

Support Vector Machines - I

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UMB

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Functions of One Real Variable

Let E be a subset of \mathbb{R} .

A function $f : E \rightarrow \mathbb{R}$ has a **maximum** M on E if there exists $x_0 \in E$ such that $f(x_0) = M$ and $f(x_1) \leq M$ for every $x_1 \in E$. The element x_0 is a **maximizer** of f on E .

Similarly, $f : E \rightarrow \mathbb{R}$ has a **minimum** m on E if there exists $x_0 \in E$ such that $f(x_0) = m$ and $f(x_1) \geq m$ for every $x_1 \in E$. The element x_0 is a **minimizer** of f on E .

- If $f : [a, b] \rightarrow \mathbb{R}$ and f is continuous, then f has a global maximum M and a global minimum m on $[a, b]$.
- If f has a derivative on $[a, b]$, and $f'(x_0) = 0$, then x_0 is a **critical point** of f .
- A local extremum (minimum or maximum) can occur only at a critical point x_0 . If $f''(x_0) < 0$, the critical point provides a local maximum; if $f''(x_0) > 0$ the critical point provides a local minimum.

The ∇f notation

(read “nabla f ”).

Let $f : X \rightarrow \mathbb{R}$, where $X \subseteq \mathbb{R}^n$, and let $\mathbf{z} \in X$. The *gradient* of f in \mathbf{z} is the vector

$$(\nabla f)(\mathbf{z}) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(\mathbf{z}) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\mathbf{z}) \end{pmatrix} \in \mathbb{R}^n.$$

Example

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be the function $f(\mathbf{x}) = x_1^2 + \cdots + x_n^2$; in other words, $f(\mathbf{x}) = \|\mathbf{x}\|^2$.

We have

$$\frac{\partial f}{\partial x_1} = 2x_1, \dots, \frac{\partial f}{\partial x_n} = 2x_n.$$

Therefore, $(\nabla f)(\mathbf{x}) = 2\mathbf{x}$.

Example

Let $\mathbf{b}_j \in \mathbb{R}^n$ and $c_j \in \mathbb{R}$ for $1 \leq j \leq n$, and let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be the function

$$f(\mathbf{x}) = \sum_{j=1}^n (\mathbf{b}'_j \mathbf{x} - c_j)^2.$$

We have $\frac{\partial f}{\partial x_i}(\mathbf{x}) = \sum_{j=1}^n 2b_{ij}(\mathbf{b}'_j \mathbf{x} - c_j)$, where $\mathbf{b}_j = (b_{1j} \cdots b_{nj})$ for $1 \leq j \leq n$. Thus, we obtain:

$$(\nabla f)(\mathbf{x}) = 2 \begin{pmatrix} \sum_{j=1}^n 2b_{1j}(\mathbf{b}'_j \mathbf{x} - c_j) \\ \vdots \\ \sum_{j=1}^n 2b_{nj}(\mathbf{b}'_j \mathbf{x} - c_j) \end{pmatrix} = 2(\mathbf{B}'\mathbf{x} - \mathbf{c}')\mathbf{B} = 2\mathbf{B}'\mathbf{x}\mathbf{B} - 2\mathbf{c}'\mathbf{B},$$

where $\mathbf{B} = (\mathbf{b}_1 \cdots \mathbf{b}_n) \in \mathbb{R}^{n \times n}$.

The matrix-valued function $H_f : \mathbb{R}^k \longrightarrow \mathbb{R}^{k \times k}$ defined by

$$H_f(\mathbf{x}) = \left(\frac{\partial^2 f}{\partial x_{i_1} \partial x_{i_2}} \right)$$

is the *Hessian matrix* of f .

Example

For the function $f(\mathbf{x}) = x_1^2 + \cdots + x_n^2$ discussed on Slide 6 we have

$$H_f(\mathbf{x}) = \begin{pmatrix} 2 & 0 & \cdots & 0 \\ 0 & 2 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & 2 \end{pmatrix}.$$

Definition

Let X be an open subset in \mathbb{R}^n and let $f : X \rightarrow \mathbb{R}$ be a function.

The point $\mathbf{x}_0 \in X$ is a *local minimum* for f if there exists $\delta > 0$ such that $B(\mathbf{x}_0, \delta) \subseteq X$ and $f(\mathbf{x}_0) \leq f(\mathbf{x})$ for every $\mathbf{x} \in B(\mathbf{x}_0, \delta)$.

The point \mathbf{x}_0 is a *strict local minimum* if $f(\mathbf{x}_0) < f(\mathbf{x})$ for every $\mathbf{x} \in B(\mathbf{x}_0, \delta) - \{\mathbf{x}_0\}$.

Definition

A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is *positive semidefinite* if $\mathbf{x}'A\mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$.

A is *positive definite* if $\mathbf{x}'A\mathbf{x} > 0$ for all $\mathbf{x} \in \mathbb{R}^n - \{\mathbf{0}_n\}$.

Example

The symmetric real matrix

$$A = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$$

is positive definite if and only if $a > 0$ and $b^2 - ac < 0$. Indeed, we have $\mathbf{x}'A\mathbf{x} > 0$ for every $\mathbf{x} \in \mathbb{R}^2 - \{\mathbf{0}\}$ if and only if $ax_1^2 + 2bx_1x_2 + cx_2^2 > 0$, where $\mathbf{x}' = (x_1 \ x_2)$; elementary algebra considerations lead to $a > 0$ and $b^2 - ac < 0$.

Is the matrix

$$A = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$$

positive definite?

No, because $(x_1 \ x_2) \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = x_1^2 + 4x_1x_2 + x_2^2$ can be made negative with $x_1 = 1$ and $x_2 = -1$.

