统计机器学习

(小班研讨)

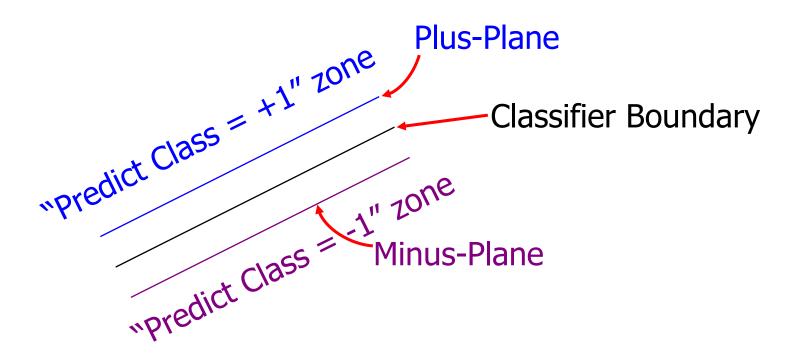


第4章 支持向量机与核方法

Support Vector Machines and Kernel Methods

线性可分支持向量机

Specifying a line and margin



- How do we represent this mathematically?
- ...in *m* input dimensions?

Specifying a line and margin

```
"Predict Class = +1" Plus-Plane
Classifier Boundary
Minus-Plane

"Predict Class = -1"

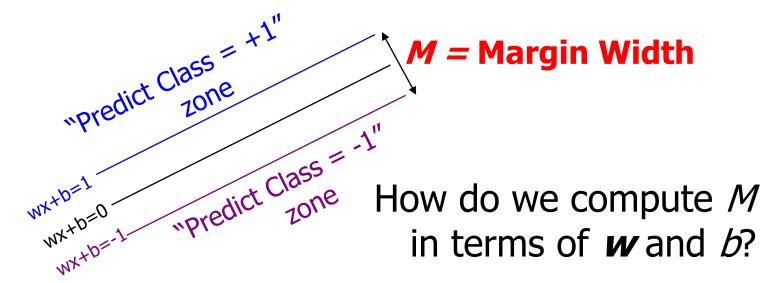
Wx+b=1 "Predict Class = -1"

Wx+b=-1 "Predict Class = -1"
```

- Plus-plane = $\{ x : w . x + b = +1 \}$
- Minus-plane = $\{ x : w . x + b = -1 \}$

Classify as.. +1 if
$$\mathbf{w} \cdot \mathbf{x} + b >= 1$$

-1 if $\mathbf{w} \cdot \mathbf{x} + b <= -1$
Universe if $-1 < \mathbf{w} \cdot \mathbf{x} + b < 1$
explodes

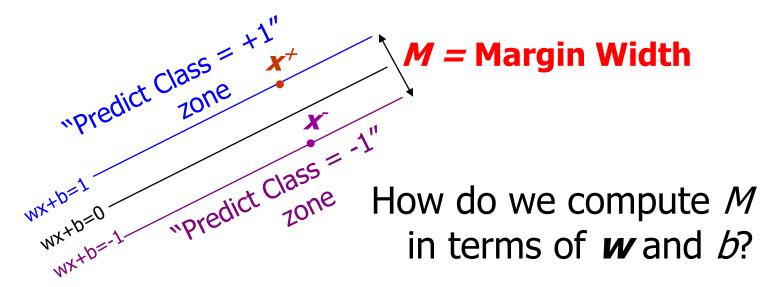


- Plus-plane = $\{ x : w . x + b = +1 \}$
- Minus-plane = $\{ x : w . x + b = -1 \}$

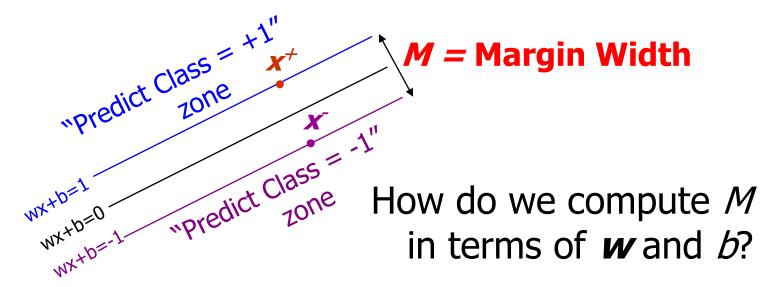
Claim: The vector w is perpendicular to the Plus Plane.

