

Support

Vector

machine

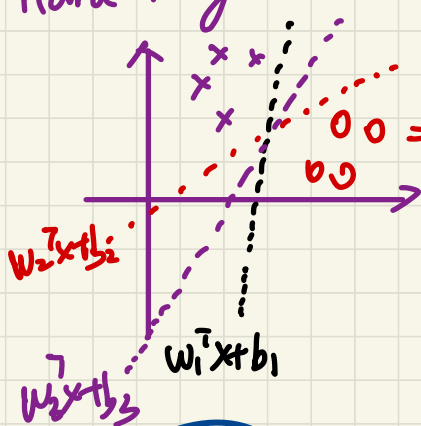
SVM

Support Vector machine

支持向量机

硬间隔 SVM

Hard-margin SVM:



$$f(w) = \text{sign}(w^T x + b)$$

⇒ 存在超平面可以对数据集进行分类。

而我们的目标是为了寻找最好的那个超平面。

寻找泛化误差最小的超平面。(优化问题)

使所有数据点到超平面的最小点的最大间隔超平面。

即: $\max \text{margin}(w, b)$

这里 $\begin{cases} \text{margin} = \min_{\substack{w, b \\ x_i, i=1 \dots N}} \frac{|w^T x_i + b|}{\|w\|} \\ \text{s.t. } y_i (w^T x_i + b) > 0 \end{cases}$

Goal function: $\max_{w, b} \min_{\substack{x_i \\ i=1 \dots N}} \frac{1}{\|w\|} |w^T x_i + b| \Rightarrow \max_{w, b} \frac{1}{\|w\|} \min_{\substack{x_i \\ i=1 \dots N}} |w^T x_i + b|$

$\text{s.t. } y_i (w^T x_i + b) > 0$

\Downarrow

$\exists \gamma > 0, \min_{\substack{x_i \\ i=1 \dots N}} y_i (w^T x_i + b) = \gamma$

$\therefore \max_{w, b} \frac{1}{\|w\|} = \max_{w, b} \frac{1}{\sum w^T w} = \min_{w, b} \sum w^T w$

令 $r=1$

\therefore goal function: $\min_{w, b} \sum \tilde{w}^T w$

约束:

由拉格朗日乘子法

$$s.t.: y_i (w^T x_i + b) \geq 1 \Leftrightarrow 1 - y_i (w^T x_i + b) \leq 0$$

for $i=1 \dots N$

$$L(w, b, \lambda) = \sum \tilde{w}^T w + \sum_{i=1}^N \underbrace{\lambda_i}_{\geq 0} \underbrace{(1 - y_i (w^T x_i + b))}_{\leq 0}$$

不约束

$$\min_{w, b} \max_{\lambda} L(w, b, \lambda)$$

把 $1 - y_i (w^T x_i + b) \leq 0$ 隐含了进来

$$s.t. \lambda_i \geq 0 \quad (拉格朗日乘子法条件)$$

$i=1 \dots N$

P.S: Reason for $\min_{w, b} \sum \tilde{w}^T w = \min_{w, b} \max_{\lambda} L(w, b, \lambda)$

if $(1 - y_i (w^T x_i + b)) > 0$, $\max_{\lambda} L(w, b, \lambda) = \infty$

if $(1 - y_i (w^T x_i + b)) \leq 0$, $\max_{\lambda} L(w, b, \lambda) = \sum \tilde{w}^T w$ ($\lambda_i = 0$)

$$\therefore \min_{w, b} \sum \tilde{w}^T w = \min_{w, b} \max_{\lambda} L(w, b, \lambda)$$

这个条件被忽略。

无约束问题: $\begin{cases} \min_{w,b} \max_{\lambda} L(w,b,\lambda) \\ \text{s.t. } \lambda_i \geq 0 \\ i=1 \dots N \end{cases}$

对偶

$\min_{w,b} \max_{\lambda} L \geq \max_{\lambda} \min_{w,b} L$ (弱对偶)
(宁为凤皇, 不为鸡头) ... '=' 时强对偶

$\begin{cases} \max_{\lambda} \min_{w,b} L(w,b,\lambda) \\ \text{s.t. } \lambda_i \geq 0 \end{cases}$

□ 优化 = 可行
强对偶 = 强对偶

$L(w,b,\lambda) = \frac{1}{2} w^T w + \sum_{i=1}^N \lambda_i (1 - y_i (w^T x_i + b))$
 $\min_{w,b} L(w,b,\lambda)$

