq 0, i \in I(\mathbf{x}^*), \\ & \mathbf{z}^T \nabla h_j(\mathbf{x}^*) = 0, j = 1, \dots, m \}.\end{aligned}$$

Note that $\bar{Z}^1(\mathbf{x}^*) \subset Z^1(\mathbf{x}^*)$.

The following theorem gives sufficient optimality conditions

Sufficient optimality conditions

Theorem

Let \mathbf{x}^* be a feasible point for problem (P). If there exist $\boldsymbol{\lambda}^* = (\lambda_1^*, \dots, \lambda_p^*)^T$, $\boldsymbol{\mu}^* = (\mu_1^*, \dots, \mu_m^*)^T$ satisfying

$$\nabla_{\mathbf{x}} L(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) = \nabla f(\mathbf{x}^*) - \sum_{i=1}^p \lambda_i^* \nabla g_i(\mathbf{x}^*) - \sum_{j=1}^m \mu_j^* \nabla h_j(\mathbf{x}^*) = \mathbf{0}, \quad (27)$$

$$\lambda_i^* g_i(\mathbf{x}^*) = 0, \quad i = 1, \dots, p, \quad (28)$$

$$\lambda^* \geq 0, \quad (29)$$

and for every $\mathbf{z} \neq \mathbf{0}$, such that $\mathbf{z} \in \bar{Z}^1(\mathbf{x}^*)$ it follows that

$$\mathbf{z}^T \left[\nabla^2 f(\mathbf{x}^*) - \sum_{i=1}^p \lambda_i^* \nabla^2 g_i(\mathbf{x}^*) - \sum_{j=1}^m \mu_j^* \nabla^2 h_j(\mathbf{x}^*) \right] \mathbf{z} = \mathbf{z}^T \nabla_{\mathbf{x}}^2 L(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) \mathbf{z} > 0, \quad (30)$$

then, \mathbf{x}^* is a strict local minimum of problem (P).

Sufficient optimality conditions (cont.)*

Proof: Assume that the conditions (27), (28), (29) and (30) hold, and that \mathbf{x}^* is not a strict local minimum. Then, there exists a sequence $\{\mathbf{z}^k\}$ of feasible points, $\mathbf{z}^k \neq \mathbf{x}^*$, convergent to \mathbf{x}^* , such that for each \mathbf{z}^k

$$f(\mathbf{x}^*) \geq f(\mathbf{z}^k). \quad (31)$$

Let $\mathbf{z}^k = \mathbf{x}^* + \theta^k \mathbf{y}^k$, with $\theta^k > 0$ and $\|\mathbf{y}^k\| = 1$. Without loss of generality, assume that the sequence $\{(\theta^k, \mathbf{y}^k)\}$ converges to $(0, \bar{\mathbf{y}})$, where $\|\bar{\mathbf{y}}\| = 1$. Since the points \mathbf{z}^k are feasible

$$g_i(\mathbf{z}^k) - g_i(\mathbf{x}^*) = \theta^k (\mathbf{y}^k)^T \nabla g_i(\mathbf{x}^* + \eta_i^k \theta^k \mathbf{y}^k) \geq 0, \quad i \in I(\mathbf{x}^*), \quad (32)$$

$$h_j(\mathbf{z}^k) - h_j(\mathbf{x}^*) = \theta^k (\mathbf{y}^k)^T \nabla h_j(\mathbf{x}^* + \bar{\eta}_j^k \theta^k \mathbf{y}^k) = 0, \quad j = 1, \dots, p, \quad (33)$$

and from (31)

$$f(\mathbf{z}^k) - f(\mathbf{x}^*) = \theta^k (\mathbf{y}^k)^T \nabla f(\mathbf{x}^* + \eta^k \theta^k \mathbf{y}^k) \leq 0 \quad (34)$$

where η^k , η_i^k and $\bar{\eta}_j^k$ are numbers between 0 and 1. Dividing (32), (33) and (34) by $\theta^k > 0$, and taking limits, we get

$$\bar{\mathbf{y}}^T \nabla g_i(\mathbf{x}^*) \geq 0, \quad i \in I(\mathbf{x}^*), \quad (35)$$

$$\bar{\mathbf{y}}^T \nabla h_j(\mathbf{x}^*) = 0, \quad j = 1, \dots, p, \quad (36)$$

