Optimality conditions. Lagrange function. Karush-Kuhn-Tucker conditions.

Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University

Background

$$f(x) \to \min_{x \in S}$$

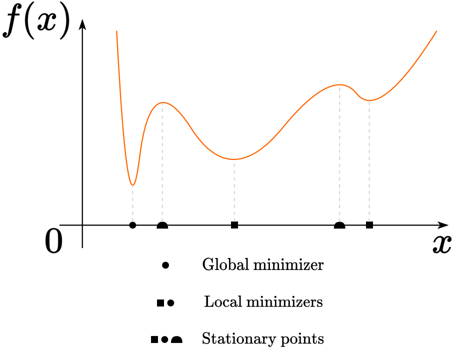

Figure 1: Illustration of different stationary (critical) points

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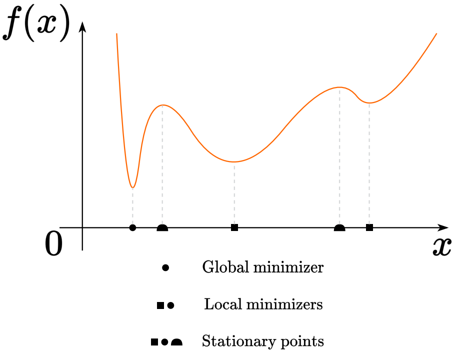

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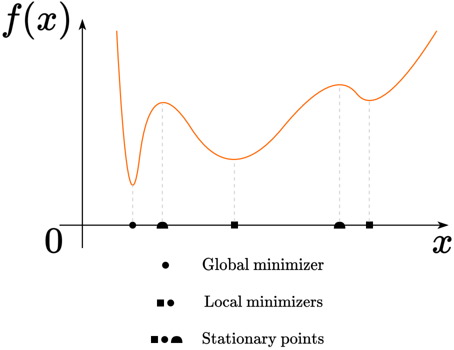

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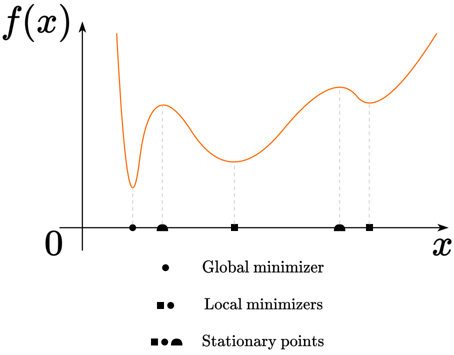

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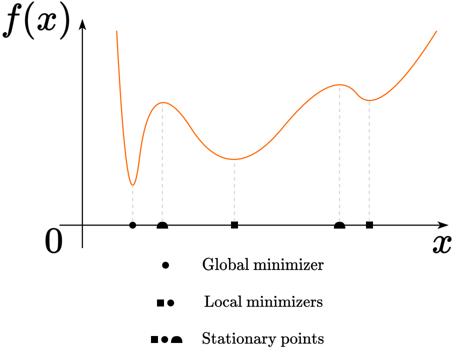

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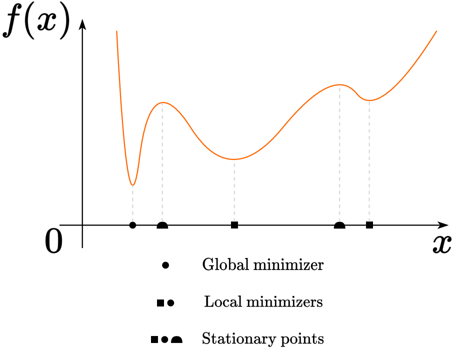

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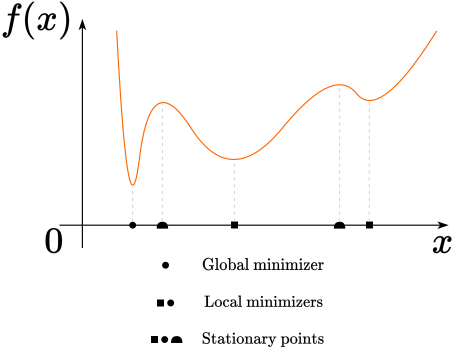

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- We call x^* a **stationary point** (or critical) if $\nabla f(x^*) = 0$. Any local minimizer of a differentiable function must be a stationary point.

Extreme value (Weierstrass) theorem

Theorem

Let $S \subset \mathbb{R}^n$ be a compact set and $f(x)$ a continuous function on S. So, the point of the global minimum of the function $f(x)$ on S exists.

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Taylor's Theorem

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and that $p \in \mathbb{R}^n$. Then we have:

$$f(x+p) = f(x) + \nabla f(x+tp)^T p \quad \text{for some } t \in (0,1)$$

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Numerical optimization
Nocedal Wright

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Moreover, if f is twice continuously differentiable, we have:

$$\nabla f(x+p) = \nabla f(x) + \int_0^1 \nabla^2 f(x+tp)p \, dt$$

$$f(x+p) = f(x) + \nabla f(x)^T p + \frac{1}{2} p^T \nabla^2 f(x+tp) p$$

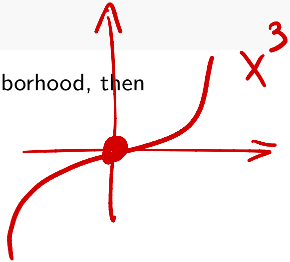
for some $t \in (0,1)$.

