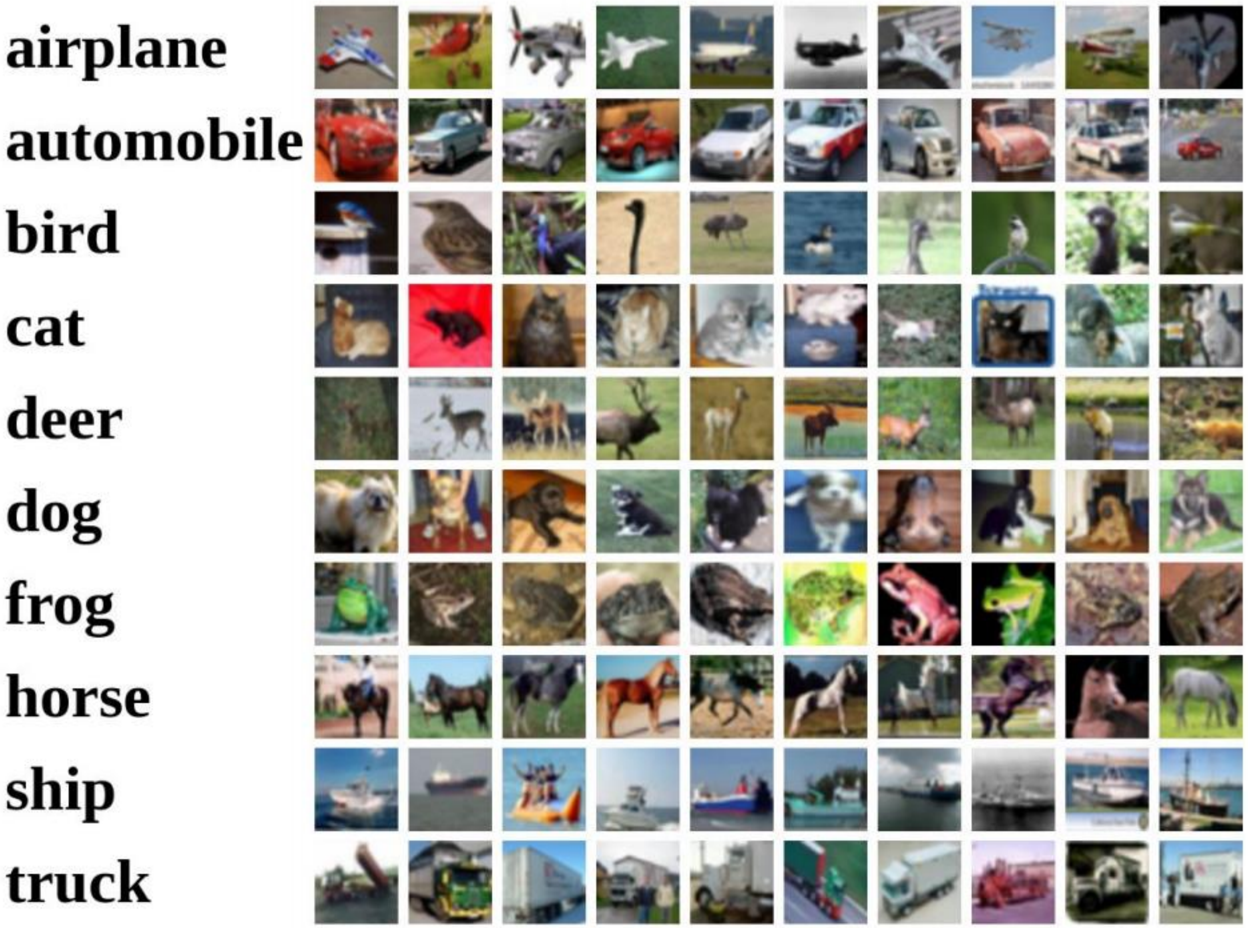
第九讲 多类别分类(*Classification for Multiclass*)

9.1 “一对多”策略的多类别分类

多类别分类问题

(*Multiclass Classification*)

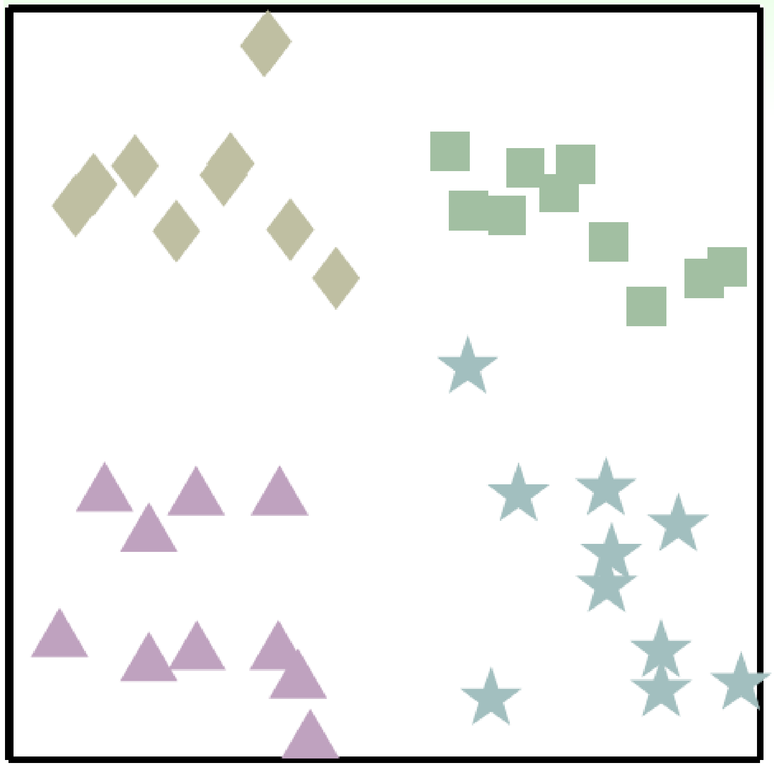


CIFAR 10 dataset

Source: CS131-stanford

9.1 “一对多”策略的多类别分类

多类别分类问题
(*Multiclass Classification*)



$\mathcal{Y} = \{$ ■, ◆, ▲, ★ $\}$ 类别数$\mathcal{K} = 4$

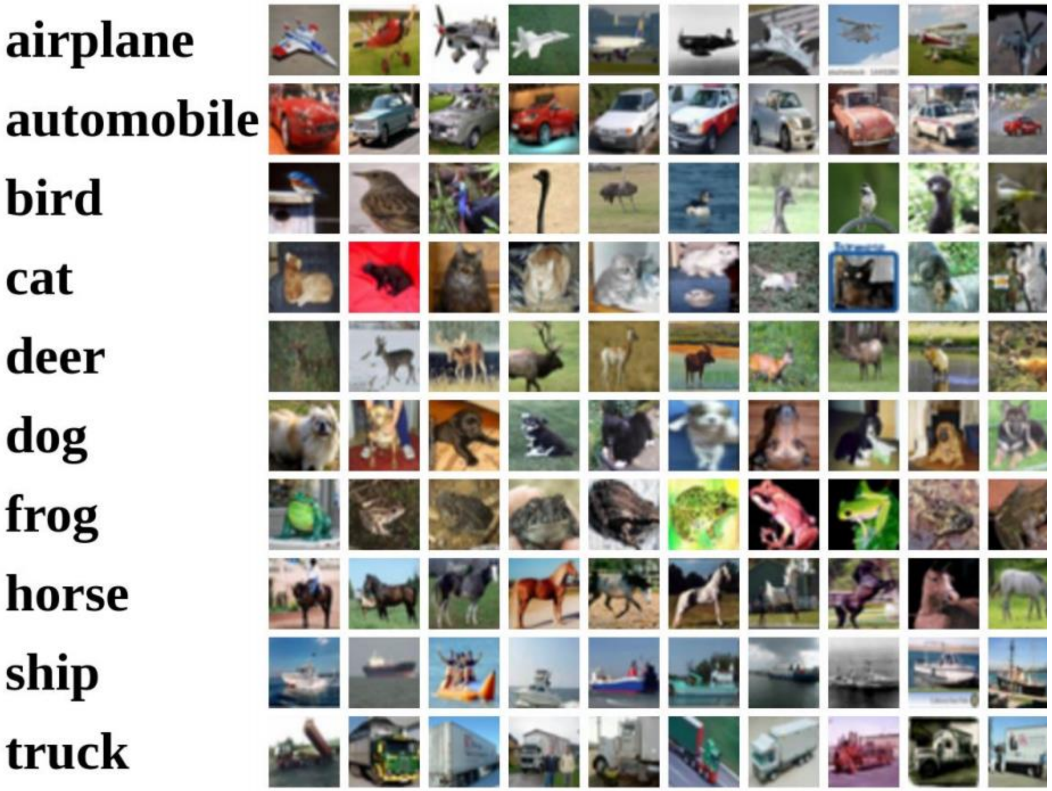
能否用二分类方法完成多分类问题?