$$\bar{\mathbf{y}}^T \nabla f(\mathbf{x}^*) \leq 0. \quad (37)$$

Sufficient optimality conditions (cont.)*

Assume now that (35) holds with a strict inequality for some $i \in \bar{I}(\mathbf{x}^*)$. Then, from (27), (35) and (36) we get

$$\bar{\mathbf{y}}^T \nabla f(\mathbf{x}^*) = \sum_{i=1}^m \lambda_i^* \bar{\mathbf{y}}^T \nabla g_i(\mathbf{x}^*) + \sum_{j=1}^p \mu_j^* \bar{\mathbf{y}}^T \nabla h_j(\mathbf{x}^*) > 0,$$

contradicting (37). Therefore $\bar{\mathbf{y}}^T \nabla g_i(\mathbf{x}^*) = 0$ for all $i \in \bar{I}(\mathbf{x}^*)$, and so $\bar{\mathbf{y}} \in \bar{Z}^1(\mathbf{x}^*)$. From Taylor's formula we obtain

$$\begin{aligned} g_i(\mathbf{z}^k) &= g_i(\mathbf{x}^*) + \theta^k (\mathbf{y}^k)^T \nabla g_i(\mathbf{x}^*) \\ &\quad + \frac{1}{2} (\theta^k)^2 (\mathbf{y}^k)^T [\nabla^2 g_i(\mathbf{x}^* + \xi_i^k \theta^k \mathbf{y}^k)] \mathbf{y}^k \geq 0, \quad i = 1, \dots, m, \end{aligned} \quad (38)$$

$$\begin{aligned} h_j(\mathbf{z}^k) &= h_j(\mathbf{x}^*) + \theta^k (\mathbf{y}^k)^T \nabla h_j(\mathbf{x}^*) \\ &\quad + \frac{1}{2} (\theta^k)^2 (\mathbf{y}^k)^T [\nabla^2 h_j(\mathbf{x}^* + \bar{\xi}_j^k \theta^k \mathbf{y}^k)] \mathbf{y}^k = 0, \quad j = 1, \dots, p, \end{aligned} \quad (39)$$

$$\begin{aligned} f(\mathbf{z}^k) - f(\mathbf{x}^*) &= \theta^k (\mathbf{y}^k)^T \nabla f(\mathbf{x}^*) \\ &\quad + \frac{1}{2} (\theta^k)^2 (\mathbf{y}^k)^T [\nabla^2 f(\mathbf{x}^* + \xi^k \theta^k \mathbf{y}^k)] \mathbf{y}^k \leq 0, \end{aligned} \quad (40)$$

where ξ^k , ξ_i^k and $\bar{\xi}_j^k$ are again numbers between 0 and 1.

Sufficient optimality conditions (cont.)*

Multiplying (38) and (39) by λ_i^* and μ_j^* , respectively, and subtracting from (40), we obtain

$$\begin{aligned} & \theta^k (\mathbf{y}^k)^T \left\{ \nabla f(\mathbf{x}^*) - \sum_{i=1}^m \lambda_i^* \nabla g_i(\mathbf{x}^*) - \sum_{j=1}^p \mu_j^* \nabla h_j(\mathbf{x}^*) \right\} \\ & + \frac{1}{2} (\theta^k)^2 (\mathbf{y}^k)^T \left[\nabla^2 f(\mathbf{x}^* + \xi^k \theta^k \mathbf{y}^k) - \sum_{i=1}^m \lambda_i^* \nabla^2 g_i(\mathbf{x}^* + \xi_i^k \theta^k \mathbf{y}^k) - \right. \\ & \quad \left. \sum_{j=1}^p \mu_j^* \nabla^2 h_j(\mathbf{x}^* + \bar{\xi}_j^k \theta^k \mathbf{y}^k) \right] \mathbf{y}^k \leq 0. \end{aligned}$$

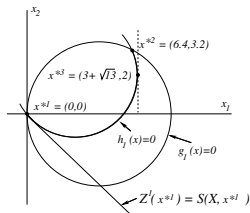
Since (27), the expression in braces (in the first line) vanishes. Dividing the remaining portion by $(\theta^k)^2/2$ and taking limits, we obtain

$$\bar{\mathbf{y}}^T \left[\nabla^2 f(\mathbf{x}^*) - \sum_{i=1}^m \lambda_i^* \nabla^2 g_i(\mathbf{x}^*) - \sum_{j=1}^p \mu_j^* \nabla^2 h_j(\mathbf{x}^*) \right] \bar{\mathbf{y}} \leq 0.$$

Since $\bar{\mathbf{y}} \neq 0$ and $\bar{\mathbf{y}} \in \bar{Z}^1(\mathbf{x}^*)$, it follows that this last inequality contradicts (30). □

The Kuhn-Tucker necessary optimality conditions

Example: Consider again the problem $\min f(x) = x_1$ of the figure



We have seen that there are (at least) three points satisfying the necessary conditions for optimality. Let us check the sufficient conditions.

