CS182 Introduction to Machine Learning

Recitation 3

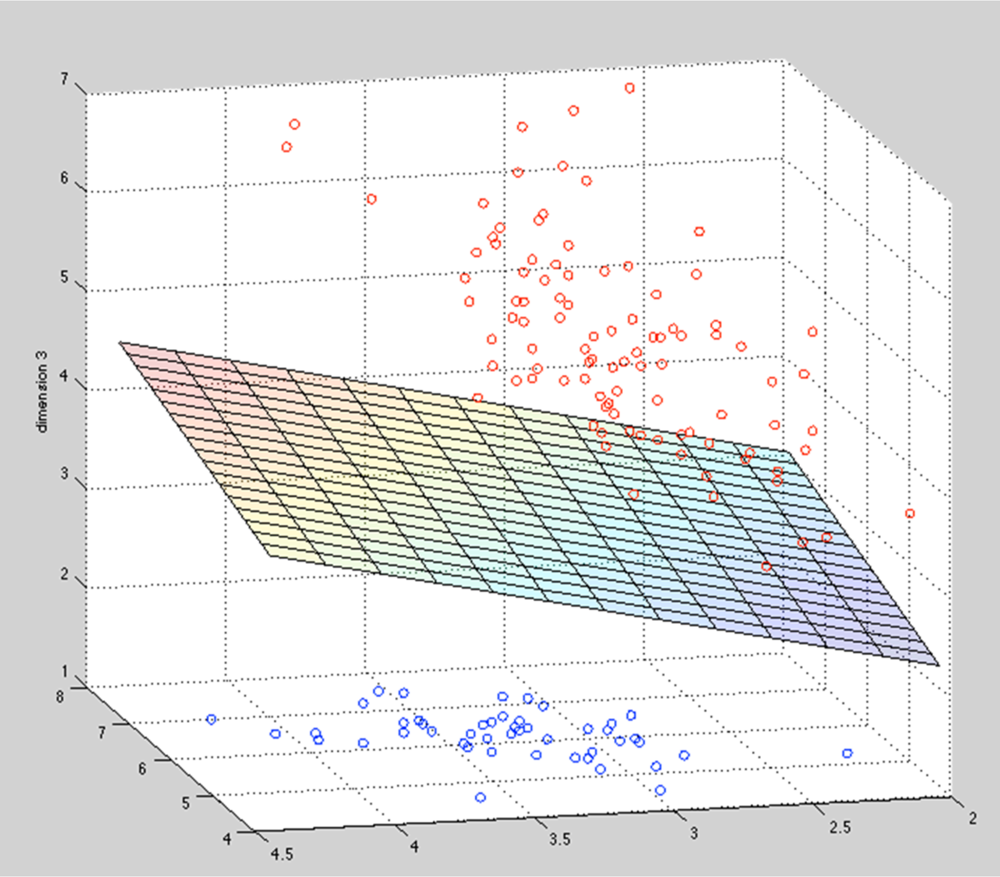
2025.3.12

Outline

- Perceptron
- Review(Preview): Optimization

Linear Classification

$$\hat{y} = \text{sign}(\mathbf{w}^\top \mathbf{x} + b) = \begin{cases} 1 & \text{if } \mathbf{w}^\top \mathbf{x} + b \geq 0 \\ -1 & \text{otherwise} \end{cases}$$



Perceptron

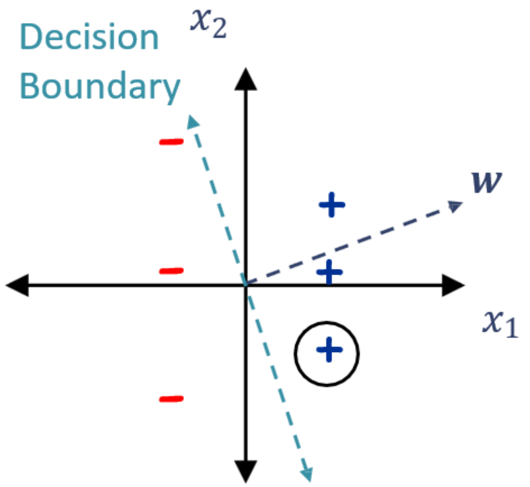
update rules

Perceptron Algorithm: (without the intercept term)

