Optimization

Màster de Fonaments de Ciència de Dades

Lecture II. Unconstrained and constrained optimization with equalities. Optimality conditions

Main issues in Optimization

- 1. Characterization of extrema (maxima/minima)
 - Necessary conditions
 - Sufficient conditions
 - ► Lagrange multiplier theory
 - ► The Karush-Kuhn-Tucker theory
- 2. Iterative algorithms for the computation of the extrema
 - Iterative descent
 - Approximation methods
 - Dual and primal-dual methods

Characterization of minima. Local and global minima

Let a function $f: \mathbb{R}^n \longrightarrow \mathbb{R}$. A point $\mathbf{x}^* \in \mathbb{R}^n$ is a:

▶ LOCAL minimum of *f* if:

there is an $\epsilon > 0$ such that $f(x^*) \le f(x)$ for all $x \in \mathbb{R}^n$ when $||x - x^*|| \le \epsilon$.

► STRICT LOCAL minimum of f if:

there is an $\epsilon > 0$ such that $f(x^*) < f(x)$ for all $x \in \mathbb{R}^n \setminus \{x^*\}$ when $||x - x^*|| \le \epsilon$.

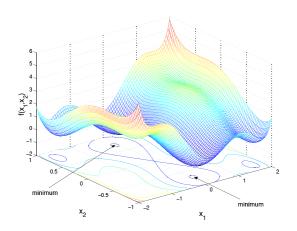
▶ GLOBAL minimum of f if:

$$f(x^*) \le f(x)$$
 for all $x \in \mathbb{R}^n$.

▶ STRICT GLOBAL minimum of f if:

$$f(\mathbf{x}^*) < f(\mathbf{x})$$
 for all $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{x}^*\}$.

Local and global minima



The function $f(x_1, x_2) = x_1^2(4 - 2.1x_1^2 + \frac{1}{3}x_1^4) + x_1x_2 + x_2^2(-4 + 4x_2^2)$ has two global minima, (0.089, -0.717) and (-0.0898, 0.717) and four local minima.

Derivatives and notation

Recall that if $x \in \mathcal{C} \subset \mathbb{R}^n$ is a point where the real function

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

is differentiable then:

▶ We define the gradient of f at x as the vector $\nabla f(x)$ given by:

$$\nabla f(\mathbf{x}) = \left(\frac{\partial f(\mathbf{x})}{\partial x_1}, ..., \frac{\partial f(\mathbf{x})}{\partial x_n}\right)^T.$$

▶ If f is twice continuously differentiable at x we define the Hessian matrix of f at x as the $n \times n$ symmetric matrix $\nabla^2 f(x)$ given by:

$$\nabla^2 f(\mathbf{x}) = \left(\frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j}\right), \quad i, j = 1, ..., n.$$

▶ The directional derivative $D_u f(x)$ of the function f, at point $x \in \mathcal{C}$, in the direction $u \in \mathbb{R}^n$ (||u|| = 1) is defined as

$$D_{\boldsymbol{u}}f(\boldsymbol{x}) = \lim_{\lambda \to 0} \frac{f(\boldsymbol{x} + \lambda \boldsymbol{u}) - f(\boldsymbol{x})}{\lambda} = \nabla f(\boldsymbol{x}) \cdot \boldsymbol{u} = \nabla f(\boldsymbol{x})^{\mathsf{T}} \boldsymbol{u}$$

One must be careful with necessary and sufficient conditions.

Theorem: Let $c \in (a; b)$ and f be a real valued **continuous** function at c. If for some $\delta > 0$, f is increasing on $(c - \delta, c)$ and decreasing on $(c, c + \delta)$, then f has a local maximum at c.

Proof: Choose any x_1 and x such that $c - \delta < x_1 < x < c$. Then $f(x_1) \le f(x)$ and by the continuity of f at c we have:

$$f(x_1) \leq \lim_{x \to c^-} f(x) = f(c).$$

Similarly, if $c < x < x_2 < c + \delta$, then

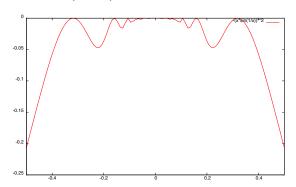
$$f(x_2) \leq \lim_{x \to c^+} f(x) = f(c).$$

This proves the result.

Remark: This Theorem gives a sufficient condition of maximum but not a necessary one.

Remark: The converse of the above Theorem is not true, i.e.: If f is continuous at c and f has a local maximum at c, then f need not be increasing on $(c-\delta,c)$ or decreasing on $(c,c+\delta)$ for any $\delta>0$. Take, for example, c=0 and

$$f(x) = -\left(x\sin\frac{1}{x}\right)^2$$
 if $x \neq 0$, and $f(0) = 0$.



Theorem (Necessary condition)

Let $f: \mathcal{C} \to \mathbb{R}$ and \mathbf{x}^* an interior point of $\mathcal{C} \subset \mathbb{R}^n$ at which f has a local minimum (or a local maximum). If f is **differentiable** at \mathbf{x}^* then:

$$\nabla f(\mathbf{x}^*) = 0.$$

Proof. As x^* is a local minimum, one has:

$$f(\mathbf{x}^*) \leq f(\mathbf{x}^* + \lambda \mathbf{s})$$
 for all $\mathbf{s} \in \mathbb{R}^n$, $\|\mathbf{s}\| = 1$ and $\lambda \in \mathbb{R}$ small enough.

Fix s and define $F(\lambda) = f(x^* + \lambda s)$, which is continuous at $\lambda = 0$. Then the above inequality becomes

$$F(0) \le F(\lambda), \quad \forall |\lambda| < \delta.$$

From the Mean Value Theorem, we have

$$F(\lambda) = F(0) + F'(\theta \lambda)\lambda,$$

where $\theta \in [0, 1]$.

Now...



Now...

– If F'(0)>0, then, by the continuity assumptions, there exists an $\epsilon>0$ such that:

$$F'(\theta\lambda) > 0$$
, $\forall \theta \in [0,1]$, and $\forall \lambda$ s.t. $|\lambda| < \epsilon$.

