Support Vector Machines-Preliminaries

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Functions of One Real Variable

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

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

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

- If $f:[a,b] \longrightarrow \mathbb{R}$ 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 $f: X \longrightarrow \mathbb{R}$, where $X \subseteq \mathbb{R}^n$, and let $\mathbf{z} \in X$. The *gradient* of f in \mathbf{z} is the vector

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

Let $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ 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, $(\nabla f)(\mathbf{x}) = 2\mathbf{x}$.

Let $\mathbf{b}_j \in \mathbb{R}^n$ and $c_j \in \mathbb{R}$ for $1 \leqslant j \leqslant n$, and let $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ 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 $\mathbf{b}_j = \left(b_{1j} \cdots b_{nj}\right)$ for $1 \leqslant j \leqslant n$. Thus, we obtain:

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

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

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.

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

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

Definition

Let X be a open subset in \mathbb{R}^n and let $f: X \longrightarrow \mathbb{R}$ 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 $f(\mathbf{x}_0) \leqslant f(\mathbf{x})$ 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 $\mathbf{x}' A \mathbf{x} \geqslant 0$ for all $\mathbf{x} \in \mathbb{R}^n$.

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

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 $f: B(\mathbf{x}_0, r) \longrightarrow \mathbb{R}$ 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 $f: \mathbb{R}^2 \longrightarrow \mathbb{R}$ 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

$$\mathbf{h}' H_f(\mathbf{x}_0) \mathbf{h} = a_{11} h_1^2 + 2 a_{12} h_1 h_2 + a_{22} h_2^2$$

= $h_2^2 (a_{11} \xi^2 + 2 a_{12} \xi + a_{22}),$

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

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

- i $\mathbf{h}' H_f(\mathbf{x}_0) \mathbf{h} \geqslant 0$ 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;
- iii $\mathbf{h}' H_f(\mathbf{x}_0) \mathbf{h} \leq 0$ 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;
- iii if $a_{12}^2 a_{11}a_{22} \ge 0$; 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.

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

Example (cont'd)

We have

$$f(\mathbf{x}) = m \| \mathbf{x} \|^2 - 2 \sum_{i=1}^m \mathbf{a}_i' \mathbf{x} + \sum_{i=1}^m \| \mathbf{a}_i \|^2$$
$$= m(x_1^2 + \dots + x_n^2) - 2 \sum_{i=1}^n \sum_{i=1}^m \mathbf{a}_{ij} x_j + \sum_{i=1}^m \| \mathbf{a}_i \|^2,$$

which implies

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

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

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

for $1 \leq i \leq n$.

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 $\{\mathbf{a}_1, \ldots, \mathbf{a}_m\}$.

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

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

Here c specifies *inequality constraints* placed on x, while d defines *equality constraints*.

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

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

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:

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

Let $x \in R_c$. The set of active constraints at x is

$$ACT(R_c, c, x) = \{i \in \{1, ..., m\} \mid c_i(x) = 0\}.$$

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

Definition

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

minimize
$$f(\mathbf{x})$$
, where $\mathbf{x} \in \mathbb{R}^n$, subject to $\mathbf{x} \in R_c$.

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 $MP(f, \mathbf{c})$.

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

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

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

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

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

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

Then

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

Theorem

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

- \blacksquare 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, rank $((D\mathbf{h})(\mathbf{x})) = m < n$.

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 $(\nabla h_1)(\mathbf{x}_0), \ldots, (\nabla h_m)(\mathbf{x}_0)$.

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

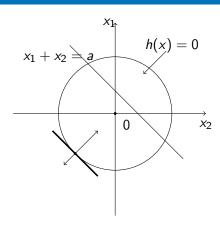
$$h(\mathbf{x}) = x_1^2 + x_2^2 - 2 = 0.$$

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 con'd)



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

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

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.