- Set t=1, start with all-zeroes weight vector w_1.
- Given example x, predict positive iff $w_t \cdot x \geq 0$.
- On a mistake, update as follows:
  - Mistake on positive, update $w_{t+1} \leftarrow w_t + x$
  - Mistake on negative, update $w_{t+1} \leftarrow w_t - x$

x_1	x_2	$\hat{y}$	y	Mistake?
-1	2	$+$	$-$	Yes
1	0	$+$	$+$	No
1	1	$-$	$+$	Yes
-1	0	$-$	$-$	No
-1	-2	$+$	$-$	Yes
1	-1	$+$	$+$	No

$$\boldsymbol{w} = \begin{bmatrix} 3 \\ 1 \end{bmatrix}$$



Perceptron Convergence

Given dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{N}$, suppose:

1. Finite size inputs: $||x^{(i)}|| \leq R$
2. Linearly separable data: $\exists \boldsymbol{\theta}^*$ and $\boldsymbol{\gamma} > 0$ s.t. $||\boldsymbol{\theta}^*|| = 1$ and $y^{(i)}(\boldsymbol{\theta}^* \cdot x^{(i)}) \geq \boldsymbol{\gamma}, \forall i$

Then, the number of mistakes k made by the perceptron algorithm on $\mathcal{D}$ is bounded by $(R/\boldsymbol{\gamma})^2$.

Proof:
Part 1: For some A, $Ak \leq ||\boldsymbol{\theta}^{(k+1)}||$

$$\begin{aligned}
\boldsymbol{\theta}^{(k+1)} \cdot \boldsymbol{\theta}^* &= (\boldsymbol{\theta}^{(k)} + y^{(i)}x^{(i)}) \cdot \boldsymbol{\theta}^*, \text{ Perceptron algorithm update} \\
&= \boldsymbol{\theta}^{(k)} \cdot \boldsymbol{\theta}^* + y^{(i)}(\boldsymbol{\theta}^* \cdot x^{(i)})) \\
&\geq \boldsymbol{\theta}^{(k)} \cdot \boldsymbol{\theta}^* + \boldsymbol{\gamma}, \text{ by assumption} \\
\implies \boldsymbol{\theta}^{(k+1)} \cdot \boldsymbol{\theta}^* &\geq k\boldsymbol{\gamma}, \text{ by induction on k since } \boldsymbol{\theta}^{(1)} = 0 \\
\implies ||\boldsymbol{\theta}^{(k+1)}|| &\geq k\boldsymbol{\gamma}, \text{ since } ||w|| \times ||u|| \geq w \cdot u \text{ and } ||\boldsymbol{\theta}^*|| = 1
\end{aligned}$$

Part 2: For some B, $||\boldsymbol{\theta}^{(k+1)}|| \leq B\sqrt{k}$

$$\begin{aligned}
||\boldsymbol{\theta}^{(k+1)}||^2 &= ||\boldsymbol{\theta}^{(k)} + y^{(i)}x^{(i)}||^2, \text{ Perceptron algorithm update} \\
&= ||\boldsymbol{\theta}^{(k)}||^2 + (y^{(i)})^2||x^{(i)}||^2 + 2y^{(i)}(\boldsymbol{\theta}^{(k)} \cdot x^{(i)}) \\
&\leq ||\boldsymbol{\theta}^{(k)}||^2 + (y^{(i)})^2||x^{(i)}||^2, \text{ since } k^{th} \text{ mistake } \implies y^{(i)}(\boldsymbol{\theta}^{(k)} \cdot x^{(i)}) \leq 0 \\
&= ||\boldsymbol{\theta}^{(k)}||^2 + R^2, \text{ since } (y^{(i)})^2||x^{(i)}||^2 = ||x^{(i)}||^2 \leq R^2, \text{ by assumption and } (y^{(i)})^2 = 1 \\
\implies ||\boldsymbol{\theta}^{(k+1)}||^2 &\leq kR^2, \text{ by induction on k since } (\theta^{(i)})^2 = 0 \\
\implies ||\boldsymbol{\theta}^{(k+1)}|| &\leq \sqrt{k}R
\end{aligned}$$

Part 3: Combine the bounds

$$\begin{aligned}
k\boldsymbol{\gamma} \leq ||\boldsymbol{\theta}^{(k+1)}|| &\leq \sqrt{k}R \\
\implies k &\leq (R/\boldsymbol{\gamma})^2
\end{aligned}$$

- Perceptron will not converge.
- However, we can achieve a similar bound on the number of mistakes made in one pass (Freund, Schapire)

Main Takeaway: For linearly separable data, if the perceptron algorithm repeatedly cycles through the data, it will converge in a finite number of steps.

