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

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> The reader will find no ~~figures~~ PROOFS in this work. The methods which I set forth do not require either constructions or geometrical or mechanical reasonings: but only algebraic operations, subject to a regular and uniform rule of procedure.

Preface to Mécanique analytique

Figure 1: Joseph-Louis Lagrange

$$\min_{x \in S} f_0(x)$$

Optimality conditions

$S = \mathbb{R}^n$ — безусловная оптимизация

$$S = \left\{ x \in \mathbb{R}^n : \begin{array}{ll} f_i(x) \leq 0, & i \in [1, m] \\ g_j(x) = 0, & j \in [m+1, k] \end{array} \right\}$$

Background

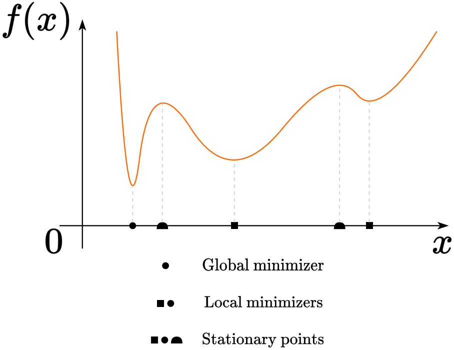

Figure 2: Illustration of different stationary (critical) points

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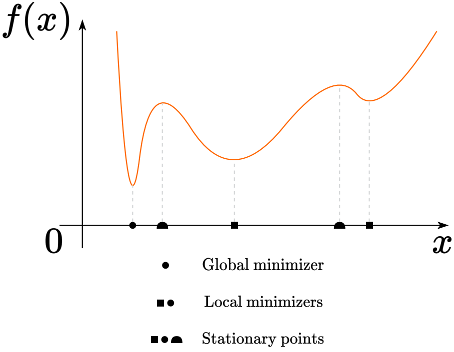

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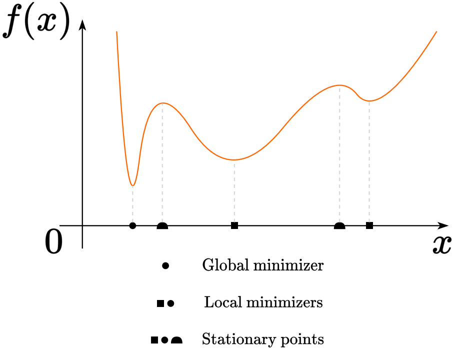

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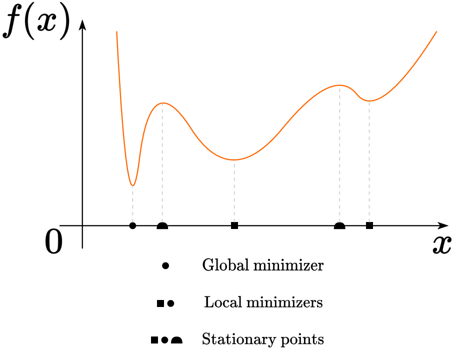

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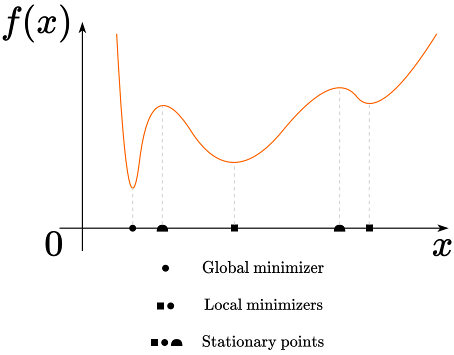

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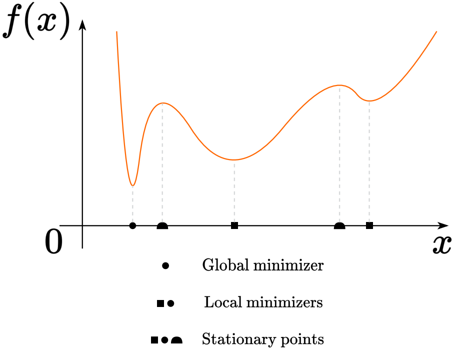

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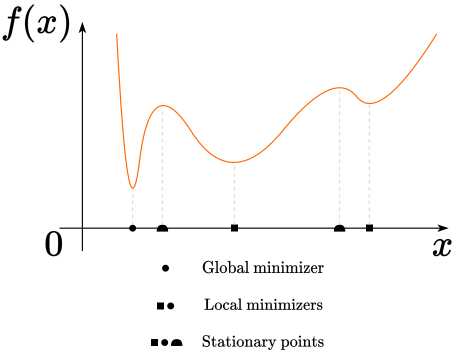

