Chapter 5: Constrained nonlinear optimization

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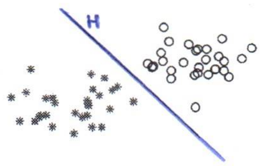
5.1 Example: Design linear classifiers and train SVMs

Support Vector Machines (SVMs) for binary classification.

Training set $T = \{(\underline{x}^i, y^i) : \underline{x}^i \in \mathbb{R}^n, y^i \in \{-1, 1\}, i = 1, \dots, p\}$.

Linear classifier: an hyperplane H that separates the points of the two classes.



If convex hulls of two classes are disjoints, T is linearly separable. ← algebraically, what does it mean? :

$\exists\, \underline{w} \in \mathbb{R}^n, b \in \mathbb{R}$: that defines an hyperplane (denoted by H) which separates the points of the two classes

$H(\underline{w}, b) = \{\underline{x} \in \mathbb{R}^n : \underline{w}^t\underline{x} = b\}$ separates the points of the two classes if

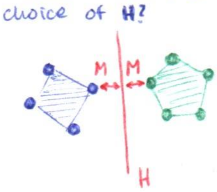
$$\begin{cases} \underline{w}^t\underline{x}^i - b \geq 1 & \text{for } y^i = +1 \\ \underline{w}^t\underline{x}^i - b \leq 1 & \text{for } y^i = -1 \end{cases}$$

we should just say $\geq 0, \leq 0$ but we want to separate them

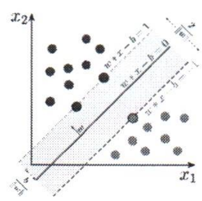
not unique.

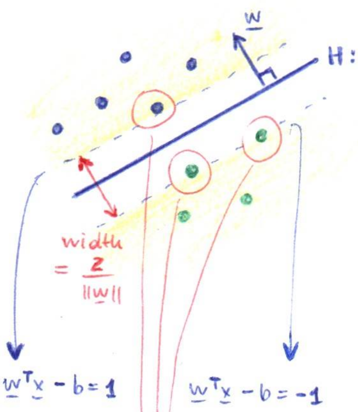
If T is linearly separable, H with **largest margin** (min distance from H to any $\underline{x}^i$) is the most robust w.r.t. noise.

Which is the most robust choice of H?



The one that guarantees the largest margin M





SUPPORT VECTORS
only those three points are determining the hyperplane

Since width $= \frac{2}{\|\underline{w}\|}$, hard-margin linear SVM training: (Primal)

$$\boxed{\begin{array}{ll} \min\limits_{\underline{w} \in \mathbb{R}^n, b \in \mathbb{R}} & \|\underline{w}\|^2 \\ \text{s.t.} & y^i(\underline{w}^t\underline{x}^i - b) \geq 1 \quad i = 1, \dots, p. \end{array}}$$

we want to maximize the width $:= 2/\|\underline{w}\|$ so we want to minimize $\|\underline{w}\|$ subjected to the fact that all the points are properly classified

$$\begin{cases} y^i = 1 \Rightarrow \underline{w}^T\underline{x}^i - b \geq 1 \\ y^i = -1 \Rightarrow \underline{w}^T\underline{x}^i - b \leq 1 \end{cases}$$

→ in a compact way: $y^i(\underline{w}^T\underline{x}^i - b) \geq 1 \quad \forall i$

strictly convex function and linear constraints.

Remark: The maximum margin hyperplane H is completely determined by the *support vectors* (closest $\underline{x}^i$ to H).

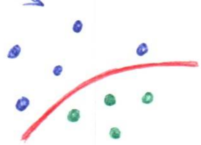
In general T is not linearly separable

Extensions:

1) Soft margin for nonlinearly separable T (not convex)

2) Nonlinear classifiers by applying kernels.

See computer lab 5.



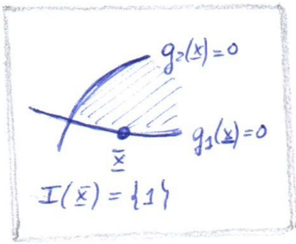
5.2 Necessary optimality conditions

Consider

$$\begin{array}{lll} \min & f(x) & \\ \text{s.t.} & g_i(\underline{x}) \le \underline{0} & i \in I = \{1, \dots, m\} \\ & \underline{x} \in \mathbb{R}^n & \end{array} \qquad (1)$$

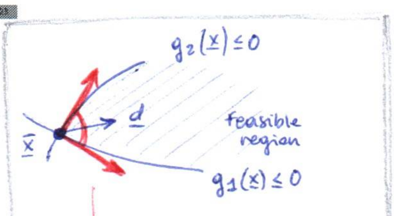
where $f, g_i \in C^1$.

Assumption: Feasible region $S = \{\, \underline{x} \in \mathbb{R}^n : g_i(x) \le 0, \forall i \in I \,\} \neq \emptyset$ but its interior can be empty.



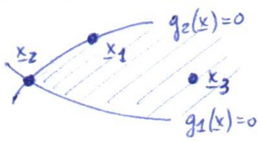
Definitions: For each $\overline{\underline{x}} \in S$

- $\mathscr{D}(\overline{\underline{x}}) = \{\, \underline{d} \in \mathbb{R}^n : \exists\, \overline{\alpha} > 0 \text{ such that } \overline{\underline{x}} + \alpha \underline{d} \in S,\ \forall \alpha \in [0, \overline{\alpha}] \,\}$
  cone of the **feasible directions**.
- $I(\overline{\underline{x}}) = \{\, i \in I : g_i(\overline{\underline{x}}) = 0 \,\} \subseteq I$ set of **indices** of the **active constraints**.
- $\mathrm{D}(\overline{\underline{x}}) = \{\, \underline{d} \in \mathbb{R}^n : \nabla^t g_i(\overline{\underline{x}}) \underline{d} \le 0, \forall i \in I(\overline{\underline{x}}) \,\}$
  cone of the **directions constrained by the gradients of the active constraints**.



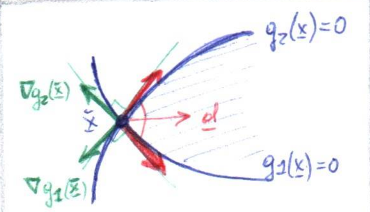
the cone generated by these two vectors is the cone (set) of all the feasible directions $:= \mathscr{D}(\overline{\underline{x}})$

At $\underline{x}_1$ second constraint is active
At $\underline{x}_2$ both constraints are active
At $\underline{x}_3$ no constraint is active



Notice that: for interior points $\underline{x}^*$ (for example $\underline{x}_3$) any direction belongs to $\mathrm{D}(\underline{x}^*)$ (as well to $\mathscr{D}(\underline{x}^*)$)

N.B.: Cone $\mathscr{D}(\overline{\underline{x}})$ can be (topologically) open.



In this case the whole $\mathscr{D}(\overline{\underline{x}})$ is the cone of the directions constrained by the gradients of the active constraints $:= \mathrm{D}(\overline{\underline{x}})$

Property: $\overline{\mathscr{D}}(\overline{\underline{x}}) \subseteq \mathrm{D}(\overline{\underline{x}})$ for all $\overline{\underline{x}} \in S$.

Proof:

Given any $\underline{d} \in \mathscr{D}(\overline{\underline{x}})$, for sufficiently small α we have

$0 \ge g_i(\overline{\underline{x}} + \alpha \underline{d}) = g_i(\overline{\underline{x}}) + \alpha \nabla^t g_i(\overline{\underline{x}}) \underline{d} + o(\alpha) \quad \forall i \in I(\overline{\underline{x}})$ with $g_i(\overline{\underline{x}}) = 0$.

Therefore $\nabla^t g_i(\overline{\underline{x}}) \underline{d} \le 0 \quad \forall i \in I(\overline{\underline{x}})$

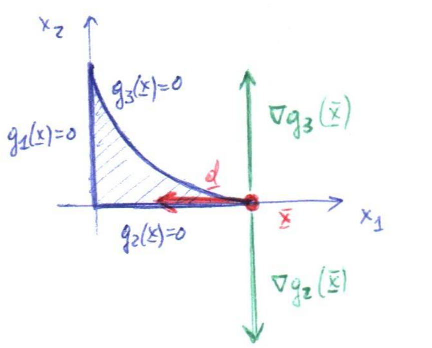
that is $\underline{d} \in \mathrm{D}(\overline{\underline{x}})$ and hence $\mathscr{D}(\overline{\underline{x}}) \subseteq \mathrm{D}(\overline{\underline{x}})$.

Since $\mathrm{D}(\overline{\underline{x}})$ is closed, we also have $\overline{\mathscr{D}}(\overline{\underline{x}}) \subseteq \mathrm{D}(\overline{\underline{x}})$. □

Not all $\underline{d} \in \mathrm{D}(\overline{\underline{x}})$ are feasible directions.

Example:

$$g_1(\underline{x}) = -x_1 \le 0$$
$$g_2(\underline{x}) = -x_2 \le 0$$
$$g_3(\underline{x}) = -(1 - x_1)^3 + x_2 \le 0$$



At $\overline{\underline{x}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ we have $I(\overline{\underline{x}}) = \{2, 3\}$

$\mathscr{D}(\overline{\underline{x}}) = \{\, (\alpha, 0) : \alpha < 0 \,\}$

Since $\nabla g_2(\overline{\underline{x}}) = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$ and $\nabla g_3(\overline{\underline{x}}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$,

$\underline{d} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ satisfies $\begin{pmatrix} -d_2 \le 0 \\ d_2 \le 0 \end{pmatrix}$ but is not a feasible direction at $\overline{\underline{x}}$.

Hence $\overline{\mathscr{D}}(\overline{\underline{x}}) \subset \mathrm{D}(\overline{\underline{x}}) = \{\, (\alpha, 0) : \alpha \in \mathbb{R} \,\}$.

the only feasible directions are the vectors of the form: $\underline{d} = [\alpha \ \ 0]^T \quad \alpha < 0$

$\underline{d} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \in \mathrm{D}(\overline{\underline{x}})$

$\underline{d} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \notin \mathscr{D}(\overline{\underline{x}})$

$\Rightarrow \mathscr{D}(\overline{\underline{x}}) \subsetneq \mathrm{D}(\overline{\underline{x}})$

$(\mathscr{D}(\overline{\underline{x}}) = \mathbb{R}^-, \ \mathrm{D}(\overline{\underline{x}}) = \mathbb{R})$

Theorem: (Extension of first order necessary optimality conditions)

If $f \in C^1$ on S and $\underline{x} \in S$ is a local minimum of f on S, then

$$\nabla f^t(\underline{x})\underline{d} \geq 0 \qquad \forall \underline{d} \in \overline{\mathscr{D}}(\underline{x}).$$

that is, all feasible directions are ascent directions. $\Longrightarrow$ if we move in $\forall$ direction we increase the objective function

Proof:

The result holds $\forall \underline{d} \in \mathscr{D}(\underline{x})$.

For every $\underline{d} \in \overline{\mathscr{D}}(\underline{x})$, $\exists$ a sequence $\{\underline{d}^k\}$ with $\underline{d}^k \in \mathscr{D}(\underline{x})$ such that $\lim_{k\to\infty} \underline{d}^k = \underline{d}$.

Since $\nabla f^t(\underline{x})\underline{d}^k \geq 0, \forall \underline{k}$, then $\lim_{k\to\infty} \nabla f^t(\underline{x})\underline{d}^k = \nabla f^t(\underline{x})\underline{d} \geq 0$. ∎

But $\overline{\mathscr{D}}(\underline{x})$ is difficult to characterize.

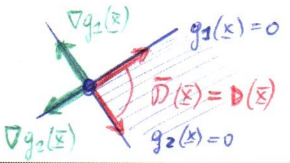
Since $\mathrm{D}(\underline{x})$ is well characterized, we introduce further conditions.

Definition: (Constraint Qualification CQ – Zangwill)

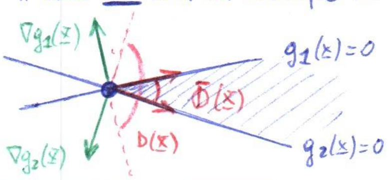
The constraint qualification assumption holds at $\underline{x} \in S$ if $\overline{\mathscr{D}}(\underline{x}) = \mathrm{D}(\underline{x})$

(For example, in the previous example the constraint qualification does not hold for $\underline{x} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$)

It holds for example in:



It does not hold for example in:



$\overline{\mathrm{D}}(\underline{x}) \subsetneq \mathrm{D}(\underline{x})$.

Theorem: (Karush-Kuhn-Tucker necessary optimality conditions) (necessary conditions for local optimality)

Suppose $f, g_i \in C^1$ and CQ assumption holds at $\underline{x} \in \{\underline{x} \in \mathbb{R}^n : g_i(\underline{x}) \leq 0, \forall i \in I\}$.

If $\underline{x}$ is a local minimum of f over S then $\exists\, u_1, \ldots, u_m \geq 0$ (KKT-multipliers) such that:

$$\boxed{\nabla f(\underline{x}) + \sum_{i \in I(\underline{x})} u_i \nabla g_i(\underline{x}) = \underline{0} \Leftrightarrow \begin{cases} \nabla f(\underline{x}) + \sum_{i=1}^m u_i \nabla g_i(\underline{x}) = \underline{0} \\ u_i g_i(\underline{x}) = 0 \quad \forall i \in I \quad (u_i = 0 \;\; \forall i \in I \text{ s.t. } g_i(\underline{x}) < 0) \end{cases}}$$

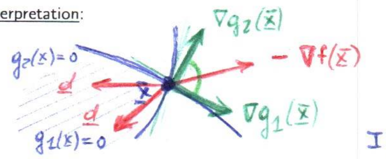
$\rightarrow$ if the constraint is not active then the coefficient is $=0$ (and so either $u_i = 0$ or $g_i(\underline{x}) = 0$, so $u_i g_i(\underline{x}) = 0 \quad \forall i$)

$$\boxed{\sum_{i \in I(\underline{x})} u_i \nabla g_i(\underline{x}) = -\nabla f(\underline{x})}$$

so the direction of the fastest decrease of the function at $\underline{x}$ ($= -\nabla f(\underline{x})$) can be expressed as a linear combination of the gradients of the constraints (only the active constraints)

$\underline{x}$ must also satisfy all the constraints $g_i(\underline{x}) \leq 0, \forall i \in I$.

Geometric interpretation:



$I(\underline{x}) = \{1, 2\}$

So $-\nabla f(\underline{x})$ can be expressed as a linear combination of $\nabla g_1(\underline{x})$ and $\nabla g_2(\underline{x})$, which means that it belongs to the cone generated by the two gradients ($\triangleleft$).

Any feasible direction $\underline{d}$ is such that: $(\underline{d})^T(-\nabla f(\underline{x})) \leq 0$

so, any feasible direction is an ascent direction.

For $\underline{x}$ to be a local min, $-\nabla f(\underline{x})$ must be expressible as a linear combination with coefficients $u_i \geq 0$ of $\nabla g_i(\underline{x})$, $\forall i \in I(\underline{x})$, i.e., must form an obtuse angle with all the feasible directions.

Proof:

Assuming CQ holds at $\underline{x}$, we have $\overline{\mathscr{D}}(\underline{x}) = \mathrm{D}(\underline{x})$.

NC for $\underline{x}$ to be a local minimum of f over S is

$$\nabla f^t(\underline{x})\underline{d} \geq 0, \quad \forall \underline{d} \text{ such that } \nabla g_i^t(\underline{x})\underline{d} \leq 0 \quad \forall i \in I(\underline{x}). \qquad (2)$$

Farkas Lemma:

$$\begin{cases} A\underline{u} = \underline{b} \\ \underline{u} \geq 0 \end{cases} \text{has a solution} \Leftrightarrow \begin{cases} \underline{b}^t \underline{d} \geq 0 \\ \forall \underline{d} \text{ such that } \underline{d}^t A \geq 0 \end{cases} \text{has a solution.}$$

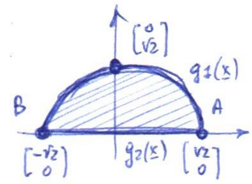
Taking $\underline{b} = \nabla f(\underline{x})$ and $A = (-\nabla g_{i_1}(\underline{x}), \ldots, -\nabla g_{i_\ell}(\underline{x}))$ ($i_j \in I(\underline{x})$) with n rows and $|I(\underline{x})|$ columns, we have that (2) is equivalent to $\underline{b}^T\underline{d} \geq 0 \quad \forall \underline{d} \in \mathbb{R}^n$ such that $\underline{d}^T A \geq \underline{0}$ which is equivalent (by Farkas Lemma) to:

$\exists\, u_i \geq 0 \quad \forall i \in I(\underline{x})$ s.t. $\nabla f(\underline{x}) = \sum_{i \in I(\underline{x})} u_i (-\nabla g_i(\underline{x}))$.

Then take $u_i = 0$ for all the constraints that are not active ($i \in I \setminus I(\underline{x})$). ∎

Example 1:

$$\begin{array}{ll} \min & f(\underline{x}) = x_1 + x_2 \\ \text{s.t.} & g_1(\underline{x}) = x_1^2 + x_2^2 \leq 2 \\ & g_2(\underline{x}) = -x_2 \leq 0 \end{array}$$



Any local optimal solution of the problem satisfies these conditions (necessary conditions)

KKT conditions: $u_1, u_2 \geq 0$ such that $\nabla f(\underline{x}) + \sum_{i \in I(\overline{\underline{x}})} u_i \nabla g_i(\underline{x}) = \underline{0}$

- $\begin{pmatrix} 1 \\ 1 \end{pmatrix} + u_1 \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix} + u_2 \begin{pmatrix} 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ ⟵ this is general ($\forall i \in I$) we need to specify $u_i = 0 \quad \forall i \in I \setminus I(\overline{\underline{x}})$
- $u_1(x_1^2 + x_2^2 - 2) = 0$, $u_2(-x_2) = 0$ ⟵ these are the conditions that guarantee $u_i = 0 \quad \forall i \in I \setminus I(\overline{\underline{x}})$
- $x_1^2 + x_2^2 \leq 2$, $-x_2 \leq 0$ ⟵ we have to specify that $\overline{\underline{x}}$ must be a feasible solution
- $u_1 \geq 0, u_2 \geq 0$

we look now for possible solutions (we have to find both $\underline{u}$ and $\underline{x}$)

Consider all four cases...