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 $\mathbf{0}_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$. At that point, we have

$$(\nabla f)(\mathbf{0}_2) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, (\nabla h_1)(\mathbf{0}_2) = \begin{pmatrix} -2 \\ 0 \end{pmatrix}, (\nabla h_2)(\mathbf{0}_2) = \begin{pmatrix} -4 \\ 0 \end{pmatrix}.$$

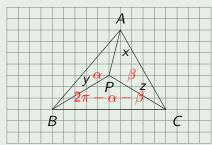
The gradients $(\nabla h_1)(\mathbf{0}_2), (\nabla h_2)(\mathbf{0}_2)$ are not linearly independent because $2(\nabla h_1)(\mathbf{0}_2) + (\nabla h_2)(\mathbf{0}_2) = \mathbf{0}_2$, so $\mathbf{0}_2$ is not a regular point and Lagrange's multipliers do not exist.

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix and let $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ 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.

Let ABC be a triangle having no angle greater than $\frac{2\pi}{3}$, P a point inside ABC and let x, y, z be the lengths of the segments PA, PB and PC, respectively. The Toricelli point of the triangle is defined as the point for which x + y + z is minimal.

Let the angle *BPA* be α , the angle *APC* be β and the angle *CPB* be $2\pi - \alpha - \beta$.



Example cont'd

The constraints are

$$x^{2} + y^{2} - 2xy \cos \alpha - c^{2} = 0,$$

$$x^{2} + z^{2} - 2xz \cos \beta - b^{2} = 0,$$

$$y^{2} + z^{2} - 2yx \cos(2\pi - \alpha - \beta) - a^{2} = 0.$$

and the expresssion to be minimized is x + y + z.

Example cont'd

Thus, the Lagrangean is

$$L = x + y + z + \lambda_1(x^2 + y^2 - 2xy\cos\alpha - c^2)$$

$$+ \lambda_2(x^2 + z^2 - 2xz\cos\beta - b^2)$$

$$+ \lambda_3(y^2 + z^2 - 2yz\cos(2\pi - \alpha - \beta) - a^2).$$

The optimality conditions are:

$$\begin{array}{l} \frac{\partial L}{\partial x} = 0, \frac{\partial L}{\partial y} = 0, \frac{\partial L}{\partial z} = 0, \\ \frac{\partial L}{\partial \alpha} = 0, \frac{\partial L}{\partial \beta} = 0. \end{array}$$

Example cont'd

We have:

$$\begin{array}{ll} \frac{\partial L}{\partial x} & = & 1 + 2x\lambda_1 - 2y\cos\alpha + 2x\lambda_2 - 2z\cos\beta = 0 \\ \frac{\partial L}{\partial y} & = & 1 + 2y\lambda_1 - 2x\cos\alpha + 2y\lambda_3 - 2z\cos(2\pi - \alpha - \beta) = 0 \\ \frac{\partial L}{\partial z} & = & 1 + 2z\lambda_2 - 2x\cos\beta + 2z\lambda_3 - 2y\cos(2\pi - \alpha - \beta) = 0 \\ \frac{\partial L}{\partial \alpha} & = & 2xy\lambda_1\sin\alpha - 2yz\lambda_3\sin(2\pi - \alpha - \beta) = 0 \\ \frac{\partial L}{\partial \beta} & = & 2xz\lambda_2\sin\beta - 2yz\lambda_3\sin(2\pi - \alpha - \beta) = 0. \end{array}$$

Regard the first three equations as a system in λ_1, λ_2 , and λ_3 :

$$\lambda_1 + \lambda_2 = \frac{-1 + 2y\cos\alpha + 2z\cos\beta}{2x},$$

$$\lambda_1 + \lambda_3 = \frac{-1 + 2x\cos\alpha + 2z\cos(2\pi - \alpha - \beta)}{2y},$$

$$\lambda_2 + \lambda_3 = \frac{-1 + 2x\cos\beta + 2yy\cos(2\pi - \alpha - \beta)}{2z}$$

The last two equations are:

$$2y(x\lambda_1\sin\alpha - z\lambda_3\sin(2\pi - \alpha - \beta)) = 0$$

$$2z(x\lambda_2\sin\beta - y\lambda_3\sin(2\pi - \alpha - \beta)) = 0.$$

Example cont'd

Eliminating
$$\lambda_1, \lambda_2$$
 and λ_3 yields $\sin \alpha = \sin \beta$ and $\sin(\alpha + \beta) = -\sin \beta$, so $\alpha = \beta = \frac{2\pi}{3}$.

