Machine Learning
(機器學習)

Lecture 10: Support Vector Machine (1)

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Roadmap

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn Better?
5. Embedding Numerous Features: Kernel Models

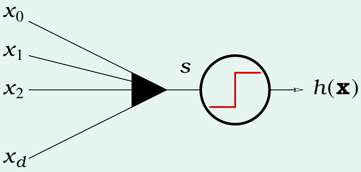
Lecture 10: Support Vector Machine (1)

- Large-Margin Separating Hyperplane
- Standard Large-Margin Problem
- Support Vector Machine
- Motivation of Dual SVM
- Lagrange Dual SVM
- Solving Dual SVM
- Messages behind Dual SVM

Linear Classification Revisited

PLA/pocket

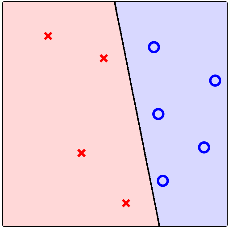
$$h(\mathbf{x}) = \text{sign}(s)$$



plausible err = 0/1

(small flipping noise)

minimize **specially**



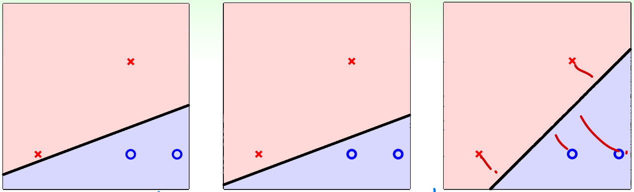
(linear separable)

data是线性可分

linear (hyperplane) classifiers:

$$h(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x})$$

Which Line Is Best?



↑答案不是唯一的 那條線好

- PLA? depending on randomness →不一定
- VC bound? whichever you like!

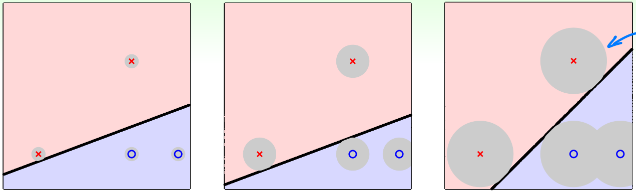
弱

$$E_{\text{out}}(\mathbf{w}) \le \underbrace{E_{\text{in}}(\mathbf{w})}_{0} + \underbrace{\Omega(\mathcal{H})}_{d_{\text{VC}}=d+1}$$

parameter都一樣.

You? **rightmost one, possibly :-)**

Why Rightmost Hyperplane?



noise tolenrence.

informal argument

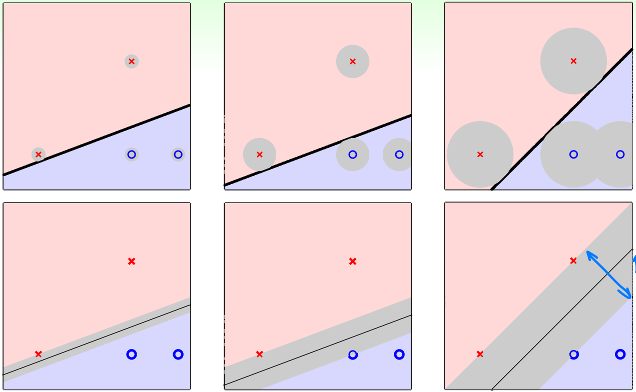
add noise.

if (Gaussian-like) noise on future $\mathbf{x} \approx \mathbf{x}_n$: 原始data.

$\mathbf{x}_n$ further from hyperplane	distance to closest $\mathbf{x}_n$
$\Longleftrightarrow$ tolerate more noise	$\Longleftrightarrow$ amount of noise tolerance
$\Longleftrightarrow$ more robust to overfitting	$\Longleftrightarrow$ robustness of hyperplane

rightmost one: **more robust**
because of **larger distance to closest $\mathbf{x}_n$**

Fat Hyperplane

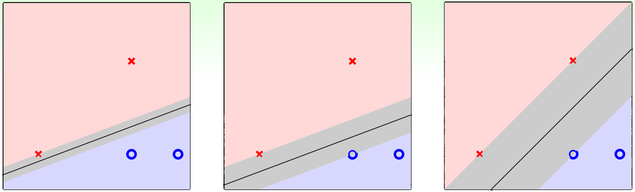


胖线较好.