Why?

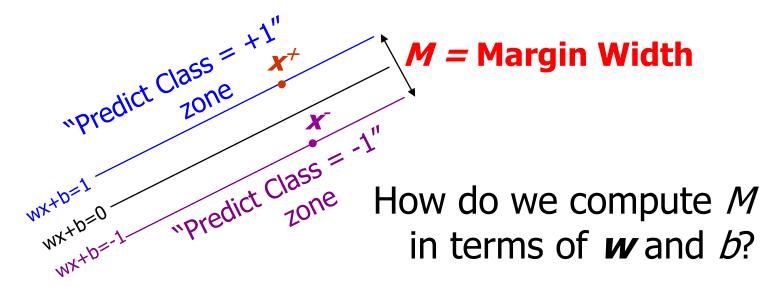
- Let \mathbf{u} and \mathbf{v} be two vectors on the Plus Plane. What is \mathbf{w} . $(\mathbf{u} \mathbf{v})$?
- And so of course the vector **w** is also perpendicular to the Minus Plane



- Plus-plane = $\{x: w.x + b = +1\}$
- Minus-plane = $\{ x : w . x + b = -1 \}$
- The vector w is perpendicular to the Plus Plane
- Let x be any point on the minus plane
 - Any location in R^m: not necessarily a datapoint
- Let **x**⁺ be the closest plus-plane-point to **x**⁻.
- Claim: $x^+ = x^- + \lambda w$ for some value of λ . Why?



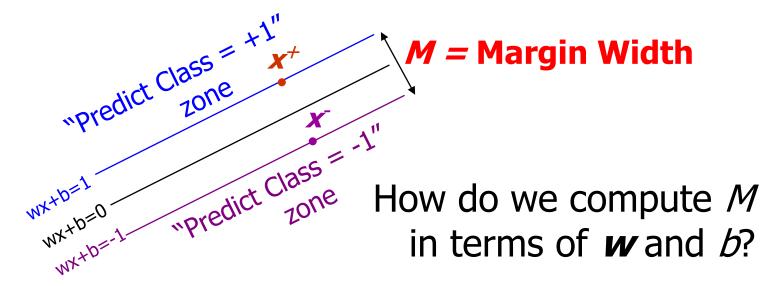
- Plus-plane = $\{ x : w . x + b = +1 \}$
- Minus-plane = $\{ x : w . x + b = -1 \}$
- Claim: $x^+ = x^- + \lambda w$ for some value of λ . Why?
 - The line from x to x is perpendicular to the planes.
 - So to get from x to x travel some distance in direction w.



What we know:

$$\mathbf{w} \cdot \mathbf{x}^+ + b = +1 \qquad \mathbf{w} \cdot \mathbf{x}^- + b = -1$$
$$\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w} \qquad \|\mathbf{x}^+ - \mathbf{x}^-\|_2 = M$$

It's now easy to get M in terms of w and b



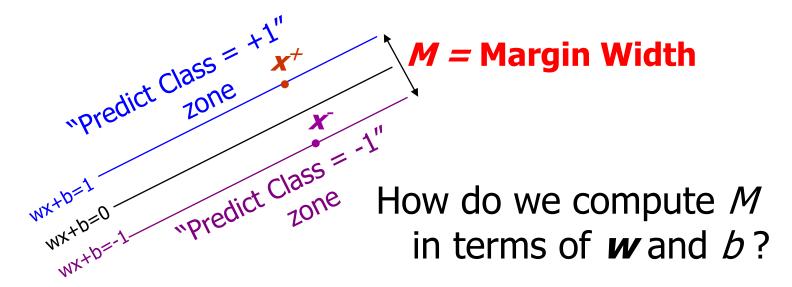
What we know:

$$\mathbf{w} \cdot \mathbf{x}^{+} + b = +1 \qquad \mathbf{w} \cdot (\mathbf{x}^{-} + \lambda \mathbf{w}) + b = 1$$

$$\mathbf{w} \cdot \mathbf{x}^{-} + b = -1 \qquad \mathbf{w} \cdot \mathbf{x}^{-} + b + \lambda \mathbf{w} \cdot \mathbf{w} = 1$$

$$\mathbf{x}^{+} = \mathbf{x}^{-} + \lambda \mathbf{w} \qquad -1 + \lambda \mathbf{w} \cdot \mathbf{w} = 1$$

$$\|\mathbf{x}^{+} - \mathbf{x}^{-}\|_{2} = M \qquad \lambda = \frac{2}{\|\mathbf{w}\|_{2}^{2}}$$