Necessary Conditions

First-Order Necessary Conditions

If x^* is a local minimizer and f is continuously differentiable in an open neighborhood, then

$$\nabla f(x^*) = 0$$



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For any $\bar{t} \in (0, T]$, we have by Taylor's theorem that

$$f(x^* + \bar{t}p) = f(x^*) + \bar{t}p^T \nabla f(x^* + tp), \text{ for some } t \in (0, \bar{t})$$

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Therefore, $f(x^* + \bar{t}p) < f(x^*)$ for all $\bar{t} \in (0, T]$. We have found a direction from x^* along which f decreases, so x^* is not a local minimizer, leading to a contradiction.

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Suppose that $\nabla^2 f$ is continuous in an open neighborhood of x^* and that

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where $z = x^* + tp$ for some $t \in (0, 1)$. Since $z \in B$, we have $p^T \nabla^2 f(z) p > 0$, and therefore $f(x^* + p) > f(x^*)$, giving the result.

Peano counterexample

Note, that if $\nabla f(x^*) = 0, \nabla^2 f(x^*) \succeq 0$, i.e. the hessian is positive *semidefinite*, we cannot be sure if x^* is a local minimum.

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Although the surface does not have a local minimizer at the origin, its intersection with any vertical plane through the origin (a plane with equation $y = mx$ or $x = 0$) is a curve that has a local minimum at the origin. In other words, if a point starts at the origin $(0,0)$ of the plane, and moves away from the origin along any straight line, the value of $(2x^2 - y)(x^2 - y)$ will increase at the start of the motion. Nevertheless, $(0,0)$ is not a local minimizer of the function, because moving along a parabola such as $y = \sqrt{2}x^2$ will cause the function value to decrease.

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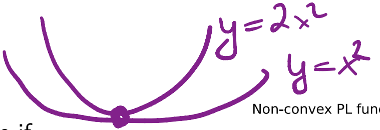

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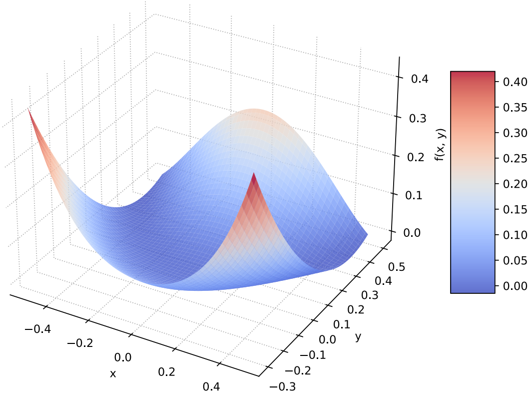
Non-convex PL function



General first-order local optimality condition

допустимое

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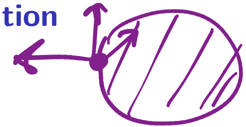

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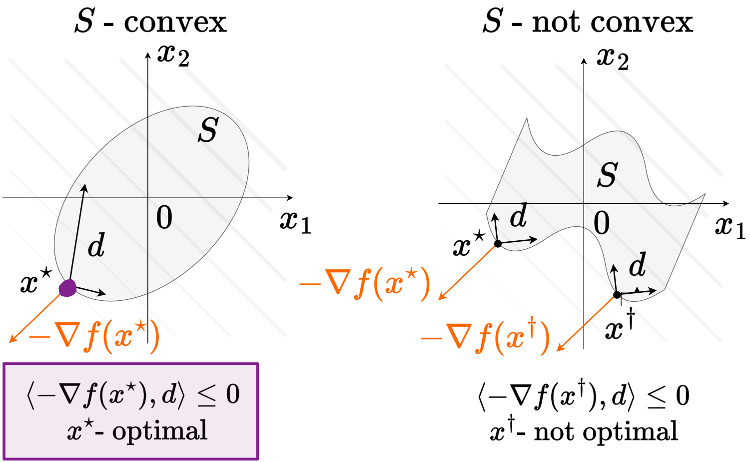

Figure 3: General first order local optimality condition

Convex case

НЕОБХ

$\nabla f = 0$

дост.

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$\nabla^2 f > 0$

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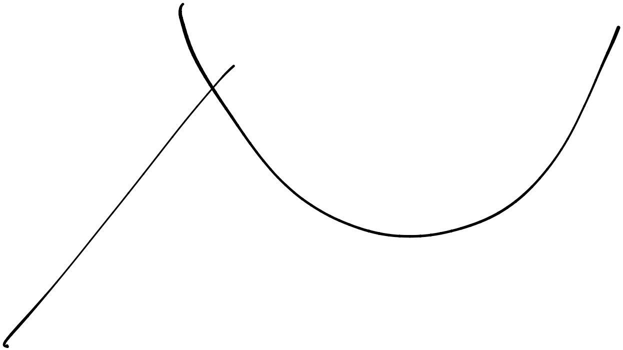

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- Any local minima is the global one.
- The set of the local minimizers S^* is convex.
- If $f(x)$ - strictly or strongly convex function, then S^* contains only one single point $S^* = \{x^*\}$.