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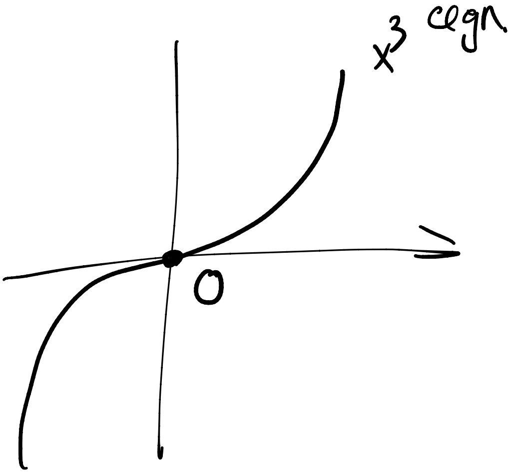
- We call x^* a **stationary point** (or critical) if $\nabla f(x^*) = 0$. Any local minimizer of a differentiable function must be a stationary point.

Extreme value (Weierstrass) theorem



> **Theorem**
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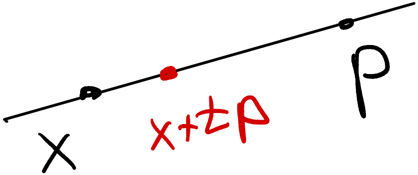
Taylor's Theorem

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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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 $t \in (0,1)$.

Unconstrained optimization

Necessary Conditions

First-Order Necessary Conditions

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

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Если x^* min

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

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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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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.

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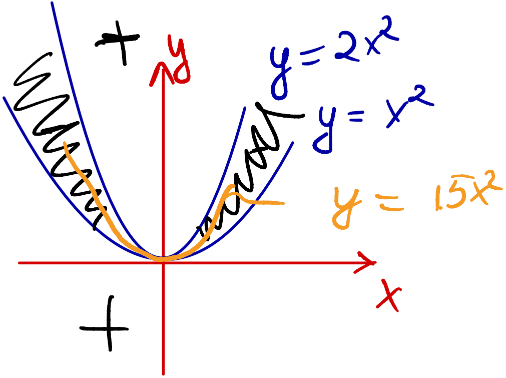

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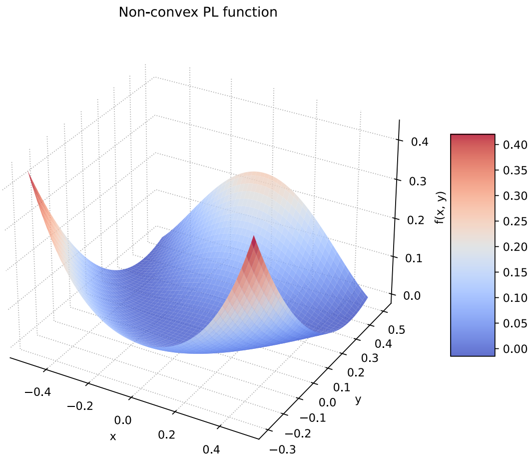

Constrained optimization

General first-order local optimality condition

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

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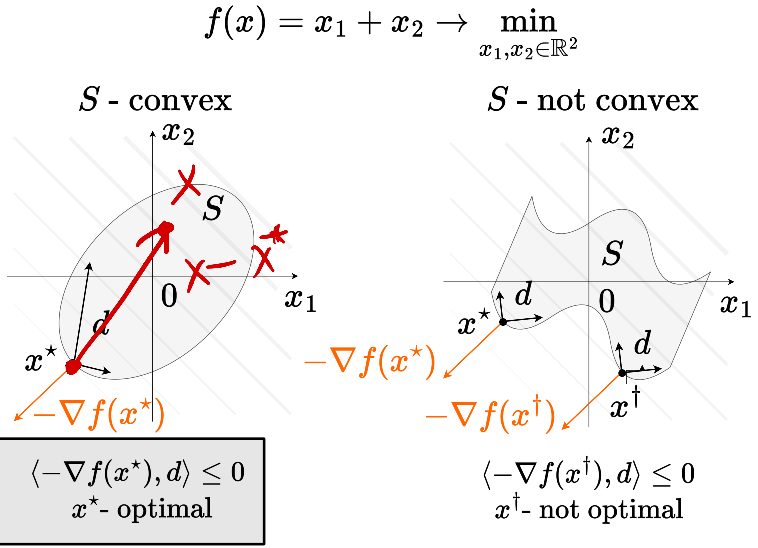

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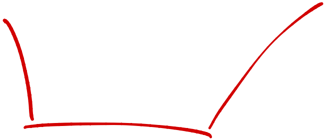

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- The set of the local minimizers S^* is convex.
- If $f(x)$ - strictly or strongly convex function, then S^* contains only one single point $S^* = \{x^*\}$.