Hence, we can find a $\lambda < 0$, such that $|\lambda| < \delta$, and, since:

$$F(\lambda) = F(0) + F'(\theta \lambda)\lambda \Rightarrow F(0) > F(\lambda),$$
 contradiction!!

– Assuming F'(0) < 0 would lead to a similar contradiction (taking $\lambda > 0$).

Thus

$$F'(0) = \nabla f(\mathbf{x}^*)^T \mathbf{s} = 0.$$

Since s is an arbitrary nonzero vector (||s|| = 1), we must have:

$$\nabla f(\mathbf{x}^*)^T = 0.$$

Theorem (Sufficient conditions)

Let x^* be an interior point of $\mathcal C$ at which f is twice continuously differentiable. If

$$\nabla f(\mathbf{x}^*) = 0, \quad \mathbf{z}^T \nabla^2 f(\mathbf{x}^*) \mathbf{z} > 0, \quad \forall \mathbf{z} \neq \mathbf{0},$$

then f has a local minimum at x^* . If

$$\nabla f(\mathbf{x}^*) = 0, \quad \mathbf{z}^T \nabla^2 f(\mathbf{x}^*) \mathbf{z} < 0, \quad \forall \mathbf{z} \neq \mathbf{0},$$

then f has a local maximum at x^* .

Moreover, the extrema are strict local extrema.

Proof. Use the Taylor expansion of f arounf x^* .

Remark. Note that the converses of the above assertions are not true. For instance, $f(x) = -x^4$, has a maximum at $x^* = 0$, is twice differentiable at 0 but $\nabla f(0) = f''(0) = 0$, which is not strictly less than 0.

Remark. The condition $\mathbf{z}^T \nabla^2 f(\mathbf{x}^*) \mathbf{z} > 0$, $\forall \mathbf{z} \neq 0$ means that $\nabla^2 f(\mathbf{x}^*)$ is positive definite.

Example. Let

$$f(x) = x^{2p}, \quad x \in \mathbb{R}, \quad p \in \mathbb{Z}_+,$$

and let C be the whole real line.

► The gradient of *f* is

$$\nabla f(x) = f'(x) = 2px^{2p-1}.$$

Clearly $\nabla f(0) = 0$, that is x = 0 satisfies the necessary condition for a minimum or a maximum.

▶ The Hessian of f is

$$\nabla^2 f(x) = f''(x) = (2p - 1)2px^{2p - 2}.$$

For p=1, $\nabla^2 f(0)=2>0$, that is, the sufficient conditions for a strict local minimum are satisfied.

If we take p > 1, then $\nabla^2 f(0) = 0$ and the sufficient conditions for a local minimum are not satisfied, yet f has a minimum at the origin.

By taking any neighborhood of the origin, it can be verifiyed that all the conditions for a local minimum given in the next Theorem are satisfied for this example.

Theorem

Let x^* be an interior point of C and assume that f is twice continuously differentiable on C, then:

(a) Necessary conditions for a local minimum of f at x^* are:

$$\nabla f(\mathbf{x}^*) = 0, \quad \mathbf{z}^T \nabla^2 f(\mathbf{x}^*) \mathbf{z} \geq 0, \quad \forall \mathbf{z} \in \mathbb{R}^n.$$

(b) Sufficient conditions for a local minimum are:

$$\nabla f(\mathbf{x}^*) = 0,$$

and that for every x in some neighborhood $N_{\epsilon}(x^*)$ and for every $z \in \mathbb{R}^n$, we have:

$$\mathbf{z}^T \nabla^2 f(\mathbf{x}) \mathbf{z} \geq 0.$$

(c) If the sense of the inequalities is reversed, then the theorem applies to a local maximum.



Proof of the Theorem

Proof

(a) The first order condition for local minimum

$$x^*$$
 minimum $\Rightarrow \nabla f(x^*) = 0$,

has already been proved (pages 8 and 9).

Turning to the second-order conditions, we have by Taylor's theorem applied to the function $F(\theta) = f(x^* + \theta s)$, with ||s|| = 1 fixed,

$$F(\theta) = F(0) + \nabla F(0)\theta + \frac{1}{2}\nabla^2 F(\lambda\theta)\theta^2, \quad \lambda \in (0,1).$$

If $\nabla^2 F(0) < 0$, then, by continuity, there exists $\epsilon' > 0$ such that $\nabla^2 F(\lambda \theta) < 0$ for $\lambda \in (0,1)$ and $|\theta| < \epsilon'$. Since $\nabla F(0) = 0$, this inequality implies that for such a θ :

$$F(\theta) < F(0),$$

which is a contradiction. Consequently

$$\nabla^2 F(0) = \mathbf{s}^T \nabla^2 f(\mathbf{x}^*) \mathbf{s} \ge 0.$$

Since this inequality holds for all unitary vector s, it must hold for all vector z.



Proof of the Theorem (cont.)

(b) Assume that $\nabla f(\mathbf{x}^*) = 0$ and that $\mathbf{z}^T \nabla^2 f(\mathbf{x}^*) \mathbf{z} \geq 0$ for all $\mathbf{x} \in N_\delta(\mathbf{x}^*)$ and all $\mathbf{z} \in \mathbb{R}^n$, but that \mathbf{x}^* is not a local minimum.

Then there exists a $\mathbf{w} \in N_{\delta}(\mathbf{x}^*)$ such that $f(\mathbf{w}) < f(\mathbf{x}^*)$.

Write $\mathbf{w} = \mathbf{x}^* + \theta \mathbf{y}$, with $\|\mathbf{y}\| = 1$ and $\theta > 0$. By Taylor's theorem:

$$f(\mathbf{w}) = f(\mathbf{x}^*) + \theta \nabla f(\mathbf{x}^*)^T \mathbf{y} + \frac{1}{2} \theta^2 \mathbf{y}^T \nabla^2 f(\mathbf{x}^* + \lambda \theta \mathbf{y}) \mathbf{y},$$

with $\lambda \in (0,1)$. Our assumptions lead then to

$$\mathbf{y}^T \nabla^2 f(\mathbf{x}^* + \lambda \theta \mathbf{y}) \mathbf{y} < 0,$$

contradicting the hypothesis, since $\mathbf{x}^* + \lambda \theta \mathbf{y} \in N_{\delta}(\mathbf{x}^*)$.