- **robust** separating hyperplane: **fat**
  —far from both sides of examples
- **robustness** $\equiv$ **fatness**: distance to closest $\mathbf{x}_n$

goal: find fattest separating hyperplane

Large-Margin Separating Hyperplane



$$\max_{\mathbf{w}} \quad \text{fatness}(\mathbf{w})$$

找最胖的线

是線性可分的

subject to $\quad \mathbf{w}$ classifies every $(\mathbf{x}_n, y_n)$ correctly

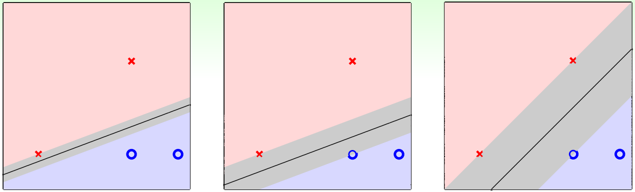
$$\text{fatness}(\mathbf{w}) = \boxed{\min_{n=1,\ldots,N} \text{distance}(\mathbf{x}_n, \mathbf{w})}$$

找最小距離

- fatness: formally called **margin**
- correctness: $y_n = \text{sign}(\mathbf{w}^T \mathbf{x}_n)$ ← 所有in-sample都是对的

goal: find **largest-margin**
separating hyperplane

Large-Margin Separating Hyperplane



$$\max_{\mathbf{w}} \quad \text{margin}(\mathbf{w})$$

subject to every $y_n \mathbf{w}^T \mathbf{x}_n > 0$ ←correctness

$$\text{margin}(\mathbf{w}) = \min_{n=1,\ldots,N} \text{distance}(\mathbf{x}_n, \mathbf{w})$$

- fatness: formally called **margin**
- correctness: $y_n = \text{sign}(\mathbf{w}^T \mathbf{x}_n)$

goal: find **largest-margin** **separating** hyperplane

Questions?

Distance to Hyperplane: Preliminary

$$\max_{\mathbf{w}} \quad \text{margin}(\mathbf{w})$$

subject to every $y_n \mathbf{w}^T \mathbf{x}_n > 0$

$$\text{margin}(\mathbf{w}) = \min_{n=1,\ldots,N} \text{distance}(\mathbf{x}_n, \mathbf{w})$$

截距

'shorten' x and w

distance needs w_0 and $(w_1, \ldots, w_d)$ differently (to be derived)

bias 分开 不把 w_0 放进去

$$b = w_0 \qquad ; \qquad \cancel{x_0 = 1}$$

$$\begin{bmatrix} | \\ \mathbf{w} \\ | \end{bmatrix} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix} ; \begin{bmatrix} | \\ \mathbf{x} \\ | \end{bmatrix} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$

for this part: $h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$

Distance to Hyperplane

want: distance($\mathbf{x}, b, \mathbf{w}$), with hyperplane $\mathbf{w}^T\mathbf{x}' + b = 0$

因為方程式要滿足

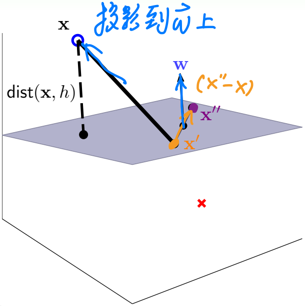
consider $\mathbf{x}'$, $\mathbf{x}''$ on hyperplane

1. $\mathbf{w}^T\mathbf{x}' = -b$, $\mathbf{w}^T\mathbf{x}'' = -b$
2. $\mathbf{w} \perp$ hyperplane:

平面的法向量

$$\left(\mathbf{w}^T \underbrace{(\mathbf{x}'' - \mathbf{x}')}_{\text{vector on hyperplane}} \right) = 0 \qquad -b-(-b)$$

3. distance = project $(\mathbf{x} - \mathbf{x}')$ to $\perp$ hyperplane



$$-\frac{w^T}{\|w\|}x' = \frac{+b}{\|w\|}$$

$$\text{distance}(\mathbf{x}, b, \mathbf{w}) = \underbrace{\left| \frac{\mathbf{w}^T}{\|\mathbf{w}\|}(\mathbf{x} - \mathbf{x}') \right|}_{\text{投影}} \overset{(1)}{=} \frac{1}{\|\mathbf{w}\|} |\mathbf{w}^T\mathbf{x} + b|$$

Distance to Separating Hyperplane

$$\text{distance}(\mathbf{x}, b, \mathbf{w}) = \frac{1}{\|\mathbf{w}\|}|\mathbf{w}^T\mathbf{x} + b|$$

- **separating** hyperplane: for every n

correctness

$$y_n(\mathbf{w}^T\mathbf{x}_n + b) > 0$$

- distance to **separating** hyperplane:

乘上y_n後 abs 可以拿掉

$$\text{distance}(\mathbf{x}_n, b, \mathbf{w}) = \frac{1}{\|\mathbf{w}\|}y_n(\mathbf{w}^T\mathbf{x}_n + b)$$

$$(\alpha_n x_n^2 + b)\frac{1}{\|\Sigma\|}$$

$$\Sigma \alpha_n y_n x_n$$

$$\max_{b,\mathbf{w}} \quad \text{margin}(b, \mathbf{w})$$

subject to every $y_n(\mathbf{w}^T\mathbf{x}_n + b) > 0$

$$\text{margin}(b, \mathbf{w}) = \min_{n=1,\ldots,N} \frac{1}{\|\mathbf{w}\|}y_n(\mathbf{w}^T\mathbf{x}_n + b)$$