Theorem

A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is positive definite if and only if all its leading principal minors are positive.

The leading minors of the previous matrix are 1 and $\begin{vmatrix} 1 & 2 \\ 2 & 1 \end{vmatrix} = -3$.

Theorem

Let $f : B(\mathbf{x}_0, r) \rightarrow \mathbb{R}$ be a function that belongs to the class $C^2(B(\mathbf{x}_0, r))$, where $B(\mathbf{x}_0, r) \subseteq \mathbb{R}^k$ and \mathbf{x}_0 is a critical point for f . If the Hessian matrix $H_f(\mathbf{x}_0)$ is positive semidefinite, then \mathbf{x}_0 is a local minimum for f ; if $H_f(\mathbf{x}_0)$ is negative semidefinite, then \mathbf{x}_0 is a local maximum for f .

Let $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ be a function in $C^2(B(\mathbf{x}_0, r))$. The Hessian matrix in \mathbf{x}_0 is

$$H_f(\mathbf{x}_0) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{pmatrix}(\mathbf{x}_0).$$

Let $a_{11} = \frac{\partial^2 f}{\partial x_1^2}(\mathbf{x}_0)$, $a_{12} = \frac{\partial^2 f}{\partial x_1 \partial x_2}(\mathbf{x}_0)$, and $a_{22} = \frac{\partial^2 f}{\partial x_2^2}(\mathbf{x}_0)$. Note that

$$\begin{aligned} \mathbf{h}' H_f(\mathbf{x}_0) \mathbf{h} &= a_{11} h_1^2 + 2a_{12} h_1 h_2 + a_{22} h_2^2 \\ &= h_2^2 (a_{11} \xi^2 + 2a_{12} \xi + a_{22}), \end{aligned}$$

where $\xi = \frac{h_1}{h_2}$.

For a critical point \mathbf{x}_0 we have:

- $\mathbf{h}'H_f(\mathbf{x}_0)\mathbf{h} \geq 0$ for every \mathbf{h} if $a_{11} > 0$ and $a_{12}^2 - a_{11}a_{22} < 0$; in this case, $H_f(\mathbf{x}_0)$ is positive semidefinite and \mathbf{x}_0 is a local minimum;
- $\mathbf{h}'H_f(\mathbf{x}_0)\mathbf{h} \leq 0$ for every \mathbf{h} if $a_{11} < 0$ and $a_{12}^2 - a_{11}a_{22} < 0$; in this case, $H_f(\mathbf{x}_0)$ is negative semidefinite and \mathbf{x}_0 is a local maximum;
- if $a_{12}^2 - a_{11}a_{22} \geq 0$; in this case, $H_f(\mathbf{x}_0)$ is neither positive nor negative definite, so \mathbf{x}_0 is a saddle point.

Note that in the first two previous cases we have $a_{12}^2 < a_{11}a_{22}$, so a_{11} and a_{22} have the same sign.

Example

Let $\mathbf{a}_1, \dots, \mathbf{a}_m$ be m points in \mathbb{R}^n . The function $f(\mathbf{x}) = \sum_{i=1}^m \|\mathbf{x} - \mathbf{a}_i\|^2$ gives the sum of squares of the distances between \mathbf{x} and the points $\mathbf{a}_1, \dots, \mathbf{a}_m$. We will prove that this sum has a global minimum obtained when \mathbf{x} is the barycenter of the set $\{\mathbf{a}_1, \dots, \mathbf{a}_m\}$.

Example (cont'd)

We have

$$\begin{aligned} f(\mathbf{x}) &= m \|\mathbf{x}\|^2 - 2 \sum_{i=1}^m \mathbf{a}'_i \mathbf{x} + \sum_{i=1}^m \|\mathbf{a}_i\|^2 \\ &= m(x_1^2 + \cdots + x_n^2) - 2 \sum_{j=1}^n \sum_{i=1}^m a_{ij} x_j + \sum_{i=1}^m \|\mathbf{a}_i\|^2, \end{aligned}$$

which implies

$$\frac{\partial f}{\partial x_j} = 2mx_j - 2 \sum_{i=1}^m a_{ij}$$

for $1 \leq j \leq n$. Thus, there exists only one critical point given by

$$x_j = \frac{1}{m} \sum_{i=1}^m a_{ij}$$

for $1 \leq j \leq n$.

The Hessian matrix $H_f = 2mI_n$ is positive definite, so the critical point is a local minimum and, in view of convexity of f , the global minimum. This point is the barycenter of the set $\{\mathbf{a}_1, \dots, \mathbf{a}_m\}$.

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $\mathbf{c} : \mathbb{R}^n \rightarrow \mathbb{R}^m$, and $\mathbf{d} : \mathbb{R}^n \rightarrow \mathbb{R}^p$ be three functions defined on \mathbb{R}^n . A general formulation of a *constrained optimization problem* is:

$$\begin{aligned} & \text{minimize } f(\mathbf{x}), \text{ where } \mathbf{x} \in \mathbb{R}^n, \\ & \text{subject to } \mathbf{c}(\mathbf{x}) \leq \mathbf{0}_m, \text{ where } \mathbf{c} : \mathbb{R}^n \rightarrow \mathbb{R}^m, \\ & \text{and } \mathbf{d}(\mathbf{x}) = \mathbf{0}_p, \text{ where } \mathbf{d} : \mathbb{R}^n \rightarrow \mathbb{R}^p. \end{aligned}$$

Here \mathbf{c} specifies *inequality constraints* placed on \mathbf{x} , while \mathbf{d} defines *equality constraints*.

