

Mathematical Foundations: Optimization Primer

Prof. Ziping Zhao

School of Information Science and Technology
ShanghaiTech University, Shanghai, China

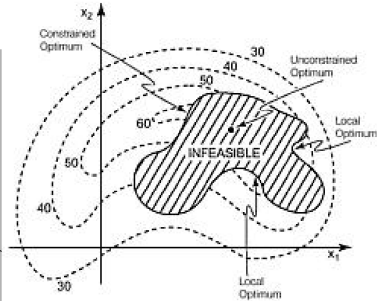
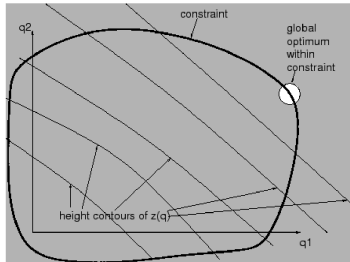
CS182: Introduction to Machine Learning (Fall 2021)
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Optimization Problem

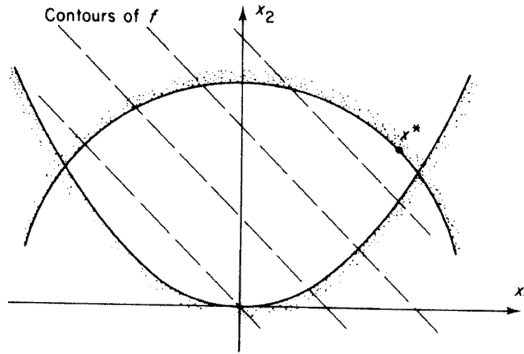
minimize $f_0(\mathbf{x})$ (objective function)

subject to $f_i(\mathbf{x}) \leq 0, \quad i = 1, \dots, m$ (inequality constraints)

$h_i(\mathbf{x}) = 0, \quad i = 1, \dots, p$ (equality constraints)



Active Constraint



A constraint is **active** at \mathbf{x}

► \mathbf{x} is on the **boundary** of its feasible region ($f_i(\mathbf{x}) = 0$)

\mathcal{A}^* : set of active constraints at the solution. The remaining constraints can be **ignored** and the problem can be treated as an **equality constraint** problem with constraints \mathcal{A}^* .

Lagrangian

standard form problem (without equality constraints)

$$\begin{aligned} & \underset{\mathbf{x}}{\text{minimize}} && f_0(\mathbf{x}) \\ & \text{subject to} && f_i(\mathbf{x}) \leq 0, \quad i = 1, \dots, m \end{aligned}$$

- ▶ primal problem
- ▶ optimal value p^*

(assume $\mathbf{x} \in \mathbb{R}^n$) **Lagrangian** $\mathcal{L} : \mathbb{R}^{n+m} \rightarrow \mathbb{R}$

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f_0(\mathbf{x}) + \lambda_1 f_1(\mathbf{x}) + \dots + \lambda_m f_m(\mathbf{x}) = f_0(\mathbf{x}) + \sum_i \lambda_i f_i(\mathbf{x})$$

- ▶ λ_i : Lagrange multipliers or dual variables
- ▶ objective is augmented with weighted sum of constraint functions

Lagrange Dual Function

(Lagrange) dual function $g : \mathbb{R}^m \rightarrow \mathbb{R} \cup \{-\infty\}$

$$g(\boldsymbol{\lambda}) = \inf_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = \inf_{\mathbf{x}} (f_0(\mathbf{x}) + \lambda_1 f_1(\mathbf{x}) + \cdots + \lambda_m f_m(\mathbf{x}))$$

- ▶ minimum of augmented cost as function of weights
- ▶ can be $-\infty$ for some $\boldsymbol{\lambda}$

Example: linear programming (LP)

$$\underset{\mathbf{x}}{\text{minimize}} \quad \mathbf{c}^T \mathbf{x} \quad \text{subject to} \quad \mathbf{a}_i^T \mathbf{x} - b_i \leq 0, \quad i = 1, \dots, m$$

