

Machine Learning Foundations

(機器學習基石)



Lecture 11: Linear Models for Classification

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Roadmap

- 1 When Can Machines Learn?
- 2 Why Can Machines Learn?
- 3 **How** Can Machines Learn?

Lecture 10: Logistic Regression

gradient descent on **cross-entropy error**
to get good **logistic hypothesis**

Lecture 11: Linear Models for Classification

- Linear Models for Binary Classification
- Stochastic Gradient Descent
- Multiclass via Logistic Regression
- Multiclass via Binary Classification

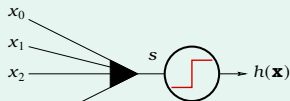
- 4 How Can Machines Learn Better?

Linear Models Revisited

linear scoring function: $\mathbf{s} = \mathbf{w}^T \mathbf{x}$

linear classification

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

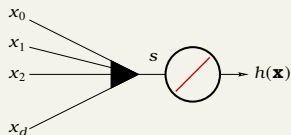


plausible err = 0/1

discrete $E_{\text{in}}(\mathbf{w})$:
NP-hard to solve

linear regression

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

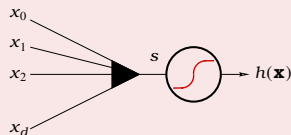


friendly err = squared

quadratic convex $E_{\text{in}}(\mathbf{w})$:
closed-form solution

logistic regression

$$h(\mathbf{x}) = \theta(\mathbf{s})$$



plausible err = cross-entropy

smooth convex $E_{\text{in}}(\mathbf{w})$:
gradient descent

can linear regression or logistic regression
help linear classification?

Error Functions Revisited

linear scoring function: $\mathbf{s} = \mathbf{w}^T \mathbf{x}$

for binary classification $y \in \{-1, +1\}$

linear classification

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

$$\text{err}(h, \mathbf{x}, y) = \mathbb{I}[h(\mathbf{x}) \neq y]$$

$$\text{err}_{0/1}(\mathbf{s}, y)$$

$$= \mathbb{I}[\text{sign}(\mathbf{s}) \neq y]$$

$$= \mathbb{I}[\text{sign}(y\mathbf{s}) \neq 1]$$

linear regression

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

$$\text{err}(h, \mathbf{x}, y) = (h(\mathbf{x}) - y)^2$$

$$\text{err}_{\text{SQR}}(\mathbf{s}, y)$$

$$= (\mathbf{s} - y)^2$$

$$= (y\mathbf{s} - 1)^2$$

logistic regression

$$h(\mathbf{x}) = \theta(\mathbf{s})$$

$$\text{err}(h, \mathbf{x}, y) = -\ln h(y\mathbf{x})$$

$$\text{err}_{\text{CE}}(\mathbf{s}, y)$$

$$= \ln(1 + \exp(-y\mathbf{s}))$$

$(y\mathbf{s})$: classification correctness score

$y\mathbf{s}$ 如果同号，表示正确，并且越大越好

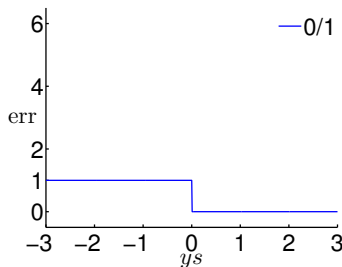
Visualizing Error Functions

$$\text{0/1 } \text{err}_{0/1}(s, y) = \mathbb{I}[\text{sign}(ys) \neq 1]$$

$$\text{sqr } \text{err}_{\text{SQR}}(s, y) = (ys - 1)^2$$

$$\text{ce } \text{err}_{\text{CE}}(s, y) = \ln(1 + \exp(-ys))$$

$$\text{scaled ce } \text{err}_{\text{SCE}}(s, y) = \log_2(1 + \exp(-ys))$$



- **0/1**: 1 iff $ys \leq 0$
- **sqr**: large if $ys \ll 1$
but over-charge $ys \gg 1$
 small $\text{err}_{\text{SQR}} \rightarrow$ small $\text{err}_{0/1}$
- **ce**: monotonic of ys
 small $\text{err}_{\text{CE}} \leftrightarrow$ small $\text{err}_{0/1}$
- **scaled ce**: a proper upper bound of **0/1**
 small $\text{err}_{\text{SCE}} \leftrightarrow$ small $\text{err}_{0/1}$

