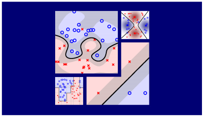
Machine Learning Techniques
(機器學習技法)



Lecture 1: Linear Support Vector Machine

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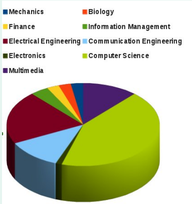
Department of Computer Science
& Information Engineering

National Taiwan University
(國立台灣大學資訊工程系)

Course History

NTU Version

- 15-17 weeks (2+ hours)
- highly-praised with **English and blackboard teaching**



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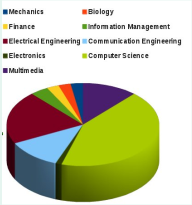

Coursera Version

- 8 weeks of 'foundations' (previous course) + 8 weeks of 'techniques' (**this course**)
- **Mandarin teaching** to reach more audience in need
- **slides teaching** improved with Coursera's quiz and homework mechanisms

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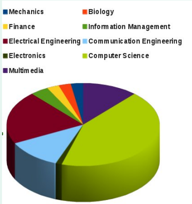

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goal: **try** making Coursera version even better than NTU version

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from Foundations to Techniques

- mixture of philosophical illustrations, key theory, core algorithms, usage in practice, and hopefully jokes :-)

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allows students to **use ML professionally**

Fun Time

Which of the following description of this course is true?

1. the course will be taught in Taiwanese
2. the course will tell me the techniques that create the android Lieutenant Commander Data in Star Trek
3. the course will be 16 weeks long
4. the course will focus on three major techniques

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Reference Answer: (4)

1. no, my Taiwanese is unfortunately not good enough for teaching (yet)
2. no, although what we teach may serve as building blocks
3. no, unless you have also joined the previous course
4. yes, **let's get started**!

Roadmap

1. Embedding Numerous Features: Kernel Models

   Lecture 1: Linear Support Vector Machine

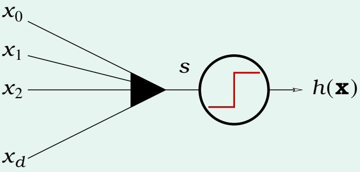
   - Course Introduction
   - Large-Margin Separating Hyperplane
   - Standard Large-Margin Problem
   - Support Vector Machine
   - Reasons behind Large-Margin Hyperplane

2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models

Linear Classification Revisited

PLA/pocket

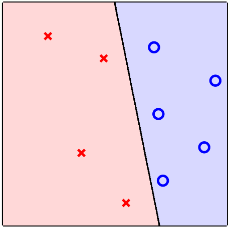
$$h(\mathbf{x}) = \text{sign}(s)$$



plausible err = 0/1

(small flipping noise)

minimize **specially**

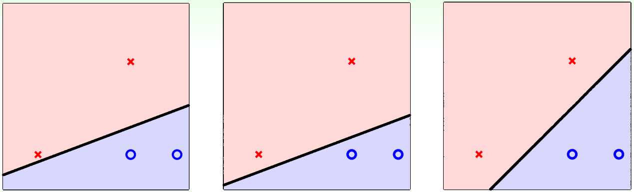


(linear separable)

linear (hyperplane) classifiers:

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

Which Line Is Best?



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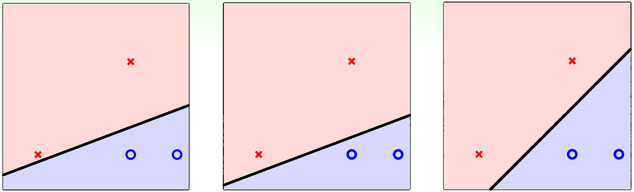

- PLA? depending on randomness

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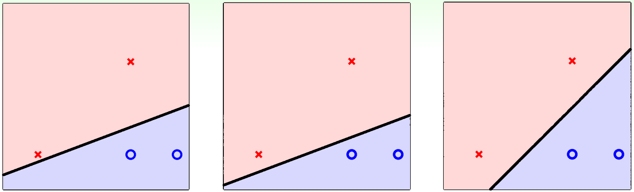

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- VC bound? whichever you like!