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = \mathbf{c}^T \mathbf{x} + \sum_{i=1}^m \lambda_i (\mathbf{a}_i^T \mathbf{x} - b_i) = -\mathbf{b}^T \boldsymbol{\lambda} + (\mathbf{A}\boldsymbol{\lambda} + \mathbf{c})^T \mathbf{x}$$

$$g(\boldsymbol{\lambda}) = \begin{cases} -\mathbf{b}^T \boldsymbol{\lambda} & \text{if } \mathbf{A}\boldsymbol{\lambda} + \mathbf{c} = \mathbf{0} \\ -\infty & \text{otherwise} \end{cases}$$

Lower Bound Property

Property

If $\lambda \geq 0$ and \mathbf{x} is primal feasible, then $g(\lambda) \leq f_0(\mathbf{x})$

Proof.

if $f_i(\mathbf{x}) \leq 0$ and $\lambda_i \geq 0$ for $i = 1, \dots, m$,

$$\begin{aligned} f_0(\mathbf{x}) &\geq f_0(\mathbf{x}) + \sum_i \lambda_i f_i(\mathbf{x}) \\ &\geq \inf_{\mathbf{z}} \left(f_0(\mathbf{z}) + \sum_i \lambda_i f_i(\mathbf{z}) \right) \\ &= g(\lambda) \end{aligned}$$



- ▶ $f_0(\mathbf{x}) - g(\boldsymbol{\lambda}) \geq 0$: **duality gap** of (primal feasible) \mathbf{x} and $\boldsymbol{\lambda} \geq 0$
- ▶ $\boldsymbol{\lambda} \in \mathbb{R}^m$ is **dual feasible** if $\boldsymbol{\lambda} \geq 0$ and $g(\boldsymbol{\lambda}) > -\infty$
- ▶ minimize $f_0(\mathbf{x}) - g(\boldsymbol{\lambda}) \geq 0$ over primal feasible \mathbf{x}

for any $\boldsymbol{\lambda} \geq 0, g(\boldsymbol{\lambda}) \leq p^*$

- dual feasible points yield **lower bounds** on optimal value!

Lagrange Dual Problem

Find the **best** lower bound on p^* :

$$\begin{array}{ll}\text{maximize} & g(\lambda) \\ \text{subject to} & \lambda \geq 0\end{array}$$

- ▶ **(Lagrange) dual problem** (associated with the primal problem)
- ▶ optimal value: d^*
- ▶ we always have $d^* \leq p^*$ (**weak duality**)
- ▶ $p^* - d^*$: **optimal duality gap**
- ▶ for convex problems, we (usually) have **strong duality** (i.e., zero duality gap):

$$d^* = p^*$$

Dual of Linear Program

primal

$$\begin{array}{ll}\text{minimize}_{\mathbf{x}} & \mathbf{c}^T \mathbf{x} \\ \text{subject to} & \mathbf{Ax} \leq \mathbf{b}\end{array}$$

- ▶ n variables, m inequality constraints

dual

$$\begin{array}{ll}\text{maximize}_{\lambda} & -\mathbf{b}^T \lambda \\ \text{subject to} & \mathbf{A}^T \lambda + \mathbf{c} = 0 \\ & \lambda \geq 0\end{array}$$

- ▶ dual of LP is also an LP
- ▶ m variables, n equality constraints, m nonnegativity constraints

Duality in Algorithms

many algorithms produce at iteration k

- ▶ a primal feasible $\mathbf{x}^{(k)}$
- ▶ and a dual feasible $\boldsymbol{\lambda}^{(k)}$

with $f_0(\mathbf{x}^{(k)}) - g(\boldsymbol{\lambda}^{(k)}) \rightarrow 0$ as $k \rightarrow \infty$

- ▶ hence at iteration k we know $p^* \in [g(\boldsymbol{\lambda}^{(k)}), f_0(\mathbf{x}^{(k)})]$
- ▶ useful for stopping criteria