(1) $u_1 = 0, \quad u_2 = 0 \quad \Longrightarrow \quad \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow$ impossible

(2) $u_1 = 0, \quad u_2 > 0 \quad \Longrightarrow \quad \begin{pmatrix} 1 \\ 1 \end{pmatrix} + u_2 \begin{pmatrix} 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ impossible

(3) $u_1 > 0, \quad u_2 = 0$

(4) $u_1 > 0, \quad u_2 > 0$

(3): $\begin{pmatrix} 1 \\ 1 \end{pmatrix} + u_1 \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \Longrightarrow \quad u_1 = -\frac{1}{2x_2}$ where $x_2 \geq 0 \Rightarrow u_1 < 0$ impossible

(4): if 2 constraints are active then it must be $\overline{\underline{x}} = \begin{bmatrix} -\sqrt{2} \\ 0 \end{bmatrix} \vee \overline{\underline{x}} = \begin{bmatrix} \sqrt{2} \\ 0 \end{bmatrix}$

since $u_1 > 0$ and $u_2 > 0$ we have:

$x_1^2 + x_2^2 - 2 = 0 \quad \wedge \quad x_2 = 0 \quad \longrightarrow \quad x_1 = \pm\sqrt{2}, \quad x_2 = 0$

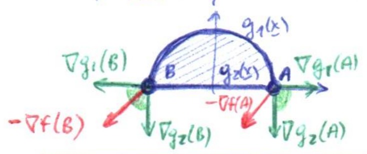
For $A = \begin{bmatrix} \sqrt{2} \\ 0 \end{bmatrix}$: $\begin{pmatrix} 1 \\ 1 \end{pmatrix} + u_1 \begin{pmatrix} 2\sqrt{2} \\ 0 \end{pmatrix} + u_2 \begin{pmatrix} 0 \\ -1 \end{pmatrix} = 0 \quad \longrightarrow \quad u_1 < 0$ ↯

$\Longrightarrow$ A does not satisfy KKT

For $B = \begin{bmatrix} -\sqrt{2} \\ 0 \end{bmatrix}$: $\begin{pmatrix} 1 \\ 1 \end{pmatrix} + u_1 \begin{pmatrix} -2\sqrt{2} \\ 0 \end{pmatrix} + u_2 \begin{pmatrix} 0 \\ -1 \end{pmatrix} = 0 \quad \Longrightarrow \quad u_1 = \frac{1}{2\sqrt{2}} > 0, \quad u_2 = 2$

$\Longrightarrow$ B does satisfy KKT

$\Longrightarrow$ the only candidate point is $\begin{pmatrix} -\sqrt{2} \\ 0 \end{pmatrix}$



Only in B the gradient of the function belongs to the cone generated by the gradients of the constraints

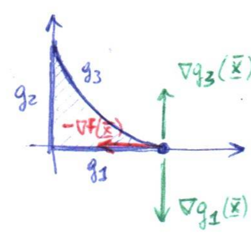
!

If CQ assumption does not hold at $\overline{\underline{x}}$, KKT conditions need not be necessary for local optimality.

It is very important to verify that $\overline{\mathcal{D}}(\overline{\underline{x}}) = D(\overline{\underline{x}})$ $\forall \overline{\underline{x}} \in$ feasible region. If for some $\underline{x}$ it does not hold, then KKT loses its importance.

Example 2:

$$\begin{array}{ll} \min & f(\underline{x}) = -x_1 \\ s.t. & g_1(\underline{x}) = -x_1 \leq 0 \\ & g_2(\underline{x}) = -x_2 \leq 0 \\ & g_3(\underline{x}) = -(1 - x_1)^3 + x_2 \leq 0 \end{array}$$



Here CQ does not hold ($\overline{\mathcal{D}}(\overline{\underline{x}}) \subsetneq D(\overline{\underline{x}})$)

We know that $D(\overline{\underline{x}}) = \{(\alpha, 0) : \alpha \in \mathbb{R}\} \neq \overline{\mathscr{D}}(\overline{\underline{x}}) = \{(\alpha, 0) : \alpha \leq 0\}$ for $\overline{\underline{x}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

Now $f(\underline{x})$ attains its global minimum at $\overline{\underline{x}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ but no multipliers exist.

Indeed u_1=0 and $\begin{pmatrix} -1 \\ 0 \end{pmatrix} + u_2 \begin{pmatrix} 0 \\ -1 \end{pmatrix} + u_3 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, that is, KKT conditions are not satisfied.

Proposition: (Sufficient conditions for Constraint Qualification)

- If
  - all g_i are linear functions (Karlin)

  or

  - all the g_i's are convex and $\exists \underline{a}$ such that $g_i(\underline{a}) < 0, \forall i \in I$, (Slater)

  CQ assumption holds at every $\underline{x} \in S$. } general (S)

- If $\nabla g_i(\overline{\underline{x}})$, $i \in I(\overline{\underline{x}})$, are linearly independent, CQ assumption holds at $\overline{\underline{x}} \in S$. } point ($\overline{\underline{x}}$)

N.B.: When the gradients of the active constraints are linearly independent, KKT multiplier vector is unique.

Theorem: (Necessary and sufficient conditions – convex problems)

= ∃ an interior point

If $f \in C^1$, $g_i \in C^1$ $\forall i \in I$ are convex, and $\exists\ \underline{a}$ such that $g_i(\underline{a}) < 0$ $\forall i \in I$, then $\underline{x}^* \in S$ is a global minimum if and only if $\exists\, u_1, \dots, u_m \geq 0$ such that :

$$\begin{cases} \nabla f(\underline{x}^*) + \sum_{i=1}^{m} u_i \nabla g_i(\underline{x}^*) = \underline{0} \\ u_i g_i(\underline{x}^*) = 0 \qquad \forall i \in I. \end{cases}$$

In this case KKT are necessary and sufficient conditions (and the optimum is global)

Proof:

$\Rightarrow$) $\underline{x}^*$ (local) minimum $\Rightarrow$ $\underline{x}^*$ satisfies KKT conditions (CQ + necessary optimality cond.)

$\Leftarrow$) KKT conditions $\Rightarrow \nabla f^t(\underline{x}^*)\underline{d} \geq 0 \quad \forall \underline{d} \in \overline{\mathscr{D}}(\underline{x}^*) = \mathrm{D}(\underline{x}^*)$ (CQ + Farkas lemma)

$\Rightarrow$ $\underline{x}^*$ (global) minimum (result for convex problems).

□

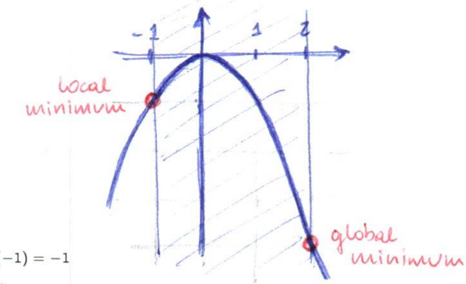
In case of Linear Programs, it amounts to the complementary slackness theorem.

Remark: Result holds under milder convexity conditions (f pseudoconvex and the g_i's quasiconvex).

If f is not convex, KKT conditions are not sufficient.

Example 3:

$$\min f(x) = -x^2$$
$$g_1(x) = -2 + x \leq 0$$
$$g_2(x) = -x - 1 \leq 0$$



For $x = -1$: $g_1(-1) = -3 \leq 0 \quad g_2(-1) = 0 \leq 0 \quad f(-1) = -1$

$$\nabla f(-1) = 2 = -u_2 \nabla g_2(-1) = u_2$$
$$u_1 g_1(-1) = -3u_1 = 0 \Rightarrow u_1 = 0$$
$$u_2 g_2(-1) = u_2 0 = 0$$

KKT conditions are verified but "candidate point" is a local minimum and not a global minimum, which is x=2.

General case

Consider

$$\begin{array}{lll} \min & f(\underline{x}) & \\ \text{s.t.} & g_i(\underline{x}) \leq 0 & i \in I = \{1, ..., m\} \\ & h_l(\underline{x}) = 0 & l \in L = \{1, ..., p\} \\ & \underline{x} \in X \subseteq \mathbb{R}^n & \end{array}$$

→ m inequality constraints
→ p equality constraints

where f, g_i, $h_l \in C^1$.

In presence of nonlinear equality constraints, usually $\mathscr{D}(\underline{x}) = \{\underline{0}\}$. →

the feasible region is the curve so ∀ step we do we go out of the curve $\Rightarrow \mathscr{D}(\bar{\underline{x}}) = \{0\}$

Extend previous results by defining cone of directions accounting for equality constraints.

⟹ to extend the results we have to consider a different cone, not the $\mathscr{D}(\bar{\underline{x}})$

$\mathscr{D}(\bar{\underline{x}}) \longrightarrow \mathrm{T}(\bar{\underline{x}})$

feasible directions — cone of the tangents

Definition: *Closed cone of the tangents* at $\bar{\underline{x}}$

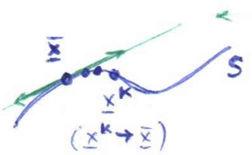
$$\mathrm{T}(\bar{\underline{x}}) = \left\{ \underline{d} \in \mathbb{R}^n : \underline{d} = \lambda \lim_{k \to \infty} \frac{\underline{x}^k - \bar{\underline{x}}}{\|\underline{x}^k - \bar{\underline{x}}\|},\ \lambda \geq 0,\ \left\{\underline{x}^k\right\} \underset{k\to\infty}{\longrightarrow} \bar{\underline{x}} \text{ with } \underline{x}^k \neq \underline{x} \right\}$$

generalization of the concept of the cone of feasible directions $\mathscr{D}(\bar{\underline{x}})$ (we should write $\mathscr{T}(\bar{\underline{x}})$)

where $\left\{\underline{x}^k\right\} \in S$ are feasible solutions.

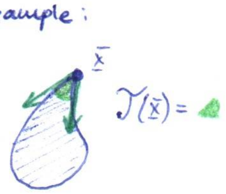
If $\underline{d} \in \mathrm{T}(\bar{\underline{x}})$ and $\exists$ sequence of feasible solutions $\left\{\underline{x}^k\right\} \to \bar{\underline{x}}$, the directions of the cords $\underline{x}^k - \underline{x}$ converge to $\underline{d}$.

Illustration:



the cone of the tangents intuitively is the set of all the vectors which "belong" to the tangent (straight line / hyperplane).

Example:

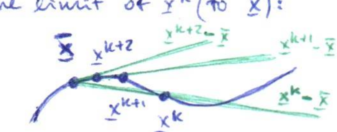


Definition: (Constraint Qualification CQ – Abadie)

The CQ assumption holds at $\bar{\underline{x}} \in S$ if $\mathrm{T}(\bar{\underline{x}}) = D(\bar{\underline{x}}) \bigcap H(\bar{\underline{x}})$ where

$\mathrm{D}(\bar{\underline{x}}) = \left\{\underline{d} \in \mathbb{R}^n : \nabla g_i^t(\bar{\underline{x}})\underline{d} \leq 0, \forall i \in I(\bar{\underline{x}})\right\}$, $H(\bar{\underline{x}}) = \left\{\underline{d} \in \mathbb{R}^n : \nabla h_l^t(\bar{\underline{x}})\underline{d} = 0, \forall l \in L\right\}$.

we're defying this considering the limit of $\underline{x}^k$ (to $\bar{\underline{x}}$):



Theorem: (General KKT necessary optimality conditions)

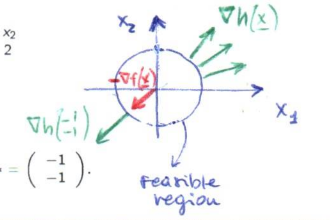
Suppose $f \in C^1$, $g_i \in C^1\ \forall i$, $h_l \in C^1\ \forall l$ and CQ assumption holds at $\overline{x} \in S$.
If $\overline{x}$ is a local minimum of f over S then $\exists\, u_i \geq 0$, $\forall i \in I(\overline{x})$ and $v_l \in \mathbb{R}$, $\forall l \in L$ such that

$$\boxed{\nabla f(\overline{x}) + \sum_{i \in I(\overline{x})} u_i \nabla g_i(\overline{x}) + \sum_{l \in L} v_l \nabla h_l(\overline{x}) = \underline{0}.}$$

N.B.: If only equality constraints, KKT conditions coincide with classical Lagrange optimality conditions.

Example:

$$\begin{array}{ll} \min & f(\underline{x}) = x_1 + x_2 \\ \text{s.t.} & x^2{}_1 + x^2{}_2 = 2 \end{array}$$



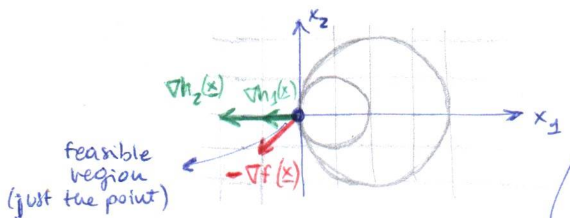
Optimal solution: $\underline{x}^* = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$.

$-\nabla f(\underline{x}) = \binom{-1}{-1}$

There is an unique optimal solution : when the gradient of $h(\underline{x})$ is collinear with $-$gradient of $f(\underline{x})$
$\Longrightarrow \underline{x}^* = \binom{-1}{-1}$

Example:

$$\begin{array}{ll} \min & f(\underline{x}) = x_1 + x_2 \\ \text{s.t.} & (x_1 - 1)^2 + x^2{}_2 - 1 = 0 \\ & (x_1 - 2)^2 + x^2{}_2 - 4 = 0 \end{array}$$



Optimal solution: $v = 1/2$ and $\underline{x}^* = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$.

Sufficient conditions for CQ are not satisfied at $\underline{x}^*$.

No multipliers v_1, v_2 exist that satisfy the KKT conditions.

Clearly we cannot express $-\nabla f(\underline{x})$ as a linear combination of $\nabla h_1(\underline{x})$ and $\nabla h_2(\underline{x})$ in $\underline{x} = \underline{0}$ (only point of the feasible region and optimal solution (as it is the only feasible point)). Notice that CQ are not satisfied (the two gradients of the two active constraints are colinear (not linearly independent)).

However $\underline{x} = \binom{0}{0}$ is optimal.

Proposition: (Sufficient conditions for CQ)

- CQ assumption holds at every $\underline{x} \in S$ if g_i convex, h_l linear and $\exists \underline{a} \in X$ such that $g_i(\underline{a}) < 0$, $\forall i \in I$ and $h_l(\underline{a}) = 0$, $\forall l \in L$. } general (S)
- CQ assumption holds at $\overline{x} \in S$ if $\nabla g_i(\overline{x})$, $\forall i \in I(\overline{x})$, and $\nabla h_l(\overline{x})$, $\forall l \in L$, are linearly independent. } point ($\overline{x}$)

5.3 Sufficient optimality conditions

Consider

$$(P) \quad \left\{ \begin{array}{lll} \min & f(\underline{x}) & \\ \text{s.t.} & g_i(\underline{x}) \leq 0 & \forall i \in I = \{1, \dots, m\} \\ & \underline{x} \in X \subseteq \mathbb{R}^n & \end{array} \right.$$

where X is an arbitrary subset (e.g., a set of points with integer coordinates like in Integer Programming).

it can even be a set of points
That's because sufficient optimality conditions do not involve the concept of gradient (of the objective function or of the constraints)
$\Longrightarrow$ very general framework

Definitions

- The **Lagrange function** associated with (P) is

  $L(\underline{x}, \underline{u}) = f(\underline{x}) + \sum_{i \in I} u_i g_i(\underline{x}) \quad \forall \underline{x} \in X$ and $\underline{u} \geq \underline{0}$

  N.B.: $\underline{u} \geq \underline{0}$ since $g_i(\underline{x}) \leq 0$.

in this way, since $g_i(\underline{x}) \leq 0$ we have $L(\underline{x}, \underline{u}) = f(\underline{x}) +$ (something that is ≤ 0)

- $(\overline{\underline{x}}, \overline{\underline{u}})$ with $\overline{\underline{x}} \in X$ and $\overline{\underline{u}} \geq \underline{0}$ is a **saddle point** of $L(\underline{x}, \underline{u})$

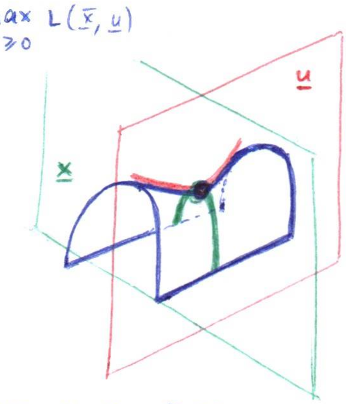
  if $L(\overline{\underline{x}}, \overline{\underline{u}}) \leq L(\underline{x}, \overline{\underline{u}}) \quad \forall \underline{x} \in X$ and $L(\overline{\underline{x}}, \underline{u}) \leq L(\overline{\underline{x}}, \overline{\underline{u}}) \quad \forall \underline{u} \geq 0$,

  that is, $\overline{\underline{x}}$ minimizes $L(\underline{x}, \overline{\underline{u}})$ over X and $\overline{\underline{u}}$ maximizes $L(\overline{\underline{x}}, \underline{u})$ over $\mathbb{R}^m$.