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

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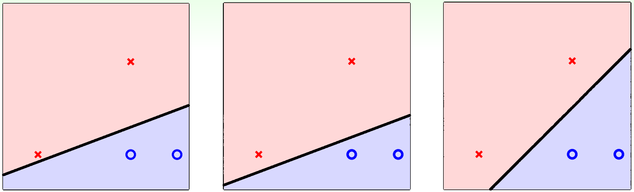

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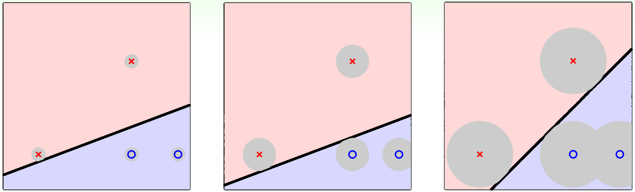
You? **rightmost one, possibly :-)**

Why Rightmost Hyperplane?



informal argument

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

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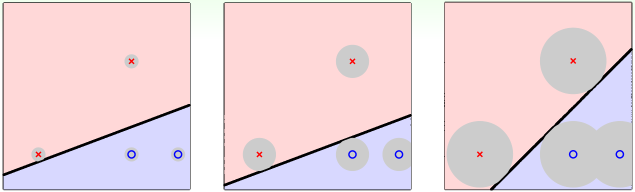

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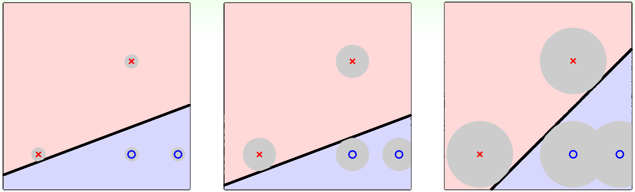

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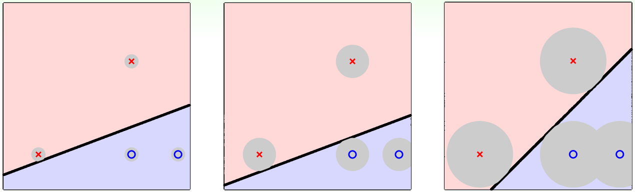

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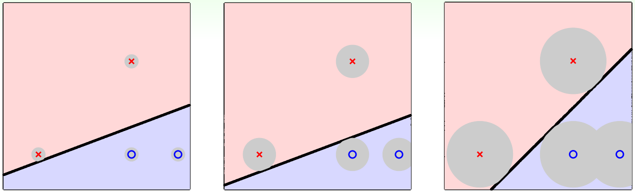

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$\Longleftrightarrow$ more robust to overfitting $\Longleftrightarrow$ robustness of hyperplane

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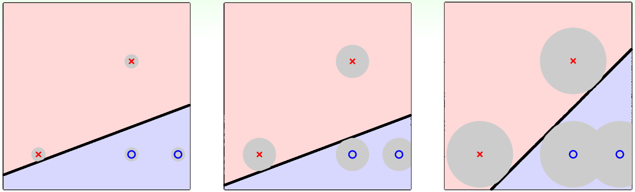

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$\Longleftrightarrow$ tolerate more noise	$\Longleftrightarrow$ amount of noise tolerance
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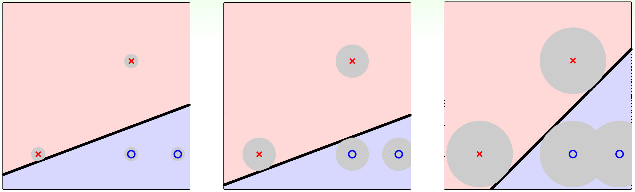

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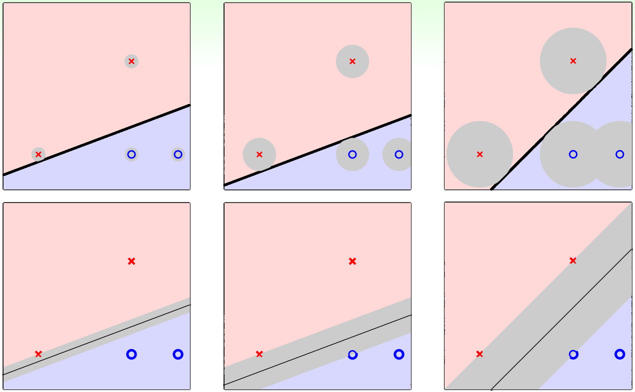
rightmost one: **more robust**
because of **larger distance to closest $\mathbf{x}_n$**