The *feasible region* of the constrained optimization problem is the set

$$R_{\mathbf{c},\mathbf{d}} = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{c}(\mathbf{x}) \leq \mathbf{0}_m \text{ and } \mathbf{d}(\mathbf{x}) = \mathbf{0}_p\}.$$

If the feasible region $R_{\mathbf{c},\mathbf{d}}$ is non-empty and bounded, then, under certain conditions a solution exists. If $R_{\mathbf{c},\mathbf{d}} = \emptyset$ we say that the constraints are *inconsistent*.

If only inequality constraints are present (as specified by the function \mathbf{c}) the feasible region is:

$$R_{\mathbf{c}} = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{c}(\mathbf{x}) \leq \mathbf{0}_m\}.$$

Let $\mathbf{x} \in R_{\mathbf{c}}$. The *set of active constraints* at \mathbf{x} is

$$\text{ACT}(R_{\mathbf{c}}, \mathbf{c}, \mathbf{x}) = \{i \in \{1, \dots, m\} \mid c_i(\mathbf{x}) = 0\}.$$

If $i \in \text{ACT}(R_{\mathbf{c}}, \mathbf{c}, \mathbf{x})$, we say that c_i is an *active constraint* or that c_i is *tight* on $\mathbf{x} \in S$; otherwise, that is, if $c_i(\mathbf{x}) < 0$, c_i is an *inactive* constraint on \mathbf{x} .

Definition

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $\mathbf{c} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be two functions. The **minimization problem $\text{MP}(f, \mathbf{c})$** is:

$$\begin{aligned} & \text{minimize } f(\mathbf{x}), \text{ where } \mathbf{x} \in \mathbb{R}^n, \\ & \text{subject to } \mathbf{x} \in R_{\mathbf{c}}. \end{aligned}$$

If \mathbf{x}_0 exists in $R_{\mathbf{c}}$ that $f(\mathbf{x}_0) = \min\{f(\mathbf{x}) \mid \mathbf{x} \in R_{\mathbf{c}}\}$ we refer to \mathbf{x}_0 as a solution of $\text{MP}(f, \mathbf{c})$.

If $\mathbf{h} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ we can write

$$\mathbf{h}(\mathbf{x}) = \begin{pmatrix} h_1(\mathbf{x}) \\ \vdots \\ h_m(\mathbf{x}) \end{pmatrix},$$

where $h_j : \mathbb{R}^n \rightarrow \mathbb{R}$ are the *components of \mathbf{h} for $1 \leq j \leq m$* . If \mathbf{h} is a differentiable function, the function $(D\mathbf{h})(\mathbf{x})$ is

$$(D\mathbf{h})(\mathbf{x}) = \begin{pmatrix} (\nabla h_1)(\mathbf{x})' \\ \vdots \\ (\nabla h_m)(\mathbf{x})' \end{pmatrix}.$$

Example

Let $\mathbf{h} : \mathbb{R}^2 \rightarrow \mathbb{R}^3$ be given by

$$\mathbf{h}(\mathbf{x}) = \begin{pmatrix} x_1 x_2 \\ x_1^2 \\ x_2^2 \end{pmatrix}$$

Then

$$(D\mathbf{h})(\mathbf{x}) = \begin{pmatrix} x_2 & x_1 \\ 2x_1 & 0 \\ 0 & 2x_2 \end{pmatrix}.$$

Observe that the rows of $(D\mathbf{h})(\mathbf{x})$ are the gradients of the components of \mathbf{h} .

Theorem

(Existence Theorem of Lagrange Multipliers) Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $\mathbf{h} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be two functions such that:

- $m < n$,
- $f \in C^1(\mathbb{R}^n)$,
- $\mathbf{h} \in C^1(\mathbb{R}^n)$, and
- the matrix $(D\mathbf{h})(\mathbf{x})$ is of full rank, that is, $\text{rank}((D\mathbf{h})(\mathbf{x})) = m < n$ (which means that the gradients $(\nabla h_1)(\mathbf{x}), \dots, (\nabla h_m)(\mathbf{x})$ are *linearly independent*).

If \mathbf{x}_0 is a regular point of \mathbf{h} and a local extremum of f subjected to the restriction $\mathbf{h}(\mathbf{x}_0) = \mathbf{0}_m$, then $(\nabla f)(\mathbf{x}_0)$ is a linear combination of $(\nabla h_1)(\mathbf{x}_0), \dots, (\nabla h_m)(\mathbf{x}_0)$.

Example

Suppose that we wish to minimize $f(\mathbf{x}) = x_1 + x_2$ subject to the condition

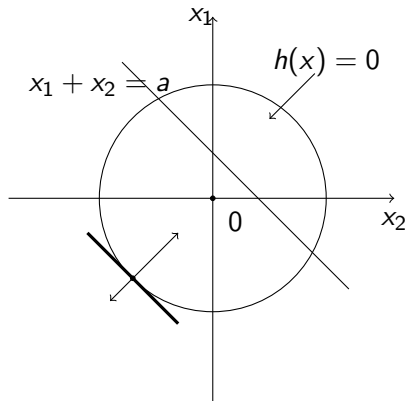
$$h(\mathbf{x}) = x_1^2 + x_2^2 = 2.$$

We have

$$(\nabla f)(\mathbf{x}) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$(\nabla h)(\mathbf{x}) = \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix}.$$

Example continued



At the local minimum $\mathbf{x}^* = (-1, -1)$
we have $(\nabla f)(\mathbf{x}^*) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and
 $(\nabla h) = \begin{pmatrix} -2 \\ -2 \end{pmatrix}$, so

$$(\nabla f)(\mathbf{x}^*) + \frac{1}{2}(\nabla h) = \mathbf{0}.$$

To apply the Lagrange multiplier technique the constraint gradients

$$(\nabla h_1)(\mathbf{x}), \dots, (\nabla h_m)(\mathbf{x})$$

must be linearly independent. In this case, \mathbf{x} is said to be **regular**.