$\overline{\underline{x}} = \min_{\underline{x} \in X} L(\underline{x}, \overline{\underline{u}})$

$\overline{\underline{u}} = \max_{\underline{u} \geq 0} L(\overline{\underline{x}}, \underline{u})$

The saddle point is maximum in the plane of $\underline{u}$ and minimum in the plane of $\underline{x}$



Proposition: (Characterization of saddle points)

$(\overline{\underline{x}}, \overline{\underline{u}})$ with $\overline{\underline{x}} \in X$ and $\overline{\underline{u}} \geq \underline{0}$ is a saddle point of $L(\underline{x}, \underline{u})$ if and only if

i) $L(\overline{\underline{x}}, \overline{\underline{u}}) = \min_{x \in X} L(\underline{x}, \overline{\underline{u}})$

ii) $g_i(\overline{\underline{x}}) \leq 0 \quad \forall i \in I$ — $\overline{\underline{x}}$ is a feasible solution of the problem (P)

iii) $\overline{u}_i g_i(\overline{\underline{x}}) = 0 \quad \forall i \in I$. — (either $\overline{u}_i = 0$ or $g_i(\overline{\underline{x}}) = 0$: if the constraint is active then $\overline{u}_i > 0$, otherwise it must be $\overline{u}_i = 0$)

Proof:

$\Rightarrow$) If $(\overline{\underline{x}}, \overline{\underline{u}})$ is a saddle point, then

i) must be true since $L(\overline{\underline{x}}, \overline{\underline{u}}) \leq L(\underline{x}, \overline{\underline{u}}) \quad \forall \underline{x} \in X$

ii) $\forall \underline{u} \geq 0 \quad L(\overline{\underline{x}}, \underline{u}) \leq L(\overline{\underline{x}}, \overline{\underline{u}}) \quad \Leftrightarrow \quad f(\overline{\underline{x}}) + \sum_{i \in I} u_i g_i(\overline{\underline{x}}) \leq f(\overline{\underline{x}}) + \sum_{i \in I} \overline{u}_i g_i(\overline{\underline{x}})$

and hence

$$\sum_{i \in I} (u_i - \overline{u}_i) g_i(\overline{\underline{x}}) \leq 0 \qquad \forall \underline{u} \geq \underline{0} \tag{1}$$

Thus $g_i(\overline{\underline{x}}) \leq 0 \quad \forall i \in I$.

Indeed, if $\exists\, i_0$ such that $g_{i_0}(\overline{\underline{x}}) > 0$, we can choose $u_{i_0} > 0$ sufficiently large so that (1) does not hold.

iii) For $\underline{u} = \underline{0}$ then (1) becomes $sum_{i \in I} \overline{u}_i g_i(\overline{\underline{x}}) \geq 0$.

But $\overline{u_i} \geq \underline{0}$ and $g_i(\overline{\underline{x}}) \leq 0$ implies that $\sum_{i \in I} \overline{u_i} g_i(\overline{\underline{x}}) = 0$

and thus $\overline{u_i} g_i(\overline{\underline{x}}) = 0 \quad \forall i \in I$.

$\Leftarrow$) If condition i) holds, $L(\overline{\underline{x}}, \overline{\underline{u}}) \leq L(\underline{x}, \overline{\underline{u}}) \quad \forall \underline{x} \in X$.

If condition iii) holds, $L(\overline{\underline{x}}, \overline{\underline{u}}) = f(\overline{\underline{x}}) + \sum_{i \in I} \overline{u}_i g_i(\overline{\underline{x}})$ with $\overline{u}_i g_i(\overline{\underline{x}}) = 0$.

Now $L(\overline{\underline{x}}, \underline{u}) = f(\overline{\underline{x}}) + \sum_{i \in I} u_i g_i(\overline{\underline{x}}) \leq f(\overline{\underline{x}}) = L(\overline{\underline{x}}, \overline{\underline{u}}) \quad \forall \underline{u} \geq \underline{0}$.

Hence $L(\overline{\underline{x}}, \underline{u}) \leq L(\overline{\underline{x}}, \overline{\underline{u}}) \leq L(\underline{x}, \overline{\underline{u}}) \quad \forall \underline{x} \in X$ and $\forall \underline{u} \geq \underline{0}$.

□

Theorem: (Sufficient optimality condition)

If $(\overline{\underline{x}}, \overline{\underline{u}})$ is a saddle point of $L(\underline{x}, \underline{u})$, then $\overline{\underline{x}}$ is a *global minimum* of problem (P).

Proof:

Condition i) of the saddle point characterization implies $L(\overline{\underline{x}}, \overline{\underline{u}}) \leq L(\underline{x}, \overline{\underline{u}}) \quad \forall \underline{x} \in X$

$\Rightarrow f(\overline{\underline{x}}) + \sum_{i \in I} \overline{u}_i g_i(\overline{\underline{x}}) \leq f(\underline{x}) + \sum_{i \in I} \overline{u}_i g_i(\underline{x}) \quad \forall \underline{x} \in X$

Condition iii) implies : $f(\overline{\underline{x}}) \leq f(\underline{x}) + \sum_{i \in I} \overline{u}_i g_i(\underline{x}) \quad \forall \underline{x} \in X$

and hence, since $\overline{\underline{u}} \geq \underline{0}$ we have : $f(\overline{\underline{x}}) \leq f(\underline{x}) \quad \forall \underline{x} \in X$ s.t. $g_i(\underline{x}) \leq 0$. ■

Observations:

- Result applies to any mathematical program (convex or not, with f and g_i differentiable or not, X continuous or discrete, ...).
- For some problems a saddle point may not exist. This is in general the case for non-convex problems.

Example:

$$\begin{array}{ll} \min & f(x) = -x^2 \\ \text{s.t.} & 2x - 1 \leq 0 \\ & 0 \leq x \leq 1 \end{array}$$

where $g_1(x) = 2x - 1$ and $X = \{x : 0 \leq x \leq 1\}$

There always exists a saddle point if the problem is convex. In general the saddle point may not exist.

$L(x, u) = -x^2 + u(2x - 1)$ is concave in x (for every fixed $u \geq 0$) implies that the minimum over [0,1] is reached either at $x = 0$ or at $x = 1$.

Optimal solution is $x^* = \frac{1}{2}$ but no saddle point of the type $(\frac{1}{2}, u)$ exists.

convex problem (P) $\rightarrow$ if (P) has an optimal solution then this solution corresponds to a saddle point for $L(\underline{x}, \underline{u})$

Theorem: (saddle point for convex problems)

Suppose f and g_i, $\forall i \in I$ are convex, $X \subseteq \mathbb{R}^n$ is convex and $\exists\, \underline{a} \in X$ such that $\underline{g}(\underline{a}) < \underline{0}$.
If (P) has an optimal solution $\overline{\underline{x}}$, $\exists\, \overline{\underline{u}} \geq \underline{0}$ such that $(\overline{\underline{x}}, \overline{\underline{u}})$ is a saddle point of $L(\underline{x}, \underline{u})$.

Connection with KKT conditions for convex problems

If f and $g_i \in C^1$ are convex, $X = \mathbb{R}^n$ and $\exists\, \underline{a} \in X$ such that $\underline{g}(\underline{a}) < \underline{0}$, then $\overline{\underline{x}}$ is an optimal solution if and only if $\overline{\underline{x}}$ satisfies the KKT conditions.

$g_i(\underline{a}) < 0 \quad \forall i$

Proof:

$\overline{\underline{x}}$ is an optimal solution $\Leftrightarrow$ $\exists\, \overline{\underline{u}} \geq \underline{0}$ such that $(\overline{\underline{x}}, \overline{\underline{u}})$ is a saddle point of $L(\underline{x}, \underline{u})$
($\Leftarrow$ Sufficient Condition, $\Rightarrow$ last theorem)

$\Leftrightarrow$ i) $L(\overline{\underline{x}}, \overline{\underline{u}}) = \min\limits_{\underline{x} \in X} L(\underline{x}, \overline{\underline{u}})$ ii) $g_i(\overline{\underline{x}}) \leq 0 \quad \forall i \in I$ iii) $\overline{u}_i g_i(\overline{\underline{x}}) = 0 \quad \forall i \in I$.

Since $L(\underline{x}, \overline{\underline{u}}) = f(\underline{x}) + \overline{\underline{u}}^t \underline{g}(\underline{x})$ is convex, due to condition i) it suffices to impose $\nabla_x L(\overline{\underline{x}}, \overline{\underline{u}}) = \underline{0}$, which coincides with the KKT conditions:

$$\nabla f(\overline{\underline{x}}) + \sum_{i \in I} \overline{u}_i \nabla g_i(\overline{\underline{x}}) = \underline{0}.$$

The CQ assumption holds at every feasible solution.

□

N.B.: 1) Without convexity assumption a stationary point $\overline{\underline{x}}$ may not minimize $L(\underline{x}, \overline{\underline{u}})$.

2) KKT multipliers are then identical to Lagrange multipliers at the saddle point.

5.4 Lagrangian duality

Consider

$$(P) \begin{cases} \min & f(\underline{x}) \\ \text{s.t.} & g_i(\underline{x}) \leq 0 \qquad \forall i \in I = \{1, \ldots, m\} \\ & \underline{x} \in X \subseteq \mathbb{R}^n \end{cases}$$

To any Nonlinear Program (NLP) with minimization we can associate a NLP with maximization such that, under some assumptions, the objective function values of respective optimal solutions coincide.

Tackle the *primal* problem (P) indirectly, by solving the second (dual) problem.

! To try to solve (P), we can look for a saddle point of the Lagrange function

Dual function:

$$w(\underline{u}) = \min_{\underline{x} \in X} L(\underline{x}, \underline{u}) \qquad \forall \underline{u} \geq \underline{0}$$

$L(\underline{x}, \underline{u}) = f(\underline{x}) + \sum_{i \in I} u_i g_i(\underline{x})$

Well-defined if, for instance, f and the g_i's are continuous and X is compact.

Search for a saddle point (if it exists):

Dual problem: $(D) \begin{cases} \max & w(\underline{u}) \\ & \underline{u} \geq \underline{0} \end{cases}$ $\leftarrow$ Lagrangian dual associated to (P) (we can always associate it to (P), even if (P) is not convex or even if the Lagrangian doesn't have a saddle point)

N.B.: $w(\underline{u})$ and (D) are defined even if no saddle point exists.

Observations:

1) We can define different Lagrangian duals of (P) depending on which $g_i(\underline{x}) \leq 0$ are dualized. Choice affects the optimal value of (D) and the complexity to evaluate $w(\underline{u})$.

dualize a $g_i(\underline{x}) \leq 0$ means bring it to the objective function (depending on which constr. we decide to Lagrangianize we obtain a different (D))

2) The Lagrangian dual is useful to solve large-scale LPs, (non)convex optimization problems, and also discrete optimization problems.

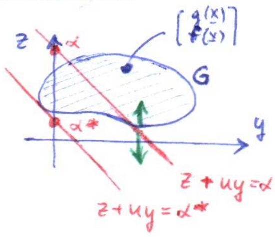
$L(x,u) = f(x) + ug(x)$
$\quad \downarrow$
$= z + uy$

Geometric interpretation: (for the Lagrangian dual)

(P) min $f(\underline{x})$ s.t. $g(\underline{x}) \leq 0, \underline{x} \in X \subseteq \mathbb{R}^n$ $\quad \longrightarrow \quad$:= min z, s.t. $y \leq 0$

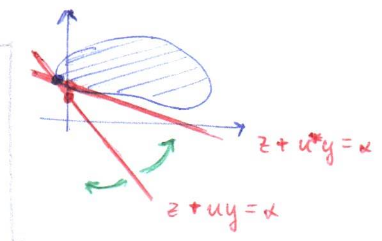
we suppose to have just one constr.

$G = \{ (y, z) : y = g(\underline{x}),\ z = f(\underline{x}) \text{ for } \underline{x} \in X \} \ldots$: G is the image of X throug (f, g)



The Lagrangian : $z + uy = \alpha$ is a line with slope $-u$ and intercept α. The primal (P) is equivalent to:
for a fixed u (= slope) : min $L(x, u)$ = min $z + uy$ over G.
This is equivalent to translate $\updownarrow$ $z + uy = \alpha$ to find the minimum α $(:= \alpha^*)$. We get $\boxed{w(u) = \alpha^*}$ $(= \min_x L(\underline{x}, \underline{u}))$.
Now there is (D): we maximize $w(u)$:
we focus on the choice of u and we find u^* s.t. $w(u^*)$ is max.
(this is equivalent to find the slope $-u$ of the supporting hyperplane (here it's a line) such that the intercept is as high as possible)

See example at beginning of Chapter 6 of M. Bazaraa, H. Sherali and C. Shetty, Nonlinear programming: Theory and Algorithms, Third edition, Wiley Interscience, 2006.



(P) min $f(\underline{x})$:
$g_i(\underline{x}) \leq 0 \ \forall i \in I$
$\underline{x} \in X \subseteq \mathbb{R}^n$

(D) max $w(\underline{u})$:
$\underline{u} \geq \underline{0}$

$w(\underline{u}) = \min_{\underline{x} \in X} L(\underline{x}, \underline{u})$

$L(\underline{x}, \underline{u}) = f(\underline{x}) + \sum_{i \in I} u_i g_i(\underline{x})$

$f(\underline{x}) \downarrow (P)$
IV
$w(\underline{u}) \uparrow (D)$

Which are the links between strong and weak duality?

Theorem: (Weak duality)

For any feasible $\underline{x}$ of (P) and $\underline{u} \geq \underline{0}$, we have $w(\underline{u}) \leq f(\underline{x})$.

Proof:

By definition of $w(\underline{u})$: $\ w(\underline{u}) \leq f(\underline{x}) + \underline{u}^t \underline{g}(\underline{x}) \quad \forall \underline{x} \in X, \ \forall \underline{u} \geq 0.$

If $\underline{g}(\underline{x}) \leq \underline{0}$ then $w(\underline{u}) \leq f(\underline{x})$ because $\underline{u} \geq 0$.

In particular, for any feasible $\underline{u} \geq 0$ of (D) the value $w(\underline{u})$ is a lower bound on the value $f(\underline{x}^*)$ of an optimal solution $\underline{x}^*$ of (P). ∎

Consequence:

If a feasible solution $\overline{\underline{x}}$ of (P) and $\overline{\underline{u}} \geq \underline{0}$ satisfy $w(\overline{\underline{u}}) = f(\overline{\underline{x}})$, $\overline{\underline{x}}$ is optimal for (P) and $\overline{\underline{u}}$ is optimal for (D).

$\Rightarrow$ $f(\underline{x}) \geq w(\underline{u})$
if $f(\underline{x}) = w(\underline{u})$ then the pair $(\underline{x}, \underline{u})$ for which it holds the "=" is optimal

For Linear Programs the objective function values of optimal solutions of the primal and the dual coincide, for Nonlinear Programs this is not always the case.

we can have a gap between the (P)-optimality and the (D)-optimality

Theorem: (Strong duality)

i) If (P) has a saddle point $(\overline{\underline{x}}, \overline{\underline{u}})$, then

$$\left\{ \begin{array}{l} \max\ w(\underline{u}) \\ \underline{u} \geq \underline{0} \end{array} \right. = w(\overline{\underline{u}}) = f(\overline{\underline{x}}) = \min \{ f(\underline{x}) : \underline{g}(\underline{x}) \leq \underline{0}, \underline{x} \in X \}.$$

if $(\overline{\underline{x}}, \overline{\underline{u}})$ is a saddle point, not only $\overline{\underline{x}}$ is optimal for (P) (as we already knew) but $\overline{\underline{u}}$ is also optimal for (D).

ii) If $\exists$ a feasible $\overline{\underline{x}}$ of (P) and $\overline{\underline{u}} \geq \underline{0}$ such that $w(\overline{\underline{u}}) = f(\overline{\underline{x}})$, then $(\overline{\underline{x}}, \overline{\underline{u}})$ is a saddle point of $L(\underline{x}, \underline{u})$.

(Weak duality: $\overline{\underline{x}}$ and $\overline{\underline{u}}$ are optimal for respective problems)

Proof:

ii) Since $(\overline{\underline{x}}, \overline{\underline{u}})$ is a saddle point $\ w(\overline{\underline{u}}) = L(\overline{\underline{x}}, \overline{\underline{u}}) = \min_{\underline{x} \in X} L(\underline{x}, \overline{\underline{u}})$

and $L(\overline{\underline{x}}, \overline{\underline{u}}) = f(\overline{\underline{x}}) + \overline{\underline{u}}^t \underline{g}(\overline{\underline{x}}) = f(\overline{\underline{x}}) = \min \{ f(\underline{x}) : \underline{g}(\underline{x}) \leq \underline{0}, \underline{x} \in X \}$.

Thus $w(\overline{\underline{u}}) = f(\overline{\underline{x}})$.

Because of weak duality $w(\underline{u}) \leq f(\overline{\underline{x}}) \quad \forall \underline{u} \geq \underline{0}$, we have $w(\overline{\underline{u}}) = \left\{ \begin{array}{l} \max\ w(\underline{u}) \\ \underline{u} \geq \underline{0}. \end{array} \right.$

ii) Let $\overline{\underline{x}}$ is a feasible solution of (P) and $\overline{\underline{u}} \geq \underline{0}$ such that $w(\overline{\underline{u}}) = f(\overline{\underline{x}})$.

By definition of $w(\underline{u})$: $\ w(\overline{\underline{u}}) \leq f(\underline{x}) + \overline{\underline{u}}^t \underline{g}(\underline{x}) \quad \forall \underline{x} \in X$.

For $\underline{x} = \overline{\underline{x}}$, we have $f(\overline{\underline{x}}) = w(\overline{\underline{u}}) \leq f(\overline{\underline{x}}) + \overline{\underline{u}}^t \underline{g}(\overline{\underline{x}})$ and hence $\overline{u}_i g_i(\overline{\underline{x}}) = 0 \ \ \forall i \in I$.