Margin of **Special** Separating Hyperplane

$$\max_{b,\mathbf{w}} \quad \text{margin}(b, \mathbf{w})$$

subject to every $y_n(\mathbf{w}^T \mathbf{x}_n + b) > 0$

$$\text{margin}(b, \mathbf{w}) = \min_{n=1,\ldots,N} \frac{1}{\|\mathbf{w}\|} \underbrace{y_n(\mathbf{w}^T \mathbf{x}_n + b)}_{=1}$$

- $\mathbf{w}^T \mathbf{x} + b = 0$ same as $3\mathbf{w}^T \mathbf{x} + 3b = 0$: scaling does not matter
- **special** scaling: only consider separating $(b, \mathbf{w})$ such that

強制scale

$$\min_{n=1,\ldots,N} y_n(\mathbf{w}^T \mathbf{x}_n + b) = 1 \Longrightarrow \text{margin}(b, \mathbf{w}) = \frac{1}{\|\mathbf{w}\|} \cdot 1$$

$$\max_{b,\mathbf{w}} \quad \frac{1}{\|\mathbf{w}\|}$$

subject to ~~every $y_n(\mathbf{w}^T \mathbf{x}_n + b) > 0$~~ 消掉了, =1 較嚴格

$$\min_{n=1,\ldots,N} y_n(\mathbf{w}^T \mathbf{x}_n + b) = 1$$

新condition.

Standard Large-Margin Hyperplane Problem

$$\max_{b,\mathbf{w}} \quad \frac{1}{\|\mathbf{w}\|} \quad \text{subject to} \quad \min_{n=1,\ldots,N} \quad y_n(\mathbf{w}^T\mathbf{x}_n + b) = 1$$

necessary constraints: $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1$ for all n

relax

放鬆條件也沒有損失

original constraint: $\min_{n=1,\ldots,N} \; y_n(\mathbf{w}^T\mathbf{x}_n + b) = 1$

want: optimal $(b, \mathbf{w})$ **here (inside)**

反證法：證不可能所有 x_n 都 >1，會取 =1

if optimal $(b, \mathbf{w})$ outside, e.g. $y_n(\mathbf{w}^T\mathbf{x}_n + b) > 1.126$ for all n

—can scale $(b, \mathbf{w})$ to "more optimal" $\left(\frac{b}{1.126}, \frac{\mathbf{w}}{1.126}\right)$ **(contradiction!)**

scale

$\|w\|\downarrow$, $\frac{1}{\|w\|}\uparrow$，這是解更好

(b,w) 不是 optimal：$\rightarrow\leftarrow$.

final change: max $\Longrightarrow$ min, remove $\sqrt{\ }$, add $\frac{1}{2}$

$\frac{1}{\|w\|} \Rightarrow \|w\| \Rightarrow w^Tw \Downarrow \frac{1}{2}w^Tw$

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

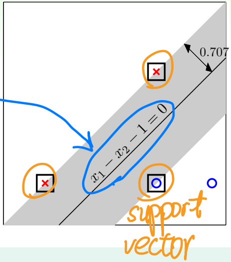
$$\text{subject to} \quad y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 \text{ for all } n$$

Questions?

Support Vector Machine (SVM)

optimal solution: $(w_1 = 1, w_2 = -1, b = -1)$

margin$(b, \mathbf{w})$ $= \frac{1}{\|\mathbf{w}\|} = \frac{1}{\sqrt{2}}$



- examples on boundary: 'locates' fattest hyperplane
  other examples: **not needed** ← 把這些点去掉也不影响
- call boundary example **support vector** (candidate)

support vector machine (SVM):
learn **fattest hyperplanes**
(with help of **support vectors**)

Solving General SVM

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

$$\text{subject to} \quad y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 \text{ for all } n$$

- **not easy manually, of course :-)**
- gradient descent? **not easy with constraints**
- luckily: 限制式:W的二次function
  - (convex) quadratic objective function of $(b, \mathbf{w})$
  - linear constraints of $(b, \mathbf{w})$

—**quadratic programming**

quadratic programming (QP):
'easy' optimization problem

Quadratic Programming

optimal $(b, \mathbf{w}) = ?$

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

subject to $\quad y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1,$

for $n = 1, 2, \ldots, N$

optimal $\mathbf{u} \leftarrow \mathrm{QP}(\mathrm{Q}, \mathbf{p}, \mathrm{A}, \mathbf{c})$

u的二次函數　　一次項係數

$$\min_{\mathbf{u}} \quad \underbrace{\frac{1}{2}\mathbf{u}^T\mathrm{Q}\mathbf{u} + \mathbf{p}^T\mathbf{u}}$$