Source: NTU-CSIE

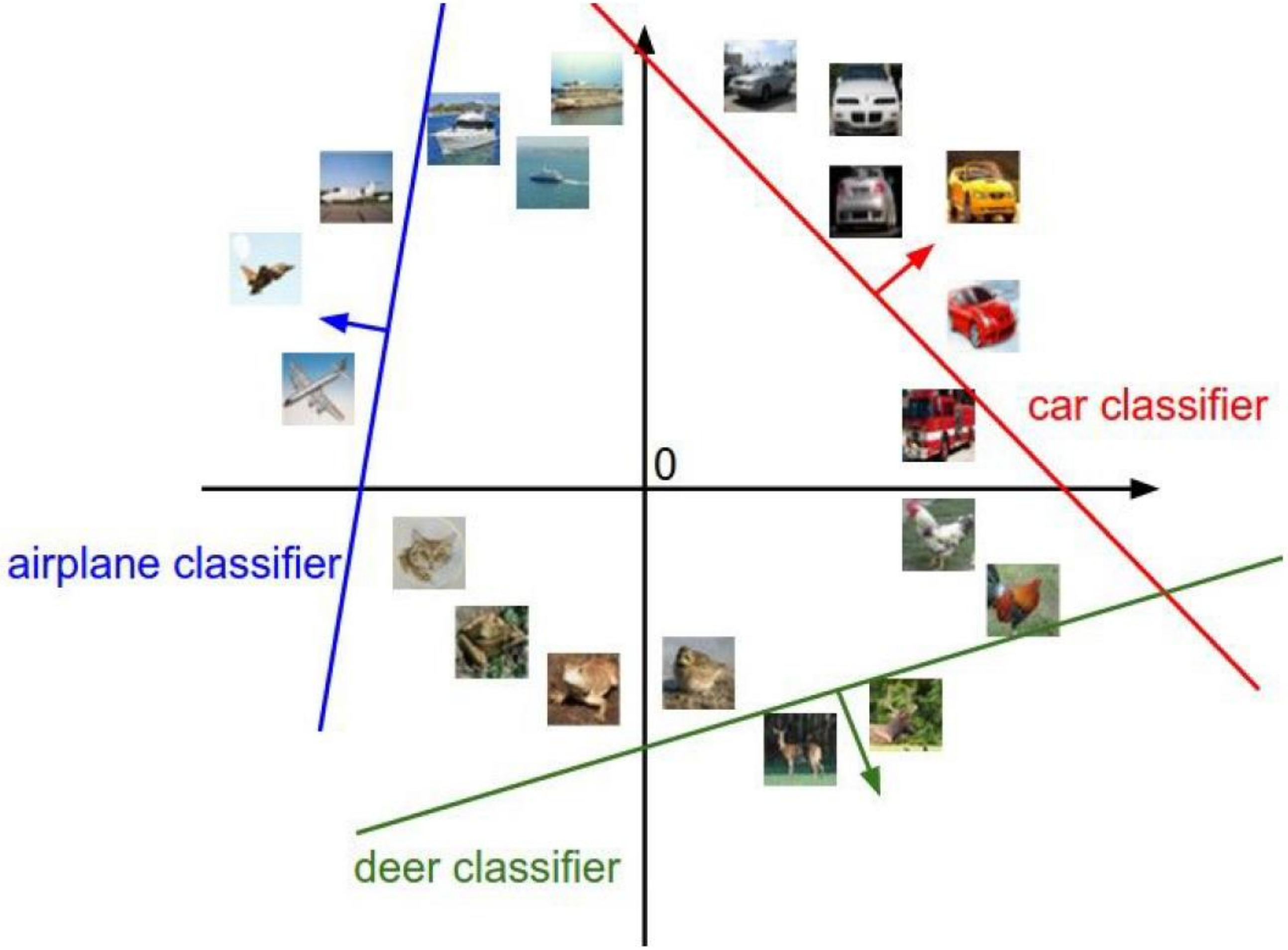
9.1 “一对多”策略的多类别分类

策略：一次只区分一个类别

(*One Class at a Time*)



CIFAR 10 dataset



Source: CS131-stanford

9.1 “一对多”策略的多类别分类

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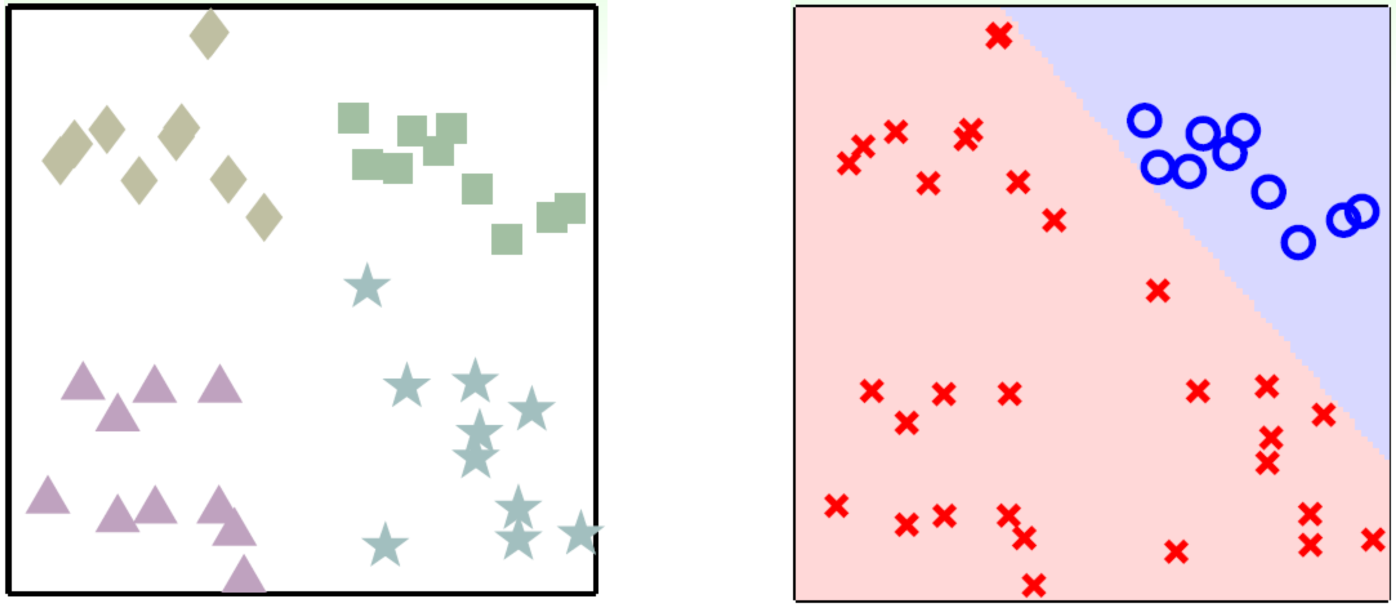
(*One Class at a Time*)