If data has margin γ and all points inside a ball of radius R, then Perceptron $\leq \left(\frac{R}{\gamma}\right)^2$ mistakes

Review(Preview): Optimization

- 通常讨论凸优化的范围
  - 凸集
  - 凸函数
  - 凸优化问题
- 优化方法
  - Lagrange Duality
  - KKT method

Review(Preview) Outline

- Matrix Derivative
- Convex Function
- Convex Problem
- Duality, KKT Condition

Matrix Derivatives 矩阵求导

Types	Scalar	Vector	Matrix
Scalar	$\frac{\mathrm{d}y}{\mathrm{d}x}$	$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}x}$	$\frac{\mathrm{d}\mathbf{Y}}{\mathrm{d}x}$
Vector	$\frac{\partial y}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$	
Matrix	$\frac{\partial y}{\partial \mathbf{X}}$		

layout

- 分子布局
  numerator layout:
  求导结果的维度以分子为主
- 分母布局
  denominator layout:
  求导结果的维度以分母为主
- 机器学习通常使用混合布局:
  向量或者矩阵对标量求导，
  则使用分子布局为准，如果是标量对向量或者矩阵求导，则以分母布局为准

具体总结如下：

自变量\因变量	标量y	列向量$\mathbf{y}$	矩阵$\mathbf{Y}$
标量x	/	$\frac{\partial \mathbf{y}}{\partial x}$ 分子布局：m维列向量（默认布局） 分母布局：m维行向量	$\frac{\partial \mathbf{Y}}{\partial x}$ 分子布局：$p \times q$矩阵（默认布局） 分母布局：$q \times p$矩阵
列向量$\mathbf{x}$	$\frac{\partial y}{\partial \mathbf{x}}$ 分子布局：n维行向量 分母布局：n维列向量（默认布局）	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$ 分子布局：$m \times n$雅克比矩阵（默认布局） 分母布局：$n \times m$梯度矩阵	/
矩阵$\mathbf{X}$	$\frac{\partial y}{\partial \mathbf{X}}$ 分子布局：$n \times m$矩阵 分母布局：$m \times n$矩阵（默认布局）	/	/

Matrix Derivatives

常见求导:

- $\dfrac{\partial \mathbf{a}^\top \mathbf{x}}{\partial \mathbf{x}} = \dfrac{\partial \mathbf{x}^\top \mathbf{a}}{\partial \mathbf{x}} = \mathbf{a}$
- $\dfrac{\partial \mathbf{x}^\top \mathbf{A} \mathbf{x}}{\partial \mathbf{x}} = (\mathbf{A} + \mathbf{A}^\top)\mathbf{x}$
- more details:

> Matrix cookbook

- Chain Rule 矩阵求导链式法则
  注意将矩阵的维度对上

> https://www.cnblogs.com/yifanrensheng/p/12639539.html

least square approximation

$$\min_{\mathbf{x}\in\mathbb{R}^n} \mathcal{L} = \|\mathbf{b} - A\mathbf{x}\|_2^2$$

$$\mathcal{L} = \|\mathbf{b} - A\mathbf{x}\|_2^2 = (\mathbf{b} - A\mathbf{x})^\top(\mathbf{b} - A\mathbf{x}) = \mathbf{b}^\top\mathbf{b} - \mathbf{b}^\top A\mathbf{x} - \mathbf{x}^\top A^\top\mathbf{b} + \mathbf{x}^\top A^\top A\mathbf{x}$$

$$\frac{\partial\mathcal{L}}{\partial\mathbf{x}} = -2A^\top\mathbf{b} + 2A^\top A\mathbf{x} = 0$$

$$\Rightarrow A^\top A\mathbf{x} = A^\top\mathbf{b}$$

Convex set

line segment between x_1 and x_2: all points

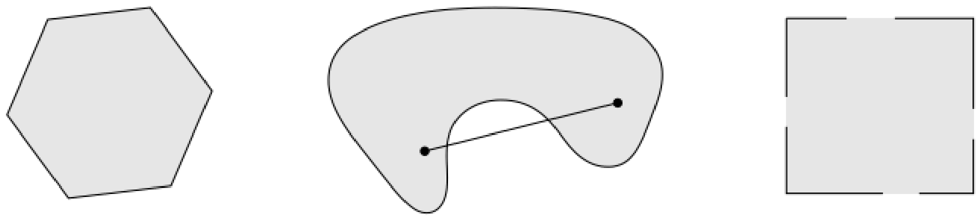
$$x = \theta x_1 + (1-\theta)x_2$$

with $0 \leq \theta \leq 1$

convex set: contains line segment between any two points in the set

$$x_1, x_2 \in C, \quad 0 \leq \theta \leq 1 \quad \Longrightarrow \quad \theta x_1 + (1-\theta)x_2 \in C$$

examples (one convex, two nonconvex sets)