$\therefore \max_{\lambda} \min_{w,b} L$
与 $\min_{w,b} \max_{\lambda} L$
同解

$\frac{\partial L}{\partial b} = - \sum_{i=1}^N \lambda_i y_i = 0 \Rightarrow \sum_{i=1}^N \lambda_i y_i = 0$ 将其代入 $L(w,b,\lambda)$

$L(w,b,\lambda) = \frac{1}{2} w^T w + \sum_{i=1}^N \lambda_i - \sum_{i=1}^N \lambda_i y_i (w^T x_i + b)$
 $= \frac{1}{2} w^T w + \sum_{i=1}^N \lambda_i - \sum_{i=1}^N \lambda_i y_i w^T x_i$

$\frac{\partial L}{\partial w} = \frac{1}{2} w - \sum_{i=1}^N \lambda_i y_i x_i \stackrel{\Delta}{=} 0 \Rightarrow w = \sum_{i=1}^N \lambda_i y_i x_i$ 代入 L

$L = \frac{1}{2} \left(\sum_{i=1}^N \lambda_i y_i x_i \right)^T \left(\sum_{j=1}^N \lambda_j y_j x_j \right) - \sum_{i=1}^N \lambda_i y_i \left(\sum_{j=1}^N \lambda_j y_j x_j \right)^T x_i + \sum_{i=1}^N \lambda_i$

$= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \lambda_i \lambda_j y_i y_j x_i^T x_j - \sum_{i=1}^N \lambda_i \lambda_j y_i y_j x_j^T x_i + \sum_{i=1}^N \lambda_i$

$= - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \lambda_i \lambda_j y_i y_j x_i^T x_j + \sum_{i=1}^N \lambda_i$

已将其代入, 故此时 $L(w,b,\lambda)$ 为最小值。

$\min_{\lambda} \min_{w, b} J(w, b, \lambda)$
 s.t. $\lambda_i \geq 0$
 for $i = 1 \dots N$

等价转换
 $\min_{\lambda} (-\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \lambda_i \lambda_j y_i y_j x_i^T x_j + \sum_{i=1}^N \lambda_i)$

s.t. $\lambda_i \geq 0$
 for $i = 1 \dots N$

$\sum_{i=1}^N \lambda_i y_i = 0$

$\min_{\lambda} (\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \lambda_i \lambda_j y_i y_j x_i^T x_j - \sum_{i=1}^N \lambda_i)$

KKT条件:

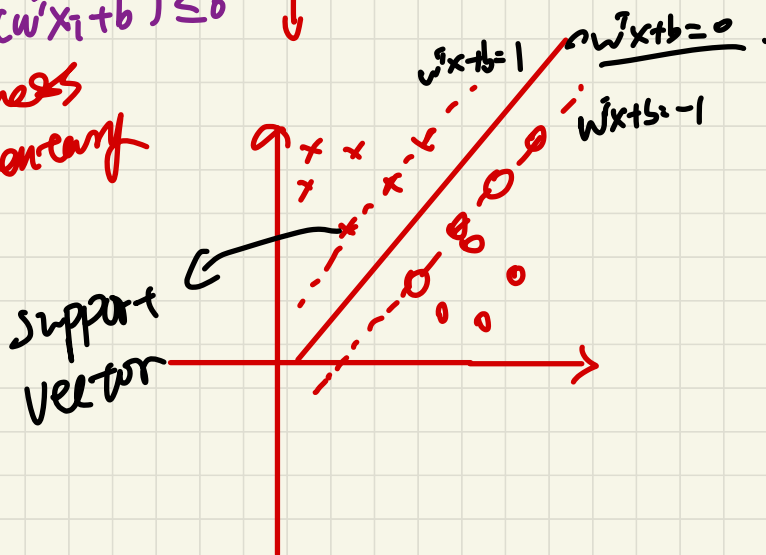
原问题, 对偶问题具有强对偶关系

\Leftrightarrow 满足 KKT 条件

$w^* = \sum_{i=0}^N \lambda_i y_i x_i$

$\frac{\partial L}{\partial w} = 0, \frac{\partial L}{\partial b} = 0$
 $\lambda_i (1 - y_i (w^T x_i + b)) = 0$
 $\lambda_i \geq 0$
 $1 - y_i (w^T x_i + b) \leq 0$