2次項係數

subject to $\quad \mathbf{a}_m^T\mathbf{u} \geq c_m,$

for $m = 1, 2, \ldots, M$

欲求的 variable.　　一次式限制

沒有一次項

objective function: $\mathbf{u} = \begin{bmatrix} b \\ \mathbf{w} \end{bmatrix}$; $\mathrm{Q} = \begin{array}{c|cc} & [b & \mathbf{w}] \\ \hline b & 0 & \mathbf{0}_d^T \\ \mathbf{w} & \mathbf{0}_d & \mathrm{I}_d \end{array}$; $\mathbf{p} = \mathbf{0}_{d+1}$

constraints: $\mathbf{a}_n^T = y_n \begin{bmatrix} 1 & \mathbf{x}_n^T \end{bmatrix}$; $c_n = 1$; $M = N$

SVM with general QP solver:
easy **if you've read the manual :-)**

wTF

SVM with QP Solver

Linear Hard-Margin SVM Algorithm

1. $Q = \begin{bmatrix} 0 & \mathbf{0}_d^T \\ \mathbf{0}_d & \mathrm{I}_d \end{bmatrix}$; $\mathbf{p} = \mathbf{0}_{d+1}$; $\mathbf{a}_n^T = y_n \begin{bmatrix} 1 & \mathbf{x}_n^T \end{bmatrix}$; $c_n = 1$
2. $\begin{bmatrix} b \\ \mathbf{w} \end{bmatrix} \leftarrow \mathrm{QP}(Q, \mathbf{p}, A, \mathbf{c})$
3. return b & $\mathbf{w}$ as g_{SVM}

坚持所有点都要分开

- **hard-margin**: nothing violate 'fat boundary'
- **linear**: $\mathbf{x}_n$ ← 找分隔线

want **non-linear**?

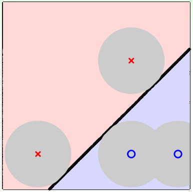
$\mathbf{z}_n = \Phi(\mathbf{x}_n)$—**remember? :-)**

Why Large-Margin Hyperplane?

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

$$\text{subject to} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 \text{ for all } n$$

転成z空間



对調

一体2面

	minimize	constraint
regularization	E_{in}	$\mathbf{w}^T\mathbf{w} \leq C$
SVM	$\mathbf{w}^T\mathbf{w}$	$E_{\text{in}} = 0$ [and more]

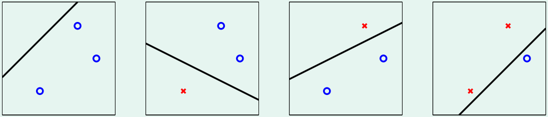
SVM (large-margin hyperplane):
'weight-decay regularization' within $E_{\text{in}} = 0$

Large-Margin Restricts Dichotomies

consider 'large-margin algorithm' $\mathcal{A}_\rho$:
either **returns g with margin$(g) \geq \rho$ (if exists)**, or 0 otherwise

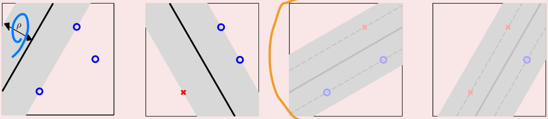
$\mathcal{A}_0$: like PLA $\Longrightarrow$ shatter 'general' 3 inputs

3 input 能 shatter



$\mathcal{A}_{1.126}$: more strict than SVM $\Longrightarrow$ cannot shatter any 3 inputs

但多了限制 ρ寬度



找到ρ=11.26 的 "linear"

fewer dichotomies $\Longrightarrow$ smaller 'VC dim.' $\Longrightarrow$ **better generalization**

VC Dimension of Large-Margin Algorithm

fewer dichotomies $\Longrightarrow$ smaller **'VC dim.'**

considers $d_{\text{VC}}(\mathcal{A}_\rho)$ [data-dependent, need more than VC]

instead of $d_{\text{VC}}(\mathcal{H})$ [data-independent, covered by VC]

generally, when $\mathcal{X}$ in radius-R hyperball:

比原本小

$$d_{\text{VC}}(\mathcal{A}_\rho) \le \min\left(\frac{R^2}{\rho^2}, d\right) + 1 \le \underbrace{d+1}_{d_{\text{VC}}(\text{perceptrons})}$$

ρ是限制的宽度

Benefits of Large-Margin Hyperplanes

	large-margin hyperplanes	hyperplanes	hyperplanes + feature transform Φ
#	even fewer	**not many**	many
boundary	simple	simple	**sophisticated**

- **not many** good, for d_{VC} and generalization
- **sophisticated** good, for possibly better E_{in}

a new possibility: non-linear SVM

	large-margin ✓ **hyperplanes + numerous feature transform Φ** ✓
#	**not many**
boundary	**sophisticated**

ŹŹ win

Questions?