Optimization with equality constraints

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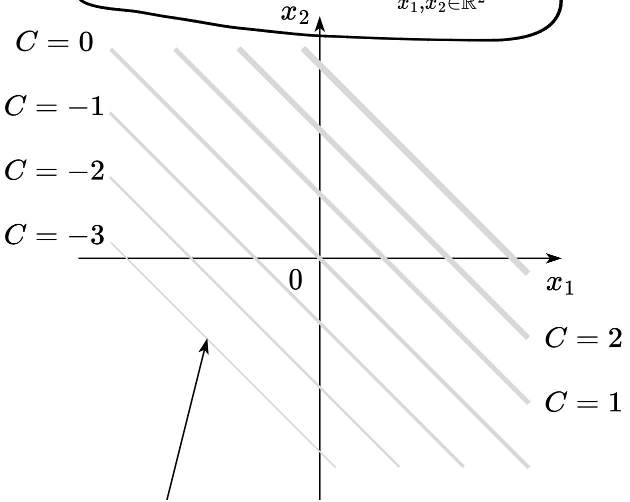
We will try to illustrate an approach to solve this problem through the simple example with $f(x) = x_1 + x_2$ and $h(x) = x_1^2 + x_2^2 - 2$.

Optimization with equality constraints

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



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

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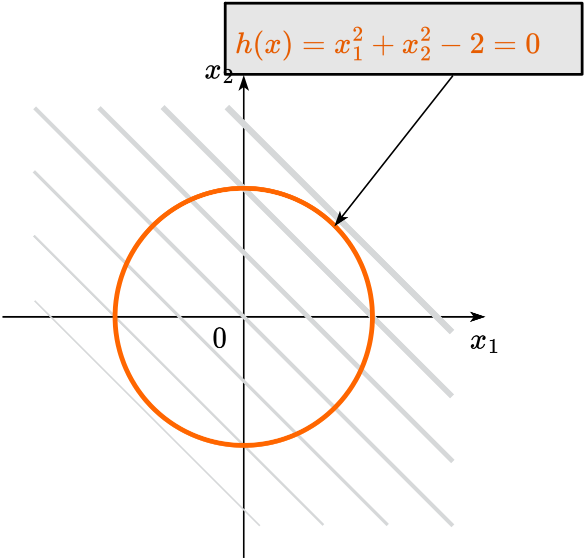

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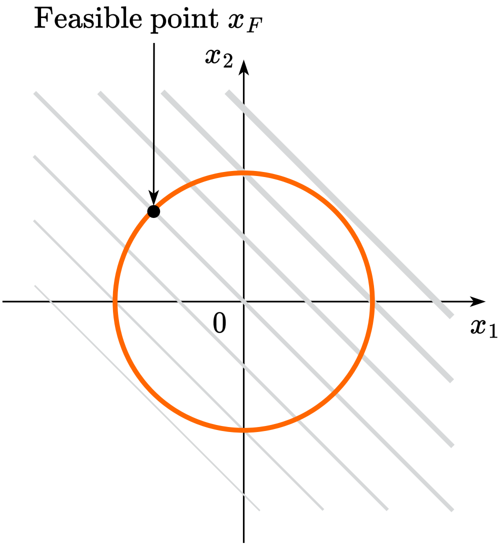

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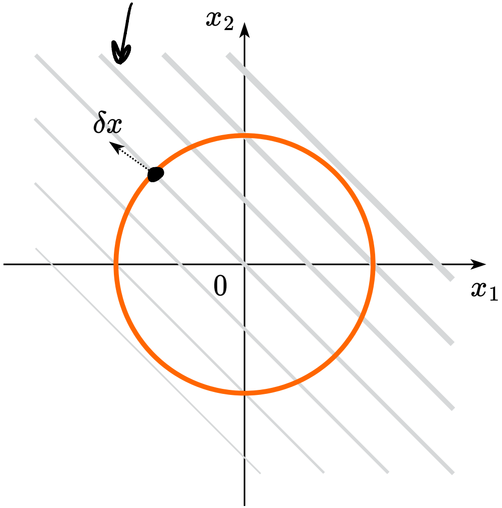
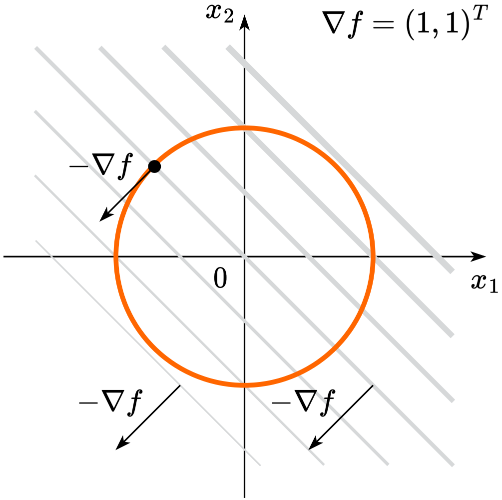