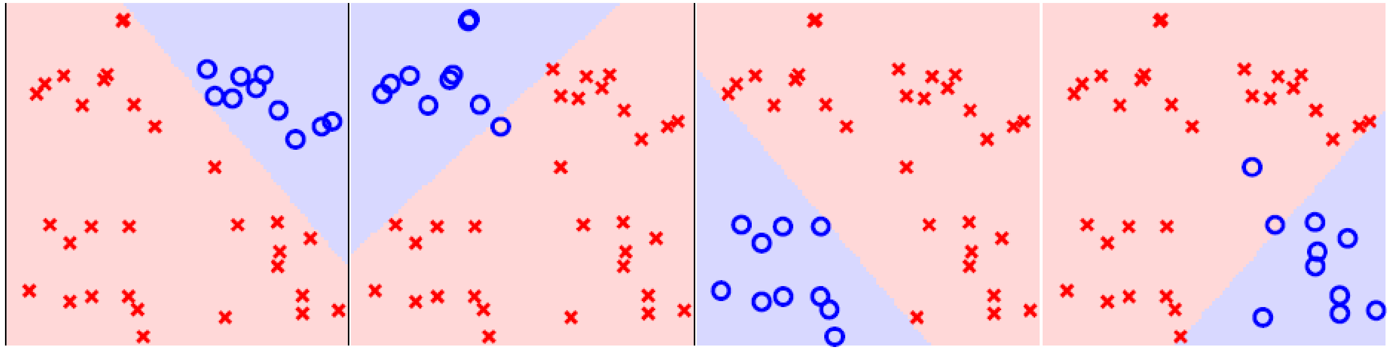
$\square$ or not? $\{\square = \circ, \Diamond = \times, \triangle = \times, \star = \times\}$

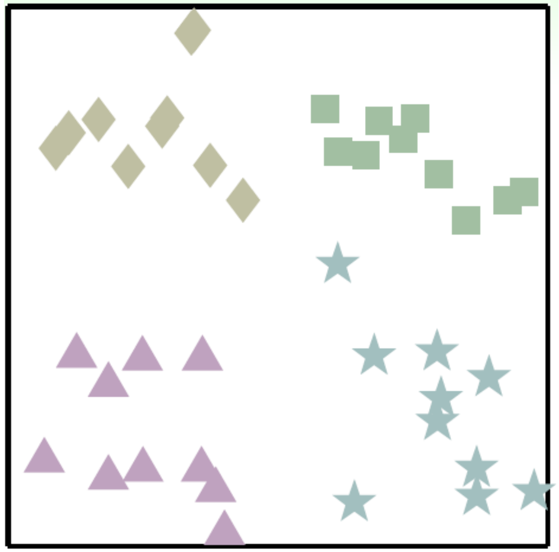
Source: NTU-CSIE

9.1 “一对多”策略的多类别分类

策略：一次只区分一个类别

(*One Class at a Time*)



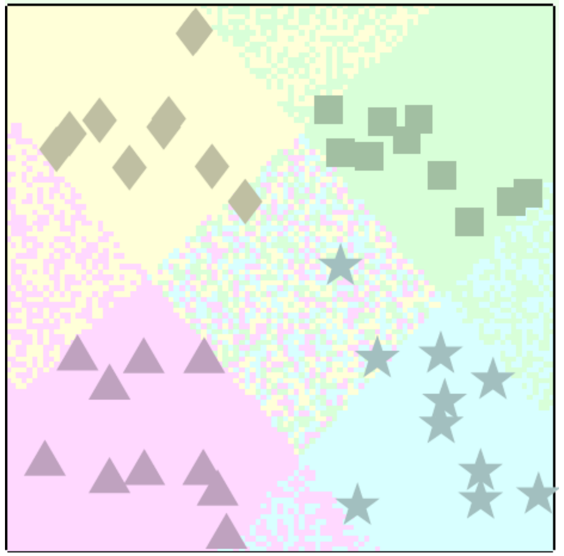


$\square$ or not? $\{\square = \circ, \Diamond = \times, \triangle = \times, \star = \times\}$

$\Diamond$ or not? $\{\square = \times, \Diamond = \circ, \triangle = \times, \star = \times\}$

$\triangle$ or not? $\{\square = \times, \Diamond = \times, \triangle = \circ, \star = \times\}$

$\star$ or not? $\{\square = \times, \Diamond = \times, \triangle = \times, \star = \circ\}$

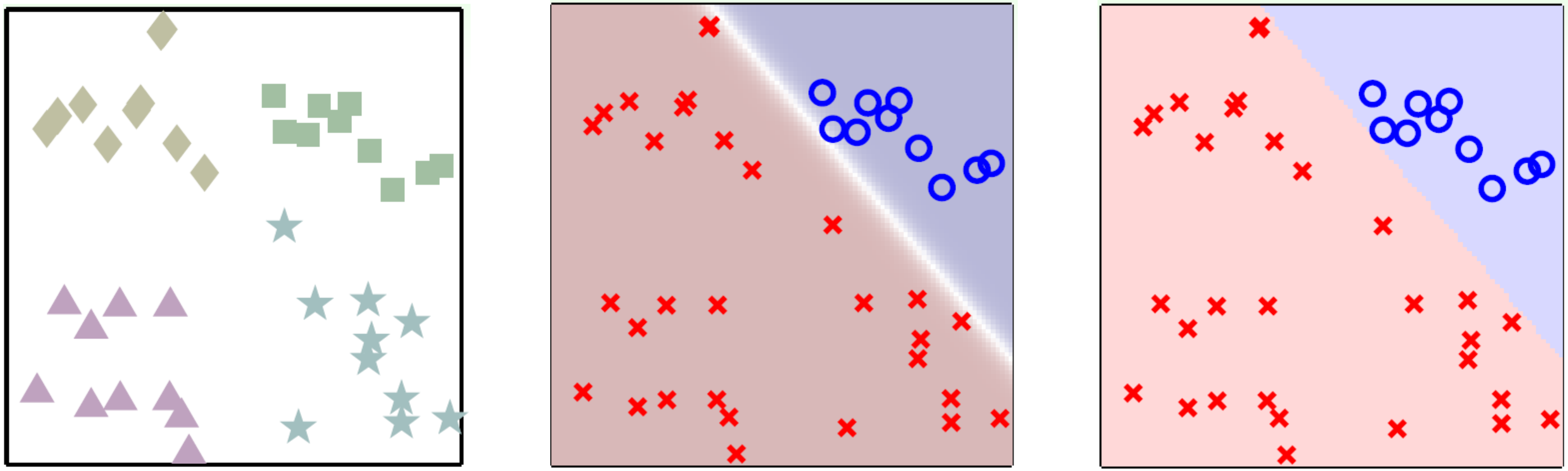


Source: NTU-CSIE

9.1 “一对多”策略的多类别分类

策略：一次只区分一个类别

(*One Class at a Time*)



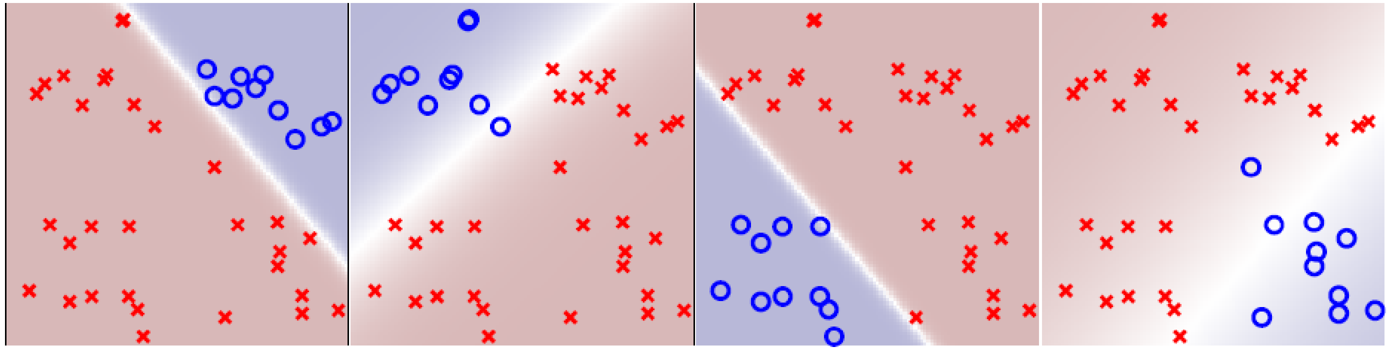
$$P(\square|\mathbf{x})?\ \{\square=\circ, \Diamond=\times, \triangle=\times, \star=\times\}$$

Source: NTU-CSIE

9.1 “一对多”策略的多类别分类

策略：一次只区分一个类别

(One Class at a Time)