Non-Linear Support Vector Machine Revisited

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

做了転換

$$\text{s. t.} \quad y_n(\mathbf{w}^T \underbrace{\mathbf{z}_n}_{\Phi(\mathbf{x}_n)} + b) \geq 1,$$

$$\text{for } n = 1, 2, \ldots, N$$

Non-Linear Hard-Margin SVM

1. $\mathrm{Q} = \begin{bmatrix} 0 & \mathbf{0}_{\tilde{d}}^T \\ \mathbf{0}_{\tilde{d}} & \mathrm{I}_{\tilde{d}} \end{bmatrix}$; $\mathbf{p} = \mathbf{0}_{\tilde{d}+1}$; $\mathbf{a}_n^T = y_n \begin{bmatrix} 1 & \mathbf{z}_n^T \end{bmatrix}$; $c_n = 1$
2. $\begin{bmatrix} b \\ \mathbf{w} \end{bmatrix} \leftarrow \mathrm{QP}(\mathrm{Q}, \mathbf{p}, \mathrm{A}, \mathbf{c})$
3. return $b \in \mathbb{R}$ & $\mathbf{w} \in \mathbb{R}^{\tilde{d}}$ with $g_{\text{SVM}}(\mathbf{x}) = \text{sign}(\mathbf{w}^T\Phi(\mathbf{x}) + b)$

控制模型複雜度

- demanded: **not many** (large-margin), but **sophisticated** boundary (feature transform)
- QP with $\tilde{d} + 1$ variables and N constraints —challenging if $\tilde{d}$ large, **or infinite?! :-)**

W dimension 很大?

goal: SVM **without dependence on $\tilde{d}$**

Todo: SVM 'without' $\tilde{d}$

Original SVM

(convex) QP of

- $\tilde{d} + 1$ variables
- N constraints

'Equivalent' SVM

(convex) QP of

- N variables
- $N + 1$ constraints

只跟N有关
N= # of data.

Warning: Heavy Math!!!!!!

- introduce some necessary math without rigor to help **understand SVM deeper**
- **'claim' some results** if details unnecessary
  —like how we 'claimed' Hoeffding

对偶問題

'Equivalent' SVM: based on some **dual problem** of Original SVM

Key Tool: Lagrange Multipliers

乘上係數的 constraint

Regularization by Constrained-Minimizing E_{in}	$\Leftrightarrow$	Regularization by Minimizing E_{aug}
$\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w})$ s.t. $\mathbf{w}^T\mathbf{w} \le C$	rid of constraint	$\min_{\mathbf{w}} E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^T\mathbf{w}$

W長度不能太大

- C equivalent to some $\lambda \geq 0$ by checking **optimality condition**

$$\nabla E_{\text{in}}(\mathbf{w}) + \frac{2\lambda}{N}\mathbf{w} = \mathbf{0}$$

- regularization: view λ as **given parameter instead of C**, and solve 'easily'
- dual SVM: view λ's as unknown given the constraints, and **solve them as variables instead** 把λ當變數

how many λ's as variables? SVM有N個constraint.

N—one per constraint

Starting Point: Constrained to 'Unconstrained'

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

$-(w^T z_n + b) \geq \rho_-$

$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1, \quad \text{for } n = 1, 2, \ldots, N$$

$\Rightarrow$

Lagrange Function

with Lagrange multipliers ~~λ_n~~ α_n,

係數

$$\mathcal{L}(b, \mathbf{w}, \boldsymbol{\alpha}) = \underbrace{\frac{1}{2}\mathbf{w}^T\mathbf{w}}_{\text{objective}} + \sum_{n=1}^{N} \alpha_n \underbrace{(1 - \cancel{y_n}(\mathbf{w}^T\mathbf{z}_n + b))}_{\text{constraint}}$$

1

$+\sum \alpha_n(\rho_- + w^T z_n + b)$

Claim

沒有constraint的最佳化

$$\text{SVM} \equiv \min_{b,\mathbf{w}} \left(\max_{\text{all } \alpha_n \geq 0} \mathcal{L}(b, \mathbf{w}, \boldsymbol{\alpha}) \right) = \min_{b,\mathbf{w}} \left(\infty \text{ if violate} ; \frac{1}{2}\mathbf{w}^T\mathbf{w} \text{ if feasible} \right)$$

調α s.t $\mathcal{L}(\ )$最大

- any 'violating' $(b, \mathbf{w})$: $\max_{\text{all } \alpha_n \geq 0} \left(\square + \sum_n \alpha_n (\text{some positive}) \right) \to \infty$ — α趕到∞

  壞(b,w)得到∞

- any 'feasible' $(b, \mathbf{w})$: $\max_{\text{all } \alpha_n \geq 0} \left(\square + \sum_n \alpha_n (\text{all non-positive}) \right) = \square$

  optimal. value.