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 $i \in ACT(S, \mathbf{c}, \mathbf{x}_0)$ 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 $f: \mathbb{R}^n \longrightarrow \mathbb{R}$ and $\mathbf{c}: \mathbb{R}^n \longrightarrow \mathbb{R}^m$. Let \mathbf{x}_0 be a local minimum in S of f subjected to the restriction $\mathbf{c}(\mathbf{x}_0) \leqslant \mathbf{0}_m$. Suppose that f is differentiable in \mathbf{x}_0 , c_i are differentiable in \mathbf{x}_0 for $i \in \mathrm{ACT}(S, \mathbf{c}, \mathbf{x}_0)$, and c_i are continuous in \mathbf{x}_0 for $i \notin \mathrm{ACT}(S, \mathbf{c}, \mathbf{x}_0)$. If $\{(\nabla c_i)(\mathbf{x}_0) \mid i \in \mathrm{ACT}(S, \mathbf{c}, \mathbf{x}_0)\}$ is a linearly independent set, then there exist non-negative numbers w_i for $i \in \mathrm{ACT}(S, \mathbf{c}, \mathbf{x}_0)$ such that

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

Theorem continued

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

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

iii
$$w'c(x_0) = 0$$
;

$$\mathbf{w}\geqslant\mathbf{0}_m$$
, where $\mathbf{w}=egin{pmatrix}w_1\ dots\ w_m\end{pmatrix}$.

The Primal Problem

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Consider the following optimization problem for an object function f: \mathbb{R}^n \longrightarrow \mathbb{R}, a subset C \subseteq \mathbb{R}^n, and the constraint functions \mathbf{c}: \mathbb{R}^n \longrightarrow \mathbb{R}^m and \mathbf{d}: \mathbb{R}^n \longrightarrow \mathbb{R}^p:

minimize f(\mathbf{x}), where \mathbf{x} \in C, subject to \mathbf{c}(\mathbf{x}) \leqslant \mathbf{0}_m and \mathbf{d}(\mathbf{x}) = \mathbf{0}_p.
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We refer to this optimization problem as the *primal problem*.

Definition

The *Lagrangian* associated to the primal problem is the function $L: \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \longrightarrow \mathbb{R}$ 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 $f(\mathbf{x}) = \sup\{L(\mathbf{x}, \mathbf{u}, \mathbf{v})\} \mid \mathbf{u} \geqslant \mathbf{0}_m, \mathbf{v} \in \mathbb{R}^p, u_i \mathbf{c}_i(\mathbf{x}) = 0 \text{ for } 1 \leqslant i \leqslant m\}.$

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

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

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

Lemma

The optimal value of the primal problem f^* is

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

Proof: Consider feasible \mathbf{x} (designated at $\mathbf{x} \in C$). In this case we have $f^* = \inf_{\mathbf{x} \in C} f(\mathbf{x}) = \inf_{\mathbf{x} \in C} \sup_{\mathbf{u} \geqslant \mathbf{0}_m, \mathbf{v}} L(\mathbf{x}, \mathbf{u}, \mathbf{v})$. When \mathbf{x} is not feasible, since $\sup_{\mathbf{u} \geqslant \mathbf{0}_m, \mathbf{v}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = \infty$ for any $\mathbf{x} \not\in C$, we have $\inf_{\mathbf{x} \not\in C} \sup_{\mathbf{u} \geqslant \mathbf{0}_m, \mathbf{v}} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = \infty$. Thus, in either case, $f^* = \inf_{\mathbf{x}} \sup_{\mathbf{u} \geqslant \mathbf{0}_m, \mathbf{v}} L(\mathbf{x}, \mathbf{u}, \mathbf{v})$.

The Dual Optimization Problem

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

$$g(\mathbf{u}, \mathbf{v}) = \inf_{\mathbf{x} \in C} L(\mathbf{x}, \mathbf{u}, \mathbf{v})$$
 (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 $\mathbf{u} \geqslant \mathbf{0}_m$.