Fat Hyperplane



- robust separating hyperplane: **fat**
  —far from both sides of examples

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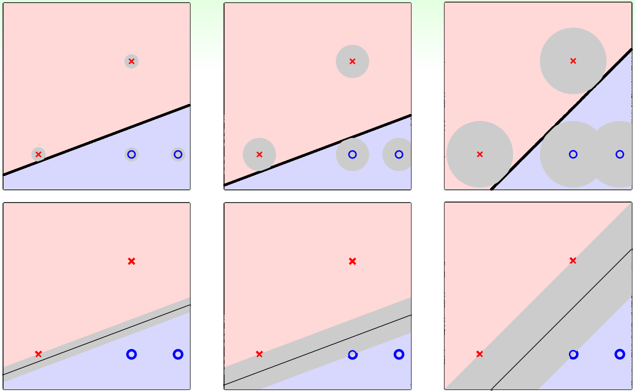

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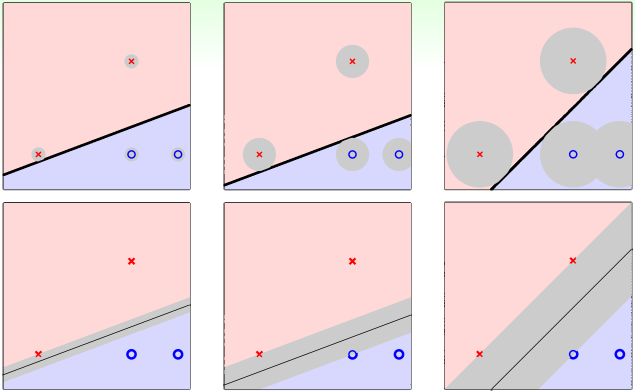

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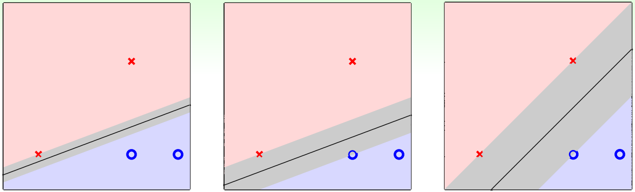
goal: find **fattest** separating hyperplane

Large-Margin Separating Hyperplane

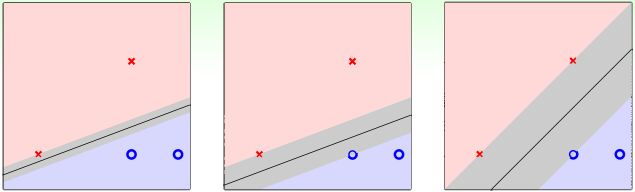


$$\max_{\mathbf{w}} \quad \text{fatness}(\mathbf{w})$$

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

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

Large-Margin Separating Hyperplane



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

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- fatness: formally called **margin**

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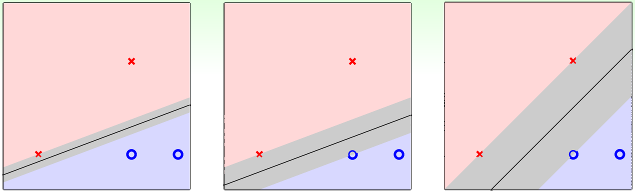
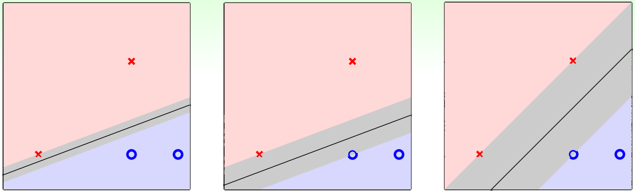


$$\max_{\mathbf{w}} \quad \text{margin}(\mathbf{w})$$
$$\text{subject to} \quad \text{every } y_n \mathbf{w}^T \mathbf{x}_n > 0$$
$$\text{margin}(\mathbf{w}) = \min_{n=1,\ldots,N} \text{distance}(\mathbf{x}_n, \mathbf{w})$$

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

Large-Margin Separating Hyperplane



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

Fun Time

Consider two examples $(\mathbf{v}, +1)$ and $(-\mathbf{v}, -1)$ where $\mathbf{v} \in \mathbb{R}^2$ (without padding the $v_0 = 1$). Which of the following hyperplane is the largest-margin separating one for the two examples? You are highly encouraged to visualize by considering, for instance, $\mathbf{v} = (3, 2)$.