Example

Let

$$f(x,y) = \frac{1}{2}x^2 + xy + 2y^2 - 4x - 4y - y^3.$$

Then

$$\nabla f(x,y) = (x+y-4, x+4y-4-3y^2)^T$$
, $H(x,y) = \begin{pmatrix} 1 & 1 \\ 1 & 4-6y \end{pmatrix}$.

 $\nabla f(x,y)=0$ has exactly two solutions, $\emph{x}_1=(4,0),\ \emph{x}_2=(3,1),$ and

$$H(x_1) = \begin{pmatrix} 1 & 1 \\ 1 & 4 \end{pmatrix}, \qquad H(x_2) = \begin{pmatrix} 1 & 1 \\ 1 & -2 \end{pmatrix}.$$

$$(x \ y) \begin{pmatrix} 1 & 1 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = x^2 + 2xy + 4y^2 = (x+y)^2 + 3y^2 > 0 \quad \text{if} \quad (x \ y) \neq (0,0).$$

$$(x y)$$
 $\begin{pmatrix} 1 & 1 \\ 1 & -2 \end{pmatrix}$ $\begin{pmatrix} x \\ y \end{pmatrix} = x^2 + 2xy - 2y^2 = (x + y)^2 - 3y^2.$

So $H(x_1)$ is positive definite and $H(x_2)$ is indefinite, therefore, the only extrema is the local minimum is x_1 .

Convexity

Convexity notions play an important role in nonlinear programming. Some reasons for that are:

- Convex optimization includes least-squares and linear programming problems, which can be solved numerically very efficiently.
- When the cost function f is convex, every local maximum/minimum is also global.
- 3. We will see that if $f(x) = x^T Q x + c^T x + d$ is such that Q is positive semidefinite, then f is convex.
- 4. The (first order) necessary condition $\nabla f(x^*) = 0$ is also sufficient for global optimality if f is convex.
- The behavior of convex functions allows for very fast algorithms to optimize them.
- 6. Many optimization problems admit a convex (re)formulation.

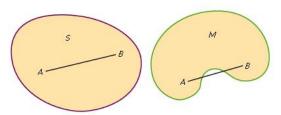
Convex sets and convex functions

▶ Let two points $x_1, x_2 \in \mathbb{R}$, and $0 \le \lambda \le 1$ be given. Then, the point

$$x = \lambda x_1 + (1 - \lambda)x_2,$$

is a convex combination of the two points x_1, x_2 .

▶ The set $\mathcal{C} \subset \mathbb{R}^n$ is called convex, if all convex combinations of any two points $x_1, x_2 \in \mathcal{C}$ are again in \mathcal{C} .

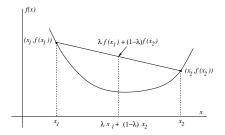


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Convex sets and convex functions

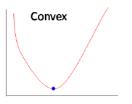
▶ A function $f: \mathcal{C} \longrightarrow \mathbb{R}$ defined on a convex set \mathcal{C} is called convex if for all $x_1, x_2 \in \mathcal{C}$ and $0 \le \lambda \le 1$ one has:

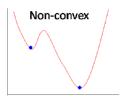
$$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda)f(x_2).$$



For a convex function, the linear interpolation $\lambda f(\mathbf{x}_1) + (1 - \lambda)f(\mathbf{x}_2)$ overstimates the function value $f(\lambda \mathbf{x}_1 + (1 - \lambda)\mathbf{x}_2)$.

Convex sets and convex functions





▶ A function $f: \mathcal{C} \longrightarrow \mathbb{R}$ defined on a convex set \mathcal{C} is called strictly convex if for all $x_1, x_2 \in \mathcal{C}$ with $x_1 \neq x_2$ and $0 < \lambda < 1$ one has.

$$f(\lambda x_1 + (1-\lambda)x_2) < \lambda f(x_1) + (1-\lambda)f(x_2).$$

- ▶ A function $f: \mathcal{C} \longrightarrow \mathbb{R}$ defined on a convex set \mathcal{C} is called concave if -f is convex.
- Remark. Recall that the domain of a convex function must be a convex set.
- ▶ Remark. Later we will give a more general definition of convex function.

Examples of convex functions

Proposition

- a) A linear function, $f(\lambda x + \mu y) = \lambda f(x) + \mu f(y)$, is convex.
- b) Any vector norm, f(x) = ||x||, is a convex function.
- c) The weighted sum of convex functions $(\sum \alpha_i f_i(\mathbf{x}))$ with positive weights $(\alpha_i > 0)$ is convex.
- d) If I is an index set, $C \subset \mathbb{R}^n$ is a convex set and $f_i : C \to \mathbb{R}$ are convex functions for each $i \in I$, then the function:

$$h: \mathcal{C} \longrightarrow (-\infty, \infty]$$

 $x \longrightarrow \sup_{i \in I} f_i(x)$

is also convex (recall that the $\sup_{i\in I} f_i(\mathbf{x})$ is the least upper bound of $\{f_i(\mathbf{x}); i\in I\}$).

Proof. a) and)c) are consequences of the definition of convexity.

b) Let $\|\cdot\|$ be a norm. Then, for any $x,y\in\mathbb{R}^n$ and any $\lambda\in[0,1]$ we have:

$$\|\lambda x + (1 - \lambda)y\| \le \|\lambda x\| + \|(1 - \lambda)y\| = \lambda \|x\| + (1 - \lambda)\|y\|.$$

d) For every $i \in I$ we have

$$f_i(\lambda \mathbf{x} + (1 - \lambda)\mathbf{y}) \leq \lambda f_i(\mathbf{x}) + (1 - \lambda)f_i(\mathbf{y}) \leq \lambda h(\mathbf{x}) + (1 - \lambda)h(\mathbf{y}).$$

Taking the supremum over all $i \in I$ we conclude:

$$h(\lambda x + (1-\lambda)y) \leq \lambda h(x) + (1-\lambda)h(y).$$

Necessary and sufficient conditions for extrema for convex functions

Theorem (Necessary condition in the convex case)

Let $f: \mathcal{C} \to \mathbb{R}$ be a convex function over the convex set $\mathcal{C} \subset \mathbb{R}^n$.