Theorem

For every primal problem the Lagrange dual function $g: \mathbb{R}^m \times \mathbb{R}^p \longrightarrow \mathbb{R}$ 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:

$$\begin{split} g(t\mathbf{u}_{1} + (1-t)\mathbf{u}_{2}, t\mathbf{v}_{1} + (1-t)\mathbf{v}_{2}) \\ &= \inf\{f(\mathbf{x}) + (t\mathbf{u}_{1}' + (1-t)\mathbf{u}_{2}')\mathbf{c}(\mathbf{x}) + (t\mathbf{v}_{1}' + (1-t)\mathbf{v}_{2}')\mathbf{d}(\mathbf{x}) \mid \mathbf{x} \in S\} \\ &= \inf\{t(f(\mathbf{x}) + \mathbf{u}_{1}'\mathbf{c} + \mathbf{v}_{1}'\mathbf{d}) \\ &+ (1-t)(f(\mathbf{x}) + \mathbf{u}_{2}'\mathbf{c}(\mathbf{x}) + \mathbf{v}_{2}'\mathbf{d}(\mathbf{x})) \mid \mathbf{x} \in S\} \\ &\geqslant t\inf\{f(\mathbf{x}) + \mathbf{u}_{1}'\mathbf{c} + \mathbf{v}_{1}'\mathbf{d} \mid \mathbf{x} \in S\} \\ &+ (1-t)\inf\{f(\mathbf{x}) + \mathbf{u}_{2}'\mathbf{c}(\mathbf{x}) + \mathbf{v}_{2}'\mathbf{d}(\mathbf{x}) \mid \mathbf{x} \in S\} \\ &= tg(\mathbf{u}_{1}, \mathbf{v}_{1}) + (1-t)g(\mathbf{u}_{2}, \mathbf{v}_{2}), \end{split}$$

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 $\mathbf{c}(\mathbf{x}_*) \leqslant \mathbf{0}_m$ and $\mathbf{d}(\mathbf{x}_*) = \mathbf{0}_p$ it follows that

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

Therefore, $g(\mathbf{u}, \mathbf{v}) = \inf_{\mathbf{x} \in C} L(\mathbf{x}, \mathbf{u}, \mathbf{v}) \leqslant f_*$ for all \mathbf{u} and \mathbf{v} . Since g_* is the optimal value of g, the last inequality implies $g_* \leqslant f_*$.

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

$$\begin{array}{rcl} \sup_{\mathbf{u}\geqslant\mathbf{0}_m,\mathbf{v}} \mathit{L}(\mathbf{x},\mathbf{u},\mathbf{v}) & = & \sup_{\mathbf{u}\geqslant\mathbf{0}_m,\mathbf{v}} \mathit{f}(\mathbf{x}) + \mathbf{u}'\mathbf{c}(\mathbf{x}) + \mathbf{v}'\mathbf{d}(\mathbf{x}) \\ & = & \begin{cases} \mathit{f}(\mathbf{x}) & \text{if } \mathbf{c}(\mathbf{x})\leqslant\mathbf{0}_m, \\ \infty & \text{otherwise} \end{cases}, \end{array}$$

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

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

Thus, the weak duality amounts to the inequality

$$\sup_{\mathbf{u}\geqslant\mathbf{0}_{m},\mathbf{v}}\inf_{\mathbf{x}\in\mathbb{R}^{n}}L(\mathbf{x},\mathbf{u},\mathbf{v})\leqslant\inf_{\mathbf{x}\in\mathbb{R}^{n}}\sup_{\mathbf{u}\geqslant\mathbf{0}_{m},\mathbf{v}}L(\mathbf{x},\mathbf{u},\mathbf{v}),$$

and the strong duality is equivalent to the equality

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

Example

Let $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ 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:

minimize
$$\mathbf{a}'\mathbf{x}$$
, where $\mathbf{x} \in \mathbb{R}^n$, subject to $\mathbf{x} \geqslant \mathbf{0}_n$ and $A\mathbf{x} - \mathbf{b} = \mathbf{0}_p$.