1. $x_1 = 0$
2. $x_2 = 0$
3. $v_1 x_1 + v_2 x_2 = 0$
4. $v_2 x_1 + v_1 x_2 = 0$

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Reference Answer: 3

Here the largest-margin separating hyperplane (line) must be a perpendicular bisector of the line segment between $\mathbf{v}$ and $-\mathbf{v}$. Hence $\mathbf{v}$ is a normal vector of the largest-margin line. The result can be extended to the more general case of $\mathbf{v} \in \mathbb{R}^d$.

Distance to Hyperplane: Preliminary

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

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'shorten' $\mathbf{x}$ and $\mathbf{w}$

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

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$$b = w_0 \qquad \sout{x_0 = 1}$$

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

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'shorten' x and w

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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 $\mathbf{w}^T\mathbf{x}' + b = 0$

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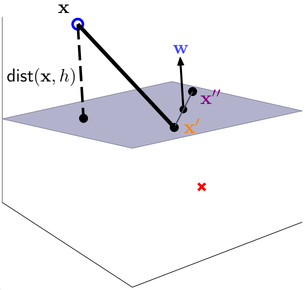
consider $\mathbf{x}'$, $\mathbf{x}''$ on hyperplane



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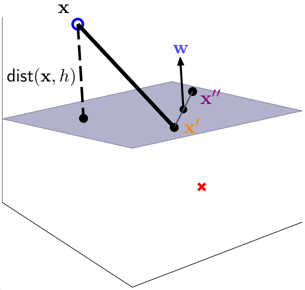

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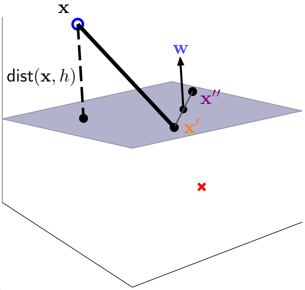

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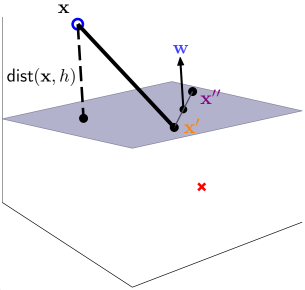
1. $\mathbf{w}^T\mathbf{x}' = -b$, $\mathbf{w}^T\mathbf{x}'' = -b$
2. $\mathbf{w} \perp$ hyperplane:

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



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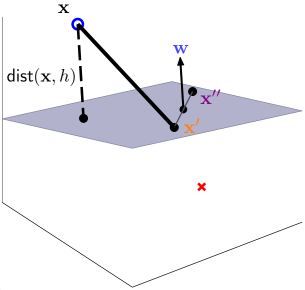

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consider $\mathbf{x}'$, $\mathbf{x}''$ on hyperplane

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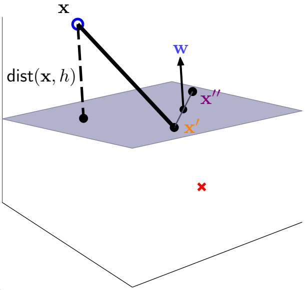
3. distance = project $(\mathbf{x} - \mathbf{x}')$ to $\perp$ hyperplane



Distance to Hyperplane

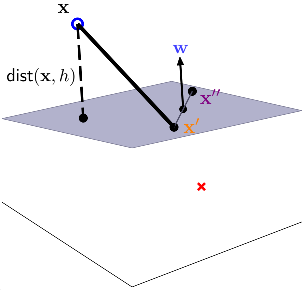
want: distance($\mathbf{x}, b, \mathbf{w}$), with hyperplane $\mathbf{w}^T\mathbf{x}' + b = 0$

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:

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

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



$$\text{distance}(\mathbf{x}, b, \mathbf{w}) = \Big| \qquad (\mathbf{x} - \mathbf{x}') \Big|$$

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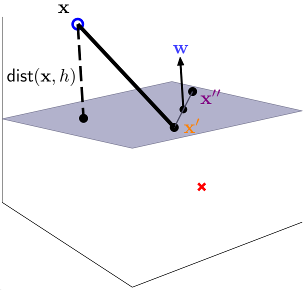

$$\text{distance}(\mathbf{x}, b, \mathbf{w}) = \left| \frac{\mathbf{w}^T}{\|\mathbf{w}\|}(\mathbf{x} - \mathbf{x}') \right|$$

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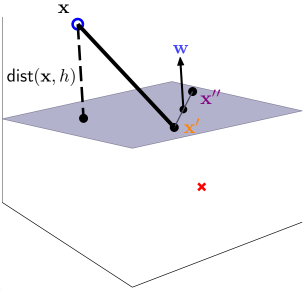

$$\text{distance}(\mathbf{x}, b, \mathbf{w}) = \left| \frac{\mathbf{w}^T}{\|\mathbf{w}\|}(\mathbf{x} - \mathbf{x}') \right| \overset{(1)}{=} \frac{1}{\|\mathbf{w}\|}|\mathbf{w}^T\mathbf{x} \quad |$$

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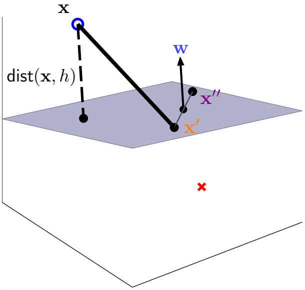

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Distance to **Separating** Hyperplane

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

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

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

$$\begin{aligned} \max_{b,\mathbf{w}} \quad & \text{margin}(b, \mathbf{w}) \\ \text{subject to} \quad & \text{every } y_n(\mathbf{w}^T\mathbf{x}_n + b) > 0 \\ & \text{margin}(b, \mathbf{w}) = \min_{n=1,\ldots,N} \text{distance}(\mathbf{x}_n, b, \mathbf{w}) \end{aligned}$$

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

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- distance to **separating** hyperplane:

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

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

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

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

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\end{aligned}$$

Margin of **Special** Separating Hyperplane

$$
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- **special** scaling: only consider separating $(b, \mathbf{w})$ such that

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

Margin of **Special** Separating Hyperplane

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Standard Large-Margin Hyperplane Problem

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

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

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

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

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final change: max $\Longrightarrow$ min, remove $\sqrt{\ }$

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$$\min_{b,\mathbf{w}} \qquad \mathbf{w}^T\mathbf{w}$$

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

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$
$$\text{subject to} \quad y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 \text{ for all } n$$

Fun Time

Consider three examples $(\mathbf{x}_1, +1)$, $(\mathbf{x}_2, +1)$, $(\mathbf{x}_3, -1)$, where $\mathbf{x}_1 = (3, 0)$, $\mathbf{x}_2 = (0, 4)$, $\mathbf{x}_3 = (0, 0)$. In addition, consider a hyperplane $x_1 + x_2 = 1$. Which of the following is not true?

1. the hyperplane is a separating one for the three examples
2. the distance from the hyperplane to $\mathbf{x}_1$ is 2
3. the distance from the hyperplane to $\mathbf{x}_3$ is $\frac{1}{\sqrt{2}}$
4. the example that is closest to the hyperplane is $\mathbf{x}_3$

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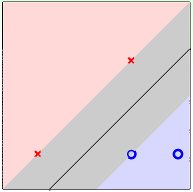
Reference Answer: 2

The distance from the hyperplane to $\mathbf{x}_1$ is $\frac{1}{\sqrt{2}}(3 + 0 - 1) = \sqrt{2}$.