- a) A local minimum of f over C is also a global minimum over C.
- b) If, in addition, f is strictly convex, then there exists at most one global minimum of f.
- c) If f is convex, the set $\mathcal C$ is open, and f is differentiable at x^* , then $\nabla f(x^*) = 0$ is a necessary (see Theorem pg. 8) and sufficient condition for $x^* \in \mathcal C$ to be a global minimum of f over $\mathcal C$.

Proof

a) Suposse that x is a local minimum of f but not a global minimum. Then there exists some $y \neq x$ such that f(y) < f(x). Since f is convex:

$$f(\alpha \mathbf{x} + (1-\alpha)\mathbf{y}) \leq \alpha f(\mathbf{x}) + (1-\alpha)f(\mathbf{y}) < \alpha f(\mathbf{x}) + (1-\alpha)f(\mathbf{x}) = f(\mathbf{x}), \ \forall \alpha \in [0,1).$$

This contradicts the assumption that x is a local minimum.

b) Suppose that two distinct global minima x and y exist (f(x) = f(y)). Then $(x + y)/2 \in \mathcal{C}$, since \mathcal{C} is convex, and also:

$$f((1/2)x + (1/2)y) < f(x),$$
 $f((1/2)x + (1/2)y) < f(y),$

and since x and y are global minima, we obtain a contradiction.



Proof (cont.)

c) By the convexity of \mathcal{C} , and using the convexity of f, we have that for all $\mathbf{x} \in \mathcal{C}$ and $\alpha \in [0,1]$:

$$\alpha \mathbf{x} + (1 - \alpha)\mathbf{x}^* = \mathbf{x}^* + \alpha(\mathbf{x} - \mathbf{x}^*) \Rightarrow f(\mathbf{x}^* + \alpha(\mathbf{x} - \mathbf{x}^*)) = f(\alpha \mathbf{x} + (1 - \alpha)\mathbf{x}^*) \le \alpha f(\mathbf{x}) + (1 - \alpha)f(\mathbf{x}^*),$$

$$f(\mathbf{x}^* + \alpha(\mathbf{x} - \mathbf{x}^*)) - f(\mathbf{x}^*) \le \alpha f(\mathbf{x}) + (1 - \alpha)f(\mathbf{x}^*) - f(\mathbf{x}^*) = \alpha(f(\mathbf{x}) - f(\mathbf{x}^*)).$$

It follows that:

$$\frac{f(\mathbf{x}^* + \alpha(\mathbf{x} - \mathbf{x}^*)) - f(\mathbf{x}^*)}{\alpha} \le f(\mathbf{x}) - f(\mathbf{x}^*).$$

Furthermore

$$\lim_{\alpha \to 0} \frac{f(\mathbf{x}^* + \alpha(\mathbf{x} - \mathbf{x}^*)) - f(\mathbf{x}^*)}{\alpha} = \nabla f(\mathbf{x}^*)^T (\mathbf{x} - \mathbf{x}^*).$$

Taking the limit as $\alpha \to 0$ in the last inequality, we get

$$\nabla f(\mathbf{x}^*)^T(\mathbf{x} - \mathbf{x}^*) \leq f(\mathbf{x}) - f(\mathbf{x}^*), \quad \forall \mathbf{x} \in \mathcal{C}.$$

If $\nabla f(\mathbf{x}^*) = 0$, we obtain

$$0 < f(x) - f(x^*) \Rightarrow f(x) > f(x^*) \quad \forall x \in C.$$

so x^* is a global minimum.



Remark

The inequality of the above page:

$$\nabla f(\mathbf{x}^*)^T(\mathbf{x} - \mathbf{x}^*) \leq f(\mathbf{x}) - f(\mathbf{x}^*), \quad \forall \mathbf{x} \in \mathcal{C},$$

can be written as:

$$f(x) \ge f(x^*) + \nabla f(x^*)^T (x - x^*), \quad \forall x \in \mathcal{C}.$$

In fact, we have proven the more general one:

$$f(x) \ge f(y) + \nabla f(y)^T (x - y), \quad \forall x, y \in \mathcal{C},$$
 (1)

since we have not used the condition $\nabla f(\mathbf{x}^*) = 0$.

The inequality is, in fact, a consequence of the following characterization of differentiable convex functions.

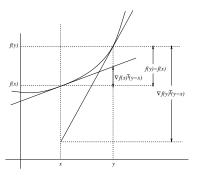
First characterization theorem of convex functions

Theorem

f is convex on $\mathcal C$ if and only if for any two points $\mathbf x, \mathbf y \in \mathcal C$ one has

$$\nabla f(\mathbf{x})^{\mathsf{T}}(\mathbf{y} - \mathbf{x}) \le f(\mathbf{y}) - f(\mathbf{x}) \le \nabla f(\mathbf{y})^{\mathsf{T}}(\mathbf{y} - \mathbf{x}). \tag{2}$$

If the inequalities are strict whenever $\mathbf{x} \neq \mathbf{y}$, then f is strictly convex over \mathcal{C} .



Remarks. As it follows from the proof, the two inequalities (2) in the Theorem can be substitued by (1) $(f(x) \ge f(y) + \nabla f(y)^T (x - y))$, since one inequality is a consequence of the other.

The proof for the strictly convex case is identical to the convex case.





Proof of the characterization theorem

Proof.

Assume that f is convex. The second inequality directly follows from (1). Interchanging the roles of x and y in (1), one gets for all $x, y \in \mathcal{C}$ that

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^{\mathsf{T}} (\mathbf{y} - \mathbf{x}), \quad \Rightarrow f(\mathbf{y}) - f(\mathbf{x}) \geq \nabla f(\mathbf{x})^{\mathsf{T}} (\mathbf{y} - \mathbf{x}),$$

which is the first inequality in (2).