At x^{*1} we have that

$$\overline{Z}^1(\mathbf{x}^{*1}) = \{0\},$$

and there are no vectors $\mathbf{z} \neq 0$ such that $\mathbf{z} \in \overline{\mathcal{Z}}^1(\mathbf{x}^{*1})$, so the sufficient conditions of the theorem are trivially satisfied. It can be seen that these conditions also hold at \mathbf{x}^{*2} .

At x^{*3} , however

$$\overline{Z}^1(\mathbf{x}^{*3}) = \{(z_1, z_2) \mid z_1 = 0\},$$

an the quadratic form that appears in the Theorem is $-(\sqrt{13}/13)\mathbf{z}^T \mathbf{z}$, which is negative for all $\mathbf{z} \neq 0$. Thus \mathbf{x}^{*3} does not satisfy the sufficient conditions.

Exercises

Exercise 7. To be delivered before 2-XII-2019 as: Ex07-YourSurname.pdf

Solve the two-dimensional problem

$$\text{minimize } (x - a)^2 + (y - b)^2 + xy,$$

$$\text{subject to } 0 \leq x \leq 1, \quad 0 \leq y \leq 1,$$

for all possible values of the scalars a and b .

Exercise 8. To be delivered before 2-XII-2019 as: Ex08-YourSurname.pdf

Given a vector \mathbf{y} , consider the problem

$$\text{maximize } \mathbf{y}^T \mathbf{x},$$

$$\text{subject to: } \mathbf{x}^T \mathbf{Q} \mathbf{x} \leq 1,$$

where \mathbf{Q} is a positive definite symmetric matrix. Show that the optimal value is $\sqrt{\mathbf{y}^T \mathbf{Q}^{-1} \mathbf{y}}$, and use this fact to establish the inequality

$$(\mathbf{x}^T \mathbf{y})^2 \leq (\mathbf{x}^T \mathbf{Q} \mathbf{x})(\mathbf{y}^T \mathbf{Q}^{-1} \mathbf{y}).$$

V'. Penalty methods for constrained optimization problems

Penalty function methods. General idea

- ▶ Consider the following **constrained optimization problem**: seek a minimum of a real-valued function f on a proper subset $X \subset \mathbb{R}^n$.
- ▶ This is problem **can be transformed into an unconstrained optimization one** after some modification of the objective function f .
- ▶ The method of **penalty functions** provides a way to attack constrained optimization problems using algorithms for unconstrained problems.
- ▶ Define

$$P(x) = \begin{cases} 0 & x \in X, \\ +\infty & x \notin X, \end{cases}$$

- ▶ Consider the unconstrained minimization of the **augmented objective function** F defined by

$$\min_{x \in \mathbb{R}^n} F(x) = \min_{x \in \mathbb{R}^n} (f(x) + P(x)),$$

where f is assumed to be defined on \mathbb{R}^n .

- ▶ The function P is called a **penalty function**, for it imposes an (infinite) penalty on points lying outside the feasible set X .
- ▶ Clearly, a point x^* minimizes F in \mathbb{R}^n if and only if it also minimizes f over X .

Penalty function methods. General idea

- ▶ In practice, the unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} (f(x) + P(x)),$$

cannot be, in general, carried out because:

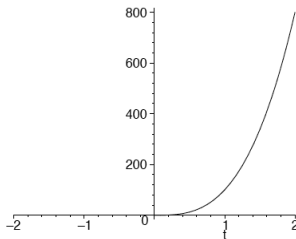
- ▶ The **discontinuity of F** on the boundary of X , and
 - ▶ The **infinite values outside X** .
- ▶ Replacing $+\infty$ by some large finite penalty will not simplify the problem, since the numerical difficulties would still remain.
 - ▶ The idea for solving these problems involves a **sequence of unconstrained minimization problems**.
 - ▶ In each problem of the sequence a **penalty parameter** is adjusted from one minimization to the next one.
 - ▶ The sequence of unconstrained minima converges to a feasible point of the constrained problem.