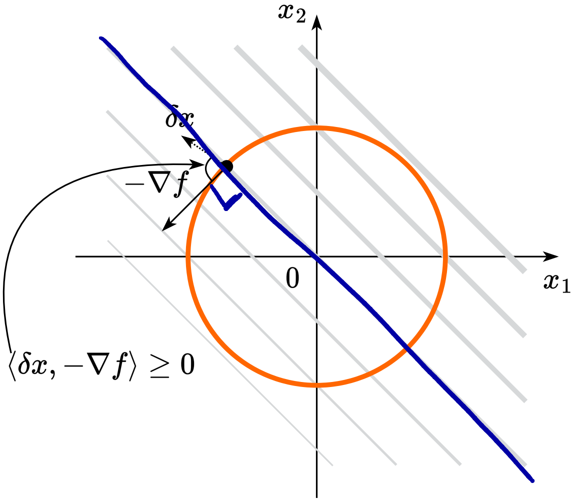
Optimization with equality constraints

$f(x_1, x_2) = x_1 + x_2 \Rightarrow \nabla f = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

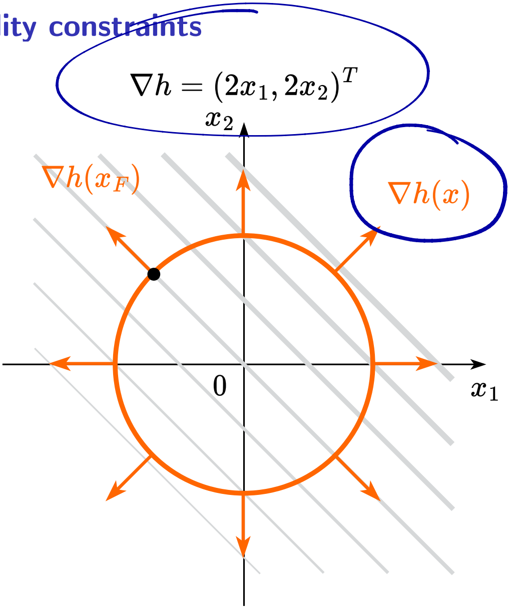


Optimization with equality constraints

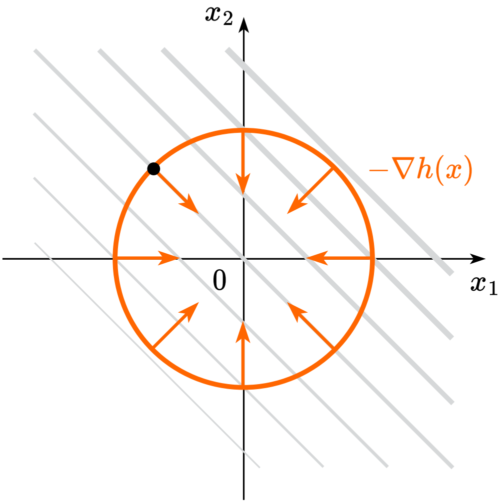
We want: $f(x_F + \delta x) \leq f(x_F)$



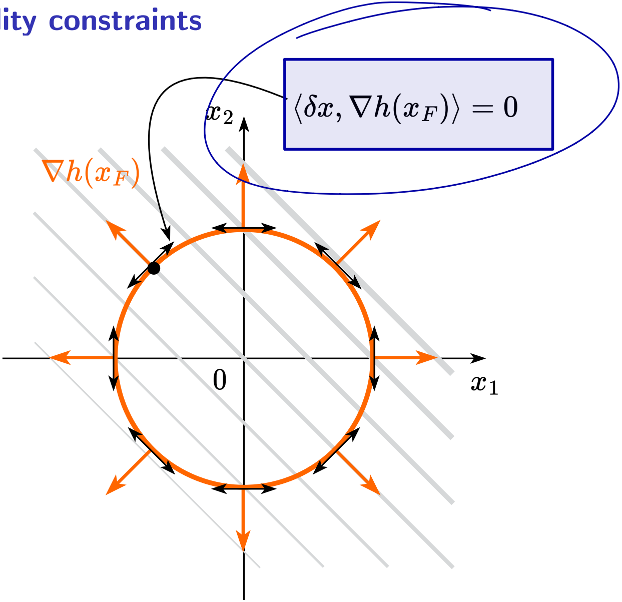
Optimization with equality constraints



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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$$\langle \delta x, \nabla h(x_F) \rangle = 0$$