使得式子看起來沒constraint

constraints now **hidden in** max

Questions?

Strong Duality of Quadratic Programming

min, max 做交換

$$\underbrace{\min_{b,\mathbf{w}}\left(\max_{\text{all }\alpha_n\ge 0}\mathcal{L}(b,\mathbf{w},\boldsymbol{\alpha})\right)}_{\text{equiv. to original (primal) SVM}} = \underbrace{\max_{\text{all }\alpha_n\ge 0}\left(\min_{b,\mathbf{w}}\mathcal{L}(b,\mathbf{w},\boldsymbol{\alpha})\right)}_{\text{Lagrange dual}}$$

- '=': **strong duality**, true for $\boxed{\text{QP}}$ if
  - convex primal
  - feasible primal (true if Φ-separable) 預
  - linear constraints, SVM 本來就線性

—called constraint qualification ⇒ 能直接解 RHS

exists primal-dual optimal solution $(b, \mathbf{w}, \boldsymbol{\alpha})$ for both sides

Solving Lagrange Dual: Simplifications (1/2)

RHS

$$\max_{\text{all } \alpha_n \geq 0} \left(\overbrace{\underbrace{\min_{b,\mathbf{w}} \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{n=1}^{N} \alpha_n (1 - y_n(\mathbf{w}^T\mathbf{z}_n + b))}_{\mathcal{L}(b,\mathbf{w},\boldsymbol{\alpha})}}^{\text{沒有條件了}} \right)$$

有條件

- inner problem 'unconstrained', at optimal:
  $\frac{\partial \mathcal{L}(b,\mathbf{w},\boldsymbol{\alpha})}{\partial b} = 0 = -\sum_{n=1}^{N} \alpha_n y_n$ 裡面微分=0
- no loss of optimality if solving with constraint $\sum_{n=1}^{N} \alpha_n y_n = 0$

but wait, b **can be removed**

只考慮微分=0的α.

变成常数.

$$\max_{\text{all } \alpha_n \geq 0, \boxed{\sum y_n \alpha_n = 0}} \left(\min_{b,\mathbf{w}} \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{n=1}^{N} \alpha_n (1 - y_n(\mathbf{w}^T\mathbf{z}_n)) - \cancel{\sum_{n=1}^{N} \alpha_n y_n \cdot b} \right)$$

Solving Lagrange Dual: Simplifications (2/2)

$$\max_{\text{all } \alpha_n \geq 0, \sum y_n \alpha_n = 0} \left(\min_{b,\mathbf{w}} \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{n=1}^{N} \alpha_n (1 - y_n(\mathbf{w}^T\mathbf{z}_n)) \right)$$ 處理 W

- inner problem 'unconstrained', at optimal:
  $\frac{\partial \mathcal{L}(b,\mathbf{w},\boldsymbol{\alpha})}{\partial w_i} = 0 = w_i - \sum_{n=1}^{N} \alpha_n y_n z_{n,i}$
- no loss of optimality if solving with constraint $\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{z}_n$

極值發生的位置

but wait!

只找極值處.

$$\max_{\text{all } \alpha_n \geq 0, \sum y_n \alpha_n = 0, \mathbf{w} = \sum \alpha_n y_n \mathbf{z}_n} \left(\boxed{\min_{b,\mathbf{w}}} \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{n=1}^{N} \alpha_n - \mathbf{w}^T\mathbf{w} \right)$$

min 也不用做了

$$\Longleftrightarrow \max_{\text{all } \alpha_n \geq 0, \sum y_n \alpha_n = 0, \mathbf{w} = \sum \alpha_n y_n \mathbf{z}_n} -\frac{1}{2}\left\| \sum_{n=1}^{N} \alpha_n y_n \mathbf{z}_n \right\|^2 + \sum_{n=1}^{N} \alpha_n$$

① ②求b ③求w

3 步 condition

KKT Optimality Conditions

人名

$\frac{1}{\|w\|}$ = distance.