To proof the converse, supose that (1) is true and we must proof that f is convex. We fix some $\mathbf{x},\mathbf{y}\in\mathcal{C}$ and some $\alpha\in[0,1]$. Let $\mathbf{z}=\alpha\mathbf{x}+(1-\alpha)\mathbf{y}$. Using the inequality twice, we get

$$f(\mathbf{x}) \geq f(\mathbf{z}) + \nabla f(\mathbf{z})^{\mathsf{T}} (\mathbf{x} - \mathbf{z}),$$

 $f(\mathbf{y}) \geq f(\mathbf{z}) + \nabla f(\mathbf{z})^{\mathsf{T}} (\mathbf{y} - \mathbf{z}).$

Multiplying the first inequality by α , the second by $(1 - \alpha)$ and adding, we obtain:

$$\alpha f(\mathbf{x}) + (1 - \alpha)f(\mathbf{y}) \ge f(\mathbf{z}) + \nabla f(\mathbf{z})^{\mathsf{T}} (\alpha \mathbf{x} + (1 - \alpha)\mathbf{y} - \mathbf{z}) = f(\mathbf{z}),$$

which proves that f is convex.



Applications

Many elementary (and and not so elementary) inequalities follow from the above Theorem.

Example: The well know inequality¹

$$e^x \geq 1 + x$$

can also be proved by using the convexity of the function $f(x) = e^x$.

Since $\nabla f(x) = f'(x) = e^x$, taking y = 0, so $\nabla f(y) = f'(0) = 1$, and using inequality (2):

$$\nabla f(x)^T (y-x) \leq f(y) - f(x) \leq \nabla f(y)^T (y-x),$$

we get:

$$e^{x}(0-x) \le 1 - e^{x} \le 0 - x \quad \Rightarrow \quad x \le e^{x} - 1 \le xe^{x}, \quad \forall x \in \mathbb{R},$$

or

$$e^x > 1 + x$$
, and $(1 - x)e^x < 1$, $\forall x \in \mathbb{R}$.

¹It can be easily be proved noting that $g(x) = e^x - (1+x)$ has a minimum at x = 0 \Rightarrow $0 < \infty$



Applications

Exercise 3. To be delivered before 4-X-2021 as: Ex03-YourSurname.pdf *Proof, whithout using the above theorem, that for any* $a \in \mathbb{R}$, $f(x) = e^{ax}$ *is a convex function.*

Characterization of convexity for twice differentiable functions

Theorem.

Let $\mathcal{C} \subset \mathbb{R}^n$ be a convex set, let $f: \mathbb{R}^n \to \mathbb{R}$ be a twice continuously differentiable function over \mathcal{C} , and let Q be a real symmetric $n \times n$ matrix.

- a) If $\nabla^2 f(x)$ is positive semidefinite for all $x \in C$, then f is convex over C.
- b) If $\nabla^2 f(x)$ is positive definite for all $x \in C$, then f is strictly convex over C.
- c) If $C = \mathbb{R}^n$ and f is convex, then $\nabla^2 f(x)$ is positive semidefinite for all $x \in C$.
- d) The quadratic function $f(x) = x^T Q x$, where Q is a symmetric matrix, is convex if and only if Q is positive semidefinite. Furthermore, f is strictly convex if and only if Q is positive definite.

Proof.

a) According to Taylor's formula, for all $x, y \in C$

$$f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^{\mathsf{T}} (\mathbf{y} - \mathbf{x}) + \frac{1}{2} (\mathbf{y} - \mathbf{x})^{\mathsf{T}} \nabla^2 f(\mathbf{x} + \alpha(\mathbf{y} - \mathbf{x})) (\mathbf{y} - \mathbf{x}),$$

for some $\alpha \in [0,1]$. Therefore, using the positive semi-definiteness of $\nabla^2 f(\mathbf{x})$, $(\mathbf{z}^T \nabla^2 f(\mathbf{x}) \mathbf{z} \geq 0, \ \forall \mathbf{z})$, we obtain

$$f(y) \ge f(x) + \nabla f(x)^{T} (y - x), \quad \forall x, y \in C,$$

from which we can conclude that f is convex.



Proof of the Theorem (cont.)

- b) Similar to the proof of part a).
- c) Suposse that $f: \mathbb{R}^n \to \mathbb{R}$ is convex and that $x \in \mathcal{C}$. For some small $\alpha > 0$ and any $y \in \mathbb{R}^n$, we have that $x + \alpha y \in \mathcal{C}$. From Taylor's formula:

$$f(\mathbf{x} + \alpha \mathbf{y}) = f(\mathbf{x}) + \alpha \nabla f(\mathbf{x})^{\mathsf{T}} \mathbf{y} + \frac{\alpha^2}{2} \mathbf{y}^{\mathsf{T}} \nabla^2 f(\mathbf{x}) \mathbf{y} + o(\|\alpha \mathbf{y}\|^2).$$

Since f is convex, we know that for any a and b:

$$f(\mathbf{a}) \ge f(\mathbf{b}) + \nabla f(\mathbf{b})^{\mathsf{T}} (\mathbf{a} - \mathbf{b}),$$

so, taking $\mathbf{a} = \mathbf{x} + \alpha \mathbf{y}$ and $\mathbf{b} = \mathbf{x}$, we get

$$f(\mathbf{x} + \alpha \mathbf{y}) \ge f(\mathbf{x}) + \alpha \nabla f(\mathbf{x})^T \mathbf{y}.$$

Therefore, we have that for any $\mathbf{y} \in \mathbb{R}^n$

$$\frac{\alpha^2}{2} \mathbf{y}^T \nabla^2 f(\mathbf{x}) \mathbf{y} + o(\|\alpha \mathbf{y}\|^2) \ge 0.$$

Dividing by $\alpha^2/2$ and taking $\alpha \to 0$, we get

$$\mathbf{y}^T \nabla^2 f(\mathbf{x}) \mathbf{y} \geq 0, \quad \forall \mathbf{y} \in \mathbb{R}^n.$$

Proof of the Theorem (cont.)

d) If $f(x) = x^T Q x$ then $\nabla^2 f(x) = 2Q$. Hence, from a) and c) it follows that f is convex if and only if Q is positive semidefinite.

For the strict convexity, supose that f is strictly convex, then, according to c), Q is positive semidefinite and it remains to show that Q is positive definite.

It can be shown that Q is positive definite if and only if all its eigenvalues are posive.