Since $\overline{\underline{u}} \geq \underline{0}$, $g_i(\overline{\underline{x}}) \leq 0 \ \ \forall i \in I$ and $w(\overline{\underline{u}}) = L(\overline{\underline{x}}, \overline{\underline{u}}) = \min_{\underline{x} \in X} L(\underline{x}, \overline{\underline{u}})$

then $(\overline{\underline{x}}, \overline{\underline{u}})$ is a saddle point. □

Consequence:

If f and g_i's convex, $X \subseteq \mathbb{R}^n$ convex and $\exists\, \underline{a}$ such that $\underline{g}(\underline{a}) < \underline{0}$, then if (P) has a finite optimal solution, $\exists$ a saddle point $(\overline{\underline{x}}, \overline{\underline{u}})$ and i) holds, that is

$$\left\{ \begin{array}{l} \max\ w(\underline{u}) \\ \underline{u} \geq \underline{0} \end{array} \right. = \min \{ f(\underline{x}) : \underline{g}(\underline{x}) \leq \underline{0}, \underline{x} \in X \}.$$

if the problem is convex (and $\exists$ an interior point) =

If the problem is convex then (P) has a finite optimal solution and we have no duality gap (between (P) and (D))

N.B.: optimal values of the objective functions coincide, we have *strong duality*.

In genereal, we can have a *duality gap*:

$$\left\{ \begin{array}{l} \max\ w(\underline{u}) \\ \underline{u} \geq \underline{0} \end{array} \right. < \min \{ f(\underline{x}) : \underline{g}(\underline{x}) \leq \underline{0}, \underline{x} \in X \}.$$

strong duality: $f(\underline{x}^*) = w(\underline{u}^*)$
weak duality: $f(\underline{x}^*) \geq w(\underline{u}^*)$

(+ Example at the end)

Since under certain conditions it is possible to solve (P) indirectly by solving (D)

we're interested in discover how difficult and how we can solve the dual problem

Property 1: The dual function $w(\underline{u})$ is concave.

That's so good!

Proof: Take any $\underline{u}_1, \underline{u}_2 \geq \underline{0}$ and $\lambda \in [0,1]$ and set $\underline{u} = \lambda \underline{u}_1 + (1-\lambda)\underline{u}_2$.

By assumption $\exists\, \overline{\underline{x}} \in X$ such that $w(\underline{u}) = f(\overline{\underline{x}}) + \underline{u}^t \underline{g}(\overline{\underline{x}})$.

By definition of $w(\underline{u})$:

$$\begin{cases} w(\underline{u}_1) \leq f(\overline{\underline{x}}) + \underline{u}_1{}^t \underline{g}(\overline{\underline{x}}) \\ w(\underline{u}_2) \leq f(\overline{\underline{x}}) + \underline{u}_2{}^t \underline{g}(\overline{\underline{x}}) \end{cases} \Rightarrow \lambda w(\underline{u}_1) + (1-\lambda) w(\underline{u}_2) \leq f(\overline{\underline{x}}) + \underline{u}^t \underline{g}(\overline{\underline{x}}) = w(\underline{u}). \quad \blacksquare$$

Observations:

If $X \subseteq \mathbb{Z}^n$ then $w(\underline{u})$ is piecewise concave:

- If $X \subseteq \mathbb{Z}^n$, $w(\underline{u})$ is not everywhere continuously differentiable. Concave piecewise linear function, lower envelope of a (in)finite family of hyperplanes in $\mathbb{R}^{n+1}$.
- In general (D) is easier than (P).
- Since $w(\underline{u})$ is concave local optima are global optima, but need for ad hoc solution method: **subgradient method**.

Since the function $w(\underline{u})$ may not be everywhere continuously differentiable we cannot use the line search method, we adapt with: **SUBGRADIENT METHOD**: we use the gradient if the point is continuously different. and the subgradient when it's not.

Property 2: For $\tilde{\underline{u}} \in \mathbb{R}^m_+$ let $X(\tilde{\underline{u}}) = \{\underline{x} \in X : f(\underline{x}) + \tilde{\underline{u}}^t \underline{g}(\underline{x}) = w(\tilde{\underline{u}})\}$ then $\underline{g}(\underline{x})$ is a subgradient of $w(\underline{u})$ for each $\underline{x} \in X(\tilde{\underline{u}})$.

all the $\underline{x} \in X$ such that: $w(\tilde{\underline{u}}) = \min_{\underline{x} \in X} L(\underline{x}, \tilde{\underline{u}})$

Is it easy to find the subgradient of $w(\underline{u})$? Yes

Proof: By definition of $w(\underline{u})$, we have $w(\underline{u}) \leq f(\underline{x}) + \underline{u}^t \underline{g}(\underline{x}) \quad \forall \underline{x} \in X \quad \forall \underline{u} \geq \underline{0}$.

For $\overline{\underline{x}} \in X(\tilde{\underline{u}})$ we have $w(\underline{u}) \leq f(\overline{\underline{x}}) + \underline{u}^t \underline{g}(\overline{\underline{x}})$.

and by definition of $X(\tilde{\underline{u}})$: $w(\tilde{\underline{u}}) \leq f(\overline{\underline{x}}) + \tilde{\underline{u}}^t \underline{g}(\overline{\underline{x}}) \Rightarrow w(\underline{u}) - w(\tilde{\underline{u}}) \leq (\underline{u}^t - \tilde{\underline{u}}^t)\, \underline{g}(\overline{\underline{x}})$. $\blacksquare$

$$\begin{bmatrix} \vdots \\ g_i(\underline{x}) \\ \vdots \end{bmatrix} \leftarrow \underline{x} \in X(\tilde{\underline{u}})$$

Observations:

- Every subgradient of $w(\underline{u})$ at $\tilde{\underline{u}}$ can be expressed as a convex combination of the subgradients $\underline{g}(\underline{x})$ with $\underline{x} \in X(\tilde{\underline{u}})$.
- If w is continuously differentiable at $\tilde{\underline{u}}$, $X(\tilde{\underline{u}})$ contains a single element $\tilde{\underline{x}}$ and $\underline{g}(\tilde{\underline{x}})$ is gradient of $w(\underline{u})$ at $\tilde{\underline{u}}$.

: it's like $\underline{g}(\underline{x})$ with $\underline{x} \in X(\tilde{\underline{u}})$ are the generators

Summary

- In general (D) is easier to solve than (P) – even if no saddle point exists.
- When saddle point exists: we can solve (D) instead of (P) and derive optimal $\underline{x}^*$ of (P) by minimizing $L(\underline{x}, \underline{u}^*)$ over X ensuring that $g_i(\underline{x}^*) \leq 0$. $\forall i \in I$, and $u_i^* g_i(\underline{x}^*) = 0 \ \ \forall i \in I$.
- When no saddle point exists: optimal $\underline{u}^*$ of (D) provides a lower bound $w(\underline{u}^*)$ for $f(\underline{x}^*)$.
- Find $\underline{u}^* \geq \underline{0}$ maximizing $w(\underline{u})$ by using the subgradient method that generates $\{\underline{u}^k\} \to \underline{u}^*$ when $k \to \infty$.
- For each $\underline{u}^k$, we have a lower bound $w(\underline{u}^k)$ for $f(\underline{x}^*)$ and we determine $\underline{x}^k$ that minimizes $L(\underline{x}, \underline{u}^k)$ over X.

5.5 Second order optimality conditions

Nonlinear program:

$$(P) \qquad \begin{array}{lll} \min & f(\underline{x}) & \\ s.t. & g_i(\underline{x}) \leq 0 & i \in I = \{1, \ldots, m\} \\ & h_l(\underline{x}) = 0 & l \in L = \{1, \ldots, k\} \\ & \underline{x} \in X \subseteq \mathbb{R}^n & \end{array}$$

with f, g_i's and h_l's of class C^2 and X open subset of $\mathbb{R}^n$.

Lagrange function:

$$L(\underline{x}, \underline{u}, \underline{v}) = f(\underline{x}) + \sum_{i=1}^{m} u_i g_i(\underline{x}) + \sum_{l=1}^{k} v_l h_l(\underline{x}) = f(\underline{x}) + \underline{u}^t \underline{g}(\underline{x}) + \underline{v}^t \underline{h}(\underline{x})$$

with $\underline{u} \geq \underline{0}$ and $\underline{v} \in \mathbb{R}^k$.

$\nabla^2_{\underline{xx}} L(\underline{x}, \underline{u}, \underline{v}) = \nabla^2 f(\underline{x}) + \sum_{i=1}^m u_i \nabla^2 g_i(\underline{x}) + \sum_{l=1}^k v_l \nabla^2 h_l(\underline{x})$ is the Hessian submatrix of $L(\underline{x}, \underline{u}, \underline{v})$ w.r.t. the variables x_j's.

Necessary conditions

$$\min f(\underline{x}) \quad \text{s.t.} \quad g_i(\underline{x}) \le 0 \quad i \in I = \{1,\dots,m\}, \quad \underline{x} \in \mathbb{R}^n$$

CQ: $\mathcal{D}(\bar{x}) = D(\bar{x})$

sufficient cond. for CQ:

- S • g_i linear
- S • g_i convex, $\exists \underline{x}^*: g_i(\underline{x}^*) < 0 \ \forall i$
- $\bar{x}$ • $\nabla g_i(\bar{x})$ are linearly $\perp\!\!\!\perp$

KKT: $u_i \ge 0$

$$\nabla f(\bar{x}) + \sum_{i \in I(\bar{x})} u_i \nabla g_i(\bar{x}) = \underline{0}$$

~~sufficient if f, gi convex and ∃x*: gi(x*)<0 ∀i~~

$$\min f(\underline{x}) \quad \text{s.t.} \quad g_i(\underline{x}) \le 0 \quad i \in I = \{1,\dots,m\}, \quad h_\ell(\underline{x}) = 0 \quad \ell \in L = \{1,\dots,p\}, \quad \underline{x} \in X \subseteq \mathbb{R}^n$$

CQ: $T(\bar{x}) = D(\bar{x}) \cap H(\bar{x})$

sufficient cond. for CQ:

- S • g_i convex, $\exists \underline{x}^*: g_i(\underline{x}^*) < 0 \ \forall i$; h_ℓ linear, $h_\ell(\underline{x}^*) = 0 \ \forall \ell$
- $\bar{x}$ • $\nabla g_i(\bar{x}), \nabla h_\ell(\bar{x})$ $\perp\!\!\!\perp$ $\forall i \forall \ell$

KKT: $u_i \ge 0, \ v_\ell \in \mathbb{R}$

$$\nabla f(\bar{x}) + \sum_{i \in I(\bar{x})} u_i \nabla g_i(\bar{x}) + \sum_{\ell \in L} v_\ell \nabla h_\ell(\bar{x}) = \underline{0}$$

Sufficient condition

$$\min f(\underline{x}) \quad \text{s.t.} \quad g_i(\underline{x}) \le 0 \quad i \in I = \{1,\dots,m\}, \quad \underline{x} \in \mathbb{R}^n$$

$:= (P)$

$$L(\underline{x}, \underline{u}) = f(\underline{x}) + \sum_{i \in I} u_i g_i(\underline{x}) \qquad u_i \ge 0$$

- $\bar{x}$ global minimum if $(\bar{x}, \bar{u})$ saddle point of $L(\underline{x}, \underline{u})$.
- f, g_i, X $(\underline{x} \in X)$ convex, $\exists \underline{x}^*: g_i(\underline{x}^*) < 0 \ \forall i$ $\longrightarrow \left[\bar{x} \text{ optimal} \Rightarrow \exists \bar{u}: (\bar{x}, \bar{u}) \text{ saddle point of } L(\bar{x}, \bar{u}) \right]$

- f, g_i, X convex, $\exists \underline{x}^*: g_i(\underline{x}^*) < 0 \ \forall i$ $\longrightarrow \left[\bar{x} \text{ optimal} \Longleftrightarrow \bar{x} \text{ KKT} \right]$

Lagrangian duality

$\min f(\underline{x})$ $g_i(\underline{x}) \leq 0 \;\; \forall i$ $\underline{x} \in X \subseteq \mathbb{R}^n$	$\max \; w(\underline{u})$ $\underline{u} \geq \underline{0}$ $w(\underline{u}) = \min_{\underline{x} \in X} L(\underline{x}, \underline{u})$ $L(\underline{x}, \underline{u}) = f(\underline{x}) + \sum_{i \in I} u_i g_i(\underline{x})$	• weak duality $f(\bar{\underline{x}}) \geq w(\bar{\underline{u}})$ • strong duality $f(\bar{\underline{x}}) = w(\bar{\underline{u}})$
(P)	(D)	

- strong duality $\iff$ $(\bar{\underline{x}}, \bar{\underline{u}})$ saddle point of $L(\underline{x}, \underline{u})$
- f, g_i, X convex, $\exists \underline{x}^* : g_i(\underline{x}^*) < 0 \;\; \forall i \implies \exists (\bar{\underline{x}}, \bar{\underline{u}})$ saddle pt., $\nexists$ duality gap
- $w(\underline{u})$ concave

QP → only equality (Null space method)

QP → equality & inequality (Active-set method)

$\boxed{\text{Active set method}}$

- $\underline{x}_0$ feasible, $W_0 \subseteq I(\underline{x}_0) \cup \{\text{eq. constr.}\}$
- $\underline{x}_k$ feasible : $\underline{d}_k \leftarrow \min \{ q(\underline{x}_k + \underline{d}_k) \; ; \; \underline{a}_i^T \underline{d}_k = 0 \;\; i \in W_k \}$
  - $\underline{d}_k \neq \underline{0}$: $\alpha_k = \min \left\{ 1, \min_{\substack{i \notin W_k : \\ \underline{a}_i^T \underline{d}_k > 0}} \frac{b_i - \underline{a}_i^T \underline{x}_k}{\underline{a}_i^T \underline{d}_k} \right\}$

    $\underline{x}_{k+1} = \underline{x}_k + \alpha_k \underline{d}_k$
  - $\underline{d}_k = \underline{0}$: $\underline{x}_{k+1} = \underline{x}_k$

    Determine u_i^k : $Q\underline{x}_k + \underline{c} + \sum_{i \in W_k} u_i^k \underline{a}_i = \underline{0}$
    - $u_i^k \geq 0 \implies \underline{x}_k$ local optimum of QP
    - $u_i^k < 0 \implies W_{k+1} = W_k \setminus \{i'\}$

      i' the most neg. u_i^k

QP: $\min \; q(\underline{x}) = \frac{1}{2} \underline{x}^T Q \underline{x} + \underline{c}^T \underline{x}$

$\underline{a}_i^T \underline{x} \leq b_i \qquad i \in I$

$\underline{a}_i^T \underline{x} = b_i \qquad i \in E$

$\underline{x} \in \mathbb{R}^n$

Second order KKT necessary conditions:

If $\underline{\overline{x}}$ is a local minimum of (P) and $\nabla g_i(\underline{\overline{x}})$, with $i \in I(\underline{\overline{x}})$, and $\nabla h_l(\underline{\overline{x}})$, with $l \in L$, are linearly independent, then $\underline{\overline{x}}$ and some $(\underline{u}, \underline{v})$ satisfy the KKT conditions:

equivalent to "CQ holds at $\overline{x}$"

$$\nabla_{\underline{x}} L(\underline{x}, \underline{u}, \underline{v}) = \nabla f(\underline{x}) + \sum_{i=1}^{m} u_i \nabla g_i(\underline{x}) + \sum_{l=1}^{k} v_l \nabla h_l(\underline{x}) = \underline{0}$$

$$\begin{aligned} g_i(\underline{x}) &\le 0 & i \in I = \{1, \dots, m\} \\ h_l(\underline{x}) &= 0 & l \in L = \{1, \dots, k\} \\ u_i g_i(\underline{x}) &= 0 & i \in I \\ \underline{u} \ge \underline{0},\ \underline{v} &\in \mathbb{R}^k. \end{aligned}$$

$\underline{x}$ is feasible

if $g_i(\underline{x})$ is not active (<0 and not $=0$) then the corresponding u_i is equal to 0

Moreover, every $\underline{d} \in \mathbb{R}^n$ such that

$$\left.\begin{aligned} \nabla^t g_i(\underline{\overline{x}}) \underline{d} &\le 0 & i \in I(\underline{\overline{x}}) \\ \nabla^t h_l(\underline{\overline{x}}) \underline{d} &= 0 & l \in L \end{aligned}\right\} (*)$$

must satisfy

$$\underline{d}^t \nabla^2_{\underline{xx}} L(\underline{\overline{x}}, \underline{u}, \underline{v}) \underline{d} \ge 0.$$

condition on the second order information

if it would have been $\forall \underline{d} \in \mathbb{R}^n$ then the Hessian matrix of the Lagrangian function at $\overline{x}$ would have been positive definite. instead, this must hold only for $\underline{d}$ s.t. $(*)$.

Second order KKT sufficient conditions:

Let $\underline{\overline{x}}$ satisfies with $(\underline{u}, \underline{v})$ the previous KKT conditions.
If

$$\underline{d}^t \nabla^2_{\underline{xx}} L(\underline{\overline{x}}, \underline{u}, \underline{v}) \underline{d} > 0$$

for each $\underline{d} \neq \underline{0}$ such that

$$\begin{aligned} \nabla^t g_i(\underline{\overline{x}}) \underline{d} &= 0 & i \in I^+ \\ \nabla^t g_i(\underline{\overline{x}}) \underline{d} &\le 0 & i \in I^0 \\ \nabla^t h_l(\underline{\overline{x}}) \underline{d} &= 0 & l = 1, \dots, k \end{aligned}$$

where $I^+ = \{i \in I \ :\ u_i > 0\}$ and $I^0 = \{i \in I \ :\ u_i = 0\}$,

then $\underline{\overline{x}}$ is a strict local minimum of (P).

5.6 Quadratic programming

Minimize a quadratic function subject to linear constraints:

$$(P) \quad \begin{aligned} \min \quad & \tfrac{1}{2}\, \underline{x}^t Q \underline{x} + \underline{c}^t \underline{x} & \\ s.t. \quad & \underline{a}_i^t \underline{x} \le b_i & i \in I \\ & \underline{a}_i^t \underline{x} = b_i & i \in E \\ & \underline{x} \in \mathbb{R}^n, & \end{aligned}$$

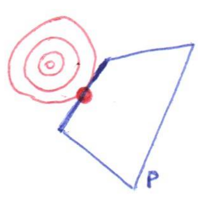
where $Q \in \mathbb{R}^{n \times n}$.