Penalty functions method. Example

- ▶ Consider minimizing the function $f(x) = x^4$ subject to the constraint $x \geq 1 \Leftrightarrow 1 - x \leq 0$.
- ▶ Here is how the method works, using the example above. Define a function $\phi(t)$ by

$$\phi(t) = \begin{cases} 0 & \text{for } t < 0 \\ kt^3 & \text{for } t \geq 0 \end{cases}$$

where k is some positive constant. The function ϕ is a penalty function. It penalizes any number t which is greater than zero (from the point of view of minimization).



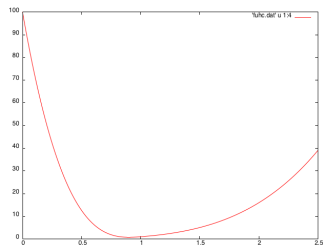
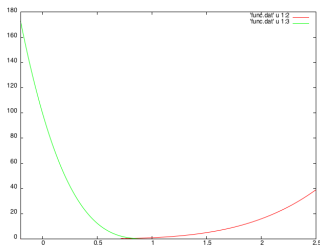
- ▶ The penalty function is also twice differentiable, even through zero.

Penalty functions method. Example

- ▶ Let's us attack the constrained problem by turning it into an unconstrained problem, as follows
- ▶ As we have already said, the constraint $x \geq 1$ is equivalent to $1 - x \leq 0$. Define a modified penalized objective function

$$\tilde{f}(x) = f(x) + \phi(1 - x) = x^4 + \phi(1 - x).$$

- ▶ The function $\tilde{f}(x)$ is identical to f if $1 - x \leq 0$, i.e., if $x \geq 1$, but rises sharply if $x < 1$. The additional $\phi(1 - x)$ term penalizes an optimization algorithm for choosing $x < 1$.



Plots of $f(x)$ and $\phi(1 - x)$ (left), and $\tilde{f}(x)$ with $k = 100$ (right)

Penalty functions method. Example

- ▶ We can approximately minimize $f(x)$ subject to the constraint $x \geq 1$ by running an unconstrained algorithm on the penalized objective function $\tilde{f}(x)$.
- ▶ The penalty term will strongly “encourage” the unconstrained algorithm to choose the best x which is greater than or equal to one.
- ▶ The penalty term is also twice differentiable, so it should not cause any trouble in an optimization algorithm which relies on first or second derivatives.
- ▶ The first and second derivatives of $\phi(t)$ are just

$$\phi'(t) = \begin{cases} 0 & \text{for } t < 0 \\ 3kt^2 & \text{for } t \geq 0 \end{cases} \quad \phi''(t) = \begin{cases} 0 & \text{for } t < 0 \\ 6kt & \text{for } t \geq 0 \end{cases}$$

- ▶ Running an unconstrained algorithm, like golden section, on $\tilde{f}(x)$ in this case (with $k = 100$) we find that the minimum is at $x = 0.9012$.

Penalty functions method. Example

- ▶ The penalty approach didn't exactly solve the problem, but it is reasonably close.
- ▶ In fact, a reasonable procedure would be to increase the constant k , say by a factor of 10, and then re-run the unconstrained algorithm on $\tilde{f}(x)$ using 0.9012 as the initial guess.
- ▶ Increasing k enforces the constrained more rigorously, while using the previous final iterate as an initial guess speeds up convergence (since we expect the minimum for the larger value of k isn't that far from the minimum for the previous value of k).
- ▶ In this case increasing k to 10^4 moves the minimum to $x = 0.989$.
- ▶ We could then increase k and use $x = 0.989$ as an initial guess, and continue this process until we obtain a reasonable estimate of the minimizer.

Penalty functions method. The general case

- ▶ In general we want to minimize a function $f(\mathbf{x})$ of n variables subject to both equality and inequality constraints of the form

$$\begin{aligned} g_i(\mathbf{x}) &\leq 0, & i = 1, \dots, m, \\ h_j(\mathbf{x}) &= 0, & j = 1, \dots, n. \end{aligned}$$

- ▶ The set of \mathbf{x} in n dimensional space which satisfy the constraints is called the **feasible set**, although it may be empty if the constraints are mutually contradictory.
- ▶ We will call $\phi(\lambda, t)$ for $\lambda \geq 0$, $t \in \mathbb{R}$ a **penalty function** if
 1. $\phi(t)$ is continuous.
 2. $\phi(\lambda, t) \geq 0$ for all λ and t .
 3. $\phi(\lambda, t) = 0$ for $t \leq 0$ and ϕ is strictly increasing for both $\lambda > 0$, $t > 0$.