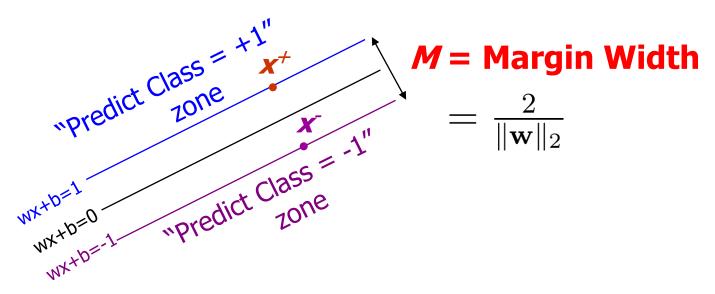
What we know:

$$\mathbf{w} \cdot \mathbf{x}^{+} + b = +1 \qquad \lambda = \frac{2}{\|\mathbf{w}\|_{2}^{2}}$$

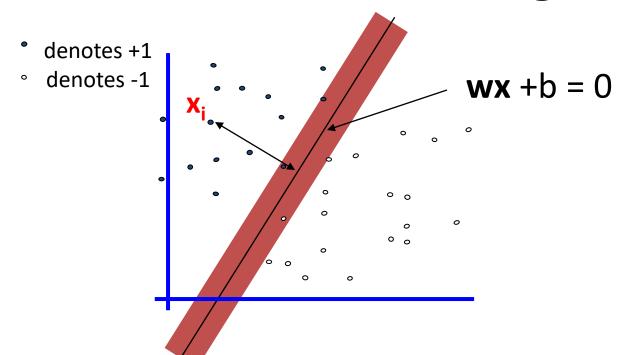
$$\mathbf{w} \cdot \mathbf{x}^{-} + b = -1 \qquad M = \|\mathbf{x}^{+} - \mathbf{x}^{-}\|_{2} = \|\lambda\mathbf{w}\|_{2} =$$

$$\mathbf{x}^{+} = \mathbf{x}^{-} + \lambda\mathbf{w} \qquad = \lambda \|\mathbf{w}\|_{2} = \lambda \sqrt{\|\mathbf{w}\|_{2}^{2}}$$

$$\|\mathbf{x}^{+} - \mathbf{x}^{-}\|_{2} = M \qquad = \frac{2\sqrt{\|\mathbf{w}\|_{2}^{2}}}{\|\mathbf{w}\|_{2}^{2}} = \frac{2}{\|\mathbf{w}\|_{2}}$$



- Given a guess of w and b we can
 - Compute whether all data points in the correct half-planes
 - Compute the width of the margin How?
- We just need to write a program to search the space of w's and b's to find the widest margin that matches all the datapoints.
 - Gradient descent? Simulated Annealing?
 - Matrix Inversion? EM? Newton's Method?



What is the distance expression for a point (x_i, y_i) to a line wx+b= 0?

$$d(\mathbf{x}_i) = \frac{y_i(\mathbf{x} \cdot \mathbf{w} + b)}{\|\mathbf{w}\|_2} = \frac{y_i(\mathbf{x} \cdot \mathbf{w} + b)}{\sqrt{\mathbf{w}^T \mathbf{w}}}$$

What is the expression for margin?

Min-max problem → game problem

Min-max problem

$$\underset{\mathbf{w},b}{\operatorname{argmax}} \quad \min_{\mathbf{x}_{i} \in D} \frac{y_{i}(\mathbf{x} \cdot \mathbf{w} + b)}{\sqrt{\mathbf{w}^{T} \mathbf{w}}}$$
subject to $\forall \mathbf{x}_{i} \in D : y_{i}(\mathbf{x}_{i} \cdot \mathbf{w} + b) \geq 0$

• 线性可分支持向量机的最优化问题

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \frac{1}{2} \mathbf{w}^T \mathbf{w}$$
 Quadratic criterion

subject to
$$\forall \mathbf{x}_i \in D : y_i (\mathbf{x}_i \cdot \mathbf{w} + b) \geq 1$$
 多少个不等式? linear constraints

How to solve it? Quadratic Programming?