Assume that zero is an eigenvalue, then there exists some $x \neq 0$ such that Qx = 0. It follows that

$$0 = f(0) = f\left(\frac{1}{2}x + \frac{1}{2}(-x)\right) = \frac{1}{2}f(x) + \frac{1}{2}f(-x) = 0,$$

which contradicts the strict convexity of f.

Optimization with equality constraints. Lagrange multiplier theory

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

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

subject only to the equality constraints

$$g_i(x) = 0, \quad i = 1, ..., m, \quad m < n,$$
 (3)

where each of the g_i is a real-valued function defined on C. This is, the problem is to find an extremum of f in the region determined by the equations (3).

- ► The first and most intuitive method of solution of such a problem involves the elimination of m variables from the problem by using equations (3).
- ▶ The conditions for such an elimination are stated by the Implicit Function Theorem, that assumes differentiability of the functions g_i and that the $n \times m$ Jacobian matrix $(\partial g_i/\partial x_i)$ has rank m.
- ► The actual solution of the unconstraint equations for m variables in terms of the remaining n - m can often be a difficult, if not impossible, task.



Optimization with equality constraints

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

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

Solution Suppose that the upper righthand corner of the rectangle is at the point (x, y), then the area of the rectangle is S = 4xy. We have:

$$\frac{2x}{a^2}dx + \frac{2y}{b^2}dy = 0 \quad \Rightarrow \quad \frac{2x}{a^2} + \frac{2y}{b^2}\frac{dy}{dx} = 0 \quad \Rightarrow \quad \frac{dy}{dx} = -\frac{b^2x}{a^2y},$$

so

$$\frac{dS}{dx} = 4y + 4x \frac{dy}{dx} = 4y - \frac{4b^2x^2}{a^2y}, \qquad \frac{dS}{dx} = 0 \quad \Rightarrow \quad y^2 = \frac{b^2x^2}{a^2}.$$

Since, according to the equation of the ellipse

$$y^2 = b^2 - \frac{b^2 x^2}{a^2},$$

we get

$$y^2 = b^2 - y^2$$
 \Rightarrow $y = \frac{b}{\sqrt{2}}$ and $x = \frac{a}{\sqrt{2}}$ \Rightarrow $S_{max} = 2ab$.

Lagrange multipliers

Another method for finding the minimum, also based on the idea of transforming a constrained problem into an unconstrained one, was proposed by Lagrange.

Before introducing this method, we present the following result:

Theorem

Let f and g_i , i=,...,m, be real-valued functions on $\mathcal{C}\subset\mathbb{R}^n$ (m< n) and continuosly differentiable on a neighborhood $N_\epsilon(x^*)\subset\mathcal{C}$. Suppose that x^* is a local minimum (or maximum) of f for all points $x\in N_\epsilon(x^*)$ that also satisfy:

$$g_i(x) = 0, \quad i = 1, ..., m.$$

Assume also that the Jacobian matrix $(\partial g_i/\partial x_j)$ at x^* has rank m. Under these hypothese, there exist real numbers λ_i^* such that

$$abla f(\mathbf{x}^*) = \sum_{i=1}^m \lambda_i^*
abla g_i(\mathbf{x}^*).$$



Before the proof. Example

Consider the problem

$$\max f(x,y) = x \ y,$$

subject to the constraint

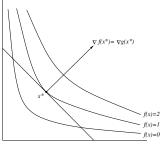
$$g(x, y) = x + y - 2 = 0.$$

The solution of this system problem is:

$$x^* = y^* = 1.$$

In this case:

$$\nabla f(\mathbf{x}^*) = \begin{pmatrix} y \\ x \end{pmatrix}_{(x,y)=(1,1)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \nabla g(\mathbf{x}^*) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}_{(x,y)=(1,1)}.$$



Proof of the Theorem

Proof. By suitable rearrangement and relabeling of rows, we can always assume that the $m \times m$ matrix formed by taking the first m rows of the Jacobian $(\partial g_i(x^*)/\partial x_j)$, is nonsingular since it has rank m.

What we want to proof is that there exist $\lambda_1^*,...,\lambda_m^*$ such that:

$$\nabla f(\mathbf{x}^*) = \lambda_1^* \nabla g_1(\mathbf{x}^*) + \lambda_2^* \nabla g_2(\mathbf{x}^*) + \dots + \lambda_m^* \nabla g_m(\mathbf{x}^*),$$

that can also be written as:

$$\begin{pmatrix} \frac{\partial f(\mathbf{x}^*)}{\partial x_1} \\ \vdots \\ \frac{\partial f(\mathbf{x}^*)}{\partial x_m} \\ \vdots \\ \frac{\partial f(\mathbf{x}^*)}{\partial x_n} \end{pmatrix} = \begin{pmatrix} \frac{\partial g_1(\mathbf{x}^*)}{\partial x_1} & \dots & \frac{\partial g_m(\mathbf{x}^*)}{\partial x_1} \\ \vdots & & \vdots \\ \frac{\partial g_1(\mathbf{x}^*)}{\partial x_m} & \dots & \frac{\partial g_m(\mathbf{x}^*)}{\partial x_m} \\ \vdots & & \vdots \\ \frac{\partial g_1(\mathbf{x}^*)}{\partial x_n} & \dots & \frac{\partial g_m(\mathbf{x}^*)}{\partial x_n} \end{pmatrix} \begin{pmatrix} \lambda_1^* \\ \vdots \\ \lambda_m^* \end{pmatrix}.$$

We will first proof that there exist $\lambda_1^*,...,\lambda_m^*$ such that:

$$\begin{pmatrix} \frac{\partial f(\mathbf{x}^*)}{\partial x_1} \\ \vdots \\ \frac{\partial f(\mathbf{x}^*)}{\partial x_m} \end{pmatrix} = \begin{pmatrix} \frac{\partial g_1(\mathbf{x}^*)}{\partial x_1} & \dots & \frac{\partial g_m(\mathbf{x}^*)}{\partial x_1} \\ \vdots & & \vdots \\ \frac{\partial g_1(\mathbf{x}^*)}{\partial x_m} & \dots & \frac{\partial g_m(\mathbf{x}^*)}{\partial x_m} \end{pmatrix} \begin{pmatrix} \lambda_1^* \\ \vdots \\ \lambda_m^* \end{pmatrix}.$$

Proof of the Theorem (cont. 1)

Since the matrix of the above linear system is non-singular, the set of linear equations $\frac{1}{2}$

$$\sum_{i=1}^{m} \frac{\partial g_i(\mathbf{x}^*)}{\partial x_j} \lambda_i = \frac{\partial f(\mathbf{x}^*)}{\partial x_j}, \quad j = 1, ..., m,$$
(4)

has a unique solution: λ_i^* , i=1,...,m. In this way we have seen that the first m components of the gradients verify the equality that we want to proof.