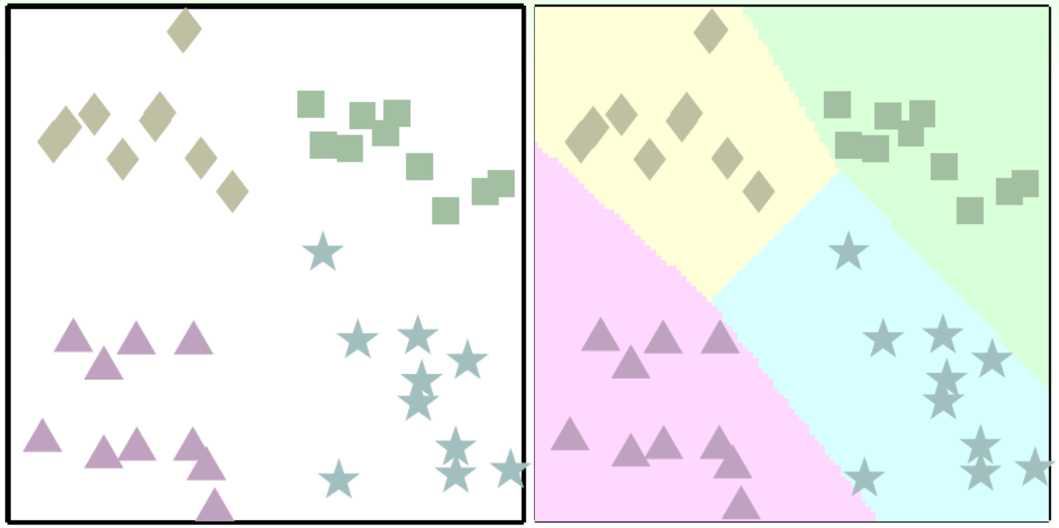


$P(\square|\mathbf{x})?\ \{\square = \circ, \diamond = \times, \triangle = \times, \star = \times\}$

$P(\diamond|\mathbf{x})?\ \{\square = \times, \diamond = \circ, \triangle = \times, \star = \times\}$

$P(\triangle|\mathbf{x})?\ \{\square = \times, \diamond = \times, \triangle = \circ, \star = \times\}$

$P(\star|\mathbf{x})?\ \{\square = \times, \diamond = \times, \triangle = \times, \star = \circ\}$



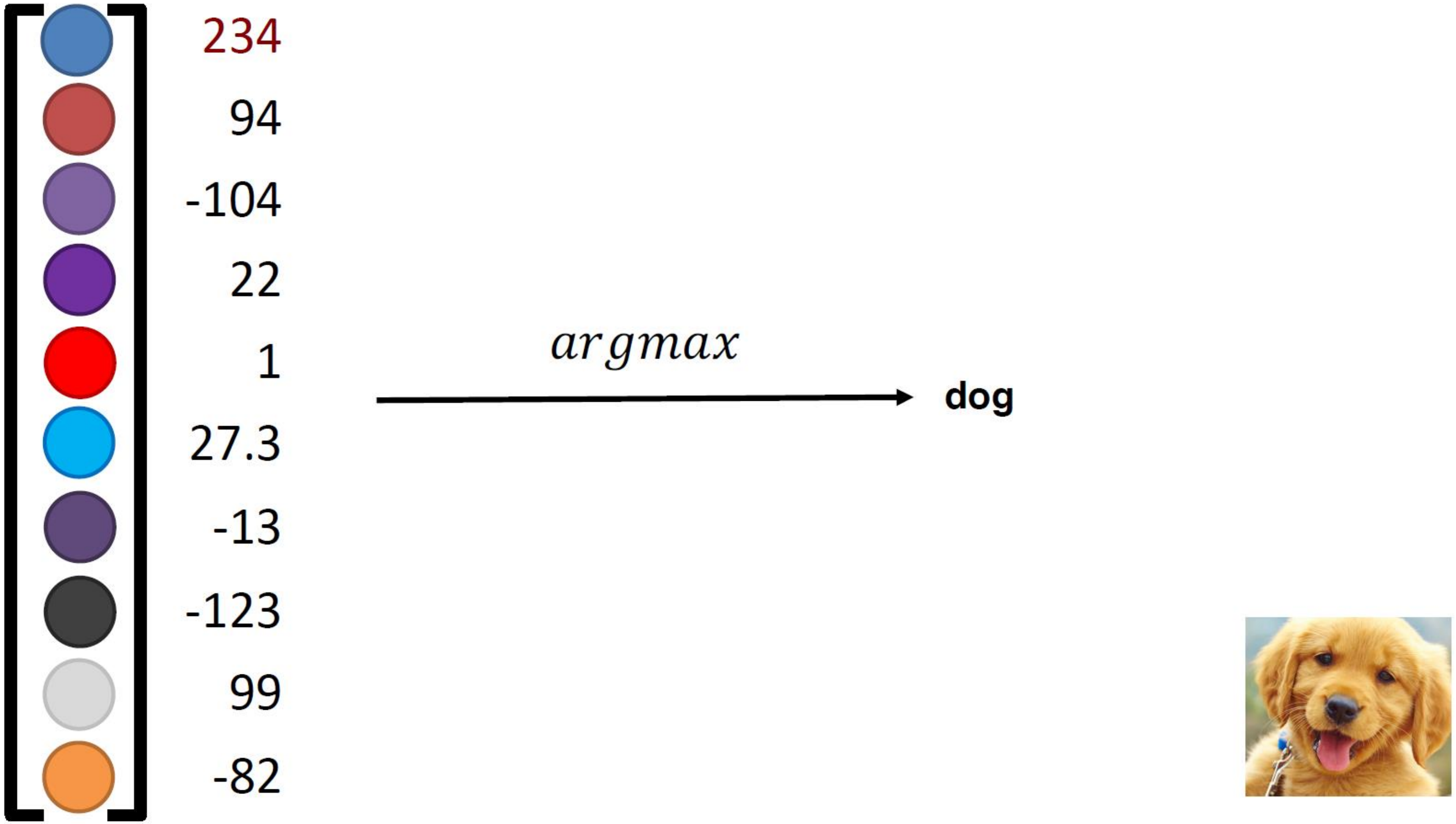
测试样本为$\mathbf{x}$时，所属类别为：

$$g(\mathbf{x}) = argmax_{k\in\mathcal{Y}}(\mathbf{w}_{[k]}^T\mathbf{x})$$

Source: NTU-CSIE

2.1 感知器模型假设空间

感知器模型的可视化：



Source: CS131-stanford

9.1 “一对多”策略的多类别分类

“One-Versus-All (OVA) ” 策略对训练样本集的重分组

① $for\ k \in \mathcal{Y}$, 对训练样本集重新分组得到 $\mathcal{D}_{[k]}$:

$$\mathcal{D}_{[k]} = \{(\mathbf{x}_n, y_n' = 2[\![y_n = k]\!] - 1)\}_{n=1}^{N}$$

② 在数据集$\mathcal{D}_{[k]}$上运行任一二分类算法，如*Logistic regression*，得到$\mathbf{w}_{[k]}$

③ 当测试样本为$\mathbf{x}$时，分类结果为： $g(\mathbf{x}) = argmax_{k \in \mathcal{Y}}(\mathbf{w}_{[k]}^T\mathbf{x})$

- 优点：简单、便于推广二分类方法实现多分类问题
- 不足：当类别数$\mathcal{K}$很大时， $\mathcal{D}_{[k]}$存在样本数不平衡问题，影响性能

不平衡问题的来源在于“一对多”的策略

Source: NTU-CSIE

9.1 “一对多”策略的多类别分类(*Multiclass via One-Versus-All*)

