Optimality conditions. Optimization with equality / inequality conditions. KKT.

Seminar

Optimization for ML. Faculty of Computer Science. HSE University

Optimality Conditions. Important notions recap

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

A set S is usually called a budget set.

- A point x^* is a global minimizer if $f(x^*) \leq f(x)$ for all x.
- A point x^* is a local minimizer if there exists a neighborhood N of x^* such that $f(x^*) \leq f(x)$ for all $x \in N$.
- A point x^* is a strict local minimizer (also called a strong local minimizer) if there exists a neighborhood N of x^* such that $f(x^*) < f(x)$ for all $x \in N$ with $x \neq x^*$.
- We call x^* a stationary point (or critical) if $\nabla f(x^*) = 0$. Any local minimizer must be a stationary point.

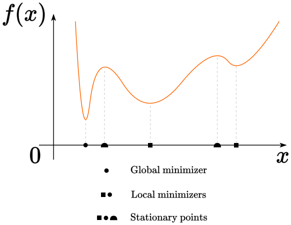

Figure 1: Illustration of different stationary (critical) points

Unconstrained optimization recap

First-Order Necessary Conditions

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

$$\nabla f(x^*) = 0 \tag{1}$$

Second-Order Sufficient Conditions

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

$$\nabla f(x^*) = 0 \quad \nabla^2 f(x^*) \succ 0. \tag{2}$$

Then x^* is a strict local minimizer of f.

Optimization with equality conditions

Consider simple yet practical case of equality constraints:

$$
\begin{split}
& f(x) \to \min\limits_{x \in \mathbb{R}^n} \\
\text{s.t. } & h_i(x) = 0, i = 1, \ldots, p
\end{split}
$$

Lagrange multipliers recap

The basic idea of Lagrange method implies the switch from conditional to unconditional optimization through increasing the dimensionality of the problem:

$$L(x, \nu) = f(x) + \sum_{i=1}^{p} \nu_i h_i(x) = f(x) + \nu^T h(x) \to \min_{x \in \mathbb{R}^n, \nu \in \mathbb{R}^p}$$

Lagrange multipliers recap

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Necessery conditions:

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

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

Sufficient conditions:

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

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

Optimization with inequality conditions

Consider simple yet practical case of inequality constraints:

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

Optimization with inequality conditions

Consider simple yet practical case of inequality constraints:

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

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

$$
g(x^*) < 0
$$
$$
\nabla f(x^*) = 0
$$
$$
\nabla^2 f(x^*) > 0
$$

$g(x) \leq 0$ **is active**. $g(x^*) = 0$:

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

General formulation

General problem of mathematical programming:

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

General formulation

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\text{s.t. } & f_i(x) \leq 0, \; i = 1, \ldots, m \\
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\end{aligned}
$$

The solution involves constructing a Lagrange function:

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

KKT 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.

KKT Necessary conditions

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$$
\begin{aligned}
&(1) \nabla_x L(x^*, \lambda^*, \nu^*) = 0 \\
&(2) \nabla_\nu L(x^*, \lambda^*, \nu^*) = 0 \\
&(3) \lambda_i^* \geq 0, i = 1, \ldots, m \\
&(4) \lambda_i^* f_i(x^*) = 0, i = 1, \ldots, m \\
&(5) f_i(x^*) \leq 0, i = 1, \ldots, m
\end{aligned}
$$

KKT Some regularity conditions

These conditions are needed in order to make KKT solutions the necessary conditions. Some of them even turn necessary conditions into sufficient. For example, Slater's condition:

KKT Some regularity conditions

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> 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 $f_i(x) < 0$ (existance of a strictly feasible point), then we have a zero duality gap and KKT conditions become necessary and sufficient.

KKT Sufficient conditions

For smooth, non-linear optimization problems, a second order sufficient condition is given as follows. The solution x^*, λ^*, ν^*, which satisfies the KKT conditions (above) is a constrained local minimum if for the Lagrangian,

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

the following conditions hold:

$$\begin{aligned}
&\langle y, \nabla^2_{xx} L(x^*, \lambda^*, \nu^*) y \rangle > 0 \\
&\forall y \neq 0 \in \mathbb{R}^n : \nabla h_i(x^*)^\top y = 0, \nabla f_0(x^*)^\top y \leq 0, \nabla f_j(x^*)^\top y = 0 \\
&i = 1, \ldots, p \quad \forall j : f_j(x^*) = 0
\end{aligned}$$

Problem 1

Question

Function $f : E \to \mathbb{R}$ is defined as

$$f(x) = \ln\left(-Q(x)\right)$$

where $E = \{x \in \mathbb{R}^n : Q(x) < 0\}$ and

$$Q(x) = \frac{1}{2}x^\top Ax + b^\top x + c$$

with $A \in \mathbb{S}^n_{++}$, $b \in \mathbb{R}^n$, $c \in \mathbb{R}$.
Find the maximizer x^* of the function f.