Complementary Slackness

suppose \mathbf{x}^* , $\boldsymbol{\lambda}^*$ are primal, dual optimal with zero duality gap

$$\begin{aligned} f_0(\mathbf{x}^*) &= g(\boldsymbol{\lambda}^*) \\ &= \inf_{\mathbf{x}} (f_0(\mathbf{x}) + \sum_{i=1}^m \lambda_i^* f_i(\mathbf{x})) \\ &\leq f_0(\mathbf{x}^*) + \sum_{i=1}^m \lambda_i^* f_i(\mathbf{x}^*) \end{aligned}$$

hence we have $\sum_{i=1}^m \lambda_i^* f_i(\mathbf{x}^*) = 0$, and so

complementary slackness condition

$$\lambda_i^* f_i(\mathbf{x}^*) = 0, \quad i = 1, \dots, m$$

- ▶ i th constraint **inactive** at optimum $\Rightarrow \lambda_i^* = 0$
- ▶ $\lambda_i^* > 0$ at optimum $\Rightarrow i$ th constraint **active** at optimum

KKT Optimality Conditions

suppose

- ▶ f_i are differentiable
- ▶ $\mathbf{x}^*, \boldsymbol{\lambda}^*$ are (primal, dual) optimal, with zero duality gap

by complementary slackness we have (from previous slide)

$$f_0(\mathbf{x}^*) + \sum_i \lambda_i^* f_i(\mathbf{x}^*) = \inf_{\mathbf{x}} \left(f_0(\mathbf{x}) + \sum_i \lambda_i^* f_i(\mathbf{x}) \right)$$

- ▶ i.e., \mathbf{x}^* minimizes $\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}^*)$ ($\because \nabla f_0(\mathbf{x}^*) + \sum_i \lambda_i^* \nabla f_i(\mathbf{x}^*) = 0$)

Karush-Kuhn-Tucker (KKT) optimality conditions:

$$f_i(\mathbf{x}^*) \leq 0$$

$$\lambda_i^* \geq 0$$

$$\lambda_i^* f_i(\mathbf{x}^*) = 0$$

$$\nabla f_0(\mathbf{x}^*) + \sum_i \lambda_i^* \nabla f_i(\mathbf{x}^*) = 0$$

Equality Constraints

$$\begin{array}{ll}\underset{\mathbf{x}}{\text{minimize}} & f_0(\mathbf{x}) \\ \text{subject to} & f_i(\mathbf{x}) \leq 0, \quad i = 1, \dots, m \\ & h_i(\mathbf{x}) = 0, \quad i = 1, \dots, p\end{array}$$

define Lagrangian $\mathcal{L} : \mathbb{R}^{n+m+p} \rightarrow \mathbb{R}$ as

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

dual function: $g(\boldsymbol{\lambda}, \boldsymbol{\nu}) = \inf_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu})$

- ▶ $(\boldsymbol{\lambda}, \boldsymbol{\nu})$ is **dual feasible** if $\boldsymbol{\lambda} \geq 0$ and $g(\boldsymbol{\lambda}, \boldsymbol{\nu}) > -\infty$
- ▶ **No** sign condition on $\boldsymbol{\nu}$

lower bound property: if \mathbf{x} is primal feasible and $(\boldsymbol{\lambda}, \boldsymbol{\nu})$ is dual feasible, then $g(\boldsymbol{\lambda}, \boldsymbol{\nu}) \leq f_0(\mathbf{x})$, hence

$$g(\boldsymbol{\lambda}, \boldsymbol{\nu}) \leq p^*$$

dual problem: find best lower bound

$$\begin{array}{ll}\text{maximize} & g(\boldsymbol{\lambda}, \boldsymbol{\nu}) \\ & \boldsymbol{\lambda}, \boldsymbol{\nu} \\ \text{subject to} & \boldsymbol{\lambda} \geq 0\end{array}$$

► note: $\boldsymbol{\nu}$ unconstrained

weak duality: $d^* \leq p^*$ always

strong duality: if primal is convex then (usually) $d^* = p^*$

KKT Optimality Conditions

assume f_i, h_i differentiable

if $\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\nu}^*$ are optimal, with zero duality gap, then they satisfy KKT conditions

$$f_i(\mathbf{x}^*) \leq 0, \quad h_i(\mathbf{x}^*) = 0$$

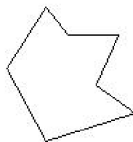
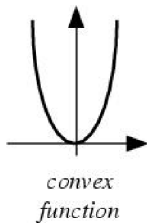
$$\lambda_i^* \geq 0$$

$$\lambda_i^* f_i(\mathbf{x}^*) = 0$$

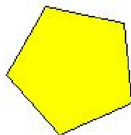
$$\nabla f_0(\mathbf{x}^*) + \sum_i \lambda_i^* \nabla f_i(\mathbf{x}^*) + \sum_i \nu_i^* \nabla h_i(\mathbf{x}^*) = 0$$