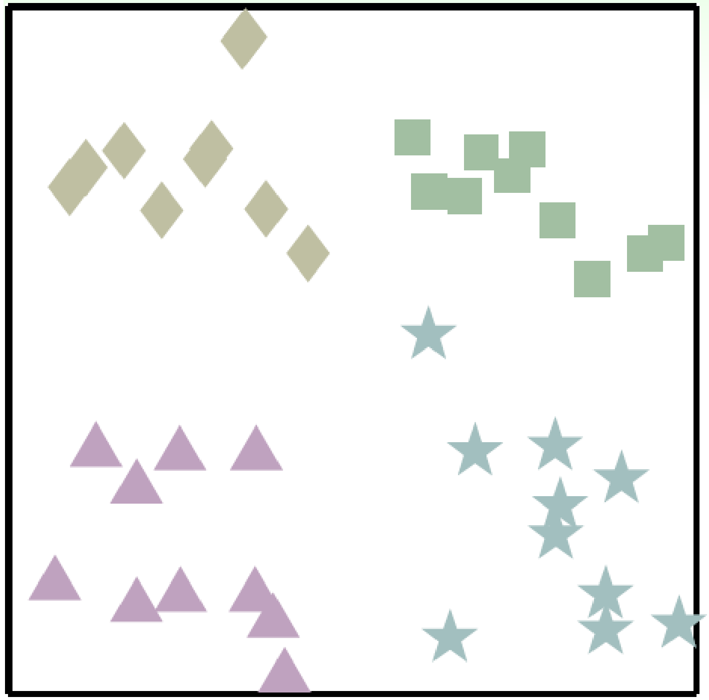
9.2 “一对一”策略的多类别分类(*Multiclass via One-Versus-One*)

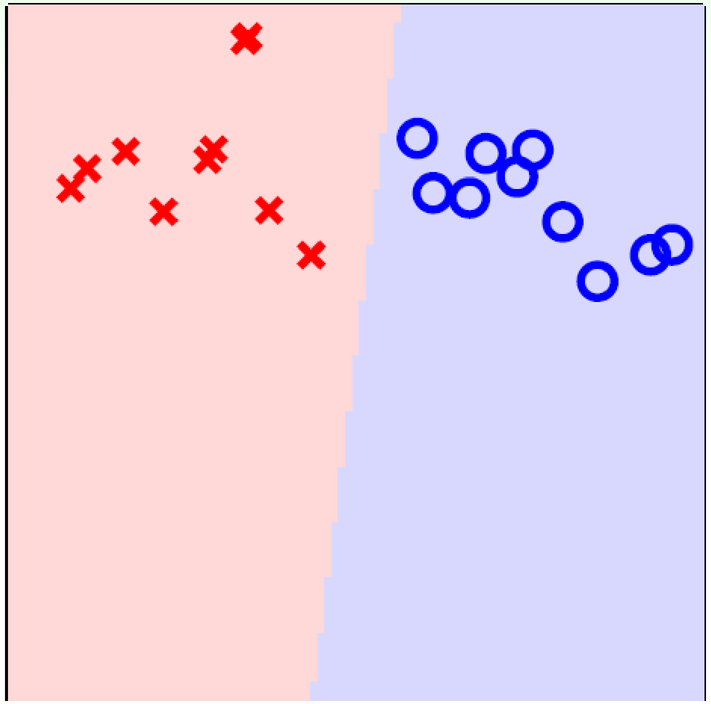
9.3 “Softmax”多类别分类(*Multiclass via Softmax*)

9.2 "一对一"策略的多类别分类

策略：一次只区分两个类别

(*One versus One at a Time*)





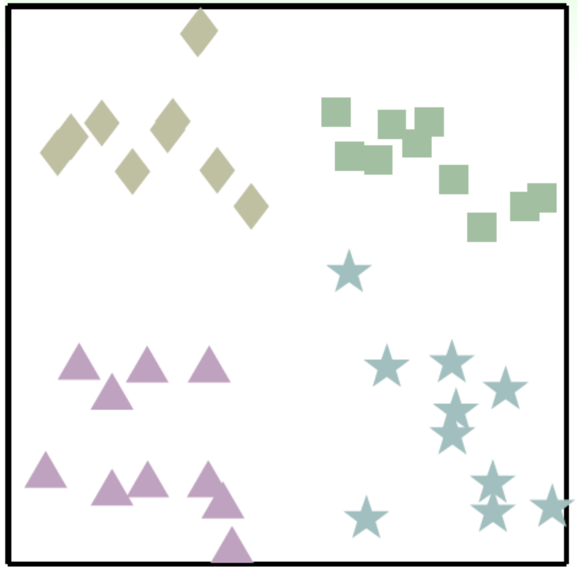
$\square$ or $\diamond$? $\{\square = \circ, \diamond = \times, \triangle = \text{nil}, \star = \text{nil}\}$

Source: NTU-CSIE

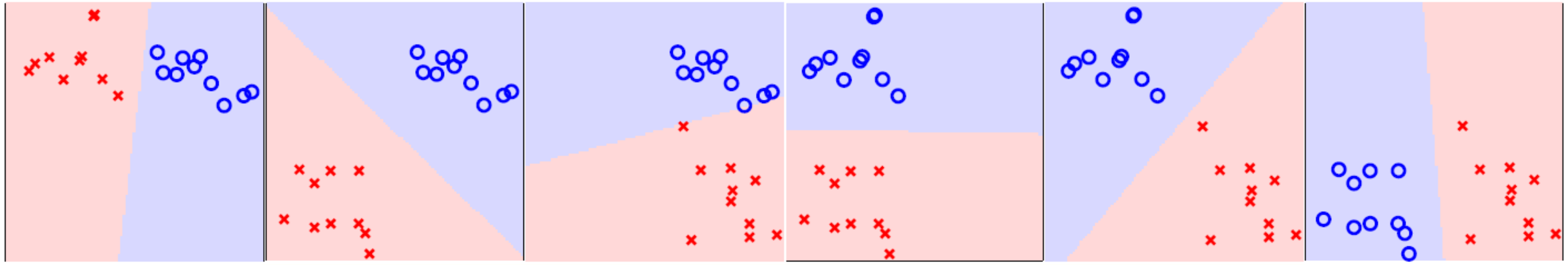
9.2 “一对一”策略的多类别分类

策略：一次只区分两个类别

(*One versus One at a Time*)



类别数两两组合，用二分类算法得到$C_{\mathcal{K}}^{2}$个分类面：$\mathbf{w}_{[k,l]}$



测试样本为$\mathbf{x}$时，所属类别为：$g(\mathbf{x}) = tournament\ champion_{k,l\in\mathcal{Y}*\mathcal{Y}}(\mathbf{w}_{[k,l]}^{T}\mathbf{x})$

样本属于得票最多的类别

Source: NTU-CSIE

9.1 “一对多”策略的多类别分类

“One-Versus-One (OVO) ”策略对训练样本集的重分组

① $for\ (k,l) \in \mathcal{Y} * \mathcal{Y}$, 对训练样本集重新分组得到 $\mathcal{D}_{[k,l]}$:

$$\mathcal{D}_{[k,l]} = \{(\mathbf{x}_n, y_n' = 2[\![y_n = k]\!] - 1): y_n = k\ or y_n = l\}_{n=1}^{N}$$

② 在数据集$\mathcal{D}_{[k]}$上运行任一二分类算法，如*Logistic regression*，得到$\mathbf{w}_{[k,l]}$

③ 当测试样本为$\mathbf{x}$时，分类结果为：$g(\mathbf{x}) = tournament\ champion_{k,l \in \mathcal{Y}*\mathcal{Y}}(\mathbf{w}_{[k,l]}^T \mathbf{x})$