Let us see that the remaining n-m components also fulfil the same equality. Let $\hat{x}=(x_{m+1},...,x_n)$, then, applying the Implicit Function Theorem to the equations $g_i(x^*)=0$, it follows that there exist real functions

$$h_j(\hat{x}) = h_j(x_{m+1}, ..., x_n), \quad j = 1, ..., m,$$

defined in an open set $\hat{D} \subset \mathbb{R}^{n-m}$ containing $oldsymbol{x}^*$ such that

$$x_j^* = h_j(\hat{\mathbf{x}}^*) = h_j(x_{m+1}^*, ..., x_n^*), \quad j = 1, ..., m,$$
 (5)

$$f(\mathbf{x}^*) = f(h_1(\hat{\mathbf{x}}^*), ..., h_m(\hat{\mathbf{x}}^*), x_{m+1}^*, ..., x_n^*).$$
 (6)

Using the same Theorem, we have also that for j = m + 1, ..., n

$$\sum_{k=1}^{m} \frac{\partial g_i(\mathbf{x}^*)}{\partial x_k} \frac{\partial h_k(\hat{\mathbf{x}}^*)}{\partial x_j} + \frac{\partial g_i(\mathbf{x}^*)}{\partial x_j} = 0, \quad i = 1, ..., m.$$
 (7)

Proof of the Theorem (cont. 2)

If x^* is a minima of f its first partial derivatives with respect to $x_{m+1},...,x_n$ must vanish at x^* . Thus

$$\frac{\partial f(\mathbf{x}^*)}{\partial x_j} = \sum_{k=1}^m \frac{\partial f(\mathbf{x}^*)}{\partial x_k} \frac{\partial h_k(\hat{\mathbf{x}}^*)}{\partial x_j} + \frac{\partial f(\mathbf{x}^*)}{\partial x_j} = 0, \quad j = m+1, ..., n.$$
 (8)

Multiplying each of the equations in (7) by λ_i^* and adding up, we get:

$$\sum_{i=1}^{m} \left(\sum_{k=1}^{m} \lambda_{i}^{*} \frac{\partial g_{i}(\mathbf{x}^{*})}{\partial x_{k}} \frac{\partial h_{k}(\hat{\mathbf{x}}^{*})}{\partial x_{j}} + \lambda_{i}^{*} \frac{\partial g_{i}(\mathbf{x}^{*})}{\partial x_{j}} \right) = 0, \quad j = m+1, ..., n.$$

Substracting this equality from (8) we get:

$$\sum_{k=1}^{m} \left[\frac{\partial f(\mathbf{x}^*)}{\partial x_k} - \sum_{i=1}^{m} \lambda_i^* \frac{\partial g_i(\mathbf{x}^*)}{\partial x_j} \right] \frac{\partial h_k(\hat{\mathbf{x}}^*)}{\partial x_j} + \frac{\partial f(\mathbf{x}^*)}{\partial x_j} - \sum_{i=1}^{m} \lambda_i^* \frac{\partial g_i(\mathbf{x}^*)}{\partial x_j} = 0,$$

for j=m+1,...,n. Since, due to (4), the expression in the brackets is zero, we get the desired result

$$\frac{\partial f(\mathbf{x}^*)}{\partial x_j} - \sum_{i=1}^m \lambda_i^* \frac{\partial g_i(\mathbf{x}^*)}{\partial x_j} = 0, \ j = m+1, ..., n.$$

Lagrange's method

Lagrange's method consists of transforming an equality constrained extremum problem into a problem of finding a stationary point of the Lagrangian function

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

Theorem (Necessary conditions)

Suppose that f and g_i , i = 1, ..., m, are real-valued functions that satisfy the hypoteses of the preceding Theorem, this is:

$$f:\mathcal{C}\subset\mathbb{R}^n\quad\longrightarrow\quad\mathbb{R},\qquad\text{and}\qquad g_i:\mathcal{C}\subset\mathbb{R}^n\quad\longrightarrow\quad\mathbb{R},\quad i=1,...,m.$$

- ▶ They are all continuosly differentiable on a neighborhood $N_{\epsilon}(\mathbf{x}^*) \subset \mathcal{C} \subset \mathbb{R}^n$.
- ▶ The Jacobian matrix $(\partial g_i(\mathbf{x}^*)/\partial x_i)$ has rank m.
- \triangleright x^* is a local minimum (or maximum) of f in $N_{\epsilon}(x^*)$.
- ▶ If $x \in N_{\epsilon}(x^*)$, then

$$g_i(x) = 0, \quad i = 1, ..., m.$$

Then, there exists a vector of multipliers $\lambda^* = (\lambda_1^*, ..., \lambda_m^*)^T$ such that $\nabla L(\mathbf{x}^*, \lambda^*) = 0$.

Proof. Follows directly from the definition of L and the preceeding Theorem.

Lagrange's method

Theorem (Sufficient conditions).

Let f, $g_1,...,g_m$ be twice continuously differentiable real-valued functions in \mathbb{R}^n . If there exist vectors $\mathbf{x}^* \in \mathbb{R}^n$, $\boldsymbol{\lambda}^* \in \mathbb{R}^m$ such that

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

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

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

it follows that

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

then, f has a strict local minimum at x^* subject to $g_i(x) = 0$, i = 1, ..., m, (similar for a maximum if $z^T \nabla_x^2 L(x^*, \lambda^*) z < 0$).

Proof of the Theorem

Proof.