Slack needs complementarity



Soft margin - SVM

model: $\begin{cases} \min_{w, b} \frac{1}{2} w^T w \\ \text{s.t. } y_i (w^T x_i + b) \geq 1 \\ \text{for } i = 1, 2, \dots, n \end{cases}$

soft = 允许一点点错误

$\min_{w, b} \frac{1}{2} w^T w + \text{loss}$

数学性质不好

① $\text{loss} = \sum_{i=1}^n \mathbb{I}(y_i (w^T x_i + b) < 1)$

没给定时数，关于 w 不连续
故不可导。

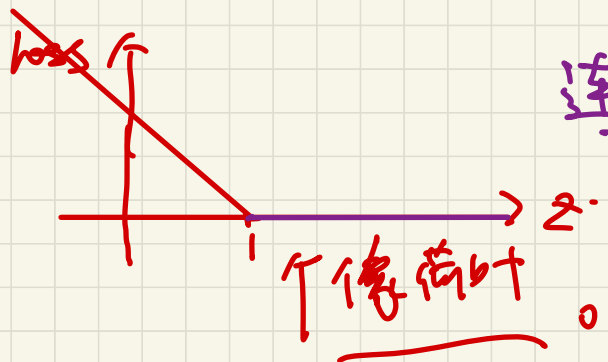
② $\text{loss} = \text{hinge loss}$

如果: $y_i (w^T x_i + b) \geq 1$. $\text{loss} = 0$

如果 $y_i (w^T x_i + b) < 1$, $\text{loss} = 1 - y_i (w^T x_i + b)$

$\text{loss} = \max \{ 0, 1 - y_i (w^T x_i + b) \}$

$\text{loss}_{\max} = \max \{ 0, 1 - z \}$



连续可导。

\therefore soft-margin \rightsquigarrow 允许存在噪声 noise

$$\begin{cases} \min_{w, b} \frac{1}{2} w^T w + c \sum_{i=1}^N \max\{0, 1 - y_i(w^T x_i + b)\} \\ \text{s.t. } y_i(w^T x_i + b) \geq 1 - \xi_i \end{cases}$$

$$\xi_i = 1 - y_i(w^T x_i + b), \xi_i \geq 0$$

$$\begin{cases} \min_{w, b} \frac{1}{2} w^T w + c \sum_{i=1}^N \xi_i \\ \text{s.t. } y_i(w^T x_i + b) \geq 1 - \xi_i \\ \xi_i \geq 0 \end{cases}$$

弱对偶性的证明:

Primal Problem

$$\begin{cases} \min_{x \in R} f(x) \\ \text{s.t. } m_i(x) \leq 0, \text{ for } i=1 \dots m \\ n_j(x) = 0, \text{ for } j=1 \dots n \end{cases}$$

拉格朗日函数: $L(x, \lambda, \eta) = f(x) + \sum_{i=1}^M \lambda_i m_i + \sum_{j=1}^N \eta_j n_j$

对偶问题

$$\begin{cases} \min_x \max_{\lambda, \eta} L(x, \lambda, \eta) \\ \text{s.t. } \lambda_i \geq 0 \end{cases}$$

$$\text{证: } \min_x \max_{\lambda, \eta} L(x, \lambda, \eta) \geq \max_{\lambda, \eta} \min_x L(x, \lambda, \eta)$$

$$\underbrace{\min_x L(x, \lambda, \eta)}_{F(\lambda, \eta)} \leq L(x, \lambda, \eta) \leq \underbrace{\max_{\lambda, \eta} L(x, \lambda, \eta)}_{G(x)}$$

$$F(\lambda, \eta) \leq G(x)$$

$$\therefore F(\lambda, \eta) \leq \min_x G(x)$$

$$\therefore \max_{\lambda, \eta} F(\lambda, \eta) \leq \min_x G(x)$$

$$\therefore \max_{\lambda, \eta} \min_x L \leq \min_x \max_{\lambda, \eta} L$$

弱对偶性

得证 //

对偶性的几何解释

为了方便表示, 我们将不等式约束是单-的而且没有等式约束。

∴ primal problem:

$$\begin{cases} \min_{x \in \mathbb{R}^n} f(x) \\ m(x) \leq 0 \end{cases}$$

$x \in D$ D 为定义域

设 $G = \{ (m(x), f(x)) \mid x \in D \}$

为了一般化, 设其图像为凸的。

而 Dual problem 为

$$\begin{cases} \max_{\lambda} \min_x L(\lambda, x) \\ \lambda \geq 0 \end{cases}$$

assuming p^* 为 primal p 的最优解

∴ $p^* = \inf \{ u \mid t \leq 0, (t, u) \in G \}$

→ 几何解释

$$\min_x L(\lambda, x) = \min_x f(x) + \lambda m(x) = \min_x \frac{u + \lambda t}{1}$$