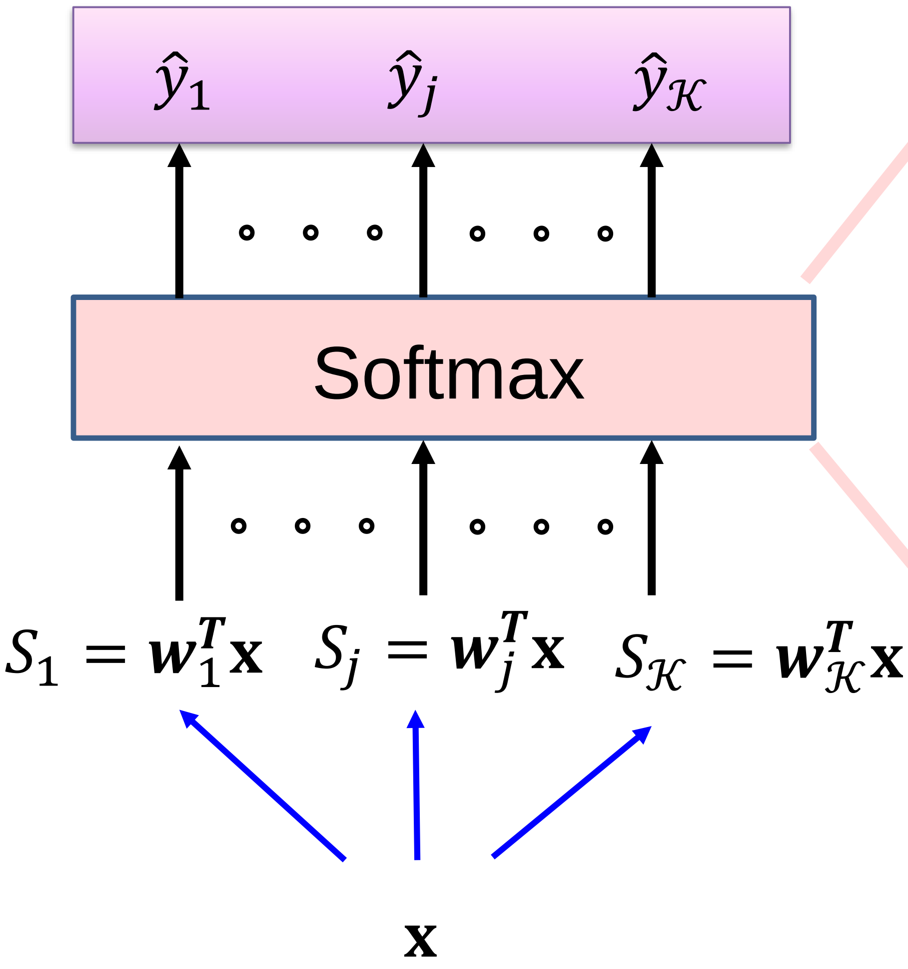
- 优点：简单、有效、稳定、便于推广二分类方法实现多分类问题
- 不足：类别组合后求解$\mathbf{w}_{[k,l]}$ 需要更多空间、更耗时

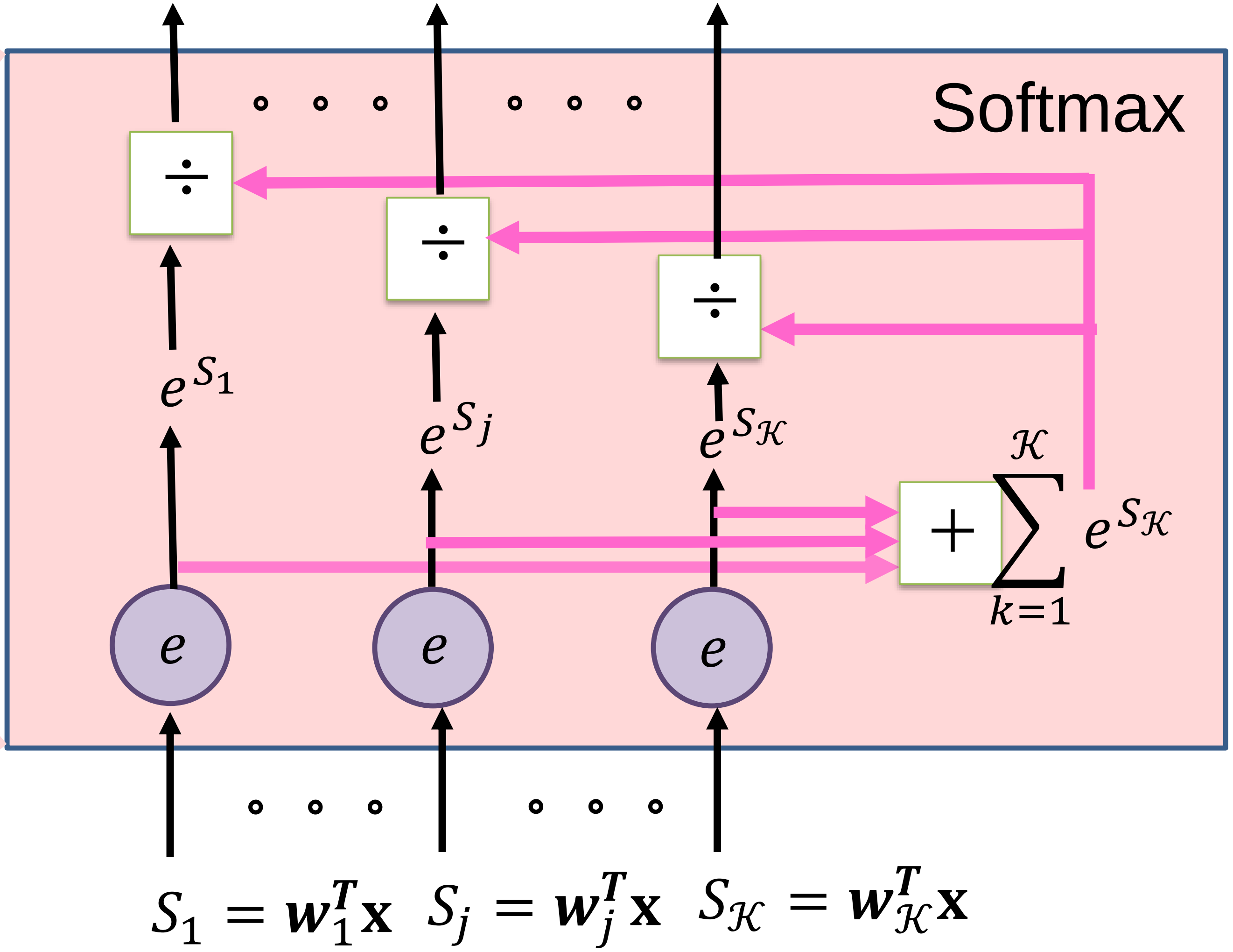
Source: NTU-CSIE

9.3 “Softmax”多类别分类

$\mathbf{y} = (y_1, y_2, \dots, y_j, \dots y_K)^T$

$$\hat{y}_1 = \frac{e^{S_1}}{\sum_k e^{S_k}} \quad \hat{y}_j = \frac{e^{S_j}}{\sum_k e^{S_k}} \quad \hat{y}_{\mathcal{K}} = \frac{e^{S_{\mathcal{K}}}}{\sum_k e^{S_k}}$$