upper bound:
 useful for designing algorithmic error $\widehat{\text{err}}$

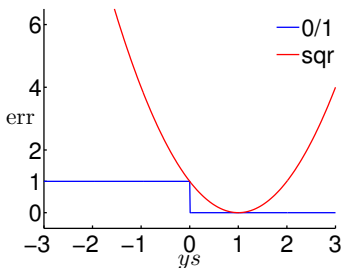
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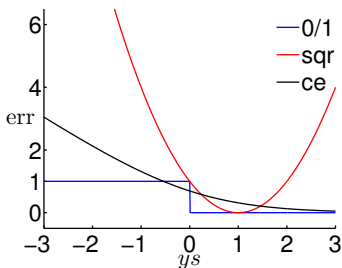
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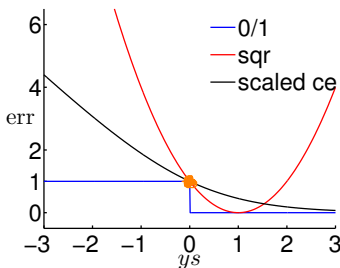
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useful for designing algorithmic error $\hat{\text{err}}$

Theoretical Implication of Upper Bound

For any $\mathbf{y}\mathbf{s}$ where $\mathbf{s} = \mathbf{w}^T \mathbf{x}$

$$\text{err}_{0/1}(\mathbf{s}, \mathbf{y}) \leq \text{err}_{\text{SCE}}(\mathbf{s}, \mathbf{y}) = \frac{1}{\ln 2} \text{err}_{\text{CE}}(\mathbf{s}, \mathbf{y}).$$

$$\Rightarrow E_{\text{in}}^{0/1}(\mathbf{w}) \leq E_{\text{in}}^{\text{SCE}}(\mathbf{w}) = \frac{1}{\ln 2} E_{\text{in}}^{\text{CE}}(\mathbf{w})$$

$$E_{\text{out}}^{0/1}(\mathbf{w}) \leq E_{\text{out}}^{\text{SCE}}(\mathbf{w}) = \frac{1}{\ln 2} E_{\text{out}}^{\text{CE}}(\mathbf{w})$$

VC on 0/1:

$$\begin{aligned} E_{\text{out}}^{0/1}(\mathbf{w}) &\leq E_{\text{in}}^{0/1}(\mathbf{w}) + \Omega^{0/1} \\ &\leq \frac{1}{\ln 2} E_{\text{in}}^{\text{CE}}(\mathbf{w}) + \Omega^{0/1} \end{aligned}$$

VC-Reg on CE :

$$\begin{aligned} E_{\text{out}}^{0/1}(\mathbf{w}) &\leq \frac{1}{\ln 2} E_{\text{out}}^{\text{CE}}(\mathbf{w}) \\ &\leq \frac{1}{\ln 2} E_{\text{in}}^{\text{CE}}(\mathbf{w}) + \frac{1}{\ln 2} \Omega^{\text{CE}} \end{aligned}$$

small $E_{\text{in}}^{\text{CE}}(\mathbf{w}) \Rightarrow$ small $E_{\text{out}}^{0/1}(\mathbf{w})$:
logistic/linear reg. for **linear classification**

Regression for Classification

- 1 run **logistic/linear reg.** on \mathcal{D} with $y_n \in \{-1, +1\}$ to get \mathbf{w}_{REG}
- 2 return $g(\mathbf{x}) = \text{sign}(\mathbf{w}_{\text{REG}}^T \mathbf{x})$

PLA

- pros: **efficient + strong guarantee if lin. separable**
- cons: works only if lin. separable, otherwise needing **pocket** heuristic

linear regression

- pros: **'easiest' optimization**
- cons: loose bound of $\text{err}_{0/1}$ for large $|y_s|$

logistic regression

- pros: **'easy' optimization**
- cons: loose bound of $\text{err}_{0/1}$ for very negative y_s

可以将线性回归得到的值当做PLA、pocket、LR的初始值 \mathbf{w}_0

- **linear regression** sometimes used to **set \mathbf{w}_0** for **PLA/pocket/logistic regression**
- **logistic regression** often preferred over **pocket**

LR和pocket效果差不多，但是一般LR更常用

Fun Time

Following the definition in the lecture, which of the following is not always $\geq \text{err}_{0/1}(y, s)$ when $y \in \{-1, +1\}$?