Without loss of generality: Q is symmetric (same function value with $\overline{Q}$ not symmetric and $Q = \frac{1}{2}(\overline{Q} + \overline{Q}^t)$).

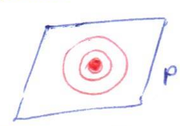
Difficulty depends on Q: if Q positive semidefinite, (P) convex and "easy" to solve, otherwise can have a large number of local optima.

Example: $\min\{-\underline{x}^t \underline{x} : -1 \le x_i \le 1,\ i = 1, \dots, n\}$ where all 2^n vertices with $x_i \in \{-1, 1\}\ \forall i$ are local minima.

Illustrations of convex Quadratic Programs (QPs):



Suppose we're optimizing on the polyhedron P. If we minimize a linear function on a polyhedron we know that the finite optimal solution is one of the vertices. If the objective function is quadratic this is no longer true: suppose that we consider a quadratic objective function which level curves are represented by —. Then the optimal belongs to the boundary but it's not an extreme point. Actually x^* could even be an interior point:



By considering a quadratic objective function we have to consider all the points of P (region on which we are optimizing).

QPs are the simplest NLP problems besides Linear Programs. Efficient QP algorithms are available.

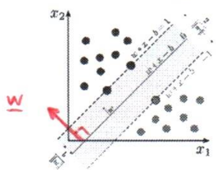
Many direct applications (for portfolio optimization see exercise 9.1).

Example: Training linear Support Vector Machines (SVMs) (SVM for classification)

Training set $T = \{(\underline{x}^i, y^i) : \underline{x}^i \in \mathbb{R}^n, y^i \in \{-1, 1\}, i = 1, \ldots, p\}$.

Linear decision function: $f(\underline{w}, b, \underline{x}) = \underline{w}^t\underline{x} + b$. The classifier is linear (characterized by $\underline{w}$ and b)

Separating hyperplane with largest margin (width $\frac{2}{\|\underline{w}\|}$) guarantees best generalization.



Hard-margin linear SVM training:

QP
$$\left\{ \begin{array}{ll} \min\limits_{\underline{w}\in\mathbb{R}^n, b\in\mathbb{R}} & \frac{1}{2}\|\underline{w}\|^2 \\ \text{s.t.} & y^i(\underline{w}^t\underline{x}^i - b - 1) \geq 0 \quad i = 1, \ldots, p. \quad (*) \end{array} \right.$$

strictly convex function but possibly huge number of linear constraints. (since we have the constraint (*) for every data in the training set)

Reformulated as QP with a single constraint using duality:

$$L(\underline{w}, b, \underline{u}) = \frac{1}{2}\|\underline{w}\|^2 - \sum_{i=1}^{p} u_i y^i(\underline{w}^t\underline{x}^i - b - 1)$$

L is convex since $\frac{1}{2}\|\underline{w}\|^2$ is convex and we're adding a linear term

lagrangian dual: $\max\limits_{\underline{u}\geq\underline{0}} \left(\min\limits_{\underline{w}, b} L(\underline{w}, b, \underline{u}) \right)$. Since L is convex we know that the necessary optimality conditions for $\min_{\underline{w},b} L(\underline{w}, b, \underline{u})$ are just the stationarity condition. So we can rewrite:

$$\max_{\underline{u}\geq\underline{0}} \left(\min_{\underline{w}, b} L(\underline{w}, b, \underline{u}) \right) \Longrightarrow \max_{\underline{u}\geq\underline{0}} L(\underline{w}, b, \underline{u}) \text{ s.t. } \nabla_{\binom{\underline{w}}{b}} L(\underline{w}, b, \underline{u}) = \underline{0}, \ \underline{u} \geq \underline{0}$$

$$\nabla_{\binom{\underline{w}}{b}} L(\underline{w}, b, \underline{u}) = \underline{0} \longrightarrow \left\{ \begin{array}{ll} \underline{w} = \sum_{i=1}^{p} u_i y^i \underline{x}^i & \longleftarrow \text{substituted in the objective function} \\ \sum_{i=1}^{p} u_i y^i = 0 & \longleftarrow \text{single equality constraint} \end{array} \right.$$

$\Longrightarrow$ We still have a QP but this is much easier to solve (since the objective function is still quadratic and convex but this time we have only one constraint (+ : $\underline{u} \geq \underline{0}$))

5.6.1 QP with only equality constraints

$A = \begin{bmatrix} \vdots \\ \underline{a}_i^T \\ \vdots \end{bmatrix}$

Consider

$$\min\{ \frac{1}{2}\underline{x}^tQ\underline{x} + \underline{c}^t\underline{x} \ : \ A\underline{x} = \underline{b} \} \qquad (1)$$

where $A \in \mathbb{R}^{m\times n}$. $(m \leq n)$

Since only linear equations, CQ assumption is satisfied at all feasible points and simple KKT conditions:

since all $g_i(\underline{x})$ are linear (This is **Karlin** sufficient condition: if all the constraints are linear then the CQ assumption is satisfied in all the points of the feasible region)

$$\nabla q(\underline{x}) \quad \left. \begin{array}{r} Q\underline{x} + \underline{c} + \sum_{i=1}^{m} u_i\underline{a}_i = \underline{0} \\ A\underline{x} = \underline{b}. \end{array} \right\} \text{KKT are much more simple}$$

N.B.: Complementary slackness constraints are automatically satisfied.

More or less direct solution of the linear system:

$$\text{KKT (matrix form)} \Longrightarrow \begin{pmatrix} Q & A^t \\ A & \underline{0} \end{pmatrix} \begin{pmatrix} \underline{x} \\ \underline{u} \end{pmatrix} = \begin{pmatrix} -\underline{c} \\ \underline{b} \end{pmatrix}. \Longrightarrow$$

finding the optimum candidate points reduces to solving a linear system. Anyway, if the problem is of large dimensions, this may not be a good way to procede, so

If A of full rank and Q is p.d. on subspace $\{\underline{x} \in \mathbb{R}^n \ : \ A\underline{x} = \underline{0}\}$, matrix is non singular.

Null-space method

Since we're interested in solving $\boxed{A\underline{x} = \underline{b}}$ we focus on a basis of $A\underline{x} = \underline{0}$:

$\dim(\text{subspace}(A\underline{x} = \underline{0})) = n - m$

Determine $Z \in \mathbb{R}^{n\times(n-m)}$ whose columns span the null space $\{\underline{x} \in \mathbb{R}^n \ : \ A\underline{x} = \underline{0}\}$ of A.

Z can be computed by (sub)matrix factorization of A (if A sparse by LU factorization).

Given feasible $\underline{x}_0$, any other feasible solution

$$\underline{x} = \underline{x}_0 + Z\underline{w}$$

for an appropriate $\underline{w} \in \mathbb{R}^{n-m}$.

$\frac{1}{2}\underline{x}^TQ\underline{x} + \underline{c}^T\underline{x}$

(1) is equivalent to unconstrained QP:

$$\frac{1}{2}(\underline{x}_0 + Z\underline{w})^TQ(\underline{x}_0 + Z\underline{w}) + \underline{c}^T(\underline{x}_0 + Z\underline{w}) \Longrightarrow \boxed{\min\{ \frac{1}{2}\underline{w}^t(Z^tQZ)\underline{w} + (Q\underline{x}_0 + \underline{c})^tZ\underline{w} : \underline{w} \in \mathbb{R}^{n-m} \}.}$$

If Z^tQZ is p.d., unique optimal solution $\underline{w}^*$ obtained by solving linear system:

$$(Z^tQZ)\underline{w} = -Z^t(Q\underline{x}_0 + \underline{c}).$$

Also other methods but null-space ones are widely used.

5.6.2 QP with equality and inequality constraints

Active-set methods

$$(P)\quad \begin{array}{lll} \min & q(\underline{x}) = \frac{1}{2}\,\underline{x}^t Q \underline{x} + \underline{c}^t \underline{x} & \\ s.t. & \underline{a}_i^t \underline{x} \le b_i & i \in I \\ & \underline{a}_i^t \underline{x} = b_i & i \in E \\ & \underline{x} \in \mathbb{R}^n & \end{array}$$

where $Q \in \mathbb{R}^{n \times n}$.

Idea: Determine the subset $I(\underline{x}^*)$ of indices that are active at an optimal solution $\underline{x}^*$, by solving a sequence of QPs with only equality constraints.

↳ if we determine these indeces we can solve a QP with these constraints imposed as equations $(“=”)$ and we can use (for instance) the Null-space method (or solve the KKT conditions directly).

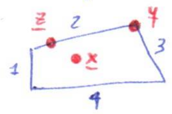
Idea: QP with only equality constraints are easier to solve, so we should try to obtain a QP-only equality

Active-set method for convex QPs

I

Initialization: Find initial feasible $\underline{x}_0$ and choose $W_0 \subseteq I(\underline{x}_0) = \{i \in I : \underline{a}_i^t \underline{x}_0 = b_i\} \cup E$ of the active constraints at $\underline{x}_0$.

“ **WORKING SET** ” subset of indeces of the active constraints at $\underline{x}_0$ and all the indeces of the equality constraints (which must be always satisfied):



$I(\underline{x}) = \{\} = \emptyset$
$I(\underline{z}) = \{2\}$
$I(\underline{y}) = \{2, 3\}$

II

Iteration k:

Given current feasible $\underline{x}_k$, determine $\underline{d}_k$ by solving the subproblem:

$$\min\{\, q(\underline{x}_k + \underline{d}) : \underline{a}_i^t(\underline{x}_k + \underline{d}) = b_i,\, i \in W_k \,\}, \tag{2}$$

where W_k is current *working* set, with $W_k \subseteq I(\underline{x}_k) = \{i \in I : \underline{a}_i^t \underline{x}_k = b_i\} \cup E$.

since $\underline{x}_k$ is a feasible point: $\underline{a}_i^T \underline{x}_k = b_i$ ⟹ we can only write: $\underline{a}_i^T \underline{d} = 0$

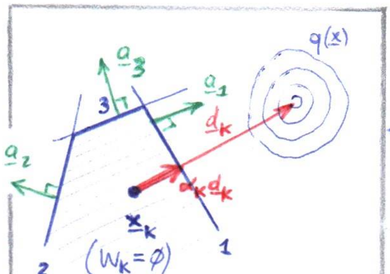
(2) is equivalent to:

$$\boxed{\min\{\, q(\underline{x}_k + \underline{d}) : \underline{a}_i^t \underline{d} = 0.\ i \in W_k \,\}.} \tag{3}$$

N.B.: If $Z^t Q Z$ is p.d. (always true if Q is p.d.), (3) has a unique solution $\underline{d}_k$.

Based on solution $\underline{d}_k$ of (3), we determine α_k, $\underline{x}_{k+1} = \underline{x}_k + \alpha_k \underline{d}_k$ and W_{k+1}.

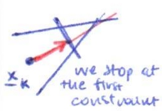
This is a QP with only equality constraints (good!)



α_k must be determined considering all the constraints (we cannot go out of the feasible region). $\underline{d}_k$ is evaluated $\perp$ of the constraints. How we check the constraints? We consider only the $\underline{a}_i$ s.t. $\underline{a}_i^T \underline{d}_k > 0$ (so in the example we just consider $\underline{a}_1$)

- If $\underline{d}_k \neq \underline{0}$, we determine the longest step length satisfying all constraints not in W_k:

$$\alpha_k = \min\{1, \min_{i \notin W_k,\ \underline{a}_i^t \underline{d}_k > 0} \frac{b_i - \underline{a}_i^t \underline{x}_k}{\underline{a}_i^t \underline{d}_k}\}.$$



and set $\underline{x}_{k+1} = \underline{x}_k + \alpha_k \underline{d}_k$.

$W_{k+1} = W_k \cup \{i'\}$ where i' is index of one constraint becoming active at $\underline{x}_{k+1}$.

- If $\underline{d}_k = \underline{0}$, $\underline{x}_k$ is a minimum over subspace defined by W_k and we set $\underline{x}_{k+1} = \underline{x}_k$.

Determine the multipliers u_i^k of 1st order optimality conditions of (3):

$$Q\underline{x}_k + \underline{c} + \sum_{i \in W_k} u_i^k \underline{a}_i = \underline{0}. \tag{4}$$

If $u_i^k \ge 0$ for every $i \in W_k \cap I$ Then $\underline{x}_k$ is a local optimum of original QP

Else $W_{k+1} = W_k \setminus \{i'\}$ where i' is the index with the most negative $u_{i'}^k$.

Notice that if $\underline{d}_k = \underline{0}$ then it doesn't mean that $\underline{x}_k$ is the ultimate optimal solution, it only means that $\underline{x}_k$ is optimal in the W_k subspace:

so to go on we have to update W_k

($\underline{x}_k$ is not necessarily the optimal solution, but it may be. How to find out? We solve (4) and look at the u_i^k.

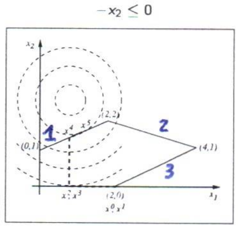
Proposition: If Q is p.d. (q is strictly convex), the metod (with anti-cycling rule) finds an optimal solution within a finite number of iterations.

Note: Finite number of working sets.

Example:

$$\begin{array}{llr} \min & q(x_1, x_2) = (x_1 - 1)^2 + (x_2 - 2.5)^2 & \\ \text{s.t.} & -x_1 + 2x_2 - 2 \le 0 & (1) \\ & x_1 + 2x_2 - 6 \le 0 & (2) \\ & x_1 - 2x_2 - 2 \le 0 & (3) \\ & -x_1 \le 0 & (4) \\ & -x_2 \le 0 & (5) \end{array}$$

Figure:



From J. Nocedal, S. Wright, Numerical Optimization, First Edition, Springer 1999, p. 462-463.

- Iteration 0:

Start from $\underline{x}_0 = \begin{pmatrix} 2 \\ 0 \end{pmatrix}$. Constraints (3) and (5) are active at $\underline{x}_0$ and we take $W_0 = \{3, 5\}$.

Since $\underline{x}_0$ is a vertex (extreme point) of the polyhedron of the feasible solutions,

$\underline{x}_0$ minimizes $q(\underline{x})$ w.r.t. W_0 (over $\{\underline{x} \in \mathbb{R}^n : \underline{a}_i^t \underline{x} = b_i,\ i \in W_0\}$) and

optimal solution of $\min\{\ q(\underline{x}_0 + \underline{d}) : \underline{a}_i^t \underline{d} = 0,\ i \in W_0\ \}$ is $\underline{d}_0 = \underline{0}$.

Thus $\underline{x}_1 = \underline{x}_0 + \alpha_0 \underline{d}_0 = \underline{x}_0$.

By solving the KKT conditions (4)

$$\nabla q(\underline{x}_0) = \begin{pmatrix} 2 \\ -5 \end{pmatrix} = u_3 \begin{pmatrix} -1 \\ 2 \end{pmatrix} + u_5 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

we obtain the multipliers $\begin{pmatrix} u_3 \\ u_5 \end{pmatrix} = \begin{pmatrix} -2 \\ -1 \end{pmatrix}$ for the active constraints.

Since $u_3 < u_5 < 0$ we delete from W_0 constraint (3), setting $W_1 = \{5\}$.

- Iteration 1:

Optimal solution of $\min\{\ q(\underline{x}_1 + \underline{d}) : \underline{a}_i^t \underline{d} = 0,\ i \in W_1\ \}$ is $\underline{d}_1 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$.

Since $\underline{d}_1$ does not violate any constraint with indices not in W_1, we have $\alpha_1 = 1$ and $\underline{x}_2 = \underline{x}_1 + \alpha_1 \underline{d}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

Since at $\underline{x}_2$ no other constraints are active, we set $W_2 = W_1 = \{5\}$.

- Iteration 2:

Optimal solution of $\min\{\ q(\underline{x}_2 + \underline{d}) : \underline{a}_i^t \underline{d} = 0,\ i \in W_2\ \}$ is $\underline{d}_2 = \underline{0}$.

By solving the KKT conditions (4), that is

$$\nabla q(\underline{x}_2) = \begin{pmatrix} 0 \\ -5 \end{pmatrix} = u_5 \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

we obtain $u_5 = -5$.

Thus $\underline{x}_3 = \underline{x}_2$ and we set $W_3 = W_2 \setminus \{5\} = \emptyset$.

- Iteration 3:

Optimal solution of $\min\{\ q(\underline{x}_3 + \underline{d}) : \underline{a}_i^t \underline{d} = 0,\ i \in W_3\ \}$ is $\underline{d}_3 = \begin{pmatrix} 0 \\ 2.5 \end{pmatrix}$.

Since $\underline{d}_3$ violates constraints (1) and (2) which are not in W_1, we have $\alpha_3 = 0.6$ and $\underline{x}_4 = \underline{x}_3 + \alpha_3 \underline{d}_3 = \begin{pmatrix} 1 \\ 1.5 \end{pmatrix}$.

Since at $\underline{x}_4$ only constraint (1) becomes active, we set $W_4 = \{1\}$.

- Iteration 4:

Optimal solution of $\min\{\ q(\underline{x}_4 + \underline{d}) : \underline{a}_i^t \underline{d} = 0,\ i \in W_4\ \}$ is $\underline{d}_4 = \begin{pmatrix} 0.4 \\ 0.2 \end{pmatrix}$.

Since $\underline{x}_4 + \underline{d}_4 = \begin{pmatrix} 1.4 \\ 1.7 \end{pmatrix}$ satisfies all the constraints with indices not in W_1, we take $\alpha_4 = 1$,

set $\underline{x}_5 = \underline{x}_4 + \underline{d}_4$ and $W_5 = W_4 = \{1\}$.