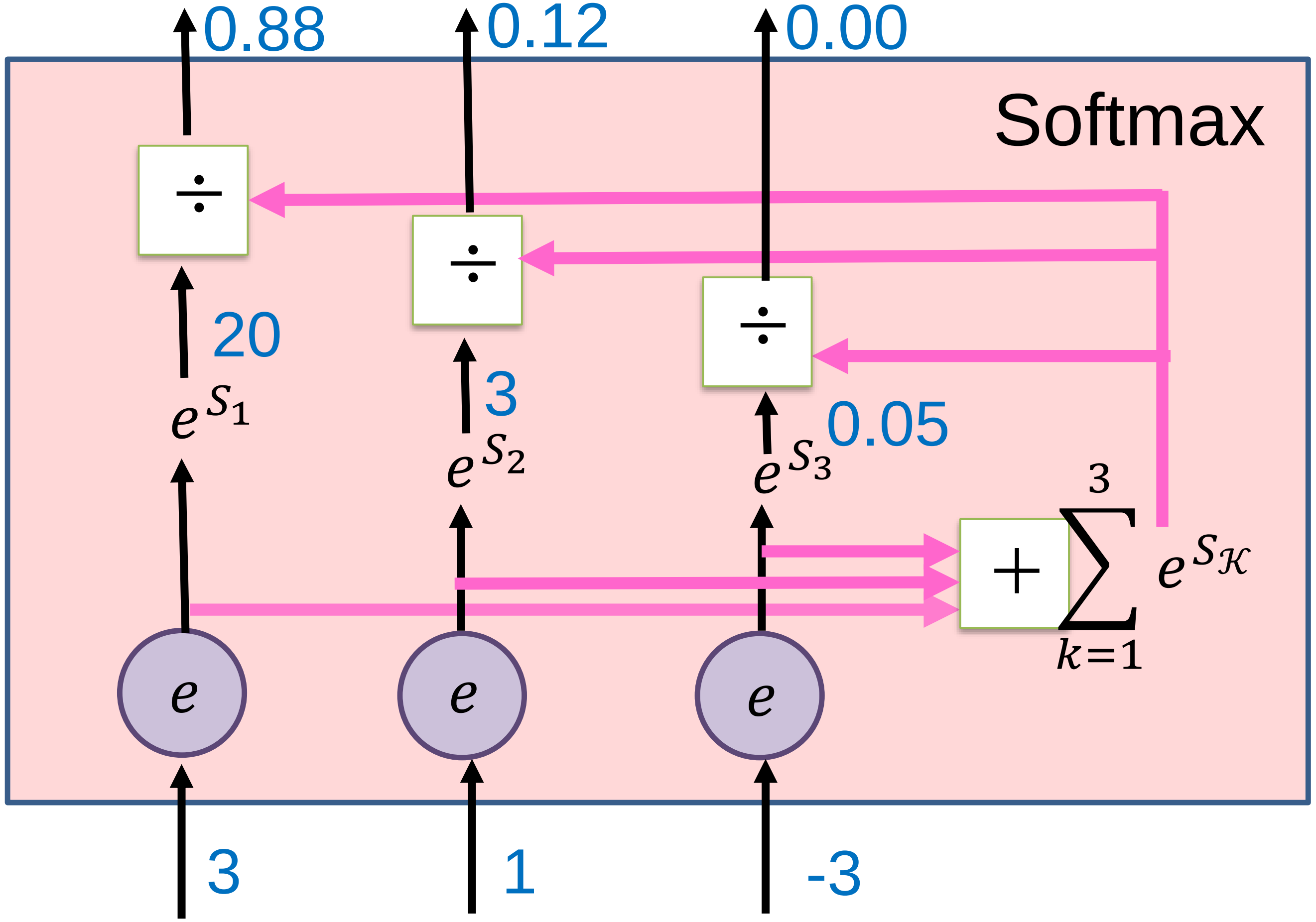




9.3 “Softmax”多类别分类

$$\hat{y}_1 = \frac{e^{S_1}}{\sum_k e^{S_k}} \qquad \hat{y}_2 = \frac{e^{S_2}}{\sum_k e^{S_k}} \qquad \hat{y}_3 = \frac{e^{S_3}}{\sum_k e^{S_k}}$$

$$\mathbf{y} = (y_1, y_2, y_3)^T$$



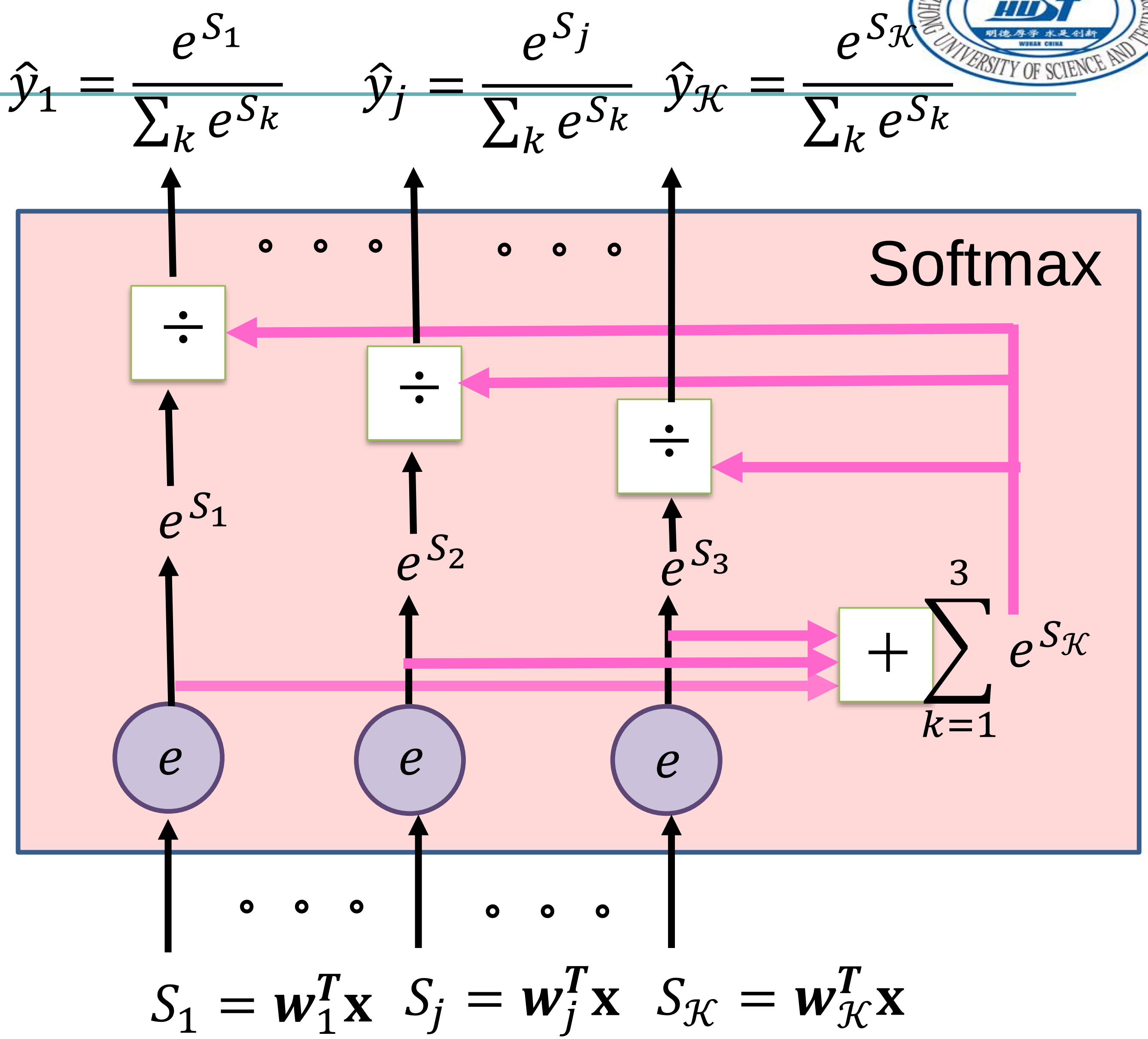
$$S_1 = \mathbf{w}_1^T\mathbf{x} \quad S_2 = \mathbf{w}_2^T\mathbf{x} \quad S_3 = \mathbf{w}_3^T\mathbf{x}$$