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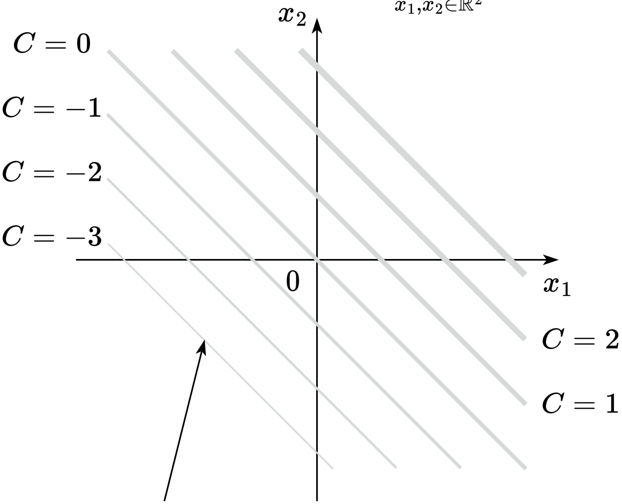
We will try to illustrate an approach to solve this problem through the simple example with $f(x) = x_1 + x_2$ and $h(x) = x_1^2 + x_2^2 - 2$.

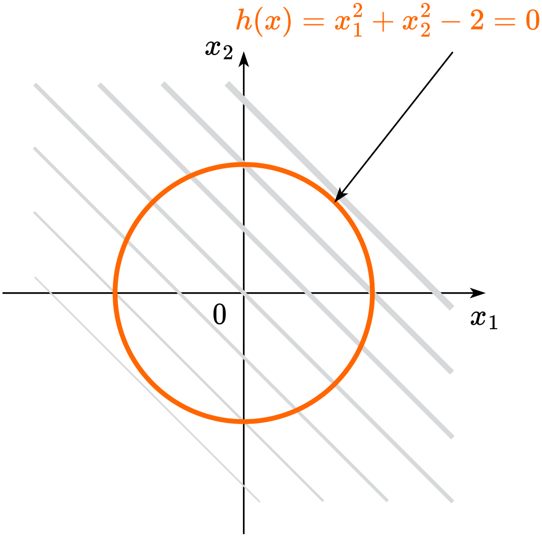
Optimization with equality constraints

$$f(x) = x_1 + x_2 \to \min_{x_1, x_2 \in \mathbb{R}^2}$$



Contour lines of $f(x) = x_1 + x_2 = C$

Optimization with equality constraints



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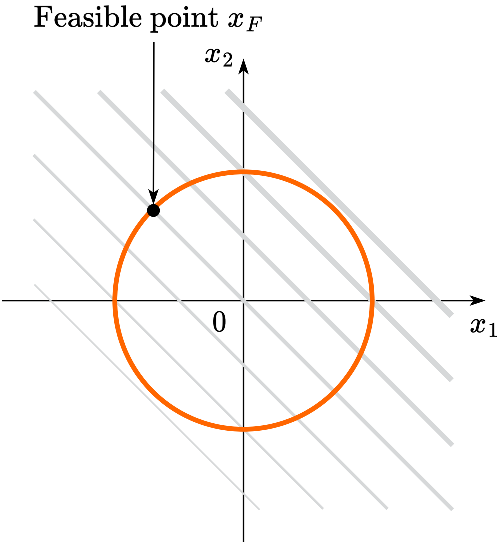

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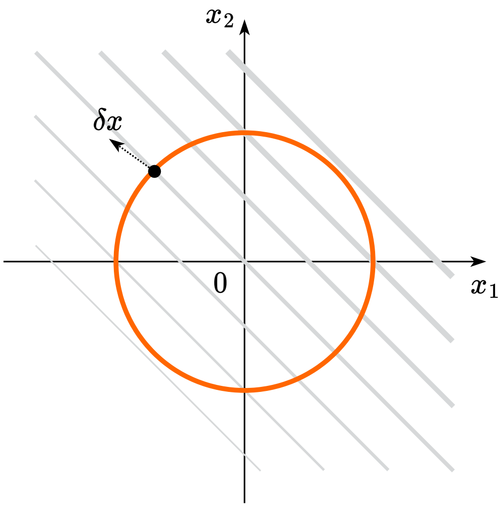

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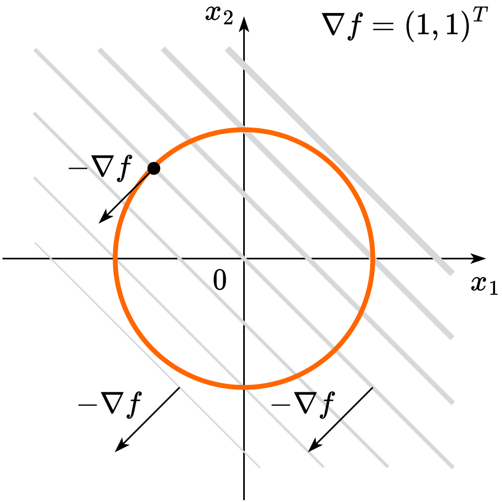