Quadratic Programming

• optimal $\mathbf{u} = QP(\mathbf{Q}, \mathbf{p}, \mathbf{A}, \mathbf{c})$

$$\min_{\mathbf{u}} \ \frac{1}{2} \mathbf{u}^T \mathbf{Q} \mathbf{u} + \mathbf{p}^T \mathbf{u}$$
subject to $\mathbf{a}_i^T \mathbf{u} \ge c_i$, for $i = 1, 2, \dots, N$

• optimal $(b, \mathbf{w}) = QP(\mathbf{Q}, \mathbf{p}, \mathbf{A}, \mathbf{c})$

$$\min_{\mathbf{u}} \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

subject to
$$y_i (\mathbf{x}_i \cdot \mathbf{w} + b) \ge 1$$
 for $i = 1, 2, \dots, N$

- objective function: $\mathbf{u} = egin{bmatrix} b \\ \mathbf{w} \end{bmatrix} \ \mathbf{Q} = egin{bmatrix} 0 & \mathbf{0}_k^T \\ \mathbf{0}_k & \mathbf{I}_k \end{bmatrix} \ \mathbf{p} = \mathbf{0}_{k+1}$
- constraints: $\mathbf{a}_i^T = y_i[1 \ \mathbf{x}_i^T]$ $c_i = 1$ $N: \# \operatorname{data} \operatorname{set}$

Quize

• objective function:
$$\mathbf{u} = egin{bmatrix} b \\ \mathbf{w} \end{bmatrix}$$
 $\mathbf{Q} = egin{bmatrix} 0 & \mathbf{0}_k^T \\ \mathbf{0}_k & \mathbf{I}_k \end{bmatrix}$ $\mathbf{p} = \mathbf{0}_{k+1}$

- constraints: $\mathbf{a}_i^T = y_i[1 \ \mathbf{x}_i^T]$ $c_i = 1$ $N: \# \operatorname{data} \operatorname{set}$
- Consider two **negative** examples with $\mathbf{x}_1 = (0,0)$ and $\mathbf{x}_2 = (2,2)$
- And two **positive** examples with $\mathbf{x}_3 = (2,0)$ and $\mathbf{x}_4 = (3,0)$
- Define u, Q, p, c as those listed above.
 Reference Answer: 4
- What are \mathbf{a}_i^T that need to be fed into the QP solver?

(1)
$$a_1^T = [-1, 0, 0], \ a_2^T = [-1, 2, 2], \ a_3^T = [-1, 2, 0], \ a_4^T = [-1, 3, 0]$$

(2)
$$a_1^T = [1, 0, 0], \ a_2^T = [1, -2, -2], \ a_3^T = [-1, 2, 0], \ a_4^T = [-1, 3, 0]$$

(3)
$$a_1^T = [1, 0, 0], \quad a_2^T = [1, 2, 2], \quad a_3^T = [1, 2, 0], \quad a_4^T = [1, 3, 0]$$

$$(4) \quad a_1^T = [-1, 0, 0], \ a_2^T = [-1, -2, -2], \ a_3^T = [1, 2, 0], \ a_4^T = [1, 3, 0]$$

QP with k + 1 variables and N constraints

$$(b, \mathbf{w}) = QP(\mathbf{Q}, \mathbf{p}, \mathbf{A}, \mathbf{c})$$
 $\mathbf{Q} = \begin{bmatrix} 0 & \mathbf{0}_k^T \\ \mathbf{0}_k & \mathbf{I}_k \end{bmatrix}$ $\mathbf{a}_i^T = y_i[1 \ \mathbf{x}_i^T]$ $c_i = 1$

- Challenging if k large? could reach infinite size in theory!
- Goal: SVM without dependence on k
 - Original SVM : convex QP of
 - k+1 variables, N constraints
 - Equivalent SVM : convex QP of
 - N variables, N+1 constraints
- How? Lagrange Multipliers
 - Build Equivalent SVM based on dual problem of Original SVM