- ① $\text{err}_{0/1}(y, s)$
- ② $\text{err}_{\text{SQR}}(y, s)$
- ③ $\text{err}_{\text{CE}}(y, s)$
- ④ $\text{err}_{\text{SCE}}(y, s)$

Reference Answer: ③

Too simple, uh? :-) Anyway, note that $\text{err}_{0/1}$ is surely an upper bound of itself.

Two Iterative Optimization Schemes

For $t = 0, 1, \dots$

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \eta \mathbf{v}$$

when stop, return last \mathbf{w} as g

PLA

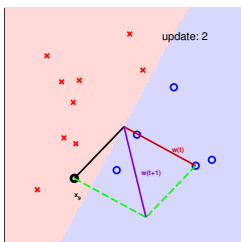
pick (\mathbf{x}_n, y_n) and decide \mathbf{w}_{t+1} by
the one example

$O(1)$ time per iteration :-)

logistic regression (pocket)

check \mathcal{D} and decide \mathbf{w}_{t+1} (or
new $\hat{\mathbf{w}}$) by **all examples**

$O(N)$ time per iteration :-)



logistic regression with
 $O(1)$ time per iteration?

Logistic Regression Revisited

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \underbrace{\eta \frac{1}{N} \sum_{n=1}^N \theta \left(-y_n \mathbf{w}_t^T \mathbf{x}_n \right) (y_n \mathbf{x}_n)}_{-\nabla E_{\text{in}}(\mathbf{w}_t)}$$

- want: update direction $\mathbf{v} \approx -\nabla E_{\text{in}}(\mathbf{w}_t)$
while computing \mathbf{v} by one single (\mathbf{x}_n, y_n)
- technique on removing $\frac{1}{N} \sum_{n=1}^N$:
view as expectation \mathcal{E} over uniform choice of n !

stochastic gradient:

$\nabla_{\mathbf{w}} \text{err}(\mathbf{w}, \mathbf{x}_n, y_n)$ with random n

true gradient:

$$\nabla_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) = \mathcal{E}_{\text{random } n} \nabla_{\mathbf{w}} \text{err}(\mathbf{w}, \mathbf{x}_n, y_n)$$

Stochastic Gradient Descent (SGD)

stochastic gradient = true gradient + zero-mean 'noise' directions

Stochastic Gradient Descent

- idea: replace true gradient by stochastic gradient
- after enough steps,
average true gradient \approx average stochastic gradient
- pros: **simple & cheaper computation :-)**
—useful for **big data** or **online learning**
- cons: less stable in nature

SGD logistic regression, **looks familiar? :-)**:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \underbrace{\eta \theta \left(-y_n \mathbf{w}_t^T \mathbf{x}_n \right) (y_n \mathbf{x}_n)}_{-\nabla \text{err}(\mathbf{w}_t, \mathbf{x}_n, y_n)}$$

PLA Revisited

SGD logistic regression:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \eta \cdot \theta \left(-y_n \mathbf{w}_t^T \mathbf{x}_n \right) (y_n \mathbf{x}_n)$$

PLA:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + 1 \cdot \left[y_n \neq \text{sign}(\mathbf{w}_t^T \mathbf{x}_n) \right] (y_n \mathbf{x}_n)$$

- SGD logistic regression \approx 'soft' PLA
- PLA \approx SGD logistic regression with $\eta = 1$ when $\mathbf{w}_t^T \mathbf{x}_n$ large

two practical rule-of-thumb:

- stopping condition? t large enough
- η ? 0.1 when \mathbf{x} in proper range

经验上来看, η 取0.1附近的时候效果不错 (前提是 \mathbf{x} 在合适的范围内)

Fun Time

Consider applying SGD on linear regression for big data. What is the update direction when using the negative stochastic gradient?