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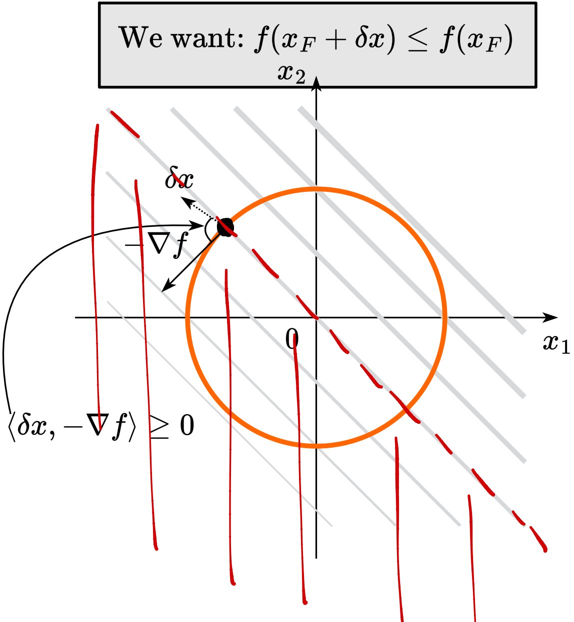
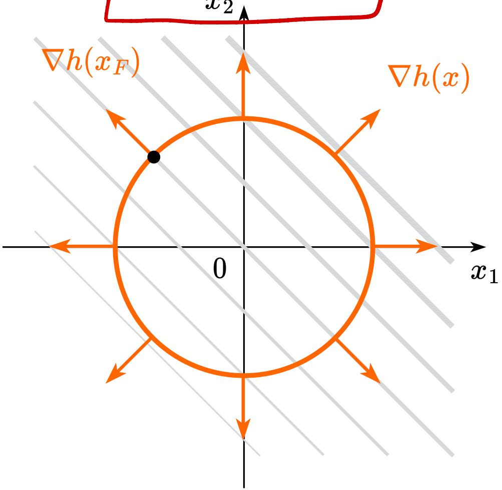


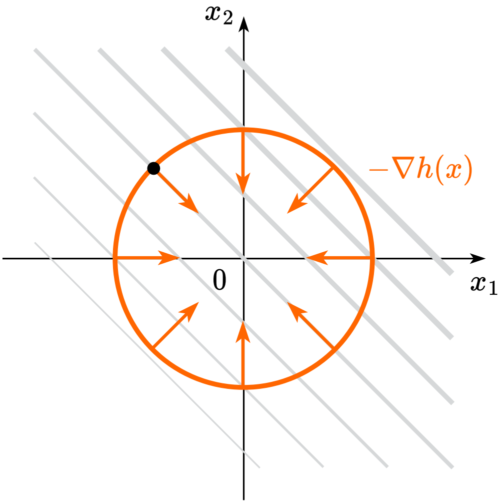
Optimization with equality constraints

$h = x_1^2 + x_2^2 - 2 = 0$

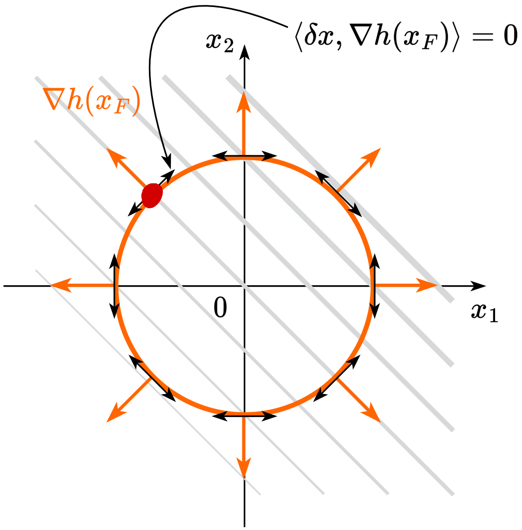
$\nabla h = (2x_1, 2x_2)^T$



Optimization with equality constraints



Optimization with equality constraints



Optimization with equality constraints

Generally: to move from x_F along the budget set toward decreasing the function, we need to guarantee two conditions:

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остаёмся в рамках S

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занимаемся min f

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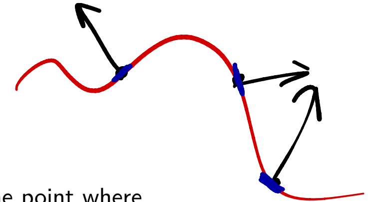

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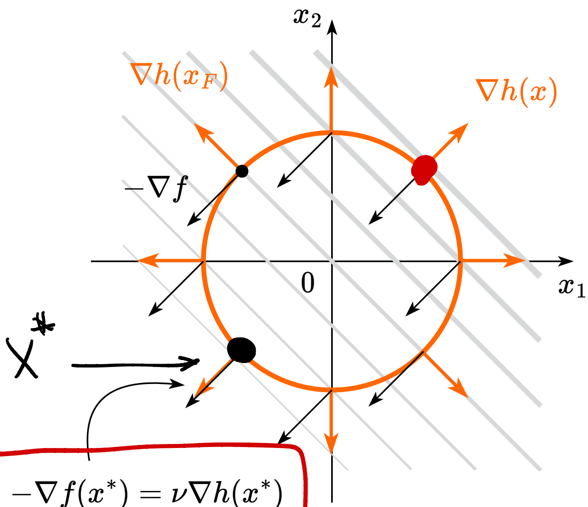
Then we came to the point of the budget set, moving from which it will not be possible to reduce our function. This is the local minimum in the constrained problem :)

Optimization with equality constraints



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Lagrangian

So let's define a Lagrange function (just for our convenience):

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We should notice that $L(x^*, \nu^*) = f(x^*)$.