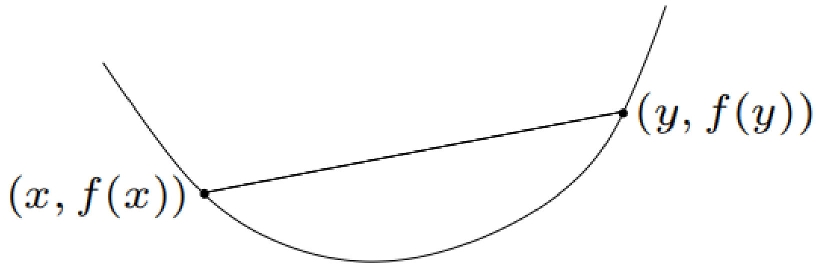


Convex function

$f : \mathbf{R}^n \to \mathbf{R}$ is convex if $\mathbf{dom}\, f$ is a convex set and

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

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



- f is concave if $-f$ is convex
- f is strictly convex if $\mathbf{dom}\, f$ is convex and

$$f(\theta x + (1-\theta)y) < \theta f(x) + (1-\theta)f(y)$$

  for $x, y \in \mathbf{dom}\, f$, $x \neq y$, $0 < \theta < 1$

多元函数微分

- ∇ 算子: $\nabla_{\mathbf{x}} f$: 函数$f(\mathbf{x})$对$\mathbf{x}$的梯度
- ∇f: 一阶导 (Jacobian matrix): $\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_n} \end{bmatrix}^\top$
- $\nabla^2 f$: 二阶导 (Hessian matrix)

$$\nabla^2 f = \nabla(\nabla f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Convex Function 凸函数

判据: $f(\mathbf{x})$是凸函数当且仅当

- $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n, \forall \theta \in [0, 1], f(\theta \mathbf{x} + (1-\theta)\mathbf{y}) \leq \theta f(\mathbf{x}) + (1-\theta) f(\mathbf{y})$
- $\forall \mathbf{x} \in \nabla^2 \mathbb{R}^n, f(\mathbf{x}) \succeq 0$
- $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n, f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x})$

> 这三条本质是等价的, 可以互相推导

Second-order conditions

f is **twice differentiable** if $\mathbf{dom}\, f$ is open and the Hessian $\nabla^2 f(x) \in \mathbf{S}^n$,

$$\nabla^2 f(x)_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}, \quad i, j = 1, \ldots, n,$$

exists at each $x \in \mathbf{dom}\, f$

2nd-order conditions: for twice differentiable f with convex domain

- f is convex if and only if

$$\nabla^2 f(x) \succeq 0 \quad \text{for all } x \in \mathbf{dom}\, f$$

- if $\nabla^2 f(x) \succ 0$ for all $x \in \mathbf{dom}\, f$, then f is strictly convex

Taylor Expansion 泰勒展开

$\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$:

- 泰勒展开

  $f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{1}{2}(\mathbf{y} - \mathbf{x})^\top \nabla^2 f(\mathbf{x})(\mathbf{y} - \mathbf{x}) + o(\|\mathbf{y} - \mathbf{x}\|^2)$
- 中值定理:

  $\exists \theta \in [0, 1], s.t.\, \mathbf{z} = \theta \mathbf{x} + (1 - \theta)\mathbf{y}$:

  $f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\mathbf{z})^\top (\mathbf{y} - \mathbf{x})$

  $f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{1}{2}(\mathbf{y} - \mathbf{x})^\top \nabla^2 f(\mathbf{z})(\mathbf{y} - \mathbf{x})$
- 凸函数 $\nabla^2 f(\mathbf{x}) \succeq 0$

  $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x})$

Jensen's Inequality

对于一个凸函数$f(x)$, 有

- 概率论角度:
  $f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)]$
- 优化角度:
  $f(\theta x+(1-\theta) y) \leq \theta f(x)+(1-\theta) f(y), \forall x, y \in \mathbb{R}^n, \theta \in[0,1]$

μ-strongly convex & L-smooth

- 如果一个函数$f(\mathbf{x})$满足: $\mu\|\mathbf{x}\|_2^2 \leq \mathbf{x}^\top \mathbf{A}\mathbf{x}$, 或写作$\mu I \preceq \mathbf{A}$, 则称$f(\mathbf{x})$是$\mu$-strongly convex 的
- 如果一个函数$f(\mathbf{x})$满足: $\mathbf{x}^\top \mathbf{A}\mathbf{x} \leq L\|\mathbf{x}\|_2^2$, 或写作 $\mathbf{A} \preceq LI$, 则称$f(\mathbf{x})$是L-smooth 的
- 一个函数的条件数(condition number)为$\kappa = \dfrac{L}{\mu}$, 这决定了Gradient Descent的收敛速度