- Iteration 5:

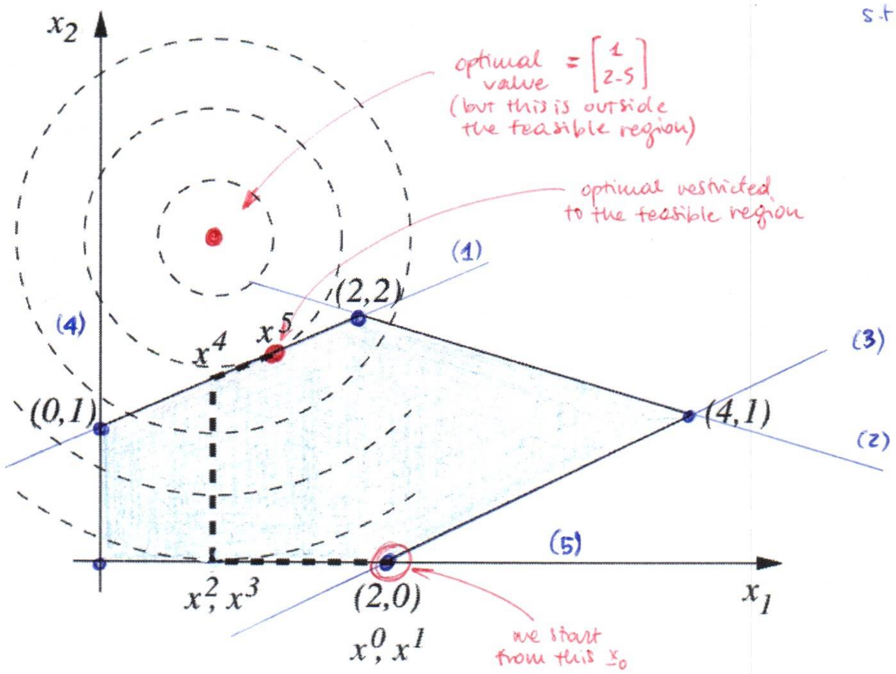
Optimal solution of $\min\{\ q(\underline{x}_5 + \underline{d}) : \underline{a}_i^t \underline{d} = 0,\ i \in W_5\ \}$ is $\underline{d}_5 = 0$.

Solving the KKT conditions (4) we obtain $u_1 = 1.25 \geq 0$.

Thus feasible solution $\underline{x}_5 = \begin{pmatrix} 1.4 \\ 1.7 \end{pmatrix}$ is optimal for the original problem.

$$\min \; q(x_1, x_2) = (x_1-1)^2 + (x_2-2.5)^2$$

$$\begin{aligned} \text{s.t.} \quad & -x_1 + 2x_2 - 2 \le 0 && (1)\\ & x_1 + 2x_2 - 6 \le 0 && (2)\\ & x_1 - 2x_2 - 2 \le 0 && (3)\\ & -x_1 \le 0 && (4)\\ & -x_2 \le 0 && (5) \end{aligned}$$



0 : We start from $\underline{x}_0 = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$, $W_0 = \{3, 5\}$

$\underline{x}_0$ is optimal in $W_0 \Longrightarrow \underline{d}_0 = \underline{0} \Longrightarrow \underline{x}_1 = \underline{x}_0 + \alpha_0 \underline{d}_0 = \underline{x}_0$

KKT conditions $(Q\underline{x}_0 + \underline{c} + \sum_{i \in W_0} u_i^0 \underline{a}_i = \underline{0}) \longrightarrow (u_3, u_5) = (-2, -1)$

$\Longrightarrow$ we delete the constraint (3) from W_0 : $W_1 = \{5\}$

1 : $\underline{x}_1 = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$, $W_1 = \{5\}$

$\min \{ q(\underline{x}_1 + \underline{d}) : \underline{a}_i^T \underline{d} = 0 \;\; i \in W_1 \} \Longrightarrow \underline{d}_1 = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$ (which does not violate constraints $\Rightarrow \alpha_1 = 1$)

$\underline{x}_2 = \underline{x}_1 + \underline{d}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

we don't have constraints (added) in $\underline{x}_2 \Longrightarrow W_2 = \{5\}$

using "all" $\underline{d}_1$ we are still in the feasible region, so we keep all $\underline{d}_1$

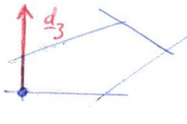
2 : $\underline{x}_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $W_2 = \{5\}$

$\underline{x}_2$ is optimal in $W_2 \longrightarrow \underline{d}_2 = \underline{0} \Longrightarrow \underline{x}_3 = \underline{x}_2$

KKT conditions $\longrightarrow u_5 = -5 \Longrightarrow W_3 = W_2 \setminus \{5\} = \{\} = \emptyset$

3 : $\underline{x}_3 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $W_3 = \emptyset$

we are determining $\underline{d}_3$ in a subspace which imposes no constraints with equality (it's an unconstrained case $\Longrightarrow$ for sure α_3 has to be analized (it'll probably be $\neq 1$))



it cannot be like that: α_3 has to be < 1

$\underline{d}_3 = \begin{bmatrix} 0 \\ 2.5 \end{bmatrix}$, $\alpha_3 = 0.6 \Longrightarrow \underline{x}_4 = \underline{x}_3 + \alpha_3 \underline{d}_3 = \begin{bmatrix} 1 \\ 1.5 \end{bmatrix}$

At $\underline{x}_4$ we have a new constraint: $W_4 = \{1\}$

4 : $\underline{x}_4 = \begin{bmatrix} 1 \\ 1.5 \end{bmatrix}$, $W_4 = \{1\}$

$\underline{d}_4 = \begin{bmatrix} 0.4 \\ 0.2 \end{bmatrix}$ ($\underline{x}_5 = \underline{x}_4 + \underline{d}_4$ does not violate constraints) $\Longrightarrow \underline{x}_5 = \underline{x}_4 + \underline{d}_4 = \begin{bmatrix} 1.4 \\ 1.7 \end{bmatrix}$

Moreover we don't have additional constraints: $W_5 = W_4 = \{1\}$

5 : $\underline{x}_5 = \begin{bmatrix} 1.4 \\ 1.7 \end{bmatrix}$, $W_5 = \{1\}$

$\underline{x}_5$ is optimal for $W_5 \Rightarrow \underline{d}_5 = \underline{0}$

KKT conditions $\longrightarrow u_1 = 1.25 \ge 0 \longrightarrow \underline{x}_5$ is optimal for the original

5.6.3 Non convex QP and solvers

If Q has some negative eigenvalues, the active-set method for convex QP can be adapted by modifying $\underline{d}_k$ and α_k in certain situations.

See J. Nocedal, S. Wright, Numerical Optimization, First edition, Springer 1999, p. 468-474.

Since W_k may change by just one index at every iteration, efficient QP solvers proceed by successive updates of the factors computed at the previous iterations.

Available active-set-based solvers: LINDO, QPOPT, NAG Library, Matlab,...

5.7 Penalty method and augmented Lagrangian method

Generic NLP problem

$$
\begin{aligned}
\min \quad & f(\underline{x}) \\
s.t. \quad & c_i(\underline{x}) \geq 0 \quad i \in I \\
& c_i(\underline{x}) = 0 \quad i \in E \\
& \underline{x} \in \mathbb{R}^n
\end{aligned}
\tag{1}
$$

where f and c_i's are of class $\mathcal{C}^1$ or $\mathcal{C}^2$.

Notation, examples and proofs: see Chapter 17 of J. Nocedal, S. Wright, Numerical Optimization, Springer, 1999, p. 491-500.

5.7.1 Quadratic penalty method

Idea: Delete constraints, add terms to objective function which penalize the constraint violation, and solve a sequence of resulting unconstrained optimization problems.

Description for

$$
\begin{aligned}
\min \quad & f(\underline{x}) \\
s.t. \quad & c_i(\underline{x}) = 0 \quad i \in E = \{1, \dots, m\} \\
& \underline{x} \in \mathbb{R}^n.
\end{aligned}
\tag{2}
$$

Definition: The **quadratic penalty function** problem associated to (2) is

$$
\boxed{\min_{\underline{x} \in \mathbb{R}^n} Q(\underline{x}, \mu) = f(\underline{x}) + \frac{1}{2\mu} \sum_{i \in E} c_i^2(\underline{x})}
\tag{3}
$$

since all the constraints are equalities we put them with the square (so every violation is equally penalized).

with the penalty parameter $\mu > 0$..

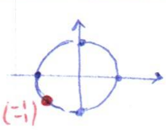
We consider $\{\mu_k\}_{k \geq 1}$ with $\lim_{k \to \infty} \mu_k = 0$ and, for each k, we determine an approximate solution $\underline{x}_k$ of (3) using an unconstrained optimization method.

If we want that eventually the equality constraints are really satisfied (with equality) we need to increase the weigth that we assign to the penalty ($\mu_k \to 0 \Rightarrow \frac{1}{2\mu_k} \to \infty$)

Example:

$$
\begin{aligned}
\min \quad & x_1 + x_2 \\
s.t. \quad & x_1^2 + x_2^2 - 2 = 0
\end{aligned}
$$

with optimal solution $(-1, -1)^t$.



$\underline{x}^* = (-1, -1)$

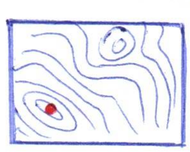
Quadratic penalty problem:

$$
\min_{\underline{x} \in \mathbb{R}^2} Q(\underline{x}, \mu) = \boxed{x_1 + x_2} + \frac{1}{2\mu} \boxed{(x_1^2 + x_2^2 - 2)^2}
$$

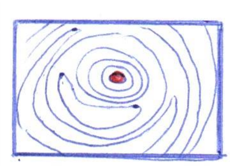
For $\mu = 1$, minimizer of $Q(\underline{x}, 1)$ is close to $(-1.1, -1.1)^t$.
For $\mu = 0.1$, minimizer of $Q(\underline{x}, 0.1)$ is much closer to $(-1, -1)^t$.

Level curves of $Q(\underline{x}, \mu)$ for different values of μ:

$\mu = 1$



$\mu = 0.1$



The optimum is much closer but the curves are becoming weirdly elongated. This is because, as $\mu \to 0$, the problem might become ill-conditionate

From J. Nocedal, S. Wright, Numerical Optimization, Springer, 1999, p. 491-492.

General scheme

accuracy parameter

at the step **k** the tolerance will be τ_k

0) Select $\varepsilon > 0$, $\mu_0 > 0$, sequence of tolerances $\{\tau_k\}_{k\geq 0}$ with $\tau_k > 0$ and $\lim_{k\to\infty} \tau_k = 0$.
Choose initial $\underline{x}_0^s$ and set $k = 0$.

1) Determine an approximate minimizer $\underline{x}_k$ of $Q(\underline{x}, \mu_k)$ starting from $\underline{x}_k^s$ and terminate when $\|\nabla Q(\underline{x}, \mu_k)\| \leq \tau_k$.

x_k^s = { **k** because is the **k**-th step, **s** because is the starting $\underline{x}_k$ (to solve the unconstrained opt. problem we use iterative methods so we have to have a solution to start from) }

2) `If` termination condition is satisfied (e.g. $|f(\underline{x}_{k-1}) - f(\underline{x}_k)| < \varepsilon$)
`Then` return solution $\underline{x}_k$
`Else` choose $\mu_{k+1} \in (0, \mu_k)$ and starting $\underline{x}_{k+1}^s$, set $k = k+1$ and `Goto 1)`

Choices:

- For convergence results, it suffices that $\lim_{k\to\infty} \tau_k = 0$.
- $\{\mu_k\}_{k\geq 0}$ generated adaptively starting from μ_0: if minimization of $Q(\underline{x}, \mu_k)$ is "difficult" set e.g. $\mu_{k+1} = 0.7\mu_k$, otherwise $\mu_{k+1} = 0.1\mu_k$.
- Judicious choice of the starting $\underline{x}_k^s$ when solving unconstrained penalty problem at each iteration: $\underline{x}_{k+1}^s := \underline{x}_k$.

Convergence

Theorem 1: Suppose each $\underline{x}_k$ is a *global minimizer* of $Q(\underline{x}, \mu_k)$ and $\lim_{k\to\infty} \mu_k = 0$, then every limit point $\underline{x}^*$ of $\{\underline{x}_k\}$ generated with above scheme ($\tau_k = 0$, $\forall k \geq 0$) is a *global minimum* of problem (2).

If we guarantee that we have the global min. for each $Q(\underline{x}, \mu_k)$ (and that $\mu_k \to 0$) then we have the guarantee that we reach the global min. of the original problem (the constrained one).

since it's the global minimizer then the tolerance is $= 0$ (we solve to optimality, not approximately)

(2) (original problem): min $f(\underline{x})$
s.t. $c_i(\underline{x}) = 0 \quad \forall i \in E$
$\underline{x} \in \mathbb{R}^n$

Proof:

Let $\overline{\underline{x}}$ be an optimal solution of (2).
Since $\underline{x}_k$ is a global minimizer of $Q(\underline{x}, \mu_k)$ and $\overline{\underline{x}}$ is feasible for (2), $Q(\underline{x}_k, \mu_k) \leq Q(\overline{\underline{x}}, \mu_k)$ namely

$$f(\underline{x}_k) + \frac{1}{2\mu_k}\sum_{i=1}^{m} c_i^2(\underline{x}_k) \leq f(\overline{\underline{x}}) + \frac{1}{2\mu_k}\sum_{i=1}^{m} c_i^2(\overline{\underline{x}}) = f(\overline{\underline{x}}) \qquad \forall k. \tag{4}$$

Thus

$$\sum_{i=1}^{m} c_i^2(\underline{x}_k) \leq 2\mu_k[f(\overline{\underline{x}}) - f(\underline{x}_k)] \qquad \forall k. \tag{5}$$

Consider any convergent subsequence of $\{\underline{x}_k\}_{k\geq 0}$ with $k \in \mathcal{K}$, such that $\lim_{k\in\mathcal{K}} x_k = \underline{x}^*$.
By taking the limit as $k \to \infty$ with $k \in \mathcal{K}$ in (5), we obtain (since $\mu_k \to 0$)

$$\sum_{i=1}^{m} c_i^2(\underline{x}^*) = \lim_{k\in\mathcal{K}} \sum_{i=1}^{m} c_i^2(\underline{x}_k) \leq \lim_{k\in\mathcal{K}} 2\mu_k[f(\overline{\underline{x}}) - f(\underline{x}_k)] = 0$$

which implies that $c_i(\underline{x}^*) = 0$

By taking the limit as $k \to \infty$ with $k \in \mathcal{K}$ in (4), we obtain (since $\mu_k \geq 0$ and $c_i(\underline{x}_k)^2 \geq 0$)

$$f(\underline{x}^*) \leq f(\underline{x}^*) + \lim_{k\in\mathcal{K}} \frac{1}{2\mu_k}\sum_{i=1}^{m} c_i^2(\underline{x}_k) \leq f(\overline{\underline{x}}),$$

namely $\underline{x}^*$ is an optimal solution of (2). □

Since unconstrained penalty problems are solved approximately, the following is more relevant.

Theorem 2: If

- tolerances $\tau_k > 0$ satisfy $\lim_{k\to\infty} \tau_k = 0$
- penalty prameters satisfy $\lim_{k\to\infty} \mu_k = 0$,

then every limit point $\underline{x}^*$ of $\{\underline{x}_k\}_{k\geq 0}$ at which all $\nabla c_i(\underline{x}^*)$, with $i \in E$, are linearly independent is a *KKT point* of problem (2).

as limit point we get a candidate local optimal point

For such points, the subsequence defined by $\mathcal{K}$ with $\lim_{k\in\mathcal{K}} \underline{x}_k = \underline{x}^*$ satisfies

$$\lim_{k\in\mathcal{K}} -\frac{c_i(\underline{x}_k)}{\mu_k} = u_i^* \qquad \forall i \in E, \tag{6}$$

where $\underline{u}^*$ satisfies with $\underline{x}^*$ the KKT conditions for problem (2).

This can (kind of) be rewritten as: $\boxed{c_i(\underline{x}_k) = -u_i^* \mu_k}$
so $\underline{x}_k$ is not respecting $c_i(\underline{x}) = 0$, but it's violating it by $-u_i^* \mu_k$
(this also explains why $\{\mu_k\}_k$ must tends to zero)

This links $c_i(\underline{x}_k)$ (which is the degree of violation of the constraints, since we have $c_i(\underline{x}) = 0 \ \forall i$), μ_k (which is the penalty parameter) and u_i^* (which is the KKT multiplier)

Observation: (6) implies that

i) The minimizer $\underline{x}_k$ of $Q(\underline{x}, \mu_k)$ does not satisfy $c_i(\underline{x}) = 0$ exactly, for all $i \in E$, namely $c_i(\underline{x}_k) = -\mu_k u_i^*$ for all $i \in E$. To obtain a feasible solution, μ_k must be driven to 0.

ii) In some circumstances $-\frac{c_i(\underline{x}_k)}{\mu_k}$ may be used as estimates of Lagrange multipliers u_i^*.

Recall: Lagrange function associated to problem (2) is

$$L(\underline{x}, \underline{u}) = f(\underline{x}) - \sum_{i=1}^{m} u_i c_i(\underline{x}) \tag{7}$$

and KKT conditions require that, apart from $c_i(\underline{x}) = 0$ for every $i \in E$,

$$\nabla_{\underline{x}} L(\underline{x}, \underline{u}) = \nabla f(\underline{x}) - \sum_{i=1}^{m} u_i \nabla c_i(\underline{x}) = \underline{0}. \tag{8}$$

By comparing

$$\nabla_{\underline{x}} Q(\underline{x}, \mu) = \nabla f(\underline{x}) + \frac{1}{\mu}\sum_{i=1}^{m} c_i(\underline{x}) \nabla c_i(\underline{x}) = \underline{0} \tag{9}$$

$\nabla_{\underline{x}} \left(f(\underline{x}) + \frac{1}{2\mu} \sum_{i\in E} c_i^2(\underline{x}) \right)$

and (8), it appears that $-\frac{c_i(\underline{x})}{\mu}$ has been substituted with u_i.

It can be proved that if $\tau_k \to 0$ then $\underline{x}_k \to \underline{x}^*$ and $-\frac{c_i(\underline{x}_k)}{\mu_k} \to u_i^*$ $\quad i = 1, 2, \dots, m$.