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$$\nabla f(x) + \nu \cdot \nabla h(x) = 0$$

$$L(x, \nu) = f(x) + \nu h(x)$$

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$\nabla_x L(x^*, \nu^*) = 0$ that's written above

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$\min f(x)$, $h(x) = 0$ $\longrightarrow$ $\min\limits_{x,\nu} L$

$$L(x, \nu) = f(x) + \nu h(x)$$

$\nabla_\nu L = h(x) = 0$

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$\langle y, \nabla^2_{xx} L(x^*, \nu^*) y \rangle > 0,$

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Sufficient conditions

$\langle y, \nabla^2_{xx} L(x^*, \nu^*) y \rangle > 0,$

$\forall y \neq 0 \in \mathbb{R}^n : \nabla h(x^*)^\top y = 0$

We should notice that $L(x^*, \nu^*) = f(x^*)$.

Equality constrained problem

$$
\begin{aligned}
& f(x) \to \min_{x \in \mathbb{R}^n} \\
& \text{s.t. } h_i(x) = 0, \; i = 1, \ldots, p
\end{aligned}
\tag{ECP}
$$

$$
L(x, \nu) = f(x) + \sum_{i=1}^{p} \nu_i h_i(x) = f(x) + \nu^\top h(x)
$$

Let $f(x)$ and $h_i(x)$ be twice differentiable at the point x^* and continuously differentiable in some neighborhood x^*. The local minimum conditions for $x \in \mathbb{R}^n, \nu \in \mathbb{R}^p$ are written as

n мерная
с огр.

ECP: Necessary conditions

$$\nabla_x L(x^*, \nu^*) = 0$$

$$\nabla_\nu L(x^*, \nu^*) = 0$$

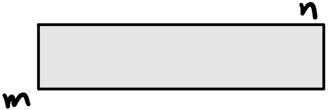
n+p
мерная

ECP: Sufficient conditions

$$\langle y, \nabla^2_{xx} L(x^*, \nu^*) y \rangle > 0,$$

$$\forall y \neq 0 \in \mathbb{R}^n : \nabla h_i(x^*)^\top y = 0$$

Linear Least Squares



$Ax = b$

$\frac{1}{2}\|x\|^2 \to \min$

$Ax = b$

задача выпуклая

Example

Pose the optimization problem and solve them for linear system $Ax = b$, $A \in \mathbb{R}^{m \times n}$ for three cases (assuming the matrix is full rank):

- $m < n$

Решение: $L(x, \nu) = \frac{1}{2}\|x\|^2 + \nu^T(Ax - b)$

$1 \times m \quad m \times 1$

$$\begin{cases} \nabla_x L = 0 \\ \nabla_\nu L = 0 \end{cases} \Rightarrow \begin{cases} x + A^T\nu = 0 \\ Ax = b \end{cases} \qquad \begin{cases} x = -A^T\nu \\ -AA^T\nu = b \end{cases} \Rightarrow \nu = -(AA^T)^{-1}b$$

$m \times m$

$$\Rightarrow \boxed{x = +A^T(AA^T)^{-1}b}$$

Linear Least Squares

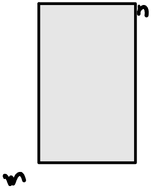
Example

Pose the optimization problem and solve them for linear system $Ax = b, A \in \mathbb{R}^{m \times n}$ for three cases (assuming the matrix is full rank):

- $m < n$
- $m = n$

$x^* = A^{-1} b$

Linear Least Squares



$$\frac{1}{2}\|Ax - b\|_2^2 \to \min_{x \in \mathbb{R}^n}$$

Example

Pose the optimization problem and solve them for linear system $Ax = b, A \in \mathbb{R}^{m \times n}$ for three cases (assuming the matrix is full rank):

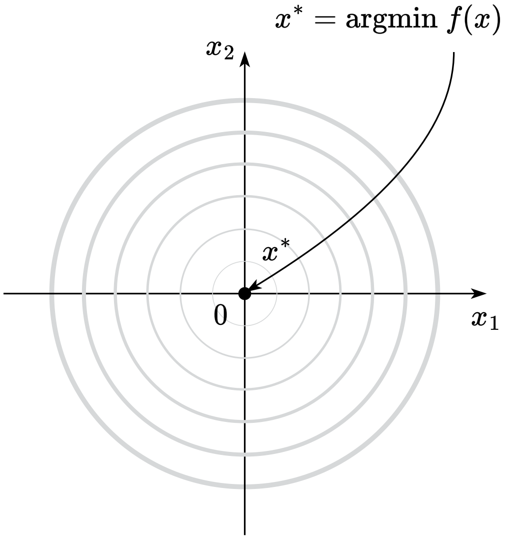
- $m < n$
- $m = n$
- $m > n$

Example of inequality constraints

$$f(x) = x_1^2 + x_2^2 \quad g(x) = x_1^2 + x_2^2 - 1$$

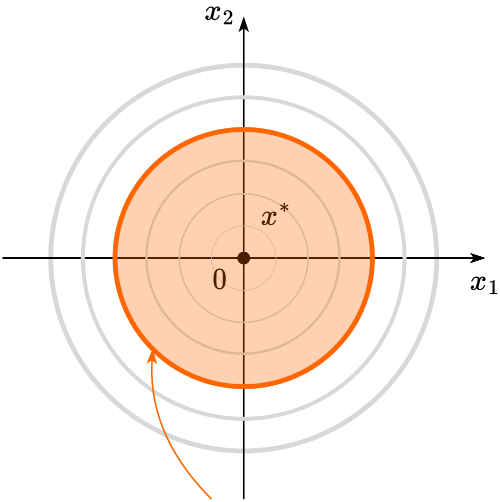
$$f(x) \to \min_{x \in \mathbb{R}^n}$$
$$\text{s.t. } g(x) \leq 0$$