Convex Problem 凸优化问题

- 对于一个优化问题:

$$
\begin{aligned}
\min_{\mathbf{x}} \quad & f_0(\mathbf{x}) \\
s.t. \quad & f_i(\mathbf{x}) \leq 0, i = 1, 2, \cdots, m \\
& h_i(\mathbf{x}) = 0, i = 1, 2, \cdots, n
\end{aligned}
$$

- 其拉格朗日函数为:

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

其中$\boldsymbol{\lambda}$和$\boldsymbol{\nu}$是拉格朗日乘子, $\lambda_i \geq 0$, ν_i无约束

- 若$f_0(\mathbf{x})$和$f_i(\mathbf{x})$是凸函数, $h_i(\mathbf{x})$是仿射/线性函数, 则原问题是凸优化问题

Example

$$\begin{aligned} \min \quad & x_1^2 + x_2^2, \\ \text{s.t.} \quad & x_2 \le \alpha, \\ & x_1 + x_2 = 1 \end{aligned}$$

其中 $(x_1, x_2) \in \mathbb{R}^2, \alpha$ 为实数

step1: 写出Lagrangigan函数

$$\mathcal{L}\left(x_1, x_2, \mu, \lambda\right) = x_1^2 + x_2^2 + \lambda\left(x_2 - \alpha\right) + \mu\left(1 - x_1 - x_2\right), \text{where } \lambda \ge 0$$

Duality 对偶性

原问题(primal problem):

$$\begin{aligned}\min_{\mathbf{x}} \quad & f_0(\mathbf{x}) \\ s.t. \quad & f_i(\mathbf{x}) \leq 0, i = 1, 2, \cdots, m \\ & h_i(\mathbf{x}) = 0, i = 1, 2, \cdots, n\end{aligned}$$

对应的对偶问题(dual problem):

$$\begin{aligned}\max_{\boldsymbol{\lambda}, \boldsymbol{\nu}} \quad & g(\boldsymbol{\lambda}, \boldsymbol{\nu}) \\ s.t. \quad & \boldsymbol{\lambda} \succeq 0 \\ & \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) \text{取到} g(\boldsymbol{\lambda}, \boldsymbol{\nu})\end{aligned}$$

> $f_0(\mathbf{x}) = \max_{\boldsymbol{\lambda} \succeq 0, \boldsymbol{\nu}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu})$, $g(\boldsymbol{\lambda}, \boldsymbol{\nu}) = \min_{\mathbf{x} \in \mathcal{D}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu})$
>
> 无论原问题是否为凸优化问题, 对偶目标函数$g(\boldsymbol{\lambda}, \boldsymbol{\nu})$ 永远是凹函数!

Duality 对偶性

> $f_0(\mathbf{x}) = \max_{\boldsymbol{\lambda}\succeq 0,\boldsymbol{\nu}} \mathcal{L}(\mathbf{x},\boldsymbol{\lambda},\boldsymbol{\nu})$, $g(\boldsymbol{\lambda},\boldsymbol{\nu}) = \min_{\mathbf{x}\in\mathcal{D}} \mathcal{L}(\mathbf{x},\boldsymbol{\lambda},\boldsymbol{\nu})$
>
> $p^* = \min_{\mathbf{x}} f_0(\mathbf{x})$
>
> $d^* = \max_{\boldsymbol{\lambda}\succeq 0,\boldsymbol{\nu}} g(\boldsymbol{\lambda},\boldsymbol{\nu})$

- Weak Duality $p^* \geq d^*$

  $g(\boldsymbol{\lambda},\boldsymbol{\nu}) = \min_{x\in\mathcal{D}} \mathcal{L}(\mathbf{x},\boldsymbol{\lambda},\boldsymbol{\nu}) \leq \mathcal{L}(\mathbf{x}^*,\boldsymbol{\lambda},\boldsymbol{\nu})$

  $= f_0(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i f_i(\mathbf{x}^*) + \sum_{i=1}^{n} \nu_i h_i(\mathbf{x}^*) \leq f_0(\mathbf{x}^*) = p^*$

  上式$\forall\boldsymbol{\lambda} \succeq 0, \boldsymbol{\nu}$成立, d^*符合该条件, 所以$d^* \leq p^*$

Duality 对偶性

- Strong Duality

  $p^* = d^*$

  假设strong duality成立, 且$\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\nu}^*$是原问题和对偶问题的最优解, 则有

  $$\begin{aligned} f_0(\mathbf{x}^*) = g(\boldsymbol{\lambda}^*, \boldsymbol{\nu}^*) &= \min_{\mathbf{x}\in\mathcal{D}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}^*, \boldsymbol{\nu}^*) \\ &= \min_{\mathbf{x}\in\mathcal{D}} \left(f_0(\mathbf{x}) + \sum_{i=1}^m \lambda_i^* f_i(\mathbf{x}) + \sum_{i=1}^n \nu_i^* h_i(\mathbf{x}) \right) \\ &\le f_0(\mathbf{x}^*) + \sum_{i=1}^m \lambda_i^* f_i(\mathbf{x}^*) + \sum_{i=1}^n \nu_i^* h_i(\mathbf{x}^*) \\ &\le f_0(\mathbf{x}^*) \end{aligned}$$