Observation: When $\mu_k \to 0$ the quadratic penalty problem (3) becomes ill conditioned.

This is the real problem of this method (quadratic penalty method). The idea of the next method (Augmented Lagrangian method) is to try to avoid $\mu_k \to 0$.

$$\nabla^2_{\underline{xx}} Q(\underline{x}, \mu_k) = \nabla^2 f(\underline{x}) + \frac{1}{\mu_k} A^t(\underline{x})\ A(\underline{x}) + \frac{1}{\mu_k} \sum_{i=1}^{m} c_i(\underline{x}) \nabla^2 c_i(\underline{x}) \tag{10}$$

where $A^t(\underline{x}) = [\nabla c_1(\underline{x}), \dots, \nabla c_m(\underline{x})]$ and $A\mathbb{R}^{m\times n}$ of full rank $m \leq n$, usually $m < n$.

When $\underline{x}$ is close to minimizer of $Q(\underline{x}, \mu_k)$ and assumptions of Theorem 2 are satisfied, (6) implies that

$$\nabla^2_{\underline{xx}} Q(\underline{x}, \mu_k) \approx \nabla^2_{\underline{xx}} L(\underline{x}, \underline{u}^*) + \frac{1}{\mu_k} A^t(\underline{x})\ A(\underline{x}). \tag{11}$$

Since $\nabla^2_{\underline{xx}} L(\underline{x}, \underline{u}^*)$ does not depend on μ_k and $\frac{1}{\mu_k} A^t(\underline{x})\ A(\underline{x})$ has $n - m$ eigenvalues of value 0 and m eigenvalues of value $O(1/\mu_k)$, numerical issues arise when $\mu_k \to 0$.

Problems with both equality and inequality constraints:

Quadratic penalty problem

$$\min_{\underline{x}\in\mathbb{R}^n} Q(\underline{x}, \mu) = f(\underline{x}) + \underbrace{\boxed{\frac{1}{2\mu} \sum_{i\in E} c_i^2(\underline{x})}}_{\text{equalities (E)}} + \underbrace{\boxed{\frac{1}{2\mu} \sum_{i\in I} ([c_i(\underline{x})]^-)^2}}_{\text{inequalities (I)}} \tag{12}$$

where $[y]^-$ denotes $\max(-y, 0)$.

Other penalty functions are available.

If only equality constraints $c_i(\underline{x}) = 0$, $i \in E$, the *exact penalty problem* is

$$\min_{\underline{x}\in\mathbb{R}^n} Q(\underline{x}, \mu) = f(\underline{x}) + \frac{1}{2\mu} \sum_{i\in E} |c_i(\underline{x})|. \tag{13}$$

N.B.: Q is not everywhere differentiable.

5.7.2 Augmented Lagrangian method

Idea: Reduce ill-conditioning issues of the unconstrained subproblems (in quadratic penalty method) by introducing explicit estimates of the Lagrange multipliers.

Description for

$$\begin{aligned} \min \quad & f(\underline{x}) \\ s.t. \quad & c_i(\underline{x}) = 0 \quad i \in E = \{1, \dots, m\} \\ & \underline{x} \in \mathbb{R}^n. \end{aligned} \tag{14}$$

Definition: The **augmented Lagrange function** associated to (14) is

$$\boxed{L_A(\underline{x}, \underline{u}, \mu) = f(\underline{x}) - \sum_{i=1}^{m} u_i c_i(\underline{x}) + \frac{1}{2\mu} \sum_{i=1}^{m} c_i^2(\underline{x})} = L(\underline{x}, \underline{u}) + \frac{1}{2\mu} \sum_{i=1}^{m} c_i^2(\underline{x}), \tag{15}$$

We mix the concepts of Lagrange function with the penalty function

where $\underline{u}$ is multiplier vector and μ the penalty parameter.

N.B.: $L_A(\underline{x}, \underline{u}, \mu)$ is a combination of $L(\underline{x}, \underline{u})$ and $Q(\underline{x}, \mu)$.

Since KKT conditions of (14) require that $\nabla_{\underline{x}} L(\underline{x}^*, \underline{u}^*) = \underline{0}$ and $c_i(\underline{x}^*) = 0\ \forall i \in E$, at optimality L_A coincides with L, and no need for $\mu \to 0$.

Similar approach:

At each iteration: $\mu_k > 0$ and determine an approximate minimizer $\underline{x}_k$ of $L_A(\underline{x}, \underline{u}^k, \mu_k)$ via an unconstrained optimization method, where $\underline{u}^k$ is an updated estimate.

Differentiating w.r.t. $\underline{x}$, we obtain

$$\nabla_{\underline{x}} L_A(\underline{x}, \underline{u}, \mu) = \nabla f(\underline{x}) - \sum_{i=1}^{m} (u_i - \frac{c_i(\underline{x})}{\mu}) \nabla c_i(\underline{x}).$$

Considerations similar to those in proof of Theorem 2 allow to establish that

$$u_i^* \approx u_i^k - \frac{c_i(\underline{x}_k)}{\mu_k} \qquad i \in E, \tag{16}$$

which is equivalent to

$$c_i(\underline{x}_k) \approx \mu_k (u_i^k - u_i^*) \qquad i \in E. \tag{17}$$

now we have 2 choices to obtain $c_i(\underline{x}_k) \to 0$ $(k \to \infty)$: either $\mu_k \to 0$ (but we want to avoid it) or $u_i^k \to u_i^*$ (KKT multiplier)

General scheme

0) Choose $\varepsilon > 0$, $\mu_0 > 0$, tolerances $\{\tau_k\}_{k\geq 0}$ with $\tau_k > 0$ and $\lim_{k\to\infty} \tau_k = 0$, $\underline{x}_0^s$ and initial $\underline{u}^0$, set $k := 0$.

1) Determine an approximate minimizer $\underline{x}_k$ of $L_A(\underline{x}, \underline{u}^k, \mu_k)$ starting from $\underline{x}_k^s$ and terminate when $\|\nabla_{\underline{x}} L_A(\underline{x}, \underline{u}^k, \mu_k)\| \leq \tau_k$.

2) `If` overall termination condition is satisfied (e.g, $|f(\underline{x}_{k-1}) - f(\underline{x}_k)| < \varepsilon$)

`Then` Stop

`Else` set
$$u_i^{k+1} = u_i^k - \frac{c_i(\underline{x}_k)}{\mu_k} \quad \text{for } i \in E \tag{18}$$

choose $\mu_{k+1} \in (0, \mu_k)$ and next starting solution $\underline{x}_{k+1}^s$

set $k := k + 1$ and `Goto 1)`

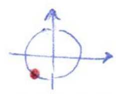
we take it from:
$u_i^* \approx u_i^k - \dfrac{c_i(x_k)}{\mu_k}$
(equation (16))

Including in L_A an additional term related to the Lagrange multipliers leads to substantial improvements w.r.t. the quadratic penalty method.

($L_A >>> Q$)
(more efficient)

Example:

$$\begin{aligned} \min \quad & x_1 + x_2 \\ s.t. \quad & x_1^2 + x_2^2 - 2 = 0 \end{aligned}$$



with optimal solution $\underline{x}^* = (-1, -1)^t$, optimal multiplier $u^* = -0.5$ and unconstrained optimization subproblem

$$\min_{\underline{x}\in\mathbb{R}^2} L_A(\underline{x}, u, \mu) = \boxed{x_1 + x_2} \boxed{- u(x_1^2 + x_2^2 - 2)} + \boxed{\frac{1}{2\mu}(x_1^2 + x_2^2 - 2)^2}$$

Suppose that $\mu_k = 1$ and estimate $u^k = -0.4$.

Contours of $L_A(\underline{x}, -0.4, 1)$ are similar to those of $Q(\underline{x}, 1)$ but the minimizer $\underline{x}^k \approx (-1.02, -1.02)^t$ of $L_A(\underline{x}, -0.4, 1)$ is much closer to $\underline{x}^*$ than the minimizer of $Q(\underline{x}, 1)$.

From J. Nocedal, S. Wright, Numerical Optimization, Springer, 1999, p. 513-514.

Theorem 3:

Let $\underline{x}^*$ be a local minimum of (14) at which the $\nabla c_i(\underline{x}^*)$, $i \in E$, are linearly independent and 2nd order sufficient optimality conditions are satisfied for $\underline{u} = \underline{u}^*$.
Then $\exists\, \overline{\mu} > 0$ such that for all $\mu \in (0, \overline{\mu}]$, $\underline{x}^*$ is a strict local minimum of $L_A(\underline{x}, \underline{u}^*, \mu)$.

we suppose to know the optimal multiplier vector $\underline{u}^*$ (this is a strong assumpt.)

N.B.: In general $\underline{u}^*$ is not known.

The next result

- concerns the more realistic case in which $\underline{u} \neq \underline{u}^*$,
- provides conditions under which $\exists$ a minimizer of L_A close to $\underline{x}^*$ and error bounds on $\underline{x}_k$ and on $\underline{u}^{k+1}$.

Theorem 4:

Suppose the assumptions of Theorem 3 are satisfied at $\underline{x}^*$ and $\underline{u}^*$, and let $\overline{\mu} > 0$ be the corresponding threshold.

Then $\exists$ scalars $\delta > 0$, $\varepsilon > 0$, and M such that

i) For all $\underline{u}^k$ and μ_k satisfying
$$\|\underline{u}^k - \underline{u}^*\| \leq \delta/\mu_k, \qquad \mu_k \leq \overline{\mu}, \tag{19}$$
the problem
$$\min_{\underline{x}\in\mathbb{R}^n:\, \|\underline{x}-\underline{x}^*\|\leq\varepsilon} L_A(\underline{x}, \underline{u}^k, \mu_k)$$
has a unique solution $\underline{x}_k$. Moreover, we have $\|\underline{x}_k - \underline{x}^*\| \leq M\mu_k \|\underline{u}^k - \underline{u}^*\|$.

ii) For all $\underline{u}^k$ and μ_k satisfying (19), we have
$$\|\underline{u}^{k+1} - \underline{u}^*\| \leq M\mu_k \|\underline{u}^k - \underline{u}^*\|,$$
where $\underline{u}^{k+1}$ is given by the formula (18).

iii) For all $\underline{u}^k$ and μ_k satisfying (19), the matrix $\nabla^2_{\underline{x}\underline{x}} L_A(\underline{x}_k, \underline{u}^k, \mu_k)$ is positive definite and the $\nabla c_i(\underline{x}_k)$, with $i \in E$, are linearly independent.

i) shows that $\underline{x}_k$ will be close to $\underline{x}^*$ if $\underline{u}^k$ is accurate or if the penalty parameter is high (so μ_k low). This approach gives us 2 ways of improving the accuracy of $\underline{x}_k$ (whereas the quadratic penalty approach gives us only one option: increasing μ_k).

ii) shows that, locally, we can ensure an improvement in the accuracy of the multipliers by choosing a sufficiently large value of μ_k

iii) shows that the second order sufficient conditions for unconstrained minimization are also satisfied for the k-th subproblem under given conditions, so we can expect good performance by applying standard unconstrained minimization techniques

Problems with also inequality constraints:

We can introduce slack variables and substitute $c_i(\underline{x}) \geq 0$, $i \in I$, with

$$c_i(\underline{x}) - s_i = 0, \qquad s_i \geq 0, \qquad i \in I.$$

In LANCELOT solver, the bounds on the variables are explicitly taken into account in the subproblem

$$\min_{\underline{l}_{inf} \leq \underline{x} \leq \underline{l}_{sup}} L_A(\underline{x}, \underline{u}^k, \mu_k).$$

"complementary" methods to the quadratic penalty (+ Lagrangian improvement) :

5.8 Barrier method

Method described for

$$\begin{array}{lll} \min & f(\underline{x}) & \\ s.t. & c_i(\underline{x}) \geq 0 \quad i \in I = \{1, \dots, m\} & (1) \\ & \underline{x} \in \mathbb{R}^n. & \end{array}$$

Notation and examples: Chapter 17 of J. Nocedal, S. Wright, Numerical Optimization, Springer, 1999, p. 498-508.

Definition: Let

$$X^o = int(\{\underline{x} \in \mathbb{R}^n \; : \; c_i(\underline{x}) \geq 0, i \in I\}) \neq \emptyset,$$

strict feasible region of the problem (= interior of the set of the feasible solutions) :

a function defined on $\mathbb{R}^n$ is a **barrier function** if it is continuous over X^o, tends to ∞ when approaching the boundary of X and has value ∞ on $\mathbb{R}^n \setminus X^o$.

The barrier function is a function that is meant to keep us away from the boundary.

Example: **Logarithmic barrier function** for $c_i(\underline{x}) \geq 0$

$$-\ln c_i(\underline{x}).$$

(natural logarithm)

Idea: Add to objective function the barrier terms associated to the constraints and solve a sequence of resulting unconstrained optimization problems.

Definition: The **logarithmic barrier problem** associated to problem (1) is

$$\min_{\underline{x} \in \mathbb{R}^n} P(\underline{x}, \mu) = f(\underline{x}) - \mu \sum_{i \in I} \ln c_i(\underline{x}), \qquad (2)$$

with barrier parameter $\mu > 0$.

N.B.: When $\mu \to 0$ the barrier term becomes negligible.

If μ is a large value we're penalizing a lot the approach to the boundary, if $\mu \to 0$ we're decreasing the penalty of approaching the boundary

sequence of barrier parameters

We consider $\{\mu_k\}$ with $\lim_{k \to \infty} \mu_k = 0$, start from $\underline{x}_0 \in X^o$ and, for each k, determine an approximate minimizer $\underline{x}_k$ of $P(\underline{x}, \mu_k)$ with an unconstrained optimization method.

Example 1:

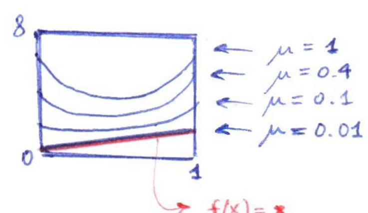
$$\begin{array}{ll} \min & x \\ s.t. & x \geq 0 \\ & 1 - x \geq 0 \end{array}$$

with optimal solution $x^* = 0$ and logarithmic barrier problem:

$$\min_{x \in \mathbb{R}} P(x, \mu) = x - \mu \ln x - \mu \ln(1 - x).$$

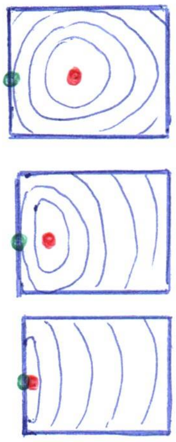
Compare contours of $P(x, \mu)$ for values of μ from 1 to 0.01.

See J. Nocedal, S. Wright, Numerical Optimization, Springer, 1999, p. 499-500.



(for μ sufficiently small (ex. $\mu = 0.01$) we cannot even distinguish the logarithmic barrier problem function from the objective function)

● = optimum we get
● = optimum we want



Example 2:

$$\begin{array}{lr} \min & (x_1+0.5)^2+(x_2-0.5)^2 \\ s.t. & x_1 \in [0,1] \\ & x_2 \in [0,1] \end{array} \longrightarrow \begin{cases} x_1 \geq 0 \\ 1-x_1 \geq 0 \end{cases}$$

with optimal solution $\underline{x}^* = (0, 0.5)^t$ and logarithmic barrier problem:

$$\min_{\underline{x}\in\mathbb{R}^2} P(\underline{x},\mu) = (x_1+0.5)^2+(x_2-0.5)^2 - \mu\,[\ln x_1 + \ln(1-x_1) + \ln x_2 + \ln(1-x_2)].$$

Compare contours of $P(\underline{x},\mu)$ for values of μ from 1 to 0.01.

For $\mu = 0.01$, shape of contours around $\underline{x}^*$ (more elongated and less elliptical) indicates prossible numerical problems.

See J. Nocedal, S. Wright, Numerical Optimization, Springer, 1999, p. 500-502.

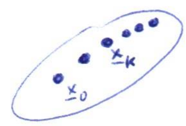
General scheme

0) Choose $\varepsilon > 0$, $\mu_0 > 0$, tolerances $\{\tau_k\}_{k\geq 0}$ with $\tau_k > 0$ and $\lim_{k\to\infty}\tau_k = 0$, initial point $\underline{x}_0^s$. Set $k := 0$.

1) Determine an approximate minimizer $\underline{x}_k$ of $P(\underline{x},\mu_k)$ starting from $\underline{x}_k^s$ and terminate when $\|\nabla P(\underline{x},\mu_k)\| \leq \tau_k$.

2) `If` overall termination condition is satisfied (e.g. $|f(\underline{x}_{k-1}) - f(\underline{x}_k)| < \varepsilon$)
   `Then` Stop
   `Else` select $\mu_{k+1} \in (0,\mu_k)$ and $\underline{x}_{k+1}^s$, set $k := k+1$ and `Goto 1)`

Since starting from $\underline{x}_0 \in X^o$ the sequence $\{\underline{x}_k\}$ remains in X^0, the algorithm is an *interior point method*.



Relation between:
min $P(\underline{x},\mu)$
and
$(\underline{x}^*, \underline{u}^*)$ satisfying KKT

Important connection between a minimum of $P(\underline{x},\mu)$, denoted $\underline{x}(\mu)$, and a point $(\underline{x}^*,\underline{u}^*)$ satisfying the KKT conditions of problem (1), namely

$\underline{x}(\mu)$ because $\underline{x}$ is different based on μ

$$\nabla_{\underline{x}} L(\underline{x},\underline{u}) = \nabla f(\underline{x}) - \sum_{i=1}^{m} u_i \nabla c_i(\underline{x}) = \underline{0} \qquad (3)$$

$$c_i(\underline{x}) \geq 0 \quad \forall i \in I \qquad (4)$$ (feasibility of $\underline{x}$)

$$u_i c_i(\underline{x}) = 0 \quad \forall i \in I \qquad (5)$$ (complementary conditions)

$$u_i \geq 0 \quad \forall i \in I. \qquad (6)$$ (since we have inequalities)

In a minimizer $\underline{x}(\mu)$ of $P(\underline{x},\mu)$, we have

$$\nabla_{\underline{x}} P(\underline{x},\mu) = \nabla f(\underline{x}) - \sum_{i=1}^{m} \frac{\mu}{c_i(\underline{x})} \nabla c_i(\underline{x}) = \underline{0}. \qquad (7)$$

$P(\underline{x},\mu) = f(\underline{x}) - \sum_{i\in I} \mu \ln(c_i(\underline{x}))$

By defining the estimates of the multipliers

(3), (7) $\Longrightarrow$

$$u_i(\mu) := \frac{\mu}{c_i(\underline{x}(\mu))} \quad \text{with } i = 1,\ldots,m, \qquad (8)$$

(7) can be rewritten as

$$\nabla f(\underline{x}) - \sum_{i=1}^{m} u_i(\mu)\nabla c_i(\underline{x}) = \underline{0} \qquad (9)$$

which is equivalent to (3).