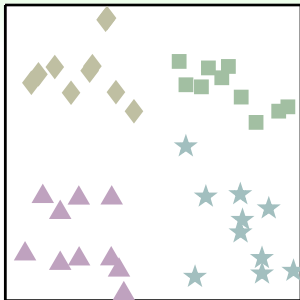
- ① \mathbf{x}_n
- ② $y_n \mathbf{x}_n$
- ③ $2(\mathbf{w}_t^T \mathbf{x}_n - y_n) \mathbf{x}_n$
- ④ $2(y_n - \mathbf{w}_t^T \mathbf{x}_n) \mathbf{x}_n$

Reference Answer: ④

Go check lecture 9 if you have forgotten about the gradient of squared error. :-)

Anyway, the update rule has a nice physical interpretation: improve \mathbf{w}_t by ‘correcting’ proportional to the residual $(y_n - \mathbf{w}_t^T \mathbf{x}_n)$.

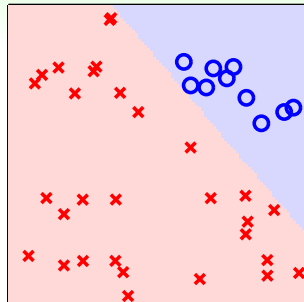
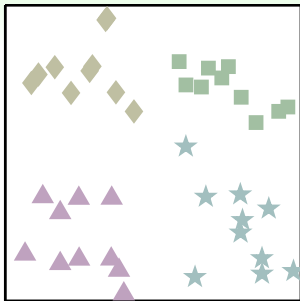
Multiclass Classification



- $\mathcal{Y} = \{\square, \diamond, \triangle, \star\}$
(4-class classification)
- **many applications** in practice, especially for 'recognition'

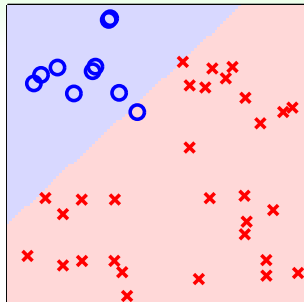
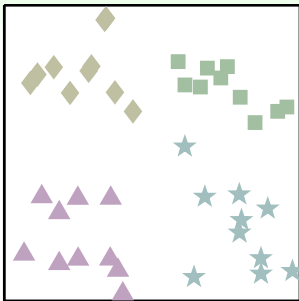
next: use **tools for $\{\times, \circ\}$ classification** to
 $\{\square, \diamond, \triangle, \star\}$ classification

One Class at a Time



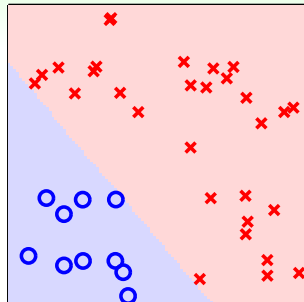
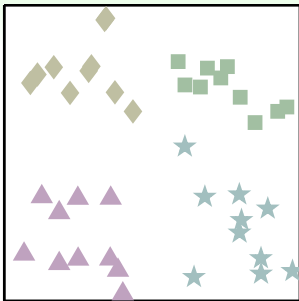
□ or not? $\{\square = \circ, \diamond = \times, \triangle = \times, \star = \times\}$

One Class at a Time



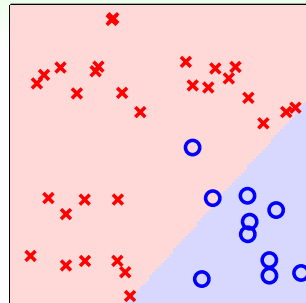
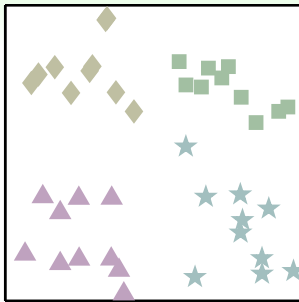
◇ or not? $\{\square = \times, \diamond = \circ, \triangle = \times, \star = \times\}$