It's also desirable if ϕ has at least one continuous derivative in t , preferably two.

Penalty functions method. The general case

- ▶ A typical **example of a penalty function** would be

$$\phi(\lambda, t) = \begin{cases} 0 & \text{for } t < 0 \\ \lambda t^n & \text{for } t \geq 0 \end{cases}$$

where $n \geq 1$.

- ▶ This function has $n - 1$ continuous derivatives in t , so taking $n = 3$ yields a C^2 penalty function.

Penalty functions method. The general case

- ▶ To minimize $f(\mathbf{x})$ subject to the above equality and inequality constraints, we define a modified objective function by

$$\tilde{f}(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^m \phi(\alpha_i, g_i(\mathbf{x})) + \sum_{j=1}^n [\phi(\beta_j, h_j(\mathbf{x})) + \phi(\beta_j, -h_j(\mathbf{x}))]$$

where the α_i and β_j are positive constants that control how strongly the constraints will be enforced.

- ▶ The penalty functions ϕ in **the first sum** modify the original objective function so that if any **inequality constraint** is violated, a large penalty is invoked; if all constraints are satisfied, no penalty.
- ▶ Similarly **the second summation** penalizes **equality constraints** which are not satisfied, by penalizing both $h_j(\mathbf{x}) < 0$ and $h_j(\mathbf{x}) > 0$.

Penalty functions method. The general case

- ▶ We minimize the function $\tilde{f}(\mathbf{x})$ with no constraints, and count on the penalty terms to keep the solution near the feasible set, although no finite choice for the penalty parameters keeps the solution in the feasible set.
- ▶ After having minimized $\tilde{f}(\mathbf{x})$ with an unconstrained method, for a given set of α_i and β_j , we may then increase the α_i and β_j and use the terminal iterate as the initial guess for a new minimization, and continue this process until we obtain a sufficiently accurate minimum.

Penalty functions method

Example:

- ▶ Let us minimize the function

$$f(x, y) = x^2 + y^2$$

subject to the inequality constraint $x + 2y \geq 6$ and the equality constraint $x - y = 3$.

- ▶ The constraints can be written as

$$\begin{aligned} g_1(x, y) &= 6 - x - 2y \leq 0, \\ h_1(x, y) &= 3 - x + y = 0. \end{aligned}$$

- ▶ We use the penalty function defined above with $\alpha_1 = 5$ and $\beta_1 = 5$ to start.
- ▶ The modified objective function is

$$\tilde{f}(x, y) = f(x, y) + \phi(5, g_1(x, y)) + \phi(5, h_1(x, y)) + \phi(5, -h_1(x, 5)).$$

Penalty functions method. Example

- ▶ Running a standard unconstrained algorithm on this we get that the minimum occurs at:

$$x = 3.506, \quad y = 1.001.$$

Note that the inequality and the equality constraints are violated:

$$6 - x - 2y = 0.449 > 0, \quad 3 - x + y = 0.494.$$

- ▶ To increase the accuracy with which the constraints are enforced we must increase the penalty parameters.
- ▶ It is convenient to use the final estimate from the previous penalty parameters as the initial guess for the larger parameters.
- ▶ With $\alpha_1 = \beta_1 = 50$ we obtain $x = 3.836$ and $y = 1.008$.
- ▶ Increasing $\alpha_1 = \beta_1 = 500$ we obtain $x = 3.947$, $y = 1.003$.
- ▶ The solution of the problem is $x = 4$, $y = 1$.

Penalty functions method. Example

- ▶ **Increasing the penalty parameters** does improve the accuracy of the final answer, but it will also **slows down the unconstrained algorithm's convergence**.
- ▶ If we **increase the values of the parameters**, then $\tilde{f}(x)$ will have a very **large gradient** and the algorithm will spend a lot of time hunting for an accurate minimum.
- ▶ Under appropriate assumptions **one can prove** that as the penalty parameters are increased without bound, **any convergent subsequence of solutions to the unconstrained penalized problems must converge to a solution of the original constrained problem**.

Pros and cons of penalty functions

Pros:

- ▶ The obvious advantage to the penalty function approach is that we obtain a **“hands-off” method for converting constrained problems of any type into unconstrained problems.**
- ▶ We **don't have to worry about finding an initial feasible point** (sometimes is a problem).
- ▶ Many constraints in the real world are “soft”, in the sense that they need not be satisfied precisely. The penalty function approach is well-suited to these type of problems.