Observation: For $\mu > 0$ the KKT conditions (3)-(6) hold except (5) because

$$u_i(\mu)c_i(\underline{x}(\mu)) = \mu \quad \text{for } i = 1,\ldots,m.$$

(by definition of the estimate (so, number (8)))

When $\mu \to 0$ a minimum $\underline{x}(\mu)$ of $P(\underline{x},\mu)$ and

the corresponding estimate

$$u_i(\mu) := \frac{\mu}{c_i(\underline{x}(\mu))} \quad \text{with } i = 1,\ldots,m,$$

tend to progressively satisfy the KKT conditions of problem (1).

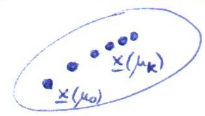
Thus we generate points on the so-called **central path**

central because is in the interior of the feasible region

$$\{(\underline{x}(\mu),\underline{u}(\mu)) \;:\; \mu > 0\}$$

defined by (8).

notice that it's not generated only $\underline{x}$ for a value μ, but a value $\underline{u}$ too (from the equation (8))



Theorem:
Suppose that $X^o \neq \emptyset$ and $\underline{x}^*$ is a local minimum of (1) at which the KKT conditions are satisfied for some $\underline{u}^*$.

Moreover, suppose that

- gradients of the active constraints at $\underline{x}^*$ are linearly independent,
- strict complementarity conditions are satisfied at $\underline{x}^*$ ($\forall i \in I$ exactly one of $c_i(\underline{x}^*)$ or u_i^* is equal to 0),
- 2nd sufficient conditions are satisfied at $(\underline{x}^*, \underline{u}^*)$.

$\longrightarrow$ $u_i = 0$ $\dot{\vee}$ $c_i(\underline{x}^*) = 0$

Then

i) $\exists$ unique continously differentiable vector function $\underline{x}(\mu)$ s.t. $\lim_{\mu \to 0_+} \underline{x}(\mu) = \underline{x}^*$. For all sufficiently small μ, $\underline{x}(\mu)$ is a local minimum of $P(\underline{x}, \mu)$ in some neigborhood of $\underline{x}^*$.

If we're sufficiently close to $\underline{x}^*$ then, by solving the logarithmic barrier associated subproblem, we get $\underline{x}(\mu)$ which is a local minimum of $P(\underline{x}, \mu)$

ii) For $\underline{x}(\mu)$ in (i), the Lagrange multiplier estimates $\underline{u}(\mu)$ defined by

$$u_i(\mu) = \mu / c_i(\underline{x}(\mu)) \qquad i = 1, \ldots, m,$$

converge to $\underline{u}^*$ when $\mu \to 0_+$.

iii) $\nabla^2_{\underline{x}\underline{x}} P(\underline{x}, \mu)$ is positive definite for all sufficiently small μ.

If also equality constraints, one may include quadratic penalty terms, obtaining a combined log-barrier/quadratic penalty function problem.

log-barrier for inequalities + quadratic penalty for equalities

Sixth computer lab: application of the logarithmic barrier method to LP.

Generic LP in standard form

$$\begin{aligned} \min \quad & \underline{c}^t \underline{x} & (10)\\ \text{s.t.} \quad & A\underline{x} = \underline{b} & (11)\\ & \underline{x} \geq \underline{0}, & (12) \end{aligned}$$

$\longleftarrow$ barrier method

an **interior point method for LP** is obtained by applying the barrier method to constraints (12) and by adapting the Newton method to account for (11).

Unlike for Simplex method, such method can be proved to provide, for any instance, an optimal solution in polynomial time w.r.t. the instance size.

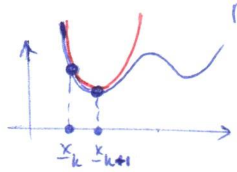
5.9 Introduction to sequential quadratic programming

Generic nonlinear program:

$$(P) \quad \begin{aligned} \min \quad & f(\underline{x}) & \\ \text{s.t.} \quad & g_i(\underline{x}) \leq 0 & i = 1, \ldots, m\\ & h_l(\underline{x}) = 0 & l = 1, \ldots, p\\ & \underline{x} \in \mathbb{R}^n & \end{aligned}$$

where f, g_i's and h_l's are of class C^2.

Newton method (unconstrained problem)



Idea: Extend the Netwon method to nonlinearly constrained problems.

Given a current iterate $\underline{x}_k$, we could try to determine an improving direction $\underline{d}_k$ by solving the quadratic approximation of (P):

$$(QA_k) \quad \begin{aligned} \min \quad & \tfrac{1}{2}\underline{d}^t \nabla^2 f(\underline{x}_k)\underline{d} + \nabla^t f(\underline{x}_k)\underline{d} + f(\underline{x}_k) & \\ s.t. \quad & \tfrac{1}{2}\underline{d}^t \nabla^2 g_i(\underline{x}_k)\underline{d} + \nabla^t g_i(\underline{x}_k)\underline{d} + g_i(\underline{x}_k) \leq 0 & i = 1, \ldots, m \quad (1)\\ & \tfrac{1}{2}\underline{d}^t \nabla^2 h_l(\underline{x}_k)\underline{d} + \nabla^t h_l(\underline{x}_k)\underline{d} + h_l(\underline{x}_k) = 0 & l = 1, \ldots, p \quad (2) \end{aligned}$$

but difficult because of the quadratic constraints.

We have to adapt it to the constraints, how?
We can, for instance, make a quadratic approximation of the constraints too.

Observation:
If $(\underline{d}^*, \underline{\eta}^*, \underline{\rho}^*)$ is a stationary point of the Lagrange function associated to (QA_k) it is also a stationary point of the Lagrange function associated to the Quadratic Program:

η multipliers of (1) in the lagrangian and ρ multipliers of (2) in the lagrangian

$$(QPA_k) \quad \begin{aligned} \min \quad & \tfrac{1}{2}\underline{d}^t \nabla^2_{\underline{x}\underline{x}} L(\underline{x}_k, \underline{\eta}^*, \underline{\rho}^*)\underline{d} + \nabla^t f(\underline{x}_k)\underline{d} + f(\underline{x}_k) & \\ s.t. \quad & \nabla^t g_i(\underline{x}_k)\underline{d} + g_i(\underline{x}_k) \leq 0 & i = 1, \ldots, m\\ & \nabla^t h_l(\underline{x}_k)\underline{d} + h_l(\underline{x}_k) = 0 & l = 1, \ldots, p \end{aligned}$$

All constraints are linear (appproximations).

To obtain a good approximation of (P) via Quadratic Programs, the objective function must include not only a quadratic model of f but also 2nd order information of the g_i's.

General scheme

Let $\underline{x}_0$, $\underline{u}_0$ and $\underline{v}_0$ be estimates of a solution of (P) and of the corresponding multipliers.

Iteration k:

Given $(\underline{x}_k, \underline{u}_k, \underline{v}_k)$ determine $\underline{d}_k$ and the corresponding multipliers $(\underline{\eta}_k, \underline{\rho}_k)$ of the quadratic program:

$$(QP_k) \quad \begin{array}{lll} \min & \frac{1}{2}\underline{d}^t \nabla^2_{\underline{x}\underline{x}} L(\underline{x}_k, \underline{u}_k, \underline{v}_k)\underline{d} + \nabla^t f(\underline{x}_k)\underline{d} & \\ s.t. & \nabla^t g_i(\underline{x}_k)\underline{d} + g_i(\underline{x}_k) \leq 0 & i = 1, \dots, m \\ & \nabla^t h_l(\underline{x}_k)\underline{d} + h_l(\underline{x}_k) = 0 & l = 1, \dots, p. \end{array}$$

we neglect $f(\underline{x}_k)$ since it's a constant

η_k

f_k

Set $\underline{x}_{k+1} := \underline{x}_k + \underline{d}_k$, $\underline{u}_{k+1} := \underline{\eta}_k$ and $\underline{v}_{k+1} := \underline{\rho}_k$

Although (QP_k) derives from (QPA_k) by subsituting the optimal multipliers with the current estimates, it can be proved that:

- feasible region of the quadratic programming subproblem (QP_k) is a *linear approximation* of that of the original problem,
- Lagrange function $L_Q(\underline{d}, \underline{\eta}, \underline{\rho})$ of (QP_k) is a *quadratic approximation* of the Lagrange function of (P).

An iteration of the *Sequential Quadratic Programming method* (SQP) is equivalent to:

- carry out one iteration of the Newton method for the Lagrange function,
- enforce feasibility with respect to the linearization of the feasible region.

The SQP method is well defined:

Proposition:
$(\underline{x}^*, \underline{u}^*, \underline{v}^*)$ is a KKT point of (P) if and only if $(\underline{d}^*, \underline{\eta}^*, \underline{\rho}^*) = (\underline{0}, \underline{u}^*, \underline{v}^*)$ is a KKT point of (QP_k).

If the only improvement step $\underline{d}^*$ is equal to $\underline{0}$ in the (QP_k) then it means that we have found a KKT point of our original problem. (Actually is a characterization, so it holds with "$\Longleftrightarrow$")

Convergence properties similar to those for Newton method:

Quadratic local convergence if

(i) Hessian matrices of the objective function and constraints are Lipschitz continuous,
(ii) constraint qualification assumption is satisfied,
(iii) 2nd order sufficient optimality conditions and strict complementarity conditions are satisfied.

if we start reasonably close to $\underline{x}^*$

if we want global convergence

To guarantee global convergence: (convergence ⇓ from the point that we take as $\underline{x}_0$)

- 1-D search that minimizes an appropriate merit function such as

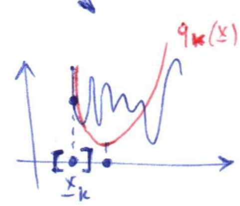
$$P(\underline{x}; \mu) = f(\underline{x}) + \frac{1}{2\mu}\left(\sum_{i=1}^{m} \max\{0, g_i(\underline{x})\} + \sum_{l=1}^{p} |h_l(\underline{x})| \right)$$

($\neq$ barrier method)

- or trust region based approach.

Quasi-Newton versions (without 2nd order derivatives) have also been investigateded.

Several SQP codes are available (SQP, NPSOL, SNOPT, Matlab,...).



since we know that $q_k(\underline{x})$ is a good approximation only in the neighborhood of $\underline{x}_k$, we should not do the Newton method blindly and consider $\underline{x}_{k+1} = \arg\min q_k(\underline{x})$, we minimize $q_k(\underline{x})$ only in a neighborhood of $\underline{x}_k$

$$\underline{x}_{k+1} = \arg\min_{\underline{x} \in B(\underline{x}_k)} q_k(\underline{x})$$

"trust region"

EXAMPLES

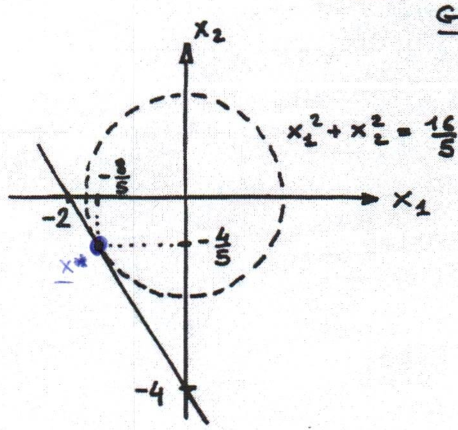
1) $\begin{cases} \text{MIN} & x_1^2 + x_2^2 \\ \text{s.c.} & 2x_1 + x_2 \leq -4 \end{cases}$

$\left. \begin{array}{l} f \,\&\, g \text{ CONVEX} \\ \underline{a} = \begin{pmatrix} -2 \\ 1 \end{pmatrix} \end{array} \right\} \Rightarrow \exists \text{ SADDLE-PT}$

$\Rightarrow$ NO DUALITY GAP

$\underline{x}^* = \left(-\frac{8}{5}, -\frac{4}{5}\right)$

$f(\underline{x}^*) = \frac{16}{5}$



$$L(\underline{x}, u) = \underbrace{\boxed{x_1^2 + x_2^2}}_{f(\underline{x})} + \underbrace{\boxed{2ux_1 + ux_2 + 4u}}_{\sum_{i \in I} u_i g_i(\underline{x})} \rightarrow \text{CONVEX}:$$

the Lagrangian is convex since we're summing convex functions

$$\begin{cases} \frac{\partial L}{\partial x_1} = 2x_1 + 2u = 0 \\ \frac{\partial L}{\partial x_2} = 2x_2 + u = 0 \end{cases} \Rightarrow \begin{cases} x_1 = -u \\ x_2 = -\frac{u}{2} \end{cases} \Rightarrow \underline{w(u)} = -\frac{5u^2}{4} + 4u$$

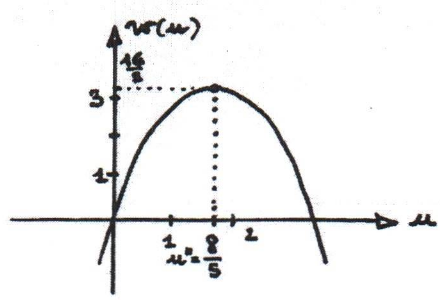
CONCAVE

$\underline{(D)}$ $\max_{u \geq 0} w(u)$ $\qquad \frac{\partial w(u)}{\partial u} = -\frac{5u}{2} + 4 \Rightarrow u^* = \frac{8}{5} \geq 0$

Thus $w(u^*) = -\frac{5}{4}\left(\frac{8}{5}\right)^2 + \frac{32}{5} = \frac{16}{5}$

$= f(\underline{x}^*)$

NO DUALITY GAP



2) $\begin{cases} \text{MIN} & -2x_1 + x_2 \\ \text{S.C.} & x_1 + x_2 - 3 = 0 \\ & \binom{x_1}{x_2} \in X = \left\{ \binom{0}{0}, \binom{0}{4}, \binom{4}{4}, \binom{4}{0}, \binom{1}{2}, \binom{2}{1} \right\} \end{cases}$

INTEGER PROGRAM

It's not a convex problem so we don't know if it exists a saddle point (in fact we'll see that a saddle point $\nexists$ and that we'll get a duality gap)

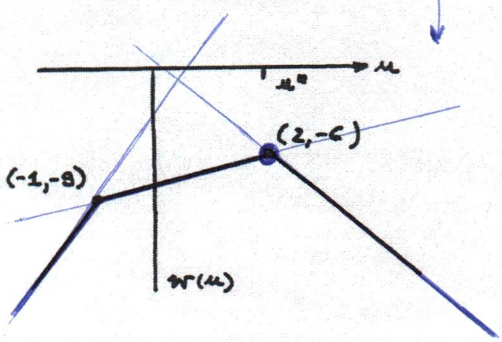
(P) : $\underline{x}^* = \binom{2}{1}$, $f(\underline{x}^*) = -3$

only two points satisfies the condition, $\binom{2}{1}$ is the optimal one

$L(\underline{x}, u) = \boxed{-2x_1 + x_2} + \boxed{u(x_1 + x_2 - 3)}$ $\quad u$ UNRESTRICTED $(u \in \mathbb{R})$

(since the constraint is an equality)

$$\underline{w(u)} = \min_{\underline{x} \in X} L(\underline{x}, u) = \begin{cases} -4 + 5u & \text{FOR } u \le -1 \\ -8 + u & \text{FOR } -1 \le u \le 2 \\ -3u & \text{FOR } u \ge 2 \end{cases}$$



$u^* = 2$, $w(u^*) = -6 < f(x^*)$

$f(x^*)$ — -3

$w(u^*)$ — -6

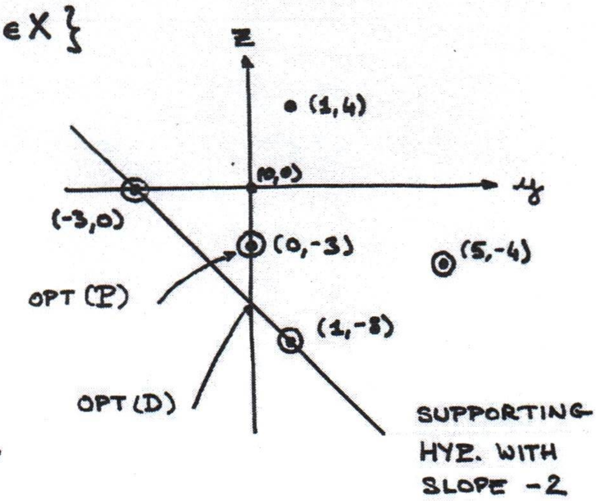
$\exists$ DUALITY $\underline{\text{GAP}}$

$(w(u^*) = -6 < -3 = f(x^*))$

we can represent the set G but we're $\underline{\text{not}}$ entering in these details

$S = \left\{ \binom{y}{z} : y = g(x), \ z = f(x) \text{ FOR SOME } x \in X \right\}$

DISCRETE



$\varphi(y) = \text{MIN}\{f(\underline{x}) : g(\underline{x}) = y, \ \underline{x} \in X\}$

$\varphi(y) = +\infty$ FOR OTHER y VALUES

NB: $\nexists \ \bar{u}$ S.T.

$$\varphi(y) \ge \varphi(0) - \bar{u}\, y \quad \forall y$$