One Class at a Time



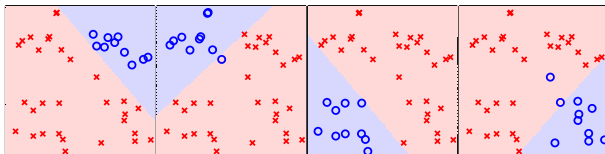
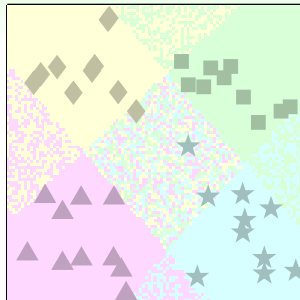
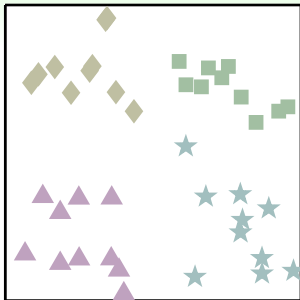
\triangle or not? $\{\square = \times, \diamond = \times, \triangle = \circ, \star = \times\}$

One Class at a Time



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

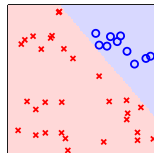
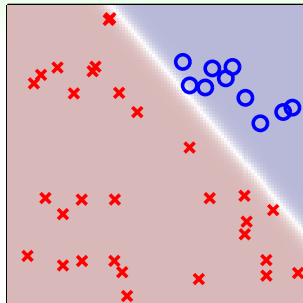
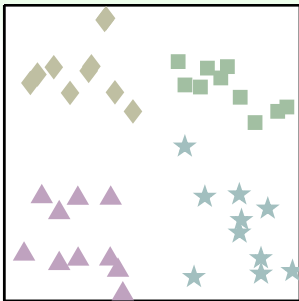
Multiclass Prediction: Combine Binary Classifiers



but **ties?** :-)

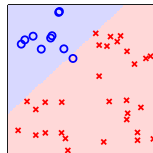
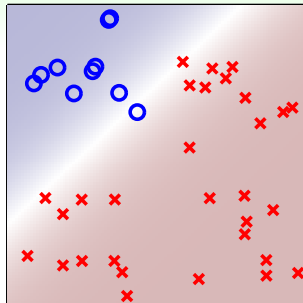
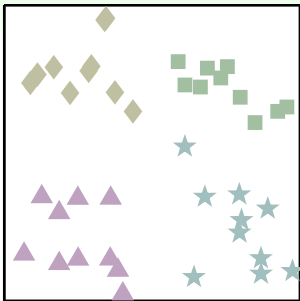
One Class at a Time **Softly**

求出属于每个类别的概率



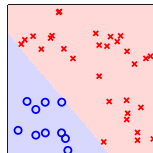
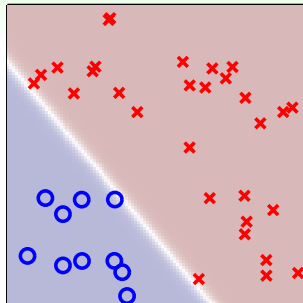
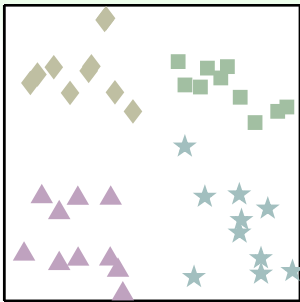
$$P(\square|\mathbf{x})? \{ \square = \circ, \diamond = \times, \triangle = \times, \star = \times \}$$