幾乎只有α

$$\max_{\text{all } \alpha_n \geq 0, \sum y_n \alpha_n = 0, \mathbf{w} = \sum \alpha_n y_n \mathbf{z}_n} \; -\frac{1}{2}\Big\|\sum_{n=1}^{N} \alpha_n y_n \mathbf{z}_n\Big\|^2 + \sum_{n=1}^{N} \alpha_n$$

$// \|w\|^2$

大於≥ 0

$-\frac{1}{2}\|w\|^2 +$

$-\frac{1}{2}\left(-\|\Sigma\|^2 + 2\Sigma\alpha\right) = \frac{1}{\|w\|}$

if primal-dual optimal $(b, \mathbf{w}, \boldsymbol{\alpha})$,

- primal feasible: $y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1$
- dual feasible: $\alpha_n \geq 0$ dual condition.
- dual-inner optimal: $\sum y_n \alpha_n = 0$; $\mathbf{w} = \sum \alpha_n y_n \mathbf{z}_n$ ← min的微分
- primal-inner optimal (at optimal all 'Lagrange terms' disappear):

↙ 2个至少有1个等於零.

$\frac{\alpha_n}{w^T z_n + b} = 0$

$$\alpha_n\big(1 - y_n(\mathbf{w}^T\mathbf{z}_n + b)\big) = 0$$

$y_n w^T z_n + y_n b = 1$

—called **Karush-Kuhn-Tucker (KKT) conditions**, necessary for optimality [& sufficient here]

will use **KKT** to 'solve' $(b, \mathbf{w})$ from optimal $\boldsymbol{\alpha}$

Questions?

Dual Formulation of Support Vector Machine

希望求min：取负

$$\max_{\text{all } \alpha_n \geq 0, \sum y_n \alpha_n = 0, \mathbf{w} = \sum \alpha_n y_n \mathbf{z}_n} -\frac{1}{2}\left\|\sum_{n=1}^{N} \alpha_n y_n \mathbf{z}_n\right\|^2 + \sum_{n=1}^{N} \alpha_n$$

standard hard-margin SVM dual

平方项展开

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{z}_n^T \mathbf{z}_m - \sum_{n=1}^{N} \alpha_n$$

subject to $\sum_{n=1}^{N} y_n \alpha_n = 0;$ ← 1个 constraint.

$\alpha_n \geq 0, \text{ for } n = 1, 2, \ldots, N$ ← N个 condition

N个α.

(convex) QP of N variables & $N+1$ constraints, as promised

how to solve? **yeah, we know QP! :-)**

Dual SVM with QP Solver

解2次

optimal $\boldsymbol{\alpha} = ?$

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_n\alpha_m y_n y_m \mathbf{z}_n^T\mathbf{z}_m - \sum_{n=1}^{N}\alpha_n$$

$$\text{subject to} \quad \sum_{n=1}^{N} y_n\alpha_n = 0;$$

$$\alpha_n \geq 0, \quad \text{for } n = 1, 2, \ldots, N$$

表示成QP

optimal $\boldsymbol{\alpha} \leftarrow \text{QP}(\mathrm{Q}, \mathbf{p}, \mathrm{A}, \mathbf{c})$

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\boldsymbol{\alpha}^T\mathrm{Q}\boldsymbol{\alpha} + \mathbf{p}^T\boldsymbol{\alpha}$$

$$\text{subject to} \quad \mathbf{a}_i^T\boldsymbol{\alpha} \geq c_i, \quad \text{for } i = 1, 2, \ldots$$

- $q_{n,m} = y_n y_m \mathbf{z}_n^T\mathbf{z}_m$ 2次項係數
- $\mathbf{p} = -\mathbf{1}_N$ 1次項係數
- $\mathbf{a}_{\geq} = \mathbf{y}$, $\mathbf{a}_{\leq} = -\mathbf{y}$; $\mathbf{a}_n^T = n$-th unit direction
- $c_{\geq} = 0$, $c_{\leq} = 0$; $c_n = 0$

特殊的bound

note: many solvers treat **equality ($\mathbf{a}_{\geq}, \mathbf{a}_{\leq}$)** & **bound ($\mathbf{a}_n$)** constraints specially for **numerical stability**

Dual SVM with Special QP Solver

dual

optimal $\boldsymbol{\alpha} \leftarrow \text{QP}(\mathrm{Q_D}, \mathbf{p}, \mathrm{A}, \mathbf{c})$

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\boldsymbol{\alpha}^T \mathrm{Q_D} \boldsymbol{\alpha} + \mathbf{p}^T \boldsymbol{\alpha}$$

subject to special equality and bound constraints

- $q_{n,m} = y_n y_m \mathbf{z}_n^T \mathbf{z}_m$, often non-zero 不稀疏
- if $N = 30,000$, dense $\mathrm{Q_D}$ (N by N symmetric) takes > 3G RAM
  3万笔，存一半
- need **special solver** for
  - not storing whole $\mathrm{Q_D}$ ← 特殊加速
  - utilizing special constraints properly

  to scale up to large N

usually better to use **special solver** in practice

Optimal $(b, \mathbf{w})$ 有α後,解得(b,w)