第一个不等号取等条件: $\mathbf{x}^*$ minimizes $\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}^*, \boldsymbol{\nu}^*)$, i.e. $\nabla_{\mathbf{x}}\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}^*, \boldsymbol{\nu}^*) = 0$

第二个不等号取等条件: $\lambda_i^* f_i(\mathbf{x}^*) = 0, i = 1, 2, \cdots, m$

KKT Condition

- primal feasibility:

$$\begin{cases} f_i(\mathbf{x}) \leq 0, i = 1, 2, \cdots, m \\ h_i(\mathbf{x}) = 0, i = 1, 2, \cdots, n \end{cases}$$

- dual feasibility:

$$\boldsymbol{\lambda} \succeq 0$$

- complementary slackness:

$$\lambda_i f_i(\mathbf{x}) = 0, i = 1, 2, \cdots, m$$

- gradient of Lagrangian:

$$\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = 0$$

> 可以注意到我们推导出KKT条件的过程中完全没有要求原问题是一个凸优化问题

Example

$$\begin{aligned} \min \quad & x_1^2 + x_2^2, \\ \text{s.t.} \quad & x_2 \le \alpha, \\ & x_1 + x_2 = 1 \end{aligned}$$

其中 $(x_1, x_2) \in \mathbb{R}^2, \alpha$ 为实数

step1: 写出Lagrangigan函数

$$\mathcal{L}(x_1, x_2, \mu, \lambda) = x_1^2 + x_2^2 + \lambda(x_2 - \alpha) + \mu(1 - x_1 - x_2), \text{where } \lambda \ge 0$$

step2: KKT condition

- primal feasibility:

$$\begin{cases} x_2 - \alpha \leq 0 \\ x_1 + x_2 = 1 \end{cases}$$

- dual feasibility:

$$\lambda \succeq 0$$

- complementary slackness:

$$\lambda \left(x_2 - \alpha \right) = 0$$

- gradient of Lagrangian:

$$\frac{\partial \mathcal{L}}{\partial x_i} = 0, \quad i = 1, 2$$

$$\frac{\partial \mathcal{L}}{\partial x_1} = 2x_1 - \mu = 0, \frac{\partial \mathcal{L}}{\partial x_2} = 2x_2 - \mu + \lambda = 0$$

step3: **Solve KKT** or construct the dual problem

由 gradient of Lagrangian: 分别解出 $x_1 = \frac{\mu}{2}$ 且 $x_2 = \frac{\mu}{2} - \frac{\lambda}{2}$ 。代入约束等式 $x_1 + x_2 = \mu - \frac{\lambda}{2} = 1$ 或 $\mu = \frac{\lambda}{2} + 1$ 。合并上面结果，

$$x_1 = \frac{\lambda}{4} + \frac{1}{2}, \quad x_2 = -\frac{\lambda}{4} + \frac{1}{2}$$

最后再加入约束不等式 $-\frac{\lambda}{4} + \frac{1}{2} \leq \alpha$ 或 $\lambda \geq 2 - 4\alpha$ 。底下分开三种情况讨论。

（1）$\alpha > \frac{1}{2}$ ：不难验证 $\lambda = 0 > 2 - 4\alpha$ 满足所有的 KKT 条件，约束不等式是无效的，$x_1^\star = x_2^\star = \frac{1}{2}$ 是内部解，目标函数的极小值是 $\frac{1}{2}$ 。

（2）$\alpha = \frac{1}{2}$ ：如同 1，$\lambda = 0 = 2 - 4\alpha$ 满足所有的KKT条件，$x_1^\star = x_2^\star = \frac{1}{2}$ 是边界解，因为 $x_2^\star = \alpha$ 。