There may not exist Lagrange multipliers for a local minimum that is not regular.

Example

Consider minimizing the function $f(\mathbf{x}) = x_1 + x_2$ subject to the constraints

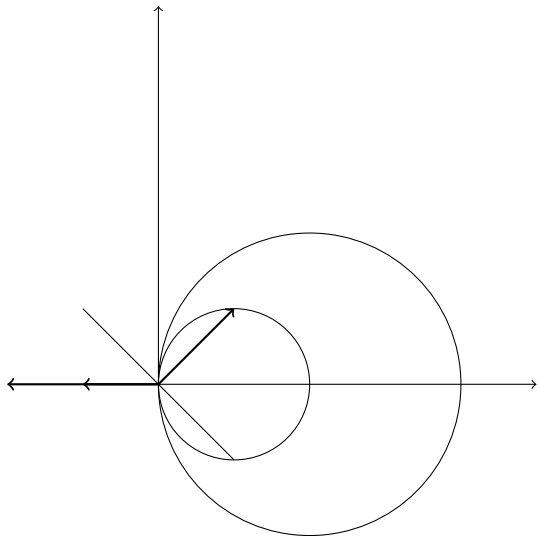
$$h_1(\mathbf{x}) = (x_1 - 1)^2 + x_2^2 - 1 = 0, h_2(\mathbf{x}) = (x_1 - 2)^2 + x_2^2 - 4 = 0.$$

We have

$$(\nabla f)(\mathbf{x}) = \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

and

$$(\nabla h_1)(\mathbf{x}) = \begin{pmatrix} 2(x_1 - 1) \\ 2x_2 \end{pmatrix}, (\nabla h_2)(\mathbf{x}) = \begin{pmatrix} 2(x_1 - 2) \\ 2x_2 \end{pmatrix}.$$



Example continued

The local minimum is at $\begin{pmatrix} 0 \\ 0 \end{pmatrix}$. At that point, we have

$$(\nabla f)(\mathbf{0}) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, (\nabla h_1)(\mathbf{0}) = \begin{pmatrix} -2 \\ 0 \end{pmatrix}, (\nabla h_2)(\mathbf{0}) = \begin{pmatrix} -4 \\ 0 \end{pmatrix}.$$

The gradients $(\nabla h_1)(\mathbf{0}), (\nabla h_2)(\mathbf{0})$ are not linearly independent, so $\mathbf{0}$ is not a regular point and Lagrange's multipliers do not exist.

Example

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix and let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be the function defined by $f(\mathbf{x}) = \mathbf{x}'A\mathbf{x}$.

Optimization problem: minimize f subjected to the restriction $\|\mathbf{x}\| = 1$, or equivalently $h(\mathbf{x}) = \|\mathbf{x}\|^2 - 1 = 0$.

Since $(\nabla f) = 2A\mathbf{x}$ and $(\nabla h)(\mathbf{x}) = 2\mathbf{x}$ there exists λ such that $2A\mathbf{x}_0 = 2\lambda\mathbf{x}_0$ for any extremum of f subjected to $\|\mathbf{x}_0\| = 1$. Thus, \mathbf{x}_0 must be a unit eigenvector of A and λ must be an eigenvalue of the same matrix.

The next theorem provides necessary conditions for optimality that

- include the linear independence of the gradients of the components of the constraint $(\nabla c_i)(\mathbf{x}_0)$ for $i \in \text{ACT}(S, \mathbf{c}, \mathbf{x}_0)$, and
- ensure that the coefficient of the gradient of the objective function $(\nabla f)(\mathbf{x}_0)$ is not null.

These conditions are known as the *Karush-Kuhn-Tucker conditions* or the *KKT conditions*.

Theorem

(Karush-Kuhn-Tucker Theorem) Let S be a non-empty open subset of \mathbb{R}^n and let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $\mathbf{c} : \mathbb{R}^n \rightarrow \mathbb{R}^m$. Let \mathbf{x}_0 be a local minimum in S of f subjected to the restriction $\mathbf{c}(\mathbf{x}_0) \leq \mathbf{0}_m$.

Suppose that f is differentiable in \mathbf{x}_0 , c_i are differentiable in \mathbf{x}_0 for $i \in \text{ACT}(S, \mathbf{c}, \mathbf{x}_0)$, and c_i are continuous in \mathbf{x}_0 for $i \notin \text{ACT}(S, \mathbf{c}, \mathbf{x}_0)$.

If $\{(\nabla c_i)(\mathbf{x}_0) \mid i \in \text{ACT}(S, \mathbf{c}, \mathbf{x}_0)\}$ is a linearly independent set, then there exist non-negative numbers w_i for $i \in \text{ACT}(S, \mathbf{c}, \mathbf{x}_0)$ such that

$$(\nabla f)(\mathbf{x}_0) + \sum \{w_i(\nabla c_i)(\mathbf{x}_0) \mid i \in \text{ACT}(S, \mathbf{c}, \mathbf{x}_0)\} = \mathbf{0}_n.$$

Theorem continued

Furthermore, if the functions c_i are differentiable in \mathbf{x}_0 for $i \notin \text{ACT}(S, \mathbf{c}, \mathbf{x}_0)$, then the previous condition can be written as:

- $(\nabla f)(\mathbf{x}_0) + \sum_{i=1}^m w_i (\nabla c_i)(\mathbf{x}_0) = \mathbf{0}_n$;
- $\mathbf{w}'\mathbf{c}(\mathbf{x}_0) = 0$;

- $\mathbf{w} \geq \mathbf{0}_m$, where $\mathbf{w} = \begin{pmatrix} w_1 \\ \vdots \\ w_m \end{pmatrix}$.