Optimization with inequality constraints



Contour lines of $f(x) = x_1^2 + x_2^2 = C$

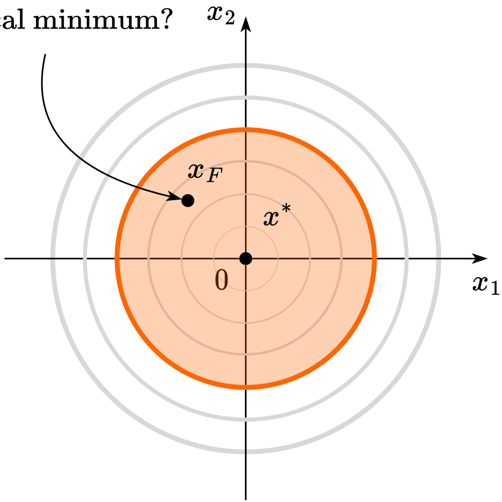
Optimization with inequality constraints



Feasible region $g(x) = x_1^2 + x_2^2 - 1 \leq 0$

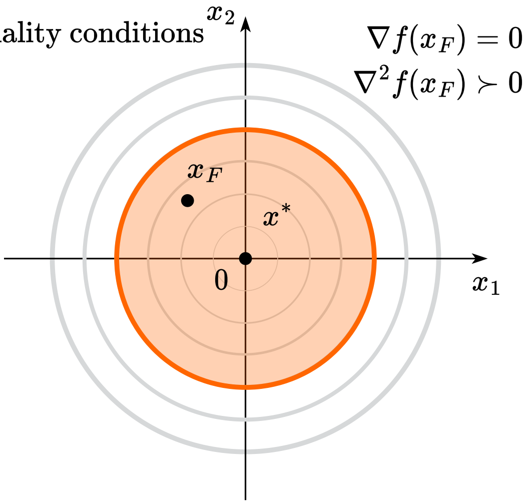
Optimization with inequality constraints

How to recognize that some feasible point is at local minimum?



Optimization with inequality constraints

Easy in this case! Just check unconstrained optimality conditions



Optimization with inequality constraints

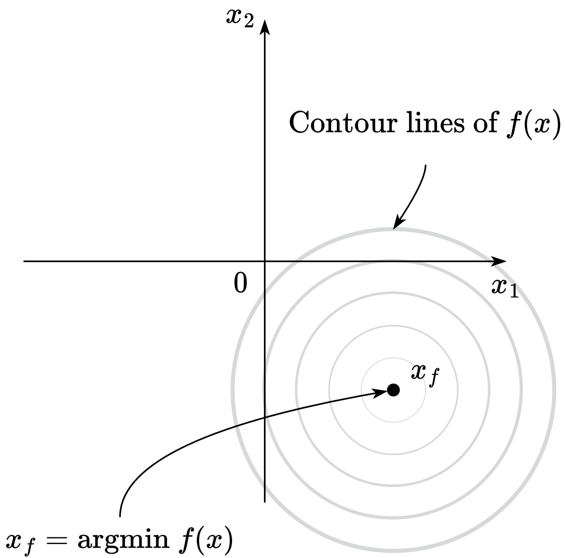
Thus, if the constraints of the type of inequalities are inactive in the constrained problem, then don't worry and write out the solution to the unconstrained problem. However, this is not the whole story. Consider the second childish example

$$f(x) = (x_1 - 1)^2 + (x_2 + 1)^2 \quad g(x) = x_1^2 + x_2^2 - 1$$

$$\begin{split} & f(x) \to \min_{x \in \mathbb{R}^n} \\ \text{s.t. } & g(x) \leq 0 \end{split}$$

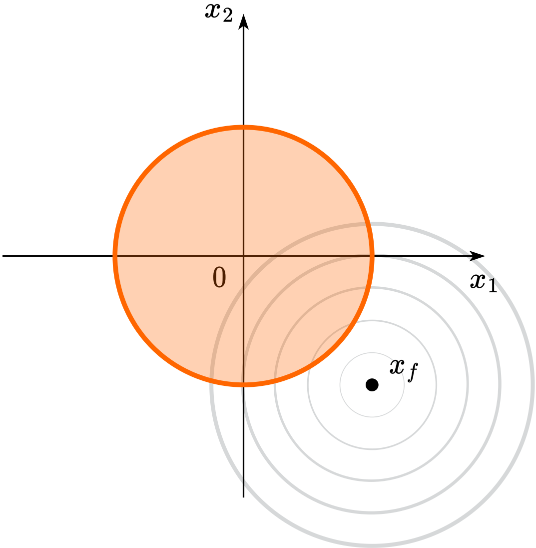
Optimization with inequality constraints

$$f(x) = (x_1 - 1)^2 + (x_2 + 1)^2 = C$$



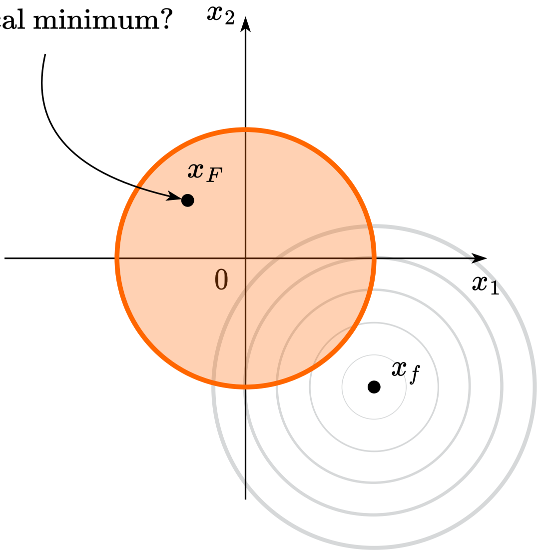
Optimization with inequality constraints