Convex Programming

minimize a **convex function** on a **convex set**



A Non-Convex Polygon



A convex Polygon

Convex Functions & Sets

- **Convex function:** A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is said to be convex if the domain, $\text{dom } f$, is convex and

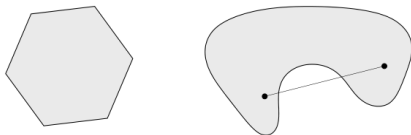
$$f(\theta \mathbf{x} + (1 - \theta) \mathbf{y}) \leq \theta f(\mathbf{x}) + (1 - \theta) f(\mathbf{y})$$

for all $\mathbf{x}, \mathbf{y} \in \text{dom } f$, $0 \leq \theta \leq 1$

- **Convex set:** A set $C \in \mathbb{R}^n$ is said to be convex if the line segment between any two points is in the set:

$$\theta \mathbf{x} + (1 - \theta) \mathbf{y} \in C$$

for all $\mathbf{x}, \mathbf{y} \in C$, $0 \leq \theta \leq 1$



Key Properties of Convex Functions

- ▶ **α -sublevel set**: sublevel sets of a convex function f are convex (converse is false)

$$C_\alpha = \{\mathbf{x} \in \text{dom } f \mid f(\mathbf{x}) \leq \alpha\}$$

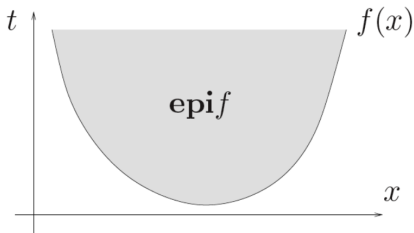
- ▶ **Epigraph**: a function f is convex if and only if its epigraph

$$\text{epi } f = \{(\mathbf{x}, t) \in \mathbb{R}^{n+1} \mid \mathbf{x} \in \text{dom } f, f(\mathbf{x}) \leq t\}$$

is a convex set

- ▶ **Relation** between convexity in sets and convexity in functions:

$$f \text{ is convex} \iff \text{epi } f \text{ is convex}$$



- **First-order condition:** a differentiable f with convex domain is convex if and only if

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) \quad \forall \mathbf{x}, \mathbf{y} \in \text{dom } f$$

- **Second-order condition:** a twice differentiable f with convex domain is convex if and only if

$$\nabla^2 f(\mathbf{x}) = \mathbf{H}(\mathbf{x}) \succeq \mathbf{0} \quad \forall \mathbf{x} \in \text{dom } f$$

- **Jensen's inequality:** if f is convex, and X is a random variable supported on $\text{dom } f$, then

$$f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)]$$

Examples

Linear programming

- ▶ linear objective function, linear constraints

$$\underset{\mathbf{x}}{\text{minimize}} \quad \mathbf{c}^T \mathbf{x} \quad \text{subject to} \quad \mathbf{a}_i^T \mathbf{x} - b_i \leq 0, \quad i = 1, \dots, m$$

Quadratic programming (QP)

- ▶ quadratic objective function, linear constraints

$$\begin{aligned} &\underset{\mathbf{x}}{\text{minimize}} \quad \frac{1}{2} \mathbf{x}^T \mathbf{G} \mathbf{x} + \mathbf{g}^T \mathbf{x} \\ &\text{subject to} \quad \begin{cases} \mathbf{a}_i^T \mathbf{x} - b_i = 0 \\ \mathbf{a}_i^T \mathbf{x} - b_i \leq 0 \end{cases} \end{aligned}$$

- ▶ \mathbf{G} : (positive semi-definite) matrix; \mathbf{g} : vector

Global Optimality

Every local solution is a **global solution**

- ▶ does not have the problem of **local optimum**