（3）$\alpha < \frac{1}{2}$: 这时约束不等式是有效的，$\lambda = 2 - 4\alpha > 0$ ，则 $x_1^\star = 1 - \alpha$ 且 $x_2^\star = \alpha$ ，目标函数的极小值是 $(1-\alpha)^2 + \alpha^2$ 。

step3: Solve KKT or **construct the dual problem**

$$
\begin{aligned}
g(\lambda, \mu) &= \min_{x_1, x_2} \mathcal{L}(x_1, x_2, \lambda, \mu) = \min_{x_1, x_2} x_1^2 + x_2^2 + \lambda(x_2 - \alpha) + \mu(1 - x_1 - x_2) \\
&= \min_{x_1, x_2} \left(x_1^2 - \mu x_1\right) + \left(x_2^2 + (\lambda - \mu) x_2\right) + \mu - \lambda\alpha \\
&= -\frac{1}{2}\mu^2 + \frac{1}{2}\mu\lambda - \frac{1}{4}\lambda^2 + \mu - \lambda\alpha
\end{aligned}
$$

Dual problem:

$$
\begin{aligned}
\max_{\mu, \lambda} \quad & -\frac{1}{2}\mu^2 + \frac{1}{2}\mu\lambda - \frac{1}{4}\lambda^2 + \mu - \lambda\alpha \\
\text{s.t.} \quad & \lambda \geq 0
\end{aligned}
$$

Example: LP

- Primal problem:

$$\begin{aligned} \min_{\mathbf{x}} \quad & \mathbf{c}^\top \mathbf{x} \\ s.t. \quad & \mathbf{A}\mathbf{x} = \mathbf{b} \\ & \mathbf{x} \succeq 0 \end{aligned}$$

- Dual problem:

$$\begin{aligned} \max_{\boldsymbol{\lambda}} \quad & \mathbf{b}^\top \boldsymbol{\lambda} \\ s.t. \quad & \mathbf{A}^\top \boldsymbol{\lambda} \preceq \mathbf{c} \end{aligned}$$

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = \mathbf{c}^\top \mathbf{x} + \boldsymbol{\lambda}^\top (\mathbf{A}\mathbf{x} - \mathbf{b}) - \boldsymbol{\nu}^\top \mathbf{x} = (\mathbf{c} + \mathbf{A}^\top \boldsymbol{\lambda} - \boldsymbol{\nu})^\top \mathbf{x} - \mathbf{b}^\top \boldsymbol{\lambda}$$

$$g(\boldsymbol{\lambda}, \boldsymbol{\nu}) = \min_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = \begin{cases} -\mathbf{b}^\top \boldsymbol{\lambda} & \text{if } \mathbf{c} - \mathbf{A}^\top \boldsymbol{\lambda} - \boldsymbol{\nu} = \mathbf{0} \\ -\infty & \text{otherwise} \end{cases}$$

Why dual problem?

- 减少变量的数量
  e.g. $\mathbf{A} \in \mathbb{R}^{m \times n}, m \ll n$
  原问题n个变量, 对偶问题只有m个变量
- 拥有更好的形式
  e.g. SVM 对偶问题引入了内积->核函数
- 对偶目标函数是凹函数, 原问题未必是凸/凹函数

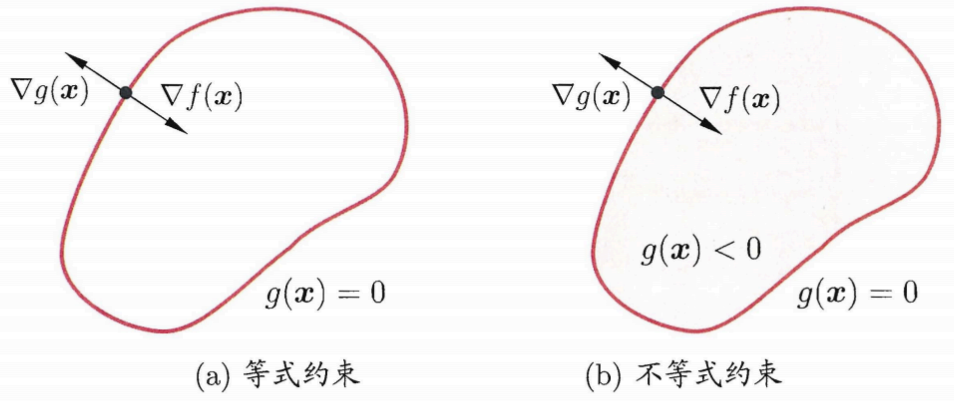
KKT condition 几何意义

对于不等式约束的互补条件

$\lambda_i f_i(\mathbf{x}) = 0, i = 1, 2, \cdots, m$

用只有一个不等式约束的情况来理解:

- 最优解在$f_i(x) < 0$处: $f_i(x) \leq 0$
  不起作用, 起作用的为$\nabla f_0(x) = 0.$
  $\lambda = 0 \Leftrightarrow \nabla \mathcal{L}(x) = \nabla f_0(x)$
- 最优解在$f_i(x) = 0$处
  一定有 $\nabla f_i(x)$与$\nabla f_0(x)$反向, i.e.
  $\exists \lambda_i > 0, s.t. \nabla \mathcal{L}(x) = \nabla f_0(x) + \lambda_i \nabla f_i(x) = 0$



附图B. 1 拉格朗日乘子法的几何含义: 在 (a) 等式约束 $g(\boldsymbol{x}) = 0$ 或 (b) 不等式约束 $g(\boldsymbol{x}) \leqslant 0$ 下, 最小化目标函数 $f(\boldsymbol{x})$. 红色曲线表示 $g(\boldsymbol{x}) = 0$ 构成的曲面, 而其围成的阴影区域表示 $g(\boldsymbol{x}) < 0$.