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

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

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

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

Example (cont'd)

The dual problem

maximize
$$g(\mathbf{u}, \mathbf{v})$$
,
subject to $\mathbf{u} \geqslant \mathbf{0}_m$.

can be expressed as:

maximize
$$-\mathbf{v}'\mathbf{b}$$
,
subject to $\mathbf{a} - \mathbf{u} + A'\mathbf{v} = \mathbf{0}_n$
and $\mathbf{u} \geqslant \mathbf{0}_m$.

In turn, this problem is equivalent to:

maximize
$$-\mathbf{v}'\mathbf{b}$$
,
subject to $\mathbf{a} + A'\mathbf{v} \geqslant \mathbf{0}_n$.

Example

The following optimization problem

minimize
$$\frac{1}{2}\mathbf{x}'Q\mathbf{x} - \mathbf{r}'\mathbf{x}$$
,
where $\mathbf{x} \in \mathbb{R}^n$,
subject to $A\mathbf{x} \geqslant \mathbf{b}$,

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 $\mathbf{u} \geqslant \mathbf{0}_m$. 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 $1\leqslant i\leqslant n$, 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 $\mathbf{u}\geqslant \mathbf{0}_p$, 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 $\mathbf{a}_1, \ldots, \mathbf{a}_m \in \mathbb{R}^n$. We seek to determine a closed sphere $B[\mathbf{x}, r]$ of minimal radius that includes all points \mathbf{a}_i for $1 \leqslant i \leqslant m$. 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 $r \geqslant 0$,
subject to $\parallel \mathbf{x} - \mathbf{a}_i \parallel \leqslant r$ for $1 \leqslant i \leqslant m$.

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

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

and the dual function is:

$$g(\mathbf{u}) = \inf_{r \in \mathbb{R}_{\geqslant 0}, \mathbf{x} \in \mathbb{R}^n} L(r, \mathbf{x}, \mathbf{u})$$

$$= \inf_{r \in \mathbb{R}_{\geqslant 0}, \mathbf{x} \in \mathbb{R}^n} r^2 \left(1 - \sum_{i=1}^m u_i \right) + \sum_{i=1}^m u_i \parallel \mathbf{x} - \mathbf{a}_i \mid^2 \parallel.$$

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 $\mathbf{a}_1, \ldots, \mathbf{a}_m$. 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 $g_i(\mathbf{x}, r) = ||\mathbf{x} - \mathbf{a}_i||^2 - r^2 \le 0$ are *not convex*.

Example

Consider the primal problem

minimize
$$x_1^2 + x_2^2$$
, where $x_1, x_2 \in \mathbb{R}$, subject to $x_1 - 1 \geqslant 0$.

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 $\sup\{g(u_1)\mid u_1\geqslant 0\}=0$ 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:

minimize
$$f(\mathbf{x}) = ax_1^2 + bx_2^2$$

subject to $px_1 + qx_2 + r \le 0$ and $x_1 \ge 0$, $x_2 \ge 0$.

The set C is $\{\mathbf{x} \in \mathbb{R}^2 \mid x_1 \geqslant 0, x_2 \geqslant 0\}$. The constraint function is $c(\mathbf{x}) = px_1 + qx_2 + r \leqslant 0$ 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

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

$$= \inf_{\mathbf{x} \in C} ax_1^2 + bx_2^2 + u(px_1 + qx_2 + r)$$

$$= \inf_{\mathbf{x} \in C} \{ax_1^2 + upx_1 \mid x_1 \ge 0\}$$

$$+ \inf_{\mathbf{x} \in C} \{bx_2^2 + uqx_2 \mid x_2 \ge 0\} + ur$$

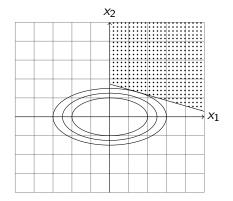
The infima are achieved when $x_1 = -\frac{up}{2a}$ and $x_2 = -\frac{uq}{2b}$ if $u \geqslant 0$ and at $\mathbf{x} = \mathbf{0}_2$ if u < 0. Thus,

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

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

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



L Duality

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.