One Class at a Time **Softly**



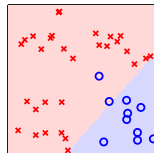
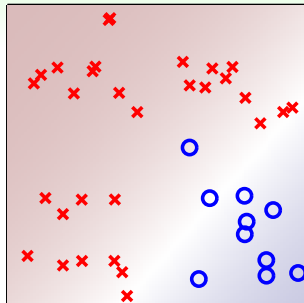
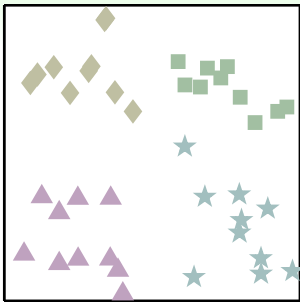
$$P(\diamond | \mathbf{x})? \{ \square = \times, \diamond = \circ, \triangle = \times, \star = \times \}$$

One Class at a Time **Softly**



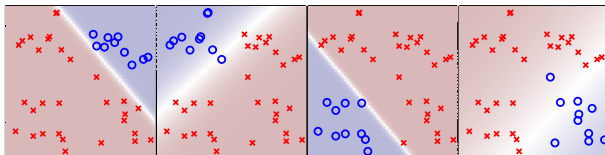
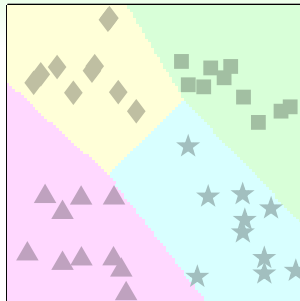
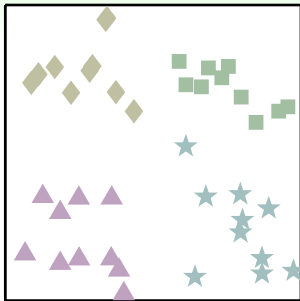
$$P(\triangle | \mathbf{x})? \{ \square = \times, \diamond = \times, \triangle = \circ, \star = \times \}$$

One Class at a Time **Softly**



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

Multiclass Prediction: Combine **Soft** Classifiers



$$g(\mathbf{x}) = \operatorname{argmax}_{k \in \mathcal{Y}} \theta \left(\mathbf{w}_{[k]}^T \mathbf{x} \right)$$

Sigmoid函数是单调的，所以不加也可以

One-Versus-All (OVA) Decomposition

- 1 for $k \in \mathcal{Y}$
obtain $\mathbf{w}_{[k]}$ by running **logistic regression** on

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

- 2 return $g(\mathbf{x}) = \operatorname{argmax}_{k \in \mathcal{Y}} (\mathbf{w}_{[k]}^T \mathbf{x})$

- pros: efficient,
can be coupled with any **logistic regression-like approaches**
- cons: often **unbalanced** $\mathcal{D}_{[k]}$ when K large 当K很大时，样本会显得
不均衡
- extension: **multinomial ('coupled') logistic regression**

LR是可以扩展到多分类的情况的

OVA: a simple multiclass **meta-algorithm**
to keep in your toolbox

Fun Time

Which of the following best describes the training effort of OVA decomposition based on logistic regression on some K -class classification data of size N ?

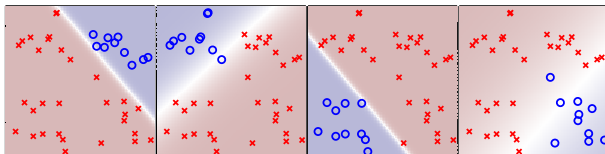
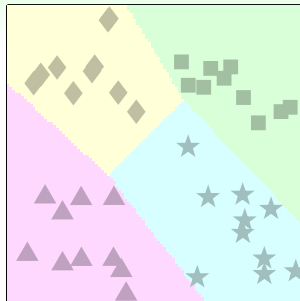
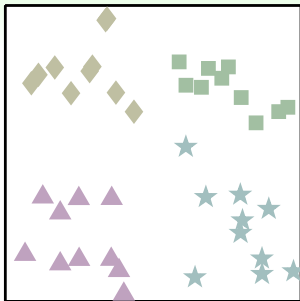
- ① learn K logistic regression hypotheses, each from data of size N/K
- ② learn K logistic regression hypotheses, each from data of size $N \ln K$
- ③ learn K logistic regression hypotheses, each from data of size N
- ④ learn K logistic regression hypotheses, each from data of size NK

Reference Answer: ③

Note that the **learning part can be easily done in parallel**, while the data is essentially of the same size as the original data.