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$$\langle \delta x, \nabla h(x_F) \rangle = 0$$ допустимость

$$\langle \delta x, -\nabla f(x_F) \rangle > 0$$ „оптимальность"

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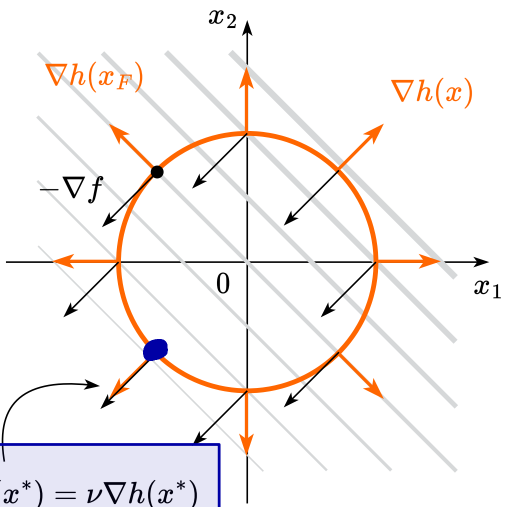
Then we reached the point of the budget set, moving from which it will not be possible to reduce our function. This is the local minimum in the constrained problem :)

Optimization with equality constraints



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

Lagrangian

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

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

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

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Necessary conditions

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

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

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

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$\nabla_\nu L(x^*, \nu^*) = 0$ budget constraint ← $h(x) = 0$

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Sufficient conditions

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

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

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

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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 of x^*. The local minimum conditions for $x \in \mathbb{R}^n, \nu \in \mathbb{R}^p$ are written as

ECP: Necessary conditions

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

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

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

$$Ax = b$$

$$x + y = 0$$

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

m ур-ий

$$a_i^T x - b_i = 0$$

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):

- $m < n$

$\underset{m\times n}{A}\underset{n\times m}{A^T}$

$\nu \in \mathbb{R}^m$ – множители Лагранжа

Решение:

1) $L(x, \nu) = \frac{1}{2}\|x\|_2^2 + \nu^T(Ax - b) =$

$$\nabla_x L = x + A^T\nu = 0 \Rightarrow x = -A^T\nu$$

$$\nabla_\nu L = Ax - b = 0 \Rightarrow A(-A^T\nu) = b$$

$$\nu = -(AA^T)^{-1} b$$

$$x^* = A^T(AA^T)^{-1} b$$

$A^+ b$

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):

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

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):

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

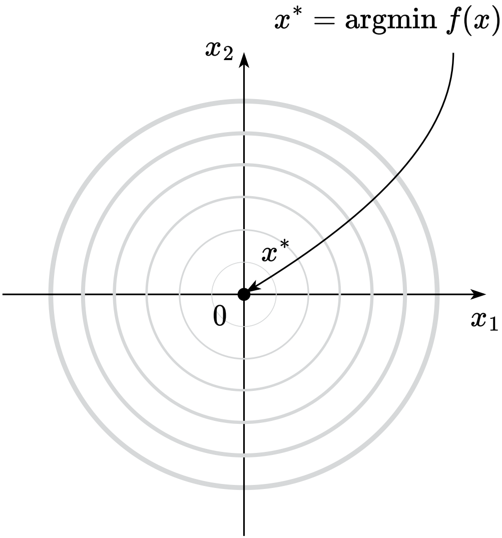
Optimization with inequality constraints

Example of inequality constraints

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

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

Optimization with inequality constraints



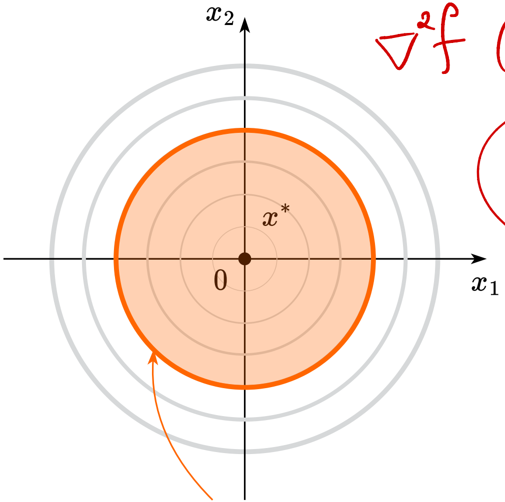
Contour lines of $f(x) = x_1^2 + x_2^2 = C$