∴ $\min_x L(\lambda, x) = \inf \{ u + \lambda t \mid (t, u) \in G \} = L^*$

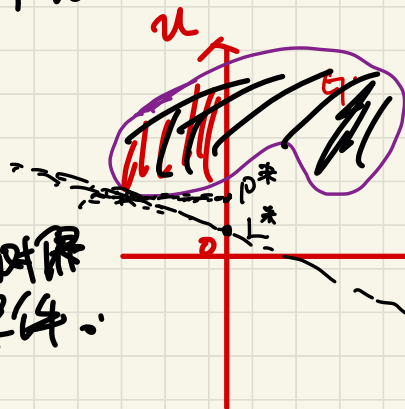
∴ $d^* = \max L^*$

∴ 可作图:

$$L^* \leq p^*$$

$$d^* \leq p^*$$

弱对偶条件



为解释为直线的直线在 u 上的值。



如果圆形 G 为凸的,

那么就有 $d^* = p^*$ \Rightarrow 强对偶条件。

Slater condition:

$Slater \text{ on } \Omega \Rightarrow$ 强对偶

$\exists \bar{x}$, 满足 $m_i(\bar{x}) < 0$

\uparrow
recting of D (D 的内部点)

可以理解为
约束函数 m_i
一阶线性函数。

放松的 Slater condition

如果 N 个不等式约束, 存在 K 个仿射函数。

则只需要 \bar{x} 满足剩下 $N-K$ 个不等式约束即可

即 $\text{for } i=1, \dots, K, m_i(\bar{x}) < 0$ 。

由于凸二次规划问题的不等式约束

都为仿射函数

所以凸二次规划问题一定是满足放松的

Slater - condition 的 \Rightarrow 一定满足强对偶条件。

KKT 条件。

primal problem:

$$\begin{cases} \min_x f(x) \end{cases}$$

$$\text{s.t. } \begin{cases} m_i(x) \leq 0, i=1, \dots, m \\ h_j(x) = 0, j=1, \dots, n \end{cases}$$

$$L(x, \lambda, \eta) = f(x) + \sum_{i=1}^m \lambda_i m_i(x) + \sum_{j=1}^n \eta_j h_j(x)$$

$$g(\lambda, \eta) = \min_x L(x, \lambda, \eta)$$

Dual prob =

$$\begin{cases} \max_{\lambda, \eta} g(\lambda, \eta) \end{cases}$$

$$\text{s.t. } \lambda_i \geq 0, \text{ for } i=1, \dots, m$$

$$(d^* = p^*)$$

convex + Slater \Rightarrow strong Duality

$$\begin{array}{c} \updownarrow \\ \text{KKT} \end{array}$$

KKT condition:

$$\begin{cases} m_i(x^*) = 0 \\ \eta_j(x^*) = 0 \\ \lambda_i^* \geq 0 \\ \sum_{i=1}^M \lambda_i^* m_i(x^*) = 0 \end{cases}$$

互补松弛条件:

$$\sum_{i=1}^M \lambda_i^* m_i(x^*) = 0$$

梯度为0:

$$\frac{\partial L(x, \lambda^*, \eta^*)}{\partial x} = 0$$

强对偶
关系

$$\begin{aligned} d^* &= \max_{\lambda, \eta} g(\lambda, \eta) = g(\lambda^*, \eta^*) \\ &= \min_x L(x, \lambda^*, \eta^*) \\ &\leq L(x^*, \lambda^*, \eta^*) \\ &= f(x^*) + \sum_{i=1}^M \lambda_i^* m_i + \sum_{j=1}^N \eta_j^* n_j \\ &= f(x^*) + \sum_{i=1}^M \lambda_i^* m_i \end{aligned}$$

$$\sum_{i=1}^M \lambda_i^* m_i, m_i(x^*) \leq 0, \lambda_i^* \geq 0$$

$$\therefore m_i(x^*) \lambda_i^* \leq 0$$

①

$$\therefore f(x^*) = p^*$$

∵ 满足强对偶条件, ∴ 不满足半强对偶条件。

$$\therefore ① f(x^*) = f(x^*) + \sum_{i=1}^M \lambda_i^* m_i(x^*)$$

$$\Rightarrow \sum_{i=1}^M \lambda_i^* m_i(x^*) = 0 \text{ in 互补松弛条件}$$

$$② \because \min_x L(x, \lambda^*, \eta^*) = L(x^*, \lambda^*, \eta^*)$$

$$\therefore \frac{\partial L(x, \lambda^*, \eta^*)}{\partial x} \Big|_{x=x^*} = 0 \text{ — 梯度为0}$$