结合两种情况可得 $\lambda_i f_i(x) = 0$

KKT解一定是最优解吗?

- 必要性:
  strong duality成立, $\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}$是原问题和对偶问题的最优解, 则他们满足KKT条件
- 充分性:
  Theorem: 若原问题是一个凸优化问题, 且Slater's condition成立, 则KKT解一定是最优解

> Slater's condition: $\exists \mathbf{x} \in \text{int } \mathcal{D}, s.t. f_i(\mathbf{x}) < 0, i = 1, 2, \cdots, m, \mathbf{A}\mathbf{x} = \mathbf{b}$
> 或者有其他的Constrain Qualification(CQ)保证KKT解是最优解

KKT 条件未必充分

$$\min_{\mathbf{x}} \quad f(\mathbf{x}) = x_1 + x_2$$

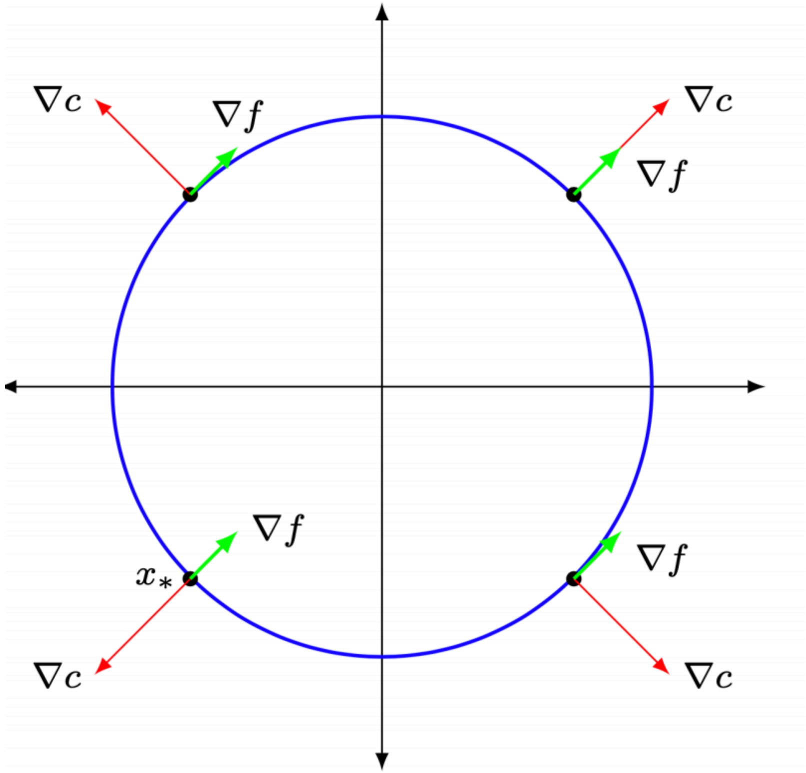
$$s.t. \quad c(\mathbf{x}) = x_1^2 + x_2^2 - 2 = 0$$

- Lagrange function:
  $\mathcal{L}(\mathbf{x}, \lambda) = x_1 + x_2 + \lambda(x_1^2 + x_2^2 - 2)$
- KKT condition: $\begin{cases} 1 + 2\lambda x_1 = 0 \\ 1 + 2\lambda x_2 = 0 \\ x_1^2 + x_2^2 - 2 = 0 \end{cases}$

  解KKT可获得两组解:

  $x = (1, 1), \lambda = -\frac{1}{2}$和$x = (-1, -1), \lambda = \frac{1}{2}$

  但是$(-1, -1)$是minimizer, $(1, 1)$是maximizer



有最优解, 但KKT条件无解

$$
\begin{aligned}
\min_x \quad & x \\
s.t. \quad & x^2 = 0
\end{aligned}
$$

- Lagrange function: $\mathcal{L}(x, \lambda) = x + \lambda x^2$
- KKT condition: $\begin{cases} 1 + 2\lambda x = 0 \\ x^2 = 0 \end{cases}$