Feasible region $g(x) = x_1^2 + x_2^2 - 1 \leq 0$



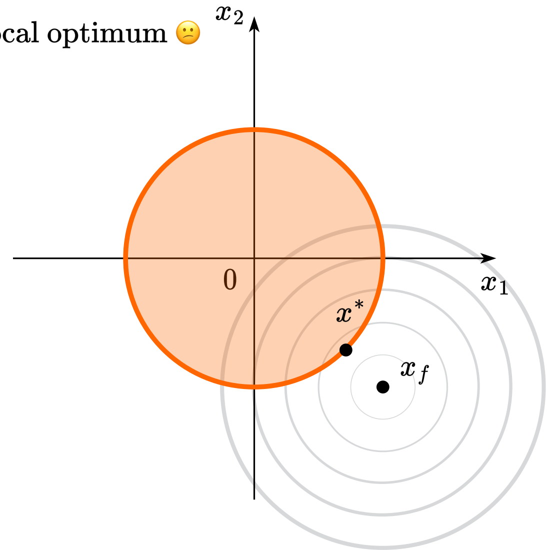
Optimization with inequality constraints

How to recognize that some feasible point is at local minimum?



Optimization with inequality constraints

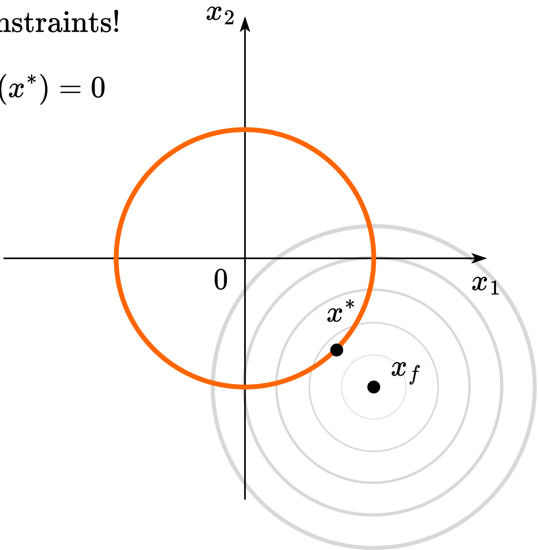
Not very easy in this case! Even gradient $\neq 0$ at local optimum 😕



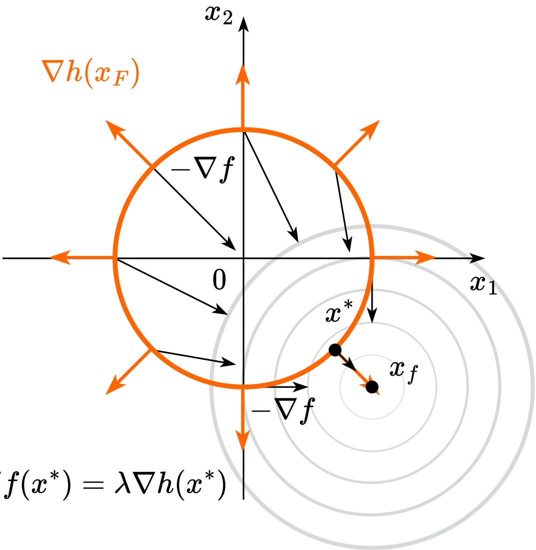
Optimization with inequality constraints

Effectively have a problem with equality constraints!

$$g(x^*) = 0$$

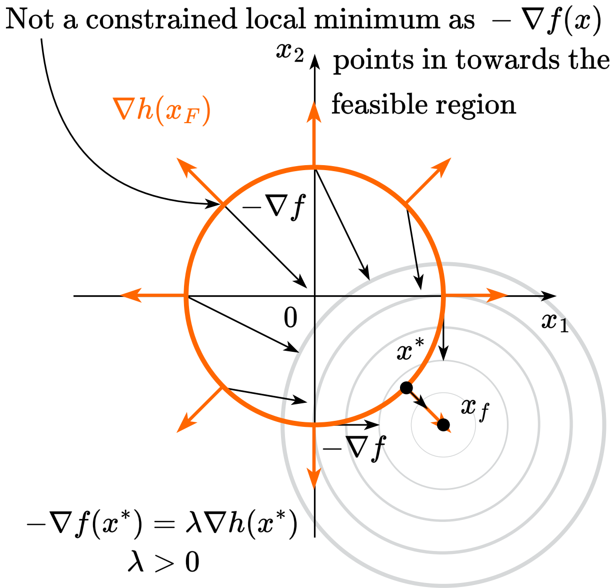


Optimization with inequality constraints



$$-\nabla f(x^*) = \lambda \nabla h(x^*)$$

Optimization with inequality constraints



$$-\nabla f(x^*) = \lambda \nabla h(x^*)$$
$$\lambda > 0$$

Optimization with inequality constraints

So, we have a problem:

$$
f(x) \to \min_{x \in \mathbb{R}^n}
$$
$$
\text{s.t. } g(x) \leq 0
$$

Two possible cases:

$g(x) \leq 0$ is inactive. $g(x^*) < 0$

- $g(x^*) < 0$

Optimization with inequality constraints

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- $\nabla f(x^*) = 0$

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- Sufficient conditions: $\langle y, \nabla^2_{xx} L(x^*, \lambda^*) y \rangle > 0, \forall y \neq 0 \in \mathbb{R}^n : \nabla g(x^*)^\top y = 0$

Lagrange function for inequality constraints

Combining two possible cases, we can write down the general conditions for the problem:

$$
\begin{aligned}
&f(x) \to \min_{x \in \mathbb{R}^n} \\
\text{s.t. } &g(x) \leq 0
\end{aligned}
$$

Let's define the Lagrange function:

$$
L(x, \lambda) = f(x) + \lambda g(x)
$$

The classical Karush-Kuhn-Tucker first and second-order optimality conditions for a local minimizer x^*, stated under some regularity conditions, can be written as follows.

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If x^* is a local minimum of the problem described above, then there exists a unique Lagrange multiplier λ^* such that:

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(1)\ \nabla_x L(x^*, \lambda^*) = 0
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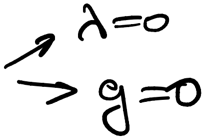

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\begin{aligned}
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&(2)\ \lambda^* \geq 0 \\
&(3)\ \lambda^* g(x^*) = 0 \\
&(4)\ g(x^*) \leq 0
\end{aligned}
$$

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$$
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(5)\ \forall y \in C(x^*) : \langle y, \nabla^2_{xx} L(x^*, \lambda^*) y \rangle > 0
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& (5) \; \forall y \in C(x^*) : \langle y, \nabla^2_{xx} L(x^*, \lambda^*) y \rangle > 0 \\
& \text{where } C(x^*) = \{y \ \in \mathbb{R}^n | \nabla f(x^*)^\top y \leq 0 \text{ and } \forall i \in I(x^*) : \nabla g_i(x^*)^T y \leq 0\}
\end{split}
$$

Lagrange function for inequality constraints

Combining two possible cases, we can write down the general conditions for the problem:

$$
f(x) \to \min_{x \in \mathbb{R}^n}
$$
$$
\text{s.t. } g(x) \leq 0
$$

Let's define the Lagrange function:

$$
L(x, \lambda) = f(x) + \lambda g(x)
$$

The classical Karush-Kuhn-Tucker first and second-order optimality conditions for a local minimizer x^*, stated under some regularity conditions, can be written as follows.

If x^* is a local minimum of the problem described above, then there exists a unique Lagrange multiplier λ^* such that:

$$
(1)\ \nabla_x L(x^*, \lambda^*) = 0
$$
$$
(2)\ \lambda^* \geq 0
$$
$$
(3)\ \lambda^* g(x^*) = 0
$$
$$
(4)\ g(x^*) \leq 0
$$
$$
(5)\ \forall y \in C(x^*) : \langle y, \nabla^2_{xx} L(x^*, \lambda^*) y \rangle > 0
$$

where $C(x^*) = \{y \ \in \mathbb{R}^n | \nabla f(x^*)^\top y \leq 0 \text{ and } \forall i \in I(x^*) : \nabla g_i(x^*)^T y \leq 0\}$

$$
I(x^*) = \{i \mid g_i(x^*) = 0\}
$$

General formulation

$$
\begin{split}
& f_0(x) \to \min_{x \in \mathbb{R}^n} \\
\text{s.t. } & f_i(x) \leq 0, \; i = 1, \ldots, m \\
& h_i(x) = 0, \; i = 1, \ldots, p
\end{split}
$$

This formulation is a general problem of mathematical programming.

The solution involves constructing a Lagrange function:

$$
L(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^m \lambda_i f_i(x) + \sum_{i=1}^p \nu_i h_i(x)
$$

Necessary conditions

Let x^*, (λ^*, ν^*) be a solution to a mathematical programming problem with zero duality gap (the optimal value for the primal problem p^* is equal to the optimal value for the dual problem d^*). Let also the functions f_0, f_i, h_i be differentiable.

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Some regularity conditions

These conditions are needed to make KKT solutions the necessary conditions. Some of them even turn necessary conditions into sufficient (for example, Slater's). Moreover, if you have regularity, you can write down necessary second order conditions $\langle y, \nabla^2_{xx} L(x^*, \lambda^*, \nu^*) y \rangle \geq 0$ with *semi-definite* hessian of Lagrangian.

- **Slater's condition.** If for a convex problem (i.e., assuming minimization, f_0, f_i are convex and h_i are affine), there exists a point x such that $h(x) = 0$ and $f_i(x) < 0$ (existence of a strictly feasible point), then we have a zero duality gap and KKT conditions become necessary and sufficient.

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- For other examples, see wiki.

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$$\min \frac{1}{2}\|\mathbf{x} - \mathbf{y}\|^2, \quad \text{s.t.} \quad \mathbf{a}^T\mathbf{x} = b.$$

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Solve the above conditions in $O(n \log n)$ time.

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- Numerical Optimization by Jorge Nocedal and Stephen J. Wright.