Problem 2

Question

Give an explicit solution of the following task.

$$
\begin{aligned}
f(x, y) = x + y &\to \min \\
\text{s.t. } x^2 + y^2 &= 1
\end{aligned}
$$

where $x, y \in \mathbb{R}$.

Problem 3

Question

Give an explicit solution of the following task.

$$
\begin{aligned}
&\langle c, x \rangle + \sum_{i=1}^n x_i \log x_i \to \min_{x \in \mathbb{R}^n} \\
\text{s.t. } &\sum_{i=1}^n x_i = 1,
\end{aligned}
$$

where $x \in \mathbb{R}^n_{++}, c \neq 0$.

Problem 4

Question

Let $A \in \mathbb{S}^n_{++}, b > 0$ show that:

$$\det(X) \to \max_{X \in \mathbb{S}^n_{++}} \text{s.t.} \langle A, X \rangle \leq b$$

Has a unique solution and find it.

Problem 5

Question

Given $y \in \{-1, 1\}$, and $X \in \mathbb{R}^{n \times p}$, the Support Vector Machine problem is:

$$
\begin{aligned}
& \frac{1}{2}||w||_2^2 + C\sum_{i=1}^{n} \xi_i \to \min_{w, w_0, \xi_i} \\
\text{s.t. } & \xi_i \geq 0, i = 1, \ldots, n \\
& y_i(x_i^T w + w_0) \geq 1 - \xi_i, i = 1, \ldots, n
\end{aligned}
$$

find the KKT stationarity condition.

Problem 6

Question

Show that the following constrained optimization task has unique solution and find it.

$$\langle C^{-1}, X\rangle - \log\det(X) \to \min_{X \in \mathbb{S}^n_{++}} \text{ s.t. } a^T X a \leq 1$$

$C \in \mathbb{S}^n_{++}, a \neq 0$
You should avoid explicit inverse of matrix C in the answer.

Problem 7 (BONUS)

For some $\Sigma, \Sigma_0 \in \mathbb{S}^n_{++}$ define a KL Divergence between two Gaussian distributions as:

$$D(\Sigma, \Sigma_0) = \frac{1}{2}(\langle \Sigma_0^{-1}, \Sigma \rangle - \log \det(\Sigma_0^{-1}\Sigma) - n)$$

Now let $H \in \mathbb{S}^n_{++}$ and $y, x \in \mathbb{R}^n : \langle y, s \rangle > 0$

We would like to solve the following constrained minimization task.

$$\min_{X \in \mathbb{S}^n_{++}} \{D(X^{-1}, H^{-1}) | Xy = s\}$$

Prove that it hass a unique sollution and it is equal to:

$$(I_n - \frac{sy^T}{y^T s})H(I_n - \frac{ys^T}{y^T s}) + \frac{ss^T}{y^T s}$$

Problem 8 (BONUS)

Question

Let $e_1, \dots, e_n$ be a standart basis in $\mathbb{R}^n$. Show that:

$$\max_{X \in \mathbb{S}^n_{++}} \det(X) : ||Xe_i|| \leq 1 \forall i \in 1, \dots, n$$

Has a unique solution I_n, and derive the Hadamard inequality:

$$\det(X) \leq \prod_{i=1}^{n} ||Xe_i|| \forall X \in \mathbb{S}^n_{++}$$

Adversarial Attacks

Definition: Adversarial attacks are techniques used to fool DL models by adding small perturbations to the input data. We can frame adversarial attacks as a constrained optimization problem where the goal is to minimize/maximize the loss function while keeping the perturbation within a certain limit (norm constraint).

The Fast Gradient Sign Method (FGSM) is the most simple such technique, that generates adversarial examples by applying a small perturbation in the direction of the gradient of the loss function. Formally:

$$x' = x + \varepsilon \cdot \text{sgn}(\nabla_x L(x, y)), \text{s.t. } ||x - x'|| \leq \varepsilon$$

So in a nutshell we perfrom a gradient ascent on an image (== maximizing loss w.r.t to that image).

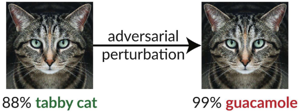

Figure 2: Illustration of different stationary (critical) points

Here is the code to try it out yourself!