Recap: Linear SVM

Min-max problem

$$\underset{\mathbf{w},b}{\operatorname{argmax}} \quad \min_{\mathbf{x}_{i} \in D} \frac{y_{i}(\mathbf{x} \cdot \mathbf{w} + b)}{\sqrt{\mathbf{w}^{T} \mathbf{w}}}$$
subject to $\forall \mathbf{x}_{i} \in D : y_{i}(\mathbf{x}_{i} \cdot \mathbf{w} + b) \geq 0$

• 线性可分支持向量机的最优化问题

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \frac{1}{2} \mathbf{w}^T \mathbf{w}$$
 Quadratic criterion

subject to
$$\forall \mathbf{x}_i \in D : y_i (\mathbf{x}_i \cdot \mathbf{w} + b) \geq 1$$

linear constraints

How to solve it? Quadratic Programming?

Lagrange Dual Problem

• 定义拉格朗日函数:引入拉格朗日乘子 $\alpha_i \geq 0, i = 1, \ldots, N$

$$\mathcal{L}(\mathbf{w}, b, \alpha) = \frac{1}{2} ||\mathbf{w}||_2^2 - \sum_{i=1}^N \alpha_i \left\{ 1 - y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \right\}$$

• 固定 (\mathbf{w}, b) , 对于任意给定的 α' (其中 $\alpha'_i \geq 0$)

$$\min_{\mathbf{w},b} \left(\max_{all \ \alpha_i \ge 0} \mathcal{L}(\mathbf{w},b,\alpha) \right) \ge \min_{\mathbf{w},b} \ \mathcal{L}(\mathbf{w},b,\alpha')$$

• 对于上式右侧的最优 α' (其中 $\alpha'_i \geq 0$) , 有:

$$\min_{\mathbf{w},b} \left(\max_{all \ \alpha_i \geq 0} \mathcal{L}(\mathbf{w},b,\alpha) \right) \geq \max_{all \ \alpha_i' \geq 0} \left(\min_{\mathbf{w},b} \ \mathcal{L}(\mathbf{w},b,\alpha') \right)$$

- 拉格朗日对偶问题:
 - 外层是关于 α 的最大化问题,内层则是原始问题的下界

• 由拉格朗日对偶性可知:原始问题的对偶问题是max-min问题

$$\min_{\mathbf{w},b} \left(\max_{all \ \alpha_i \geq 0} \mathcal{L}(\mathbf{w},b,\alpha) \right) \geq \max_{all \ \alpha'_i \geq 0} \left(\min_{\mathbf{w},b} \ \mathcal{L}(\mathbf{w},b,\alpha') \right)$$

- 强对偶性: 若QP问题满足以下条件 (constraint qualification)
 - convex primal
 - feasible primal (true if $\Phi(\mathbf{x})$ separable)
 - linear constraints
- 满足强对偶性: 因此求解对偶问题即可
 - 思考: 如何求解上式右侧的二次规划问题?

Solving Lagrange Dual

$$\max_{all \ \alpha_i \ge 0} \left(\min_{\mathbf{w}, b} \ \frac{1}{2} \mathbf{w}^T \mathbf{w} + \sum_{i=1}^{N} \alpha_i (1 - y_i (\mathbf{w}^T \mathbf{x}_i + b)) \right)$$

- 注意到内部的最小化问题是无约束的
- 求解该对偶问题,应首先求得 \mathcal{L} 对 \mathbf{w}, b 的极小,再求对 \mathcal{L} 的极大

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, b, \alpha) = \mathbf{w} - \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i = 0 \implies \mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

$$\nabla_b \mathcal{L}(\mathbf{w}, b, \alpha) = -\sum_{i=1}^N \alpha_i y_i = 0$$
 $\Rightarrow \sum_{i=1}^N \alpha_i y_i = 0$

Solving Lagrange Dual

• 代入拉格朗日函数得到:

$$\mathcal{L}(\mathbf{w}, b, \alpha) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j) - \sum_{i=1}^{N} \alpha_i y_i \left(\left(\sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \right) \cdot \mathbf{x}_i + b \right) + \sum_{i=1}^{N} \alpha_i$$

$$= -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j) + \sum_{i=1}^{N} \alpha_i \qquad b \sum_{j=1}^{N} \alpha_j y_j = 0$$