The Primal Problem

Consider the following optimization problem for an object function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, a subset $C \subseteq \mathbb{R}^n$, and the constraint functions

$\mathbf{c} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ and $\mathbf{d} : \mathbb{R}^n \rightarrow \mathbb{R}^p$:

$$\begin{aligned} & \text{minimize } f(\mathbf{x}), \text{ where } \mathbf{x} \in C, \\ & \text{subject to } \mathbf{c}(\mathbf{x}) \leq \mathbf{0}_m \\ & \text{and } \mathbf{d}(\mathbf{x}) = \mathbf{0}_p. \end{aligned}$$

We refer to this optimization problem as the *primal problem*.

Definition

The *Lagrangian* associated to the primal problem is the function $L : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \rightarrow \mathbb{R}$ given by:

$$L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = f(\mathbf{x}) + \mathbf{u}'\mathbf{c}(\mathbf{x}) + \mathbf{v}'\mathbf{d}(\mathbf{x})$$

for $\mathbf{x} \in C$, $\mathbf{u} \in \mathbb{R}^m$, and $\mathbf{v} \in \mathbb{R}^p$.

The component u_i of \mathbf{u} is the *Lagrangian multiplier* corresponding to the constraint $c_i(\mathbf{x}) \leq 0$; the component v_j of \mathbf{v} is the *Lagrangian multiplier* corresponding to the constraint $d_j(\mathbf{x}) = 0$.

Lemma

At each feasible \mathbf{x} we have

$$f(\mathbf{x}) = \sup\{L(\mathbf{x}, \mathbf{u}, \mathbf{v}) \mid \mathbf{u} \geq \mathbf{0}_m, \mathbf{v} \in \mathbb{R}^p, u_i c_i(\mathbf{x}) = 0 \text{ for } 1 \leq i \leq m\}.$$

Proof: at each feasible \mathbf{x} we have $c_i(\mathbf{x}) \leq 0$ and $d_i(\mathbf{x}) = 0$, hence

$$L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = f(\mathbf{x}) + \mathbf{u}'\mathbf{c}(\mathbf{x}) + \mathbf{v}'\mathbf{d}(\mathbf{x}) \leq f(\mathbf{x}).$$

The last inequality becomes an equality if $u_i c_i(\mathbf{x}) = 0$ for $1 \leq i \leq m$.

Lemma

The optimal value of the primal problem f^* is

$$f^* = \inf_{\mathbf{x}} \sup_{\mathbf{u} \geq \mathbf{0}_{m,\mathbf{v}}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}).$$

Proof: Consider feasible \mathbf{x} (designated as $\mathbf{x} \in C$). In this case we have

$$f^* = \inf_{\mathbf{x} \in C} f(\mathbf{x}) = \inf_{\mathbf{x} \in C} \sup_{\mathbf{u} \geq \mathbf{0}_{m,\mathbf{v}}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}).$$

When \mathbf{x} is not feasible, since $\sup_{\mathbf{u} \geq \mathbf{0}_{m,\mathbf{v}}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = \infty$ for any $\mathbf{x} \notin C$, we have $\inf_{\mathbf{x} \notin C} \sup_{\mathbf{u} \geq \mathbf{0}_{m,\mathbf{v}}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = \infty$. Thus, in either case,

$$f^* = \inf_{\mathbf{x}} \sup_{\mathbf{u} \geq \mathbf{0}_{m,\mathbf{v}}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}).$$

The Dual Optimization Problem

The *dual optimization problem* starts with the *Lagrange dual function* $g : \mathbb{R}^m \times \mathbb{R}^p \rightarrow \mathbb{R}$ defined by

$$g(\mathbf{u}, \mathbf{v}) = \inf_{\mathbf{x} \in C} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) \quad (1)$$

and consists of

maximize $g(\mathbf{u}, \mathbf{v})$, where $\mathbf{u} \in \mathbb{R}^m$ and $\mathbf{v} \in \mathbb{R}^p$,
subject to $\mathbf{u} \geq \mathbf{0}_m$.

Theorem

For every primal problem the Lagrange dual function $g : \mathbb{R}^m \times \mathbb{R}^p \rightarrow \mathbb{R}$ defined by Equality (1) is **always concave** over $\mathbb{R}^m \times \mathbb{R}^p$.

Proof

For $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^m$ and $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^p$ we have:

$$\begin{aligned} & g(t\mathbf{u}_1 + (1-t)\mathbf{u}_2, t\mathbf{v}_1 + (1-t)\mathbf{v}_2) \\ &= \inf\{f(\mathbf{x}) + (t\mathbf{u}'_1 + (1-t)\mathbf{u}'_2)\mathbf{c}(\mathbf{x}) + (t\mathbf{v}'_1 + (1-t)\mathbf{v}'_2)\mathbf{d}(\mathbf{x}) \mid \mathbf{x} \in S\} \\ &= \inf\{t(f(\mathbf{x}) + \mathbf{u}'_1\mathbf{c} + \mathbf{v}'_1\mathbf{d}) + (1-t)(f(\mathbf{x}) + \mathbf{u}'_2\mathbf{c}(\mathbf{x}) + \mathbf{v}'_2\mathbf{d}(\mathbf{x})) \mid \mathbf{x} \in S\} \\ &\geq t \inf\{f(\mathbf{x}) + \mathbf{u}'_1\mathbf{c} + \mathbf{v}'_1\mathbf{d} \mid \mathbf{x} \in S\} \\ &\quad + (1-t) \inf\{f(\mathbf{x}) + \mathbf{u}'_2\mathbf{c}(\mathbf{x}) + \mathbf{v}'_2\mathbf{d}(\mathbf{x}) \mid \mathbf{x} \in S\} \\ &= tg(\mathbf{u}_1, \mathbf{v}_1) + (1-t)g(\mathbf{u}_2, \mathbf{v}_2), \end{aligned}$$

which shows that g is concave.