Optimization with inequality constraints

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

$$\nabla^2 f(x^*) \succ 0$$

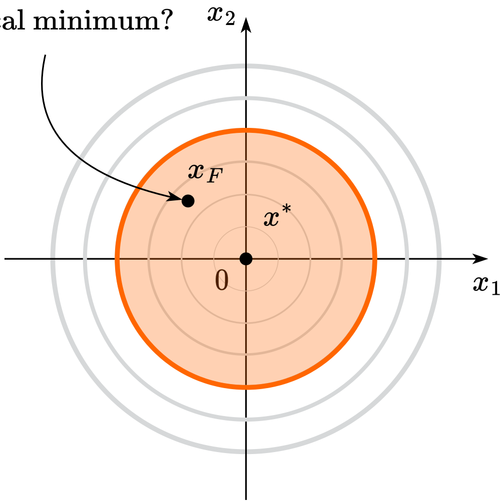
$$g(x^*) \leq 0$$



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

Optimization with inequality constraints

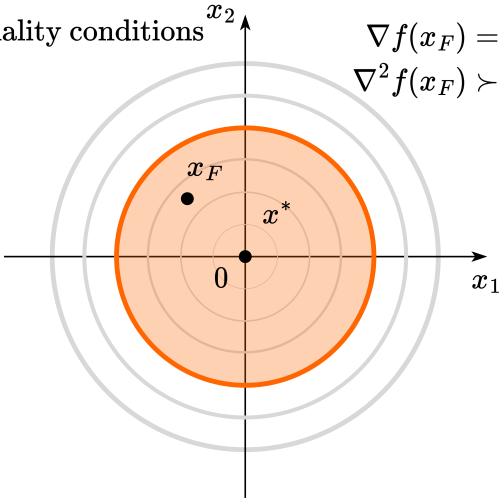
How to recognize that some feasible point is at local minimum?



Optimization with inequality constraints

Easy in this case! Just check unconstrained optimality conditions

$$\nabla f(x_F) = 0$$
$$\nabla^2 f(x_F) \succ 0$$



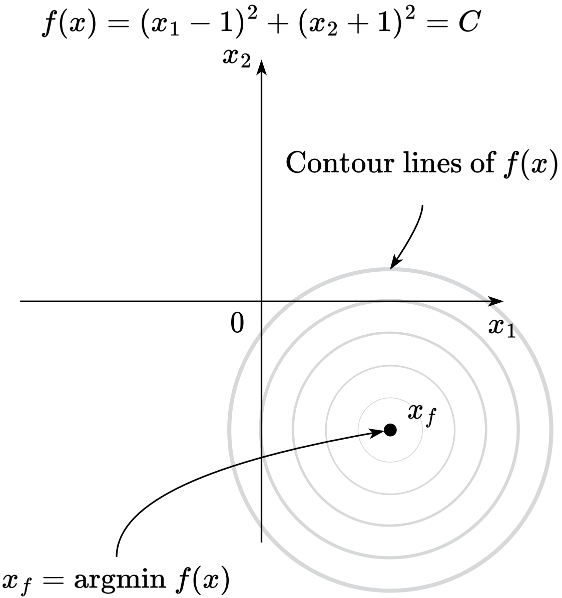
Optimization with inequality constraints

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

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

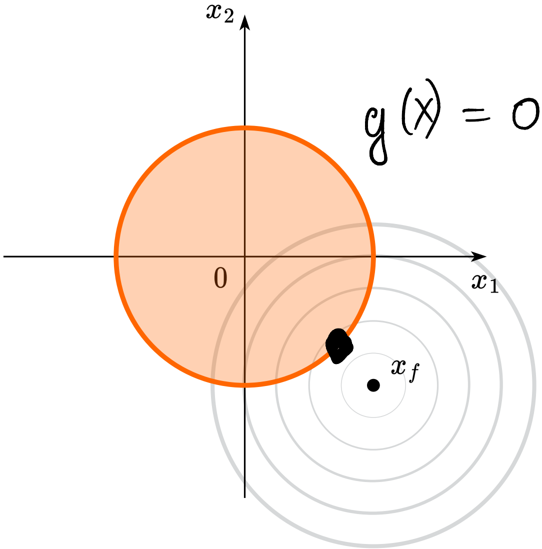
$$f(x) \to \min_{x \in \mathbb{R}^n}$$
$$\text{s.t. } g(x) \leq 0$$

Optimization with inequality constraints



Optimization with inequality constraints

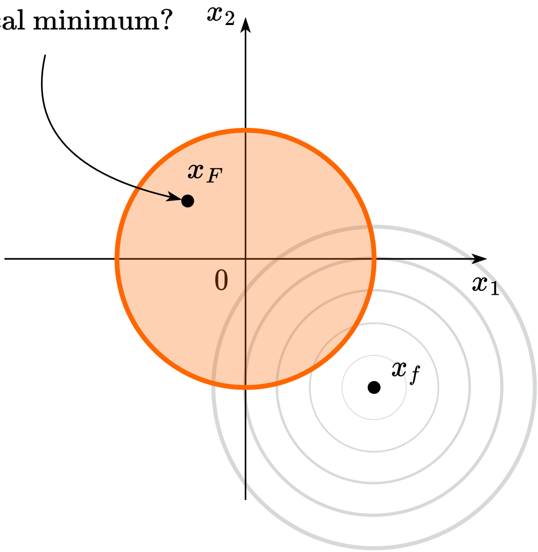
Feasible region $g(x) = x_1^2 + x_2^2 - 1 \leq 0$