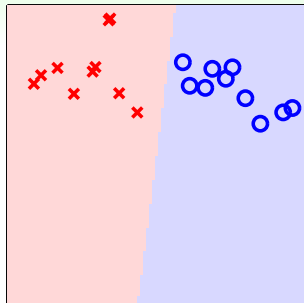
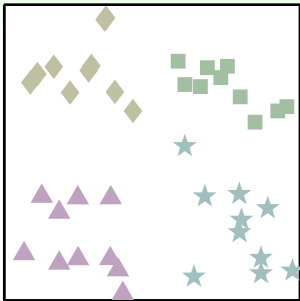
可以在K个机器上并行

Source of **Unbalance**: One versus **All**



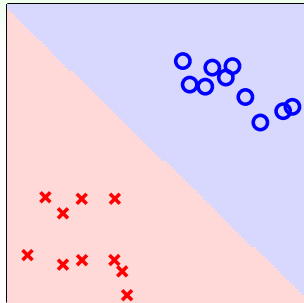
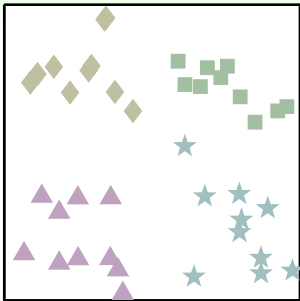
idea: make binary classification problems
more **balanced** by one versus **one**

One versus One at a Time



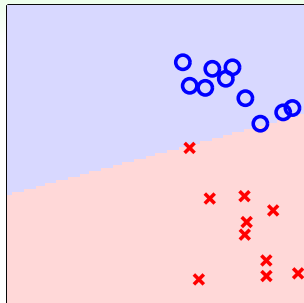
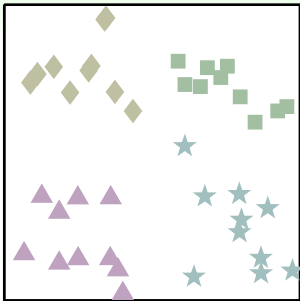
\square or \diamond ? $\{\square = \circ, \diamond = \times, \triangle = \text{nil}, \star = \text{nil}\}$

One versus One at a Time



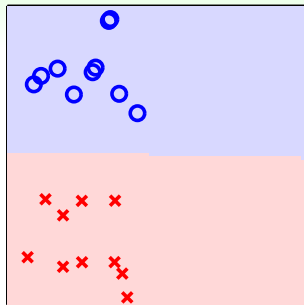
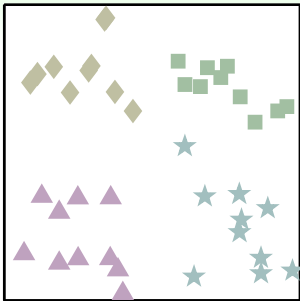
\square or \triangle ? $\{\square = \circ, \diamond = \text{nil}, \triangle = \times, \star = \text{nil}\}$

One versus One at a Time



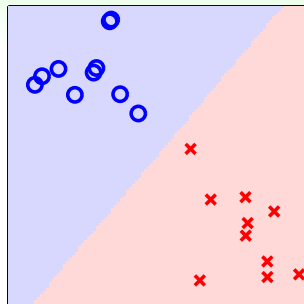
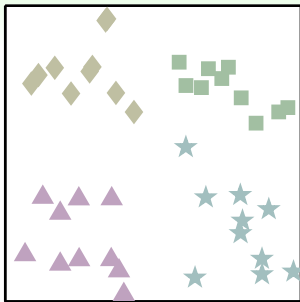
□ or ★? {□ = ○, ◇ = nil, △ = nil, ★ = ×}