Assume that x^* is not a strict local minimum. Then there exist a neighborhood $N_{\delta}(x^*)$ and a sequence $\{z^k\}_{k\in\mathbb{Z}}$, $z^k\in N_{\delta}(x^*)$, $z^k\neq x^*$, converging to x^* such that for every z^k in the sequence

$$g_i(\mathbf{z}^k) = 0, \quad i = 1, ..., m, \quad f(\mathbf{x}^*) \ge f(\mathbf{z}^k).$$
 (9)

Let $\mathbf{z}^k = \mathbf{x}^* + \theta^k \mathbf{y}^k$, where $\theta^k > 0$ and $\|\mathbf{y}^k\| = 1$. The sequence $\{(\theta^k, \mathbf{y}^k)\}_{k \in \mathbb{Z}}$ has a subsequence that converges to $(0, \overline{\mathbf{y}})$, where $\|\overline{\mathbf{y}}\| = 1$. By the Mean Value Theorem, for each k in this subsequence

$$g_i(\mathbf{z}^k) - g_i(\mathbf{x}^*) = \theta^k (\mathbf{y}^k)^T \nabla g_i(\mathbf{x}^* + \eta_i^k \theta^k \mathbf{y}^k) = 0, \quad i = 1, ..., m.$$
 (10)

with $0 < \eta_i^k < 1$ and

$$f(\mathbf{z}^k) - f(\mathbf{x}^*) = \theta^k (\mathbf{y}^k)^T \nabla f(\mathbf{x}^* + \xi^k \theta^k \mathbf{y}^k) \le 0,$$
(11)

with $0 < \xi_i^k < 1$. Dividing (10) and (11) by θ^k and taking limits as $k \to \infty$, we get

$$\overline{\mathbf{y}}^T \nabla g_i(\mathbf{x}^*) = 0, i = 1, ...m$$

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

Proof of the Theorem (cont)

From Taylor's theorem we have

$$L(\mathbf{z}^{k}, \boldsymbol{\lambda}^{*}) = L(\mathbf{x}^{*}, \boldsymbol{\lambda}^{*}) + \theta^{k} (\mathbf{y}^{k})^{T} \nabla_{\mathbf{x}} L(\mathbf{x}^{*}, \boldsymbol{\lambda}^{*}) + \frac{1}{2} (\theta^{k})^{2} (\mathbf{y}^{k})^{T} \nabla_{\mathbf{x}}^{2} L(\mathbf{x}^{*} + \eta^{k} \theta^{k} \mathbf{y}^{k}, \boldsymbol{\lambda}^{*}) \mathbf{y}^{k},$$
(12)

with $0 < \eta^k < 1$. Dividing this equality by $(\theta^k)^2/2$, using the definition of L, the hypothesis $\nabla L(\mathbf{x}^*, \boldsymbol{\lambda}^*) = 0$ and the conditions (9), we get (exercise)

$$(\mathbf{y}^k)^T \nabla_x^2 L(\mathbf{x}^* + \eta^k \theta^k \mathbf{y}^k, \boldsymbol{\lambda}^*) \mathbf{y}^k \leq 0.$$

Letting $k \to \infty$, we obtain $\overline{\mathbf{y}}$ verifying

$$\overline{\mathbf{y}}^T \nabla_{\mathbf{x}}^2 L(\mathbf{x}^*, \boldsymbol{\lambda}^*) \overline{\mathbf{y}} \leq 0.$$

This completes the proof, since $\overline{\mathbf{y}} \neq 0$ and satisfyes $\overline{\mathbf{y}}^T \nabla g_i(\mathbf{x}^*) = 0$ for i = 1, ...m.

Example

Consider again the problem

$$\max f(x,y) = x \ y,$$

subject to the constraint

$$g(x,y) = x + y - 2 = 0.$$

The Lagrangian is

$$L(x,\lambda)=xy-\lambda(x+y-2).$$

Setting $\nabla L(\mathbf{x}, \lambda) = 0$, we get:

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial x} = y - \lambda = 0,$$

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial y} = x - \lambda = 0,$$

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial \lambda} = -x - y + 2 = 0.$$

The solution of this system of equations is

$$x^* = v^* = \lambda^* = 1.$$

According to the Theorem on necessary conditions, the point $(x^*, \lambda^*) = (1, 1, 1)$ satisfies the necessary conditions for a maximum,

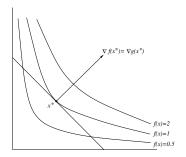
Example (cont.)

The linear dependence between ∇f and ∇g at the maxima, is clearly illustrated in the figure. In fact, in this case they concide, since

$$\nabla f(\mathbf{x}^*) = \begin{pmatrix} y \\ x \end{pmatrix}_{(x,y)=(1,1)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

and

$$abla g(\mathbf{x}^*) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}_{(\mathbf{x},\mathbf{y})=(1,1)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$



Example (cont.)

Turning to the sufficient conditions, we compute $\nabla_x^2 L(\mathbf{x}^*, \boldsymbol{\lambda}^*)$:

$$\frac{\partial^2 L(\boldsymbol{x}^*, \boldsymbol{\lambda}^*)}{\partial x \partial x} = 0, \quad \frac{\partial^2 L(\boldsymbol{x}^*, \boldsymbol{\lambda}^*)}{\partial x \partial y} = 1, \quad \frac{\partial^2 L(\boldsymbol{x}^*, \boldsymbol{\lambda}^*)}{\partial y \partial y} = 0.$$

Hence

$$\mathbf{z}^T \nabla_{\mathbf{x}}^2 L(\mathbf{x}^*, \boldsymbol{\lambda}^*) \mathbf{z} = (z_1, z_2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = 2z_1 z_2,$$

According to the last Theorem, we must determine the sign of $2z_1z_2$ for all $z \neq 0$ such that $z^T \nabla g(x^*) = 0$.

Since

$$\frac{\partial g(\mathbf{x}^*)}{\partial \mathbf{x}} = \frac{\partial g(\mathbf{x}^*)}{\partial \mathbf{y}} = 1,$$

the last condition $\mathbf{z}^T \nabla g(\mathbf{x}^*) = 0$ is equivalent to $z_1 + z_2 = 0$, from which we get

$$\mathbf{z}^T \nabla_{\mathbf{x}}^2 L(\mathbf{x}^*, \boldsymbol{\lambda}^*) \mathbf{z} = -2z_1^2 < 0.$$

Thus, (1,1) is a strict local maximum.