输出具有概率特性：

$$0 < \hat{y}_k < 1, \qquad \sum_k \hat{y}_k = 1$$

9.3 “Softmax”多类别分类

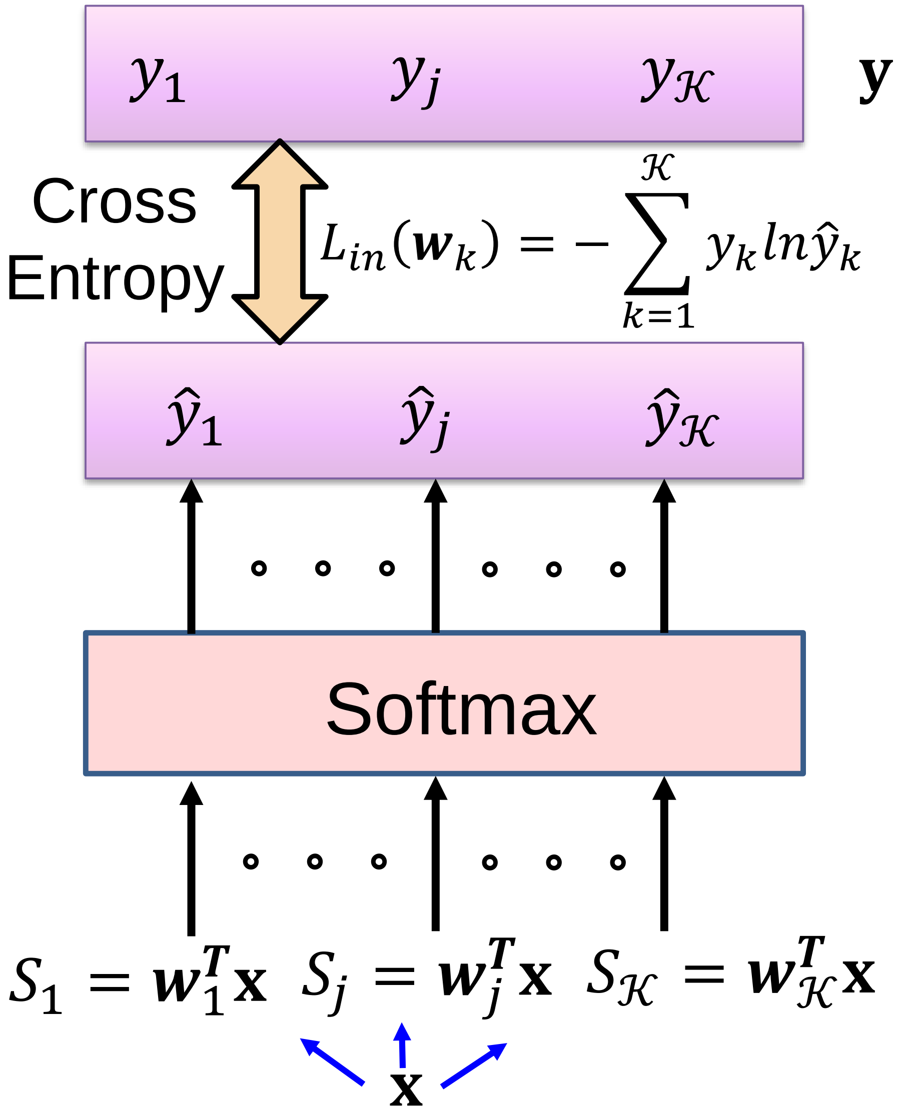
$\mathbf{y} = (y_1, y_2, y_3)^T$



输出具有概率特性：

$$0 < \hat{y}_k < 1, \qquad \sum_k \hat{y}_k = 1$$

9.3 “Softmax”多类别分类



$$\mathbf{y} = (y_1, y_2, \dots, y_j, \dots y_K)^T$$

$if \;\; \mathbf{x} \in class\ 1$

$$\mathbf{y} = \begin{pmatrix} 1 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$L_{in}(\boldsymbol{w}_1) = -ln\hat{y}_1$$

$if \;\; \mathbf{x} \in class\ j$

$$\mathbf{y} = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

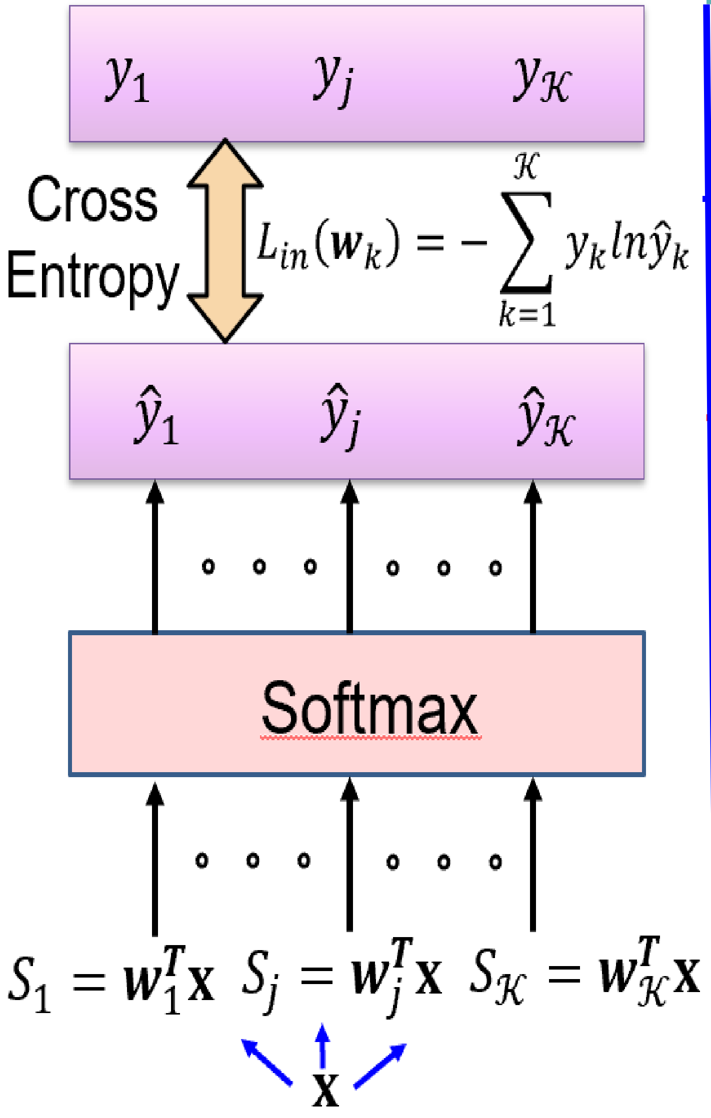
$$L_{in}(\boldsymbol{w}_j) = -ln\hat{y}_j$$

$if \;\; \mathbf{x} \in class\ \mathcal{K}$

$$\mathbf{y} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

$$L_{in}(\boldsymbol{w}_{\mathcal{K}}) = -ln\hat{y}_{\mathcal{K}}$$

9.3 “Softmax” 多类别分类



$$s_j = \mathbf{w}_j^T\mathbf{x}, \qquad \hat{y}_j = \frac{e^{s_j}}{\sum_k e^{s_k}}, \qquad L_{in}(\mathbf{w}_k) = -\sum_{k=1}^{K} y_k ln\hat{y}_k = -ln\hat{y}_k$$

$$\frac{\partial L_{in}}{\partial \mathbf{w}_j} = \frac{\partial L_{in}}{\partial \hat{y}_k}\frac{\partial \hat{y}_k}{\partial S_j}\frac{\partial S_j}{\partial \mathbf{w}_j} = -\frac{1}{\hat{y}_k}\boxed{\frac{\partial \hat{y}_k}{\partial S_j}}\mathbf{x}^T$$

$$\frac{\partial \hat{y}_k}{\partial S_j} = \frac{\partial}{\partial S_j}\left(\frac{e^{s_k}}{\sum_k e^{s_k}}\right) = \frac{(e^{s_k})'\sum_k e^{s_k} - (\sum_k e^{s_k})' e^{s_k}}{(\sum_k e^{s_k})^2} =$$

$$\begin{cases} \dfrac{e^{s_j}\sum_k e^{s_k} - e^{s_j}e^{s_j}}{(\sum_k e^{s_k})^2} = \dfrac{e^{s_j}}{\sum_k e^{s_k}} - \dfrac{e^{s_j}}{\sum_k e^{s_k}}\dfrac{e^{s_j}}{\sum_k e^{s_k}} = \hat{y}_j(1-\hat{y}_j) & j = k \\ \dfrac{0\sum_k e^{s_k} - e^{s_j}e^{s_k}}{(\sum_k e^{s_k})^2} = 0 - \dfrac{e^{s_j}}{\sum_k e^{s_k}}\dfrac{e^{s_k}}{\sum_k e^{s_k}} = -\hat{y}_j\hat{y}_k & j \neq k \end{cases}$$

$$\frac{\partial L_{in}}{\partial \mathbf{w}_j} = \frac{\partial L_{in}}{\partial \hat{y}_k}\frac{\partial \hat{y}_k}{\partial S_j}\frac{\partial S_j}{\partial \mathbf{w}_j} = -\frac{1}{\hat{y}_k}\frac{\partial \hat{y}_k}{\partial S_j}\mathbf{x}^T = \begin{cases} (\hat{y}_j - 1)\mathbf{x}^T & j = k \\ \hat{y}_j\mathbf{x}^T & j \neq k \end{cases}$$

9.3 “Softmax”多类别分类

	OVO,OVA	Softmax
Attributes	Overlap between classes	No overlap between classes
Examples	Indoor scene、 Gray images、 People photos	Indoor scene、 Outdoor urban scene、 Outdoor wilderness scene
	Vocal music、 Dance music、 Movie music、 Pop Song	Classical music、 Country music、 Rock music、 Jazz

9.1 “一对多”策略的多类别分类(Multiclass via One-Versus-All)

样本分类到概率最大的类别

9.2 “一对一”策略的多类别分类(Multiclass via One-Versus-One)

通过投票机制确定样本所属类别

9.3 “Softmax”多类别分类(Multiclass via Softmax)

用交叉熵 (cross entropy) 作为损失函数求解分类面