- The concavity of g is significant because a local optimum of g is a global optimum regardless of convexity properties of f , \mathbf{c} or \mathbf{d} .
- Although the dual function g is not given explicitly, the restrictions of the dual have a simpler form and this may be an advantage in specific cases.
- The dual function produces lower bounds for the optimal value of the primal problem.

Theorem

(The Weak Duality Theorem) Suppose that x_* is an optimum of f and $f_* = f(x_*)$, $(\mathbf{u}_*, \mathbf{v}_*)$ is an optimum for g , and $g_* = g(\mathbf{u}_*, \mathbf{v}_*)$. We have $g_* \leq f_*$.

Proof: Since $\mathbf{c}(x_*) \leq \mathbf{0}_m$ and $\mathbf{d}(x_*) = \mathbf{0}_p$ it follows that

$$L(x_*, \mathbf{u}, \mathbf{v}) = f(x_*) + \mathbf{u}'\mathbf{c}(x_*) + \mathbf{v}'\mathbf{d}(x_*) \leq f_*.$$

Therefore, $g(\mathbf{u}, \mathbf{v}) = \inf_{\mathbf{x} \in C} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) \leq f_*$ for all \mathbf{u} and \mathbf{v} .

Since g_* is the optimal value of g , the last inequality implies $g_* \leq f_*$.

The inequality of the previous theorem holds when f_* and g_* are finite or infinite. The difference $f_* - g_*$ is the *duality gap* of the primal problem. *Strong duality* holds when the duality gap is 0.

Note that for the Lagrangian function of the primal problem we can write

$$\begin{aligned}\sup_{\mathbf{u} \geq \mathbf{0}_m, \mathbf{v}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) &= \sup_{\mathbf{u} \geq \mathbf{0}_m, \mathbf{v}} f(\mathbf{x}) + \mathbf{u}'\mathbf{c}(\mathbf{x}) + \mathbf{v}'\mathbf{d}(\mathbf{x}) \\ &= \begin{cases} f(\mathbf{x}) & \text{if } \mathbf{c}(\mathbf{x}) \leq \mathbf{0}_m, \\ \infty & \text{otherwise} \end{cases},\end{aligned}$$

which implies $f_* = \inf_{\mathbf{x} \in \mathbb{R}^n} \sup_{\mathbf{u} \geq \mathbf{0}_m, \mathbf{v}} L(\mathbf{x}, \mathbf{u}, \mathbf{v})$. By the definition of g_* we also have

$$g_* = \sup_{\mathbf{u} \geq \mathbf{0}_m, \mathbf{v}} \inf_{\mathbf{x} \in \mathbb{R}^n} L(\mathbf{x}, \mathbf{u}, \mathbf{v}).$$

Thus, the weak duality amounts to the inequality

$$\sup_{\mathbf{u} \geq \mathbf{0}_m, \mathbf{v}} \inf_{\mathbf{x} \in \mathbb{R}^n} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) \leq \inf_{\mathbf{x} \in \mathbb{R}^n} \sup_{\mathbf{u} \geq \mathbf{0}_m, \mathbf{v}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}),$$

and the strong duality is equivalent to the equality

$$\sup_{\mathbf{u} \geq \mathbf{0}_m, \mathbf{v}} \inf_{\mathbf{x} \in \mathbb{R}^n} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = \inf_{\mathbf{x} \in \mathbb{R}^n} \sup_{\mathbf{u} \geq \mathbf{0}_m, \mathbf{v}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}).$$

Example

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be the linear function $f(\mathbf{x}) = \mathbf{a}'\mathbf{x}$, $A \in \mathbb{R}^{p \times n}$, and $\mathbf{b} \in \mathbb{R}^p$. Consider the primal problem:

$$\begin{aligned} & \text{minimize } \mathbf{a}'\mathbf{x}, \text{ where } \mathbf{x} \in \mathbb{R}^n, \\ & \text{subject to } \mathbf{x} \geq \mathbf{0}_n \text{ and} \\ & \mathbf{A}\mathbf{x} - \mathbf{b} = \mathbf{0}_p. \end{aligned}$$

The constraint functions are $\mathbf{c}(\mathbf{x}) = -\mathbf{x}$ and $\mathbf{d}(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b}$ and the Lagrangian L is

$$\begin{aligned} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) &= \mathbf{a}'\mathbf{x} - \mathbf{u}'\mathbf{x} + \mathbf{v}'(\mathbf{A}\mathbf{x} - \mathbf{b}) \\ &= -\mathbf{v}'\mathbf{b} + (\mathbf{a}' - \mathbf{u}' + \mathbf{v}'\mathbf{A})\mathbf{x}. \end{aligned}$$

Example (cont'd)

This yields the dual function

$$g(\mathbf{u}, \mathbf{v}) = -\mathbf{v}'\mathbf{b} + \inf_{\mathbf{x} \in \mathbb{R}^n} (\mathbf{a}' - \mathbf{u}' + \mathbf{v}'A)\mathbf{x}.$$

Unless $\mathbf{a}' - \mathbf{u}' + \mathbf{v}'A = \mathbf{0}'_n$ we have $g(\mathbf{u}, \mathbf{v}) = -\infty$. Therefore, we have

$$g(\mathbf{u}, \mathbf{v}) = \begin{cases} -\mathbf{v}'\mathbf{b} & \text{if } \mathbf{a} - \mathbf{u} + A'\mathbf{v} = \mathbf{0}_n, \\ -\infty & \text{otherwise.} \end{cases}$$

