Support Vector Machines - I supplementary material

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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

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

Example

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

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

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

Example

Let $\mathbf{b}_j \in \mathbb{R}^n$ and $c_j \in \mathbb{R}$ for $1 \leqslant j \leqslant n$, 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 $\mathbf{b}_j = \begin{pmatrix} b_{1j} \cdots b_{nj} \end{pmatrix}$ 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. Using this matrix we can write

$$((\mathbf{h}'\nabla)2f)(\mathbf{x}) = H_f(\mathbf{x}).$$

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 $x \in B(\mathbf{x}_0, \delta) - \{\mathbf{x}_0\}$.

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

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

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

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

1. $\mathbf{h}' H_f(\mathbf{x}_0)\mathbf{h} \geqslant 0$ 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;
2. $\mathbf{h}' H_f(\mathbf{x}_0)\mathbf{h} \leqslant 0$ 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;
3. if $a_{12}^2 - a_{11}a_{22} \geqslant 0$; 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 $\mathbf{a}_1, \ldots, \mathbf{a}_m$ 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

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

which implies

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

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

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

for $1 \leqslant j \leqslant n$.

The Hessian matrix $H_f = 2mI_n$ is pkarositive 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 $\{\mathbf{a}_1, \ldots, \mathbf{a}_m\}$.

Theorem

(Existence Theorem of Lagrange Multipliers) *Let* $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *and let* $\mathbf{h} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ *be two functions such that* $f \in C^1(\mathbb{R}^n)$, $\mathbf{h} \in C^1(\mathbb{R}^n)$, *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* $(\nabla h_1)(\mathbf{x}_0), \ldots, (\nabla h_m)(\mathbf{x}_0)$.

Example

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 $f(\mathbf{x}) = \mathbf{x}' A \mathbf{x}$. We seek to 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 $(\nabla h)(\mathbf{x}) = 2\mathbf{x}$, by Theorem 6 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 $f : \mathbb{R}^n \longrightarrow \mathbb{R}$, $\mathbf{c} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$, 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

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

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

Note that equality constraints can be replaced in a constrained optimization problem by inequality constraints. Indeed, a constraint of the form $\mathbf{d}(\mathbf{x}) = \mathbf{0}_p$ can be replaced by a pair of constraints $\mathbf{d}(\mathbf{x}) \leqslant \mathbf{0}_p$ and $-\mathbf{d}(\mathbf{x}) \leqslant \mathbf{0}_p$. This transformation is inapplicable if we assume that all equality constraints must be convex (or concave) because this transformation may introduce constraints that violate convexity (or concavity, respectively). On the other hand, if $\mathbf{d}$ is an affine function, replacing $\mathbf{d}(\mathbf{x}) = \mathbf{0}_p$ by both $\mathbf{d}(\mathbf{x}) \leqslant \mathbf{0}_p$ and $-\mathbf{d}(\mathbf{x}) \leqslant \mathbf{0}_p$ results in two affine restrictions that are both convex and concave functions.

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

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

If $i \in \mathtt{ACT}(R_{\mathbf{c}}, \mathbf{c}, \mathbf{x})$, 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 $\mathbf{x}$.

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

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

Theorem continued

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

1. $(\nabla f)(\mathbf{x}_0) + \sum_{i=1}^{m} w_i (\nabla c_i)(\mathbf{x}_0) = \mathbf{0}_n$;
2. $\mathbf{w}'\mathbf{c}(\mathbf{x}_0) = 0$;
3. $\mathbf{w} \geqslant \mathbf{0}_m$, where $\mathbf{w} = \begin{pmatrix} w_1 \\ \vdots \\ w_m \end{pmatrix}$.

The Primal Problem

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

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

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

Definition

The *Lagrangian* associated to the primal problem is the function $L : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \longrightarrow \mathbb{R}$ 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 $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{u} \in \mathbb{R}^m$, and $\mathbf{v} \in \mathbb{R}^p$.
The component u_i of $\mathbf{u}$ is the *Lagrangian multiplier* corresponding to the constraint $c_i(\mathbf{x}) \leqslant 0$; the component v_j of $\mathbf{v}$ is the *Lagrangian multiplier* corresponding to the constraint $d_j(\mathbf{x}) = 0$.

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

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

and consists of

$$\begin{aligned} &\textit{maximize } g(\mathbf{u}, \mathbf{v}), \textit{ where } \mathbf{u} \in \mathbb{R}^m \textit{ and } \mathbf{v} \in \mathbb{R}^p, \\ &\qquad\qquad\qquad \textit{subject to } \mathbf{u} \geqslant \mathbf{0}_m. \end{aligned}$$

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 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:

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

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 $g_* \leqslant f_*$.*

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 Theorem 11 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

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

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

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

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

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

Example (cont'd)

An equivalent of the dual problem is

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

In turn, this problem is equivalent to:

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

Example

The following optimization problem

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

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 $1 \leqslant i \leqslant n$, 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:

$$\begin{aligned} &\textit{minimize } r, \textit{ where } r \geq 0, \\ &\qquad\qquad \textit{subject to } \| \mathbf{x} - \mathbf{a}_i \| \leqslant r \textit{ for } 1 \leqslant i \leqslant m. \end{aligned}$$

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

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

and the dual function is:

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

This leads to the following conditions:

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

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

Example

Consider the primal problem

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

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:

$$\text{minimize } f(\mathbf{x}) = ax_1^2 + bx_2^2$$
$$\text{subject to } px_1 + qx_2 + r \leqslant 0 \text{ and } x_1 \geqslant 0,\ x_2 \geqslant 0.$$

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

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

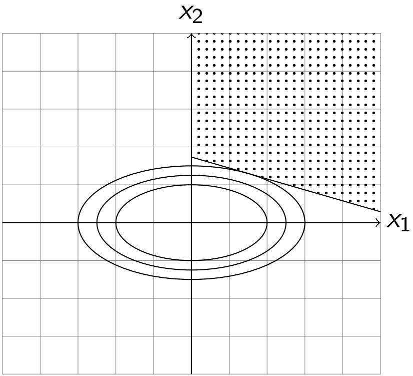
The infima are achieved when $x_1 = -\frac{up}{2a}$ and $x_2 = -\frac{uq}{2b}$ if $u \geqslant 0$ and at $\mathbf{x} = \mathbf{0}_2$ if $u < 0$. Thus,

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

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.