• 即:

$$\min_{\mathbf{w},b} \mathcal{L}(\mathbf{w},b,\alpha) = -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j) + \sum_{i=1}^{N} \alpha_i$$

• 接下来求解上式对 α 的极大,即对偶问题

Solving Lagrange Dual

求解对偶问题

$$\max_{\alpha} \left(-\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j) + \sum_{i=1}^{N} \alpha_i \right)$$

s.t.
$$\sum_{i=1}^{N} \alpha_i y_i = 0; \quad \alpha_i \ge 0, \ i = 1, 2, \dots, N$$

• 将其转化为求极小,得到如下等价(对偶)问题:

$$\min_{\alpha} \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j) - \sum_{i=1}^{N} \alpha_i$$

s.t.
$$\sum_{i=1}^{N} \alpha_i y_i = 0; \quad \alpha_i \ge 0, \ i = 1, 2, \dots, N$$

Convex QP of N variables & N + 1 constraints!

Dual SVM with QP Solver

$$\min_{\alpha} \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j) - \sum_{i=1}^{N} \alpha_i$$

s.t.
$$\sum_{i=1}^{N} \alpha_i y_i = 0; \quad \alpha_i \ge 0, \ i = 1, 2, \dots, N$$

• optimal $\alpha = QP(\mathbf{Q}, \mathbf{p}, \mathbf{A}, \mathbf{c})$

$$\min_{\alpha} \frac{1}{2} \alpha^T \mathbf{Q} \mathbf{u} + \mathbf{p}^T \alpha$$

subject to $\mathbf{a}_i^T \alpha \ge c_i$, for $i = 1, 2, \dots, N$

- where: $\mathbf{Q}_{ij} = y_i y_j \mathbf{x}_i^T \mathbf{x}_j$
- Problem: if N = 30,000, dense Q takes > 3G RAM
 - need special solver for not storing whole Q by utilizing special constraints properly to scale up to large N

Karush-Kuhn-Tucker Optimality Conditions

- 如果原始问题和对偶问题有相同的最优解 (\mathbf{w}, b, α) , 需满足:
 - primal feasible: $y_i(\mathbf{w}^T\mathbf{x}_i + b) \ge 1$
 - dual feasible: $\alpha_i \geq 0$
 - dual-inner optimal: $\sum_{i=1}^{N} \alpha_i y_i = 0 \quad \mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$
 - primal-inner optimal: complimentary slackness
 - at optimal all Lagrange terms disappear

$$\alpha_i \left(1 - y_i(\mathbf{w}^T \mathbf{x}_i + b) \right) = 0$$

$$\min_{\mathbf{w},b} \left(\max_{all \ \alpha_i \geq 0} \mathcal{L}(\mathbf{w},b,\alpha) \right) \geq \max_{all \ \alpha_i' \geq 0} \left(\min_{\mathbf{w},b} \ \mathcal{L}(\mathbf{w},b,\alpha') \right)$$

Quize

• For a single variable \mathbf{w} , consider minimizing $\frac{1}{2}\mathbf{w}^2$ subject to two linear constraints $\mathbf{w} \geq 1$ and $\mathbf{w} \leq 3$. We know that the Lagrange function $\mathcal{L}(\mathbf{w},\alpha) = \frac{1}{2}\mathbf{w}^2 + \alpha_1(1-\mathbf{w}) + \alpha_2(\mathbf{w}-3)$

- Which of the following equations that contain α are among the KKT conditions of the optimization problem?
 - (1) $\alpha_1 \geq 0$ and $\alpha_2 \geq 0$
 - (2) $\mathbf{w} = \alpha_1 \alpha_2$
 - (3) $\alpha_1(1 \mathbf{w}) = 0 \text{ and } \alpha_2(\mathbf{w} 3)$
 - (4) all of the above

Reference Answer: 4

KKT Optimality Conditions

- 根据定理2和3可知,KKT条件成立
 - 设 $\alpha^* = (\alpha_1^*, \alpha_2^*, \dots, \alpha_l^*)$ 是对偶优化问题的解,由KKT条件可知