$g(x) = 0$ - граница мн-ва $g(x) \leq 0$

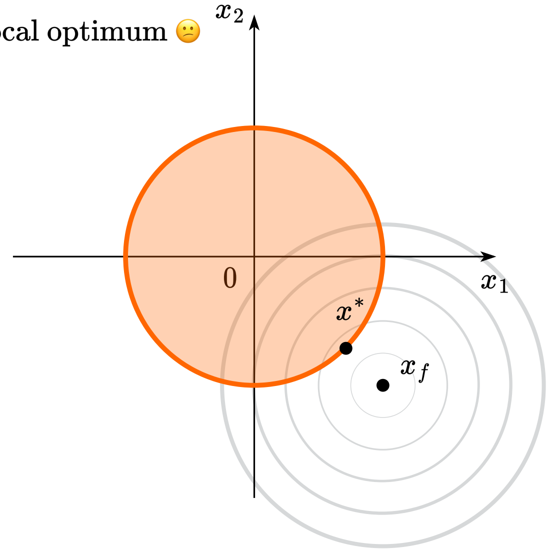
Optimization with inequality constraints

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



Optimization with inequality constraints

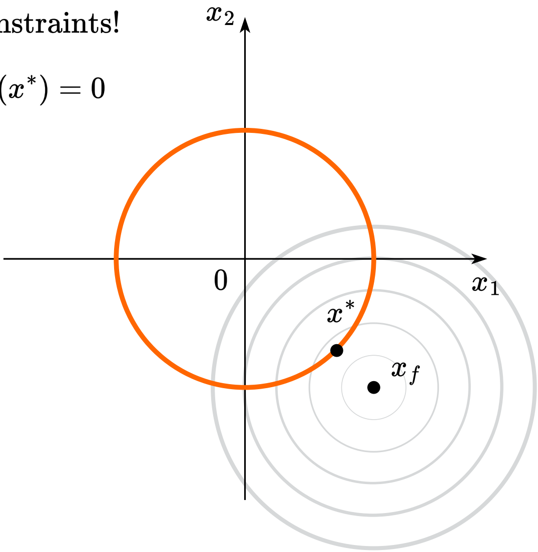
Not very easy in this case! Even gradient $\neq 0$ at local optimum 😕



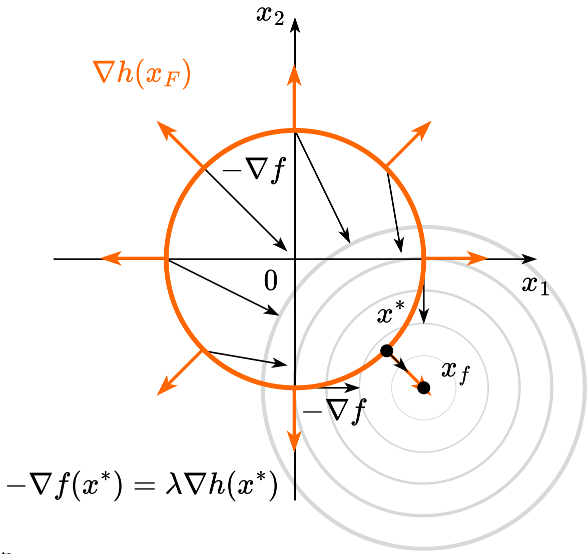
Optimization with inequality constraints

Effectively have a problem with equality constraints!

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



Optimization with inequality constraints



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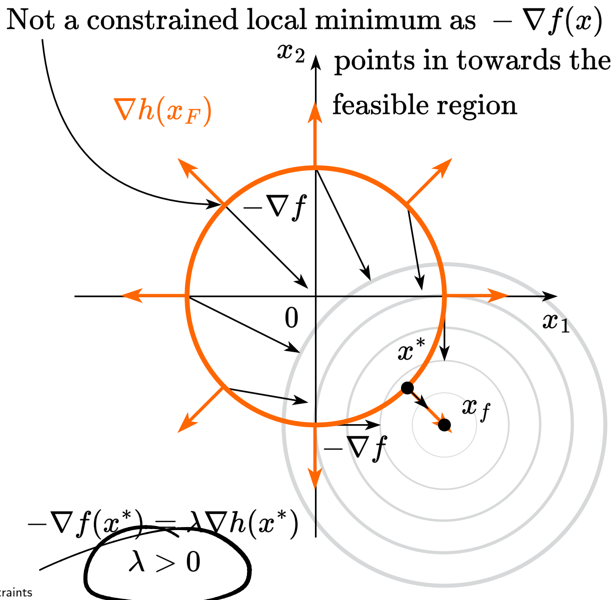