Solving a Particular Standard Problem

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$
$$\text{subject to} \quad y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 \text{ for all } n$$



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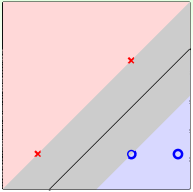

$$\mathrm{X} = \begin{bmatrix} 0 & 0 \\ 2 & 2 \\ 2 & 0 \\ 3 & 0 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} -1 \\ -1 \\ +1 \\ +1 \end{bmatrix}$$

$$\begin{array}{rrrl} & & -\, b \geq 1 & (i) \\ -2w_1 & -\, 2w_2 & -\, b \geq 1 & (ii) \\ 2w_1 & & +\, b \geq 1 & (iii) \\ 3w_1 & & +\, b \geq 1 & (iv) \end{array}$$

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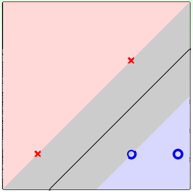

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$$\begin{aligned} -b &\geq 1 \quad (i) \\ -2w_1 - 2w_2 - b &\geq 1 \quad (ii) \\ 2w_1 + b &\geq 1 \quad (iii) \\ 3w_1 + b &\geq 1 \quad (iv) \end{aligned}$$

- $\left\{ \begin{array}{l} (i) \;\; \& \;\; (iii) \implies w_1 \geq +1 \\ \end{array} \right.$

Solving a Particular Standard Problem

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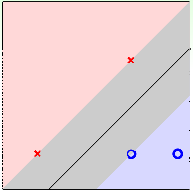

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$$\begin{aligned} -b &\geq 1 \quad (i) \\ -2w_1 - 2w_2 - b &\geq 1 \quad (ii) \\ 2w_1 + b &\geq 1 \quad (iii) \\ 3w_1 + b &\geq 1 \quad (iv) \end{aligned}$$

- $\left\{ \begin{array}{ccccc} (i) & \& & (iii) & \Longrightarrow & w_1 \geq +1 \\ (ii) & \& & (iii) & \Longrightarrow & w_2 \leq -1 \end{array} \right\} \Longrightarrow$

Solving a Particular Standard Problem

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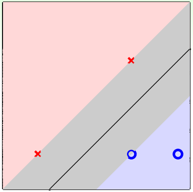

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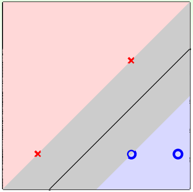

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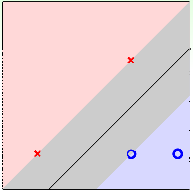

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$$g_{\text{SVM}}(\mathbf{x}) = \text{sign}(x_1 - x_2 - 1):$$

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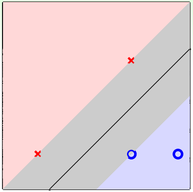

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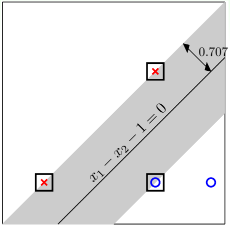
Support Vector Machine (SVM)

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

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



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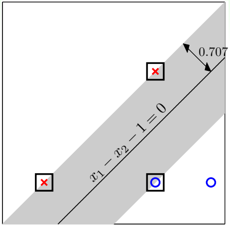

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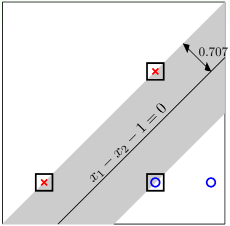

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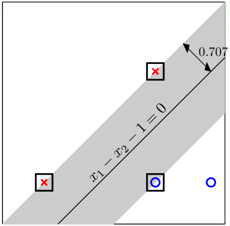

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support vector machine (SVM):
learn **fattest hyperplanes**
(with help of **support vectors**)

Solving General SVM

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

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—**quadratic programming**

quadratic programming (QP):
'easy' optimization problem

Quadratic Programming

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

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

SVM with QP Solver

Linear Hard-Margin SVM Algorithm

1. $Q = \begin{bmatrix} 0 & \mathbf{0}_d^T \\ \mathbf{0}_d & I_d \end{bmatrix}$; $\mathbf{p} = \mathbf{0}_{d+1}$; $\mathbf{a}_n^T = y_n \begin{bmatrix} 1 & \mathbf{x}_n^T \end{bmatrix}$; $c_n = 1$

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

Fun Time

Consider two negative examples with $\mathbf{x}_1 = (0, 0)$ and $\mathbf{x}_2 = (2, 2)$; two positive examples with $\mathbf{x}_3 = (2, 0)$ and $\mathbf{x}_4 = (3, 0)$, as shown on page 17 of the slides. Define $\mathbf{u}$, Q, $\mathbf{p}$, c_n as those listed on page 20 of the slides. What are $\mathbf{a}_n^T$ that need to be fed into the QP solver?