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}^*, b^*, \alpha^*) = \mathbf{w}^* - \sum_{i=1}^N \alpha_i^* y_i \mathbf{x}_i = 0$$

$$\nabla_b \mathcal{L}(\mathbf{w}^*, b^*, \alpha^*) = -\sum_{i=1}^N \alpha_i^* y_i = 0$$

$$\alpha_i^* (y_i (\mathbf{w}^* \cdot \mathbf{x}_i + b^*) - 1) = 0, \quad i = 1, 2, \dots, N$$

$$y_i (\mathbf{w}^* \cdot \mathbf{x}_i + b^*) - 1 \ge 0, \quad i = 1, 2, \dots, N$$

$$\alpha_i^* \ge 0, \quad i = 1, 2, \dots, N$$

由此可得:

$$\mathbf{w}^* = \sum_{i=1}^N \alpha_i^* y_i \mathbf{x}_i \quad b^* = y_j - \sum_{i=1}^N \alpha_i^* y_i (\mathbf{x}_i \cdot \mathbf{x}_j)$$

for any given $\alpha_i > 0$

Quize

• Consider two transformed examples $(\mathbf{x}_1, +1)$ and $(\mathbf{x}_2, -1)$ with $\mathbf{x}_1 = \mathbf{x}$ and $\mathbf{x}_2 = -\mathbf{x}$. After solving the dual problem of hard-margin SVM, assume that the optimal α_1 and α_2 are both strictly positive. What is the optimal b?

$$(1) -1 \qquad (2) 0 \qquad (3) 1$$

- (4) not certain with the descriptions above
- Hints: with the descriptions, \mathbf{x} located on the margin $y_i(\mathbf{w}^*\cdot\mathbf{x}+b^*)-1=0 \Rightarrow b^*=y_i-\mathbf{w}^*\cdot\mathbf{x}$

$$b^* = 1 - \mathbf{w}^* \cdot \mathbf{x} = -1 - \mathbf{w}^* \cdot (-\mathbf{x})$$
 Reference Answer: 2

分类超平面可以表示为:

$$\sum_{i=1}^{N} \alpha_i^* y_i(\mathbf{x} \cdot \mathbf{x}_i) + b^* = 0$$

分类决策函数可以表示为:

$$f(x) = \operatorname{sign}\left(\sum_{i=1}^{N} \alpha_i^* y_i(\mathbf{x} \cdot \mathbf{x}_i) + b^*\right)$$

- 分类决策函数只依赖于输入x和训练样本特征向量的内积
- 上式称为线性可分支持向量机的对偶形式

Support Vectors Revisited

• 将 $\alpha_i > 0$ 的样本 (\mathbf{x}_i, y_i) 称为 support vectors

$$SV$$
 (positive α_i) $\subseteq SV$ candidates (on boundary)

only SV needed to compute w:

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i = \sum_{SV} \alpha_i y_i \mathbf{x}_i$$

only SV needed to compute b:

$$b = y_i - \mathbf{w}^T \mathbf{x}_i$$
 with any SV: $(\mathbf{x}_i; y_i)$

- 支持向量机的基本思想: 求解最大边界的分类超平面
 - 方法: 通过求解对偶问题识别出支持向量

SVM与PLA的对比

SVM

PLA

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i(y_i \mathbf{x}_i)$$

$$\mathbf{w} = \sum_{i=1}^{N} \beta_i(y_i \mathbf{x}_i)$$

• α_i from dual solution

• β_i by # mistake corrections

$$\mathbf{w} = \text{linear combination of } y_i \mathbf{x}_i$$

- also true for SGD-based LogReg/LinReg when $w_0 = 0$
- call w represented by data
- SVM: represent w by support vectors only

Summary: Two Forms of Hard-Margin SVM

- Primal Hard-Margin SVM
 - k + 1 variables, N constraints
 - suitable when k small
 - physical meaning: locate specially-scaled (b, w)
- Dual Hard-Margin SVM
 - N variables, N + 1 simple constraints
 - suitable when N small思考:真的与k无关吗?
 - physical meaning: locate SVs (x_i, y_i) & their \alpha_i
- both result in optimal (b,w) for fattest hyperplane

$$g_{svm}(\mathbf{x}) = sign(\mathbf{w}^T\mathbf{x} + b)$$