Thus, the dual problem is

$$\begin{aligned} & \text{maximize } g(\mathbf{u}, \mathbf{v}), \\ & \text{subject to } \mathbf{u} \geq \mathbf{0}_m. \end{aligned}$$

Example (cont'd)

An equivalent of the dual problem is

$$\begin{aligned} & \text{maximize } -\mathbf{v}'\mathbf{b}, \\ & \text{subject to } \mathbf{a} - \mathbf{u} + A'\mathbf{v} = \mathbf{0}_n \\ & \text{and } \mathbf{u} \geq \mathbf{0}_m. \end{aligned}$$

In turn, this problem is equivalent to:

$$\begin{aligned} & \text{maximize } -\mathbf{v}'\mathbf{b}, \\ & \text{subject to } \mathbf{a} + A'\mathbf{v} \geq \mathbf{0}_n. \end{aligned}$$

Example

The following optimization problem

$$\begin{aligned} & \text{minimize } \frac{1}{2} \mathbf{x}' Q \mathbf{x} - \mathbf{r}' \mathbf{x}, \\ & \text{where } \mathbf{x} \in \mathbb{R}^n, \\ & \text{subject to } A \mathbf{x} \geq \mathbf{b}, \end{aligned}$$

where $Q \in \mathbb{R}^{n \times n}$ is a positive definite matrix, $\mathbf{r} \in \mathbb{R}^n$, $A \in \mathbb{R}^{p \times n}$, and $\mathbf{b} \in \mathbb{R}^p$ is known as a *quadratic optimization problem*.

The Lagrangian L is

$$L(\mathbf{x}, \mathbf{u}) = \frac{1}{2}\mathbf{x}'Q\mathbf{x} - \mathbf{r}'\mathbf{x} + \mathbf{u}'(A\mathbf{x} - \mathbf{b}) = \frac{1}{2}\mathbf{x}'Q\mathbf{x} + (\mathbf{u}'A - \mathbf{r}')\mathbf{x} - \mathbf{u}'\mathbf{b}$$

and the dual function is $g(\mathbf{u}) = \inf_{\mathbf{x} \in \mathbb{R}^n} L(\mathbf{x}, \mathbf{u})$ subject to $\mathbf{u} \geq \mathbf{0}_m$. Since \mathbf{x} is unconstrained in the definition of g , the minimum is attained when we have the equalities

$$\frac{\partial}{\partial x_i} \left(\frac{1}{2}\mathbf{x}'Q\mathbf{x} + (\mathbf{u}'A - \mathbf{r}')\mathbf{x} - \mathbf{u}'\mathbf{b} \right) = 0$$

for $1 \leq i \leq n$, which amount to $\mathbf{x} = Q^{-1}(\mathbf{r} - A\mathbf{u})$. The dual optimization function is: $g(\mathbf{u}) = -\frac{1}{2}\mathbf{u}'P\mathbf{u} - \mathbf{u}'\mathbf{d} - \frac{1}{2}\mathbf{r}'Q\mathbf{r}$ subject to $\mathbf{u} \geq \mathbf{0}_p$, where $P = AQ^{-1}A'$, $\mathbf{d} = \mathbf{b} - AQ^{-1}\mathbf{r}$. This shows that the dual problem of this quadratic optimization problem is itself a quadratic optimization problem.

Example

Let $\mathbf{a}_1, \dots, \mathbf{a}_m \in \mathbb{R}^n$. We seek to determine a closed sphere $B[\mathbf{x}, r]$ of minimal radius that includes all points \mathbf{a}_i for $1 \leq i \leq m$. This is the *minimum bounding sphere* problem, formulated by J. J. Sylvester. This problem amounts to solving the following primal optimization problem:

minimize r , where $r \geq 0$,

subject to $\|\mathbf{x} - \mathbf{a}_i\| \leq r$ for $1 \leq i \leq m$.

An equivalent formulation requires minimizing r^2 and stating the restrictions as $\| \mathbf{x} - \mathbf{a}_i \|^2 - r^2 \leq 0$ for $1 \leq i \leq m$. The Lagrangian of this problem is:

$$\begin{aligned} L(r, \mathbf{x}, \mathbf{u}) &= r^2 + \sum_{i=1}^m u_i (\| \mathbf{x} - \mathbf{a}_i \|^2 - r^2) \\ &= r^2 \left(1 - \sum_{i=1}^m u_i \right) + \sum_{i=1}^m u_i \| \mathbf{x} - \mathbf{a}_i \|^2 \end{aligned}$$

and the dual function is:

$$\begin{aligned} g(\mathbf{u}) &= \inf_{r \in \mathbb{R}_{\geq 0}, \mathbf{x} \in \mathbb{R}^n} L(r, \mathbf{x}, \mathbf{u}) \\ &= \inf_{r \in \mathbb{R}_{\geq 0}, \mathbf{x} \in \mathbb{R}^n} r^2 \left(1 - \sum_{i=1}^m u_i \right) + \sum_{i=1}^m u_i \| \mathbf{x} - \mathbf{a}_i \|^2 . \end{aligned}$$

This leads to the following conditions:

$$\frac{\partial L(r, \mathbf{x}, \mathbf{u})}{\partial r} = 2r \left(1 - \sum_{i=1}^m u_i \right) = 0$$

$$\frac{\partial L(r, \mathbf{x}, \mathbf{u})}{\partial x_p} = 2 \sum_{i=1}^m u_i (\mathbf{x} - \mathbf{a}_i)_p = 0 \text{ for } 1 \leq p \leq n.$$

The first equality yields $\sum_{i=1}^m u_i = 1$. Therefore, from the second equality we obtain $\mathbf{x} = \sum_{i=1}^m u_i \mathbf{a}_i$. This shows that for \mathbf{x} is a convex combination of $\mathbf{a}_1, \dots, \mathbf{a}_m$. The dual function is

$$g(\mathbf{u}) = \sum_{i=1}^m u_i \left(\sum_{h=1}^m u_h \mathbf{a}_h - \mathbf{a}_i \right) = 0$$

because $\sum_{i=1}^m u_i = 1$.