One versus One at a Time



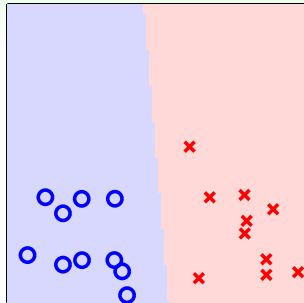
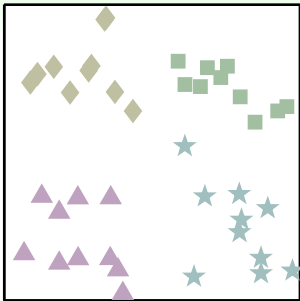
\diamond or \triangle ? $\{\square = \text{nil}, \diamond = \circ, \triangle = \times, \star = \text{nil}\}$

One versus One at a Time



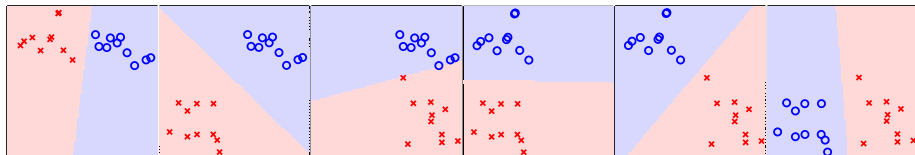
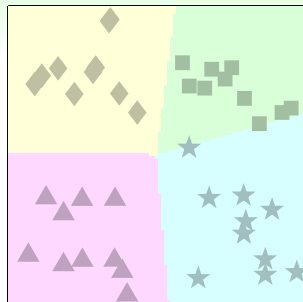
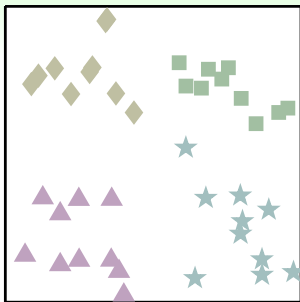
\diamond or \star ? $\{\square = \text{nil}, \diamond = \circ, \triangle = \text{nil}, \star = \times\}$

One versus One at a Time



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

Multiclass Prediction: Combine **Pairwise** Classifiers



$$g(\mathbf{x}) = \text{tournament champion} \left\{ \mathbf{w}_{[k,\ell]}^T \mathbf{x} \right\}$$

投票法

(voting of classifiers)

One-versus-one (OVO) Decomposition

- 1 for $(k, \ell) \in \mathcal{Y} \times \mathcal{Y}$
obtain $\mathbf{w}_{[k, \ell]}$ by running **linear binary classification** on

$$\mathcal{D}_{[k, \ell]} = \{(\mathbf{x}_n, y'_n = 2 \mathbb{I}[y_n = k] - 1) : y_n = k \text{ or } y_n = \ell\}$$

- 2 return $g(\mathbf{x}) = \text{tournament champion } \left\{ \mathbf{w}_{[k, \ell]}^T \mathbf{x} \right\}$

- pros: efficient ('smaller' training problems), stable,
can be coupled with any **binary classification approaches**
- cons: use $O(K^2)$ $\mathbf{w}_{[k, \ell]}$
—**more space, slower prediction, more training**

OVO: another simple multiclass
meta-algorithm to keep in your toolbox

Fun Time

Assume that some binary classification algorithm takes exactly N^3 CPU-seconds for data of size N . Also, for some 10-class multiclass classification problem, assume that there are $N/10$ examples for each class. Which of the following is total CPU-seconds needed for OVO decomposition based on the binary classification algorithm?

- 1 $\frac{9}{200} N^3$
- 2 $\frac{9}{25} N^3$
- 3 $\frac{4}{5} N^3$
- 4 N^3

Reference Answer: ②

There are 45 binary classifiers, each trained with data of size $(2N)/10$. Note that OVA decomposition with the same algorithm would take $10N^3$ time, much worse than OVO.

Summary

- 1 When Can Machines Learn?
- 2 Why Can Machines Learn?
- 3 **How** Can Machines Learn?

Lecture 10: Logistic Regression

Lecture 11: Linear Models for Classification

- Linear Models for Binary Classification
three models useful in different ways
- Stochastic Gradient Descent
follow negative stochastic gradient
- Multiclass via Logistic Regression
predict with maximum estimated $P(k|\mathbf{x})$
- Multiclass via Binary Classification
predict the tournament champion

- **next: from linear to nonlinear**

- 4 How Can Machines Learn Better?