Pros and cons of penalty functions

Cons:

- ▶ The drawback to penalty function methods is that **the solution to the unconstrained penalized problem will not be an exact solution to the original problem** (except in the limit, as mentioned above).
- ▶ In some cases, penalty methods can't be applied because the objective function is actually undefined outside the feasible set.
- ▶ As we **increase the penalty parameters** to more strictly enforce the constraints, the **unconstrained formulation becomes very illconditioned**, with large gradients and abrupt function changes.
- ▶ There are more efficient (but more elaborate and difficult) methods for approaching constrained optimization problems, we will see some of them by the end of this course.

Barrier function methods

- ▶ **Barrier function methods** are closely related to penalty function methods, and in fact might as well be considered a type of penalty function method.
- ▶ These methods are generally applicable **only to inequality constrained** optimization problems.
- ▶ Barrier methods have the advantage that they **always maintain feasible iterates**, unlike the penalty methods above.

Barrier function methods. The log barrier method

- ▶ The most common is the **log barrier** method.
- ▶ Suppose we have an objective function $f(\mathbf{x})$ with inequality constraints

$$g_i(\mathbf{x}) \leq 0, \text{ for } 1 \leq i \leq m.$$

- ▶ Construct a modified, or penalized, **objective function**:

$$\tilde{f}(\mathbf{x}) = f(\mathbf{x}) - \sum_{i=1}^m r_i \ln(-g_i(\mathbf{x})),$$

where the $r_i > 0$.

- ▶ Notice that $\tilde{f}(\mathbf{x})$ is undefined if any $g_i(\mathbf{x}) \geq 0$, so **we can only evaluate \tilde{f} in the interior of the feasible region**.
- ▶ However, even inside the feasible region the penalty term is non-zero, but it becomes an “anti-penalty” if $g_i(\mathbf{x}) \leq -1$ (recall that $\lim_{x \rightarrow \infty} \log(x) = -\infty$).
- ▶ Suppose we start some choice for the r_i and with initial feasible point \mathbf{x}_0 , and minimize \tilde{f} .

Then the terminal point \mathbf{x}_k , must be a feasible point, because the log terms in the definition of \tilde{f} form a barrier of infinite height which prevents the optimization routine from leaving the interior of the feasible region.

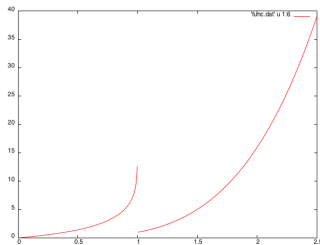
Barrier function methods

Example 1

Consider the objective function $f(t) = t^4$ and the constraint $t \geq 1$.

The penalized objective function is, taking $r_1 = 2$:

$$\tilde{f}(t) = t^4 - 2 \ln(t - 1)$$



A barrier method works in a similar way to the penalty methods above:

1. We start with some **positive** r_i and **feasible point** x_0 .
2. **Minimize** \tilde{f} using an **unconstrained algorithm**.
3. Next, **decrease the value of the** r_i and **re-optimize**, using the final iterate as an initial guess for the newly decreased r_i .
4. Continue until an acceptable minimum is found.

Barrier function methods

Example 2

Let

$$f(x, y) = x^2 + y^2$$

We want to minimize f subject to $6 - x - 2y \leq 0$.

- ▶ If we take $r_1 = 5$ in the definition of \tilde{f} , so

$$\tilde{f}(x, y) = x^2 + y^2 - 5 \ln(x + 2y - 6)$$

and start with feasible point $(5, 5)$ we obtain a minimum at $(1.53, 3.05)$.

- ▶ **Decreasing** r_i to 0.5 gives a minimum at $(1.24, 2.48)$, and decreasing r_i to 0.05 gives a minimum at $(1.204, 2.408)$
- ▶ The true minimum is at $(1.2, 2.4)$.

Remarks:

- ▶ One **issue** in using a barrier method is that of **finding an initial feasible point** which is in the interior of the feasible region. In many cases such a point will be obvious from considerations specific to the problem. If not, it can be rather difficult to find such a point.
- ▶ One idea **to find an initial point** would be to **use penalty functions, but on constraints** $g_i(\mathbf{x}) \leq -\delta < 0$ with $f = 0$. If a solution to this problem can be found with $\tilde{f}(\mathbf{a}) = 0$ then \mathbf{a} is a feasible point which is in the interior of the feasible region defined by $g_i(\mathbf{x}) \leq 0$