KKT conditions

if primal-dual optimal $(b, \mathbf{w}, \boldsymbol{\alpha})$, 中間產物

- primal feasible: $y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1$
- dual feasible: $\alpha_n \geq 0$
- dual-inner optimal: $\sum y_n \alpha_n = 0$; $\mathbf{w} = \sum \alpha_n y_n \mathbf{z}_n$
- primal-inner optimal (at optimal all 'Lagrange terms' disappear):

$$\alpha_n(1 - y_n(\mathbf{w}^T\mathbf{z}_n + b)) = 0 \text{ (complementary slackness)}$$

- optimal $\boldsymbol{\alpha} \Longrightarrow$ optimal $\mathbf{w}$? easy above!
- optimal $\boldsymbol{\alpha} \Longrightarrow$ optimal b? a range from primal feasible & equality from **comp. slackness** if one $\alpha_n > 0 \Rightarrow b = y_n - \mathbf{w}^T\mathbf{z}_n$

其中有一人=零

從一個不是零的α_n求得b.

comp. slackness:

$\alpha_n > 0 \Rightarrow$ **on fat boundary (SV!)**

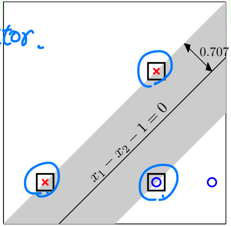
該點剛好是support vector

Questions?

Support Vectors Revisited

- on boundary: 'locates' fattest hyperplane; others: **not needed**
- examples with $\alpha_n > 0$: on boundary

  $\alpha_n > 0$, 該点為support vector.
- call $\alpha_n > 0$ examples $(\mathbf{z}_n, y_n)$ **support vectors** ~~(candidates)~~
- SV (positive α_n) $\subseteq$ SV candidates (on boundary)



α 的 linear combine.

只算SV 的α.

- only SV needed to compute $\mathbf{w}$: $\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{z}_n = \boxed{\sum_{\text{SV}} \alpha_n y_n \mathbf{z}_n}$
- only SV needed to compute b: $b = y_n - \mathbf{w}^T \mathbf{z}_n$ with any SV $(\mathbf{z}_n, y_n)$

任一个SV.

SVM: learn **fattest hyperplane** by identifying **support vectors** with **dual** optimal solution

① 找SV ② 用SV找optimal.

Summary: Two Forms of Hard-Margin SVM

Primal Hard-Margin SVM

原始的

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

sub. to $\quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1,$

for $n = 1, 2, \ldots, N$

- $\tilde{d}+1$ variables,
  N constraints
  —suitable when $\tilde{d}+1$ small
- physical meaning: locate **specially-scaled** $(b, \mathbf{w})$

Dual Hard-Margin SVM

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\boldsymbol{\alpha}^T \mathrm{Q_D} \boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha}$$

s.t. $\quad \mathbf{y}^T\boldsymbol{\alpha} = 0;$

$\alpha_n \geq 0$ for $n = 1, \ldots, N$

- N variables,
  $N+1$ simple constraints
  —suitable when N small
- physical meaning: locate **SVs** $(\mathbf{z}_n, y_n)$ & their α_n

both eventually result in optimal $(b, \mathbf{w})$ for fattest hyperplane

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

← 用(b, w) 做 求得的 prediction.

Are We Done Yet?

goal: SVM **without dependence on $\tilde{d}$**

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\boldsymbol{\alpha}^T \mathrm{Q_D} \boldsymbol{\alpha} - \mathbf{1}^T \boldsymbol{\alpha}$$

$$\text{subject to} \quad \mathbf{y}^T \boldsymbol{\alpha} = 0;$$

跟$\tilde{d}$有关

$$\alpha_n \geq 0, \text{for } n = 1, 2, \ldots, N$$

- N variables, $N + 1$ constraints: **no dependence on $\tilde{d}$?**
- $\boxed{q_{n,m} = y_n y_m \mathbf{z}_n^T \mathbf{z}_m}$: inner product in $\mathbb{R}^{\tilde{d}}$ —$O(\tilde{d})$ via naïve computation!

如何避开$\tilde{d}$的计算

no dependence only if
avoiding naïve computation **(next lecture :-))**

Questions?

Summary

1. Embedding Numerous Features: Kernel Models

Lecture 10: Support Vector Machine (1)

- Large-Margin Separating Hyperplane
  intuitively more robust against noise
- Standard Large-Margin Problem
  minimize 'length of w' at special separating scale
- Support Vector Machine
  'easy' via quadratic programming
- Motivation of Dual SVM
  want to remove dependence on $\tilde{d}$
- Lagrange Dual SVM
  KKT conditions link primal/dual
- Solving Dual SVM
  another QP, better solved with special solver
- Messages behind Dual SVM
  SVs represent fattest hyperplane