Optimization with inequality constraints

So, we have a problem:

неАктивно

$$f(x) \to \min_{x \in \mathbb{R}^n}$$

$$\text{s.t. } g(x) \leq 0$$

Two possible cases:

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

- $g(x^*) < 0$

Optimization with inequality constraints

So, we have a problem:

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f(x) \to \min_{x \in \mathbb{R}^n}
$$

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

Optimization with inequality constraints

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АКТИВНО

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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:

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

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.

Lagrange function for inequality constraints

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

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f(x) &\to \min_{x \in \mathbb{R}^n} \\
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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:

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

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

Lagrange function for inequality constraints

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

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& (1) \; \nabla_x L(x^*, \lambda^*) = 0 \\
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\begin{split}
& (1) \; \nabla_x L (x^*, \lambda^*) = 0 \\
& (2) \; \lambda^* \geq 0 \\
& (3) \; \lambda^* g(x^*) = 0
\end{split}
$$

Lagrange function for inequality constraints

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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:

$$
\begin{cases}
(1)\ \nabla_x L(x^*, \lambda^*) = 0 \\
(2)\ \lambda^* \geq 0 \\
(3)\ \lambda^* g(x^*) = 0 \\
(4)\ g(x^*) \leq 0
\end{cases}
$$

General formulation

задача мат. программиров.

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

мн-тели

↓ Лагранжа

λ_i, ν_i нто

This formulation is a general problem of mathematical programming.

The solution involves constructing a Lagrange function:

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

μ_i нто

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.

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

Necessary conditions

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- $\nabla_x L(x^*, \lambda^*, \nu^*) = 0$
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- $\nabla_x L(x^*, \lambda^*, \nu^*) = 0$
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- $\lambda^*_i \geq 0, i = 1, \ldots, m$

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.

- $\nabla_x L(x^*, \lambda^*, \nu^*) = 0$
- $\nabla_\nu L(x^*, \lambda^*, \nu^*) = 0$
- $\lambda_i^* \geq 0, i = 1, \ldots, m$
- $\lambda_i^* f_i(x^*) = 0, i = 1, \ldots, m$

Necessary conditions

для задачи с условиями регулярности

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.

- $\nabla_x L(x^*, \lambda^*, \nu^*) = 0$
- $\nabla_\nu L(x^*, \lambda^*, \nu^*) = 0$
- $\lambda^*_i \geq 0, i = 1, \dots, m$
- $\lambda^*_i f_i(x^*) = 0, i = 1, \dots, m$
- $f_i(x^*) \leq 0, i = 1, \dots, m$

KKT

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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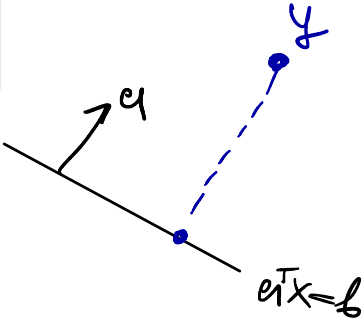
- For other examples, see wiki.

Example. Projection onto a hyperplane

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



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Derivative of L with respect to $\mathbf{x}$:

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\frac{\partial L}{\partial \mathbf{x}} = \mathbf{x} - \mathbf{y} + \nu\mathbf{a} = 0, \qquad \mathbf{x} = \mathbf{y} - \nu\mathbf{a}
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$$
a^T x = a^T y - \nu a^T a
$$

$$
\frac{\partial L}{\partial \nu} = 0 \Rightarrow a^T x = b
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$$
\min \frac{1}{2}\|x-y\|^2, \quad \text{s.t.} \quad x^\top 1 = 1, \quad x \geq 0.
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$$
f(A) = P\left(-\left(\frac{\|A^\top A x\|_2}{\|Ax\|_2} + \|Ax\|_2\right) \leq \|A\|_2\right)
$$

$x \sim \mathcal{N}(0, I)$

$= f(z_2 \ldots z_k)$ при фикс. z_1

f - симм. по z_i

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The Lagrangian is given by:

$$L = \frac{1}{2}\|x-y\|^2 - \sum_i \lambda_i x_i + \nu(x^\top 1 - 1)$$

$$\sqrt{\frac{\sum y_i^2 z_i^4}{\sum y_i^2 z_i^2}} + \sqrt{\sum y_i^2 z_i^2}$$

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Question

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

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