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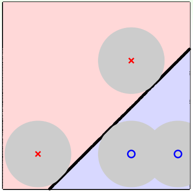
Reference Answer: (4)

We need $\mathbf{a}_n^T = y_n \begin{bmatrix} 1 & \mathbf{x}_n^T \end{bmatrix}$.

Why Large-Margin Hyperplane?

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$
$$\text{subject to} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 \text{ for all } n$$



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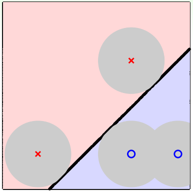

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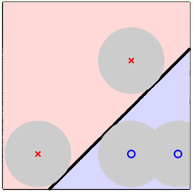

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SVM (large-margin hyperplane):
'weight-decay regularization' within $E_{\text{in}} = 0$

Large-Margin Restricts Dichotomies

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

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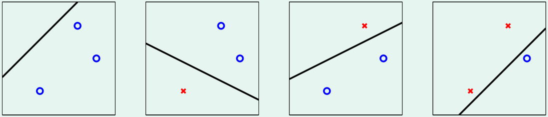

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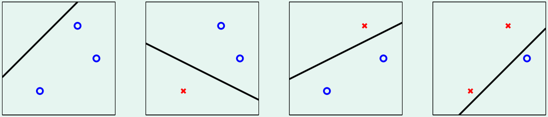
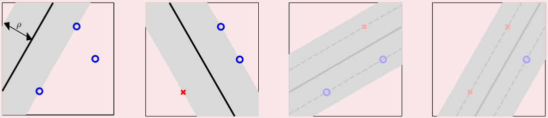


$\mathcal{A}_{1.126}$: more strict than SVM $\Longrightarrow$ cannot shatter any 3 inputs



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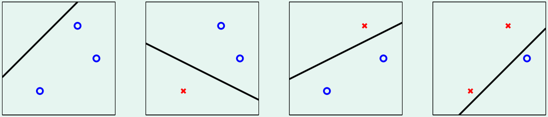

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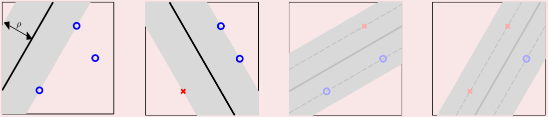

fewer dichotomies $\Longrightarrow$ smaller 'VC dim.' $\Longrightarrow$ **better generalization**

VC Dimension of Large-Margin Algorithm

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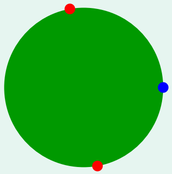

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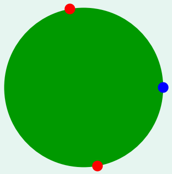

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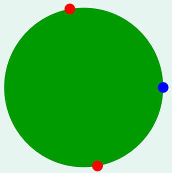

generally, when $\mathcal{X}$ in radius-R hyperball:

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

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	large-margin hyperplanes	hyperplanes	hyperplanes + feature transform $\mathbf{\Phi}$
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a new possibility: non-linear SVM

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boundary	**sophisticated**

Fun Time

Consider running the 'large-margin algorithm' $\mathcal{A}_\rho$ with $\rho = \frac{1}{4}$ on a $\mathcal{Z}$-space such that $\mathbf{z} = \mathbf{\Phi}(\mathbf{x})$ is of 1126 dimensions (excluding z_0) and $\|\mathbf{z}\| \leq 1$. What is the upper bound of $d_{\text{VC}}(\mathcal{A}_\rho)$ when calculated by $\min\left(\frac{R^2}{\rho^2}, d\right) + 1$?

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Reference Answer: ②

By the description, $d = 1126$ and $R = 1$. So the upper bound is simply 17.

Summary

1. Embedding Numerous Features: Kernel Models

Lecture 1: Linear Support Vector Machine

- Course Introduction
  from foundations to techniques
- 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
- Reasons behind Large-Margin Hyperplane
  fewer dichotomies and better generalization

- **next: solving non-linear Support Vector Machine**

2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models