Note that the restriction functions $g_i(\mathbf{x}, r) = \|\mathbf{x} - \mathbf{a}_i\|^2 - r^2 \leq 0$ are *not convex*.

Example

Consider the primal problem

$$\begin{aligned} & \text{minimize } x_1^2 + x_2^2, \text{ where } x_1, x_2 \in \mathbb{R}, \\ & \text{subject to } x_1 - 1 \geq 0. \end{aligned}$$

It is clear that the minimum of $f(\mathbf{x})$ is obtained for $x_1 = 1$ and $x_2 = 0$ and this minimum is 1. The Lagrangian is

$$L(\mathbf{u}) = x_1^2 + x_2^2 + u_1(x_1 - 1)$$

and the dual function is

$$g(\mathbf{u}) = \inf_{\mathbf{x}} \{x_1^2 + x_2^2 + u_1(x_1 - 1) \mid \mathbf{x} \in \mathbb{R}^2\} = -\frac{u_1^2}{4}.$$

Then $\sup\{g(u_1) \mid u_1 \geq 0\} = 0$ and a gap exists between the minimal value of the primal function and the maximal value of the dual function.

Example

Let $a, b > 0$, $p, q < 0$ and let $r > 0$. Consider the following primal problem:

$$\begin{aligned} \text{minimize } f(\mathbf{x}) &= ax_1^2 + bx_2^2 \\ \text{subject to } px_1 + qx_2 + r &\leq 0 \text{ and } x_1 \geq 0, x_2 \geq 0. \end{aligned}$$

The set C is $\{\mathbf{x} \in \mathbb{R}^2 \mid x_1 \geq 0, x_2 \geq 0\}$. The constraint function is $c(\mathbf{x}) = px_1 + qx_2 + r \leq 0$ and the Lagrangian of the primal problem is

$$L(\mathbf{x}, u) = ax_1^2 + bx_2^2 + u(px_1 + qx_2 + r),$$

where u is a Lagrangian multiplier.

Thus, the dual problem objective function is

$$\begin{aligned}g(u) &= \inf_{\mathbf{x} \in C} L(\mathbf{x}, u) \\&= \inf_{\mathbf{x} \in C} ax_1^2 + bx_2^2 + u(px_1 + qx_2 + r) \\&= \inf_{\mathbf{x} \in C} \{ax_1^2 + upx_1 \mid x_1 \geq 0\} \\&\quad + \inf_{\mathbf{x} \in C} \{bx_2^2 + uqx_2 \mid x_2 \geq 0\} + ur\end{aligned}$$

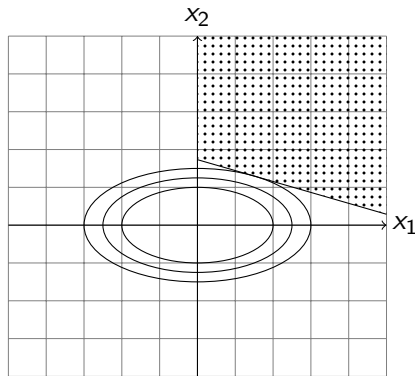
The infima are achieved when $x_1 = -\frac{up}{2a}$ and $x_2 = -\frac{uq}{2b}$ if $u \geq 0$ and at $\mathbf{x} = \mathbf{0}_2$ if $u < 0$. Thus,

$$g(u) = \begin{cases} -\left(\frac{p^2}{4a} + \frac{q^2}{4b}\right)u^2 + ru & \text{if } u \geq 0, \\ ru & \text{if } u < 0 \end{cases}$$

which is a concave function.

The maximum of $g(u)$ is achieved when $u = \frac{2r}{\frac{p^2}{a} + \frac{q^2}{b}}$ and equals

$$\frac{r^2}{\left(\frac{p^2}{a} + \frac{q^2}{b}\right)}$$



Family of Concentric Ellipses; the ellipse that “touches” the line $px_1 + qx_2 + r = 0$ gives the optimum value for f . The dotted area is the feasible region.

Note that if \mathbf{x} is located on an ellipse $ax_1^2 + bx_2^2 - k = 0$, then $f(\mathbf{x}) = k$. Thus, the minimum of f is achieved when k is chosen such that the ellipse is tangent to the line $px_1 + qx_2 + r = 0$. In other words, we seek to determine k such that the tangent of the ellipse at $\mathbf{x}_0 = \begin{pmatrix} x_{01} \\ x_{02} \end{pmatrix}$ located on the ellipse coincides with the line given by $px_1 + qx_2 + r = 0$. The equation of the tangent is

$$ax_1x_{01} + bx_2x_{02} - k = 0.$$

Therefore, we need to have:

$$\frac{ax_{01}}{p} = \frac{bx_{02}}{q} = \frac{-k}{r},$$

hence $x_{01} = -\frac{kp}{ar}$ and $x_{02} = -\frac{kq}{br}$. Substituting back these coordinates in the equation of the ellipse yields $k_1 = 0$ and $k_2 = \frac{r^2}{\frac{p^2}{a} + \frac{q^2}{b}}$. In this case no duality gap exists.