第五章 非线性方法

集成学习

（Ensemble learning）

如何获得一个更好的分类系统?

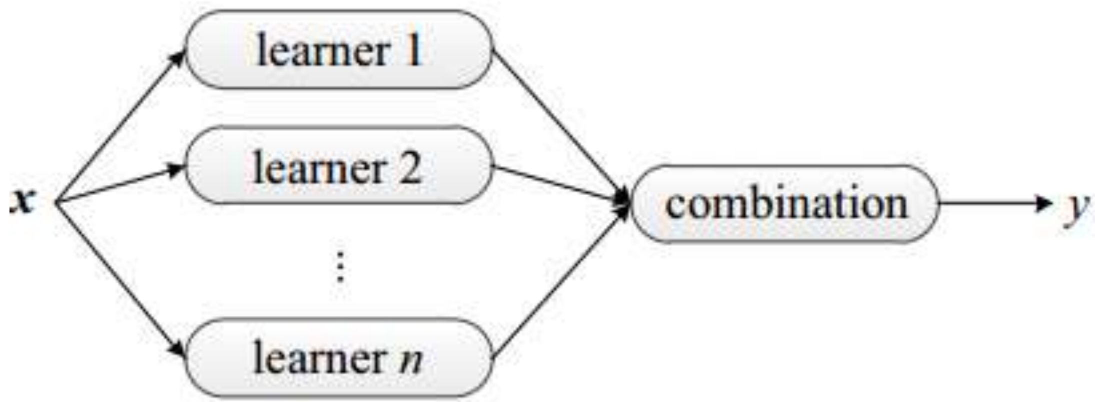
- 提取更好的特征
- 利用更强大的学习算法
- 更多的训练样本
- 样本在不同空间的映射
- 利用先验知识和上下文信息
- …
- 分类器的组合

三个臭皮匠赛过诸葛亮

社会生活中常用的原则：民主选举

Ensemble learning

若干个“弱”学习器进行结合，常获得比单一学习器显著优越的性能



基学习器（base learner）

投票： $g(\mathbf{x}) = sign\left[\sum_{k=1}^{N} h_k(\mathbf{x})\right]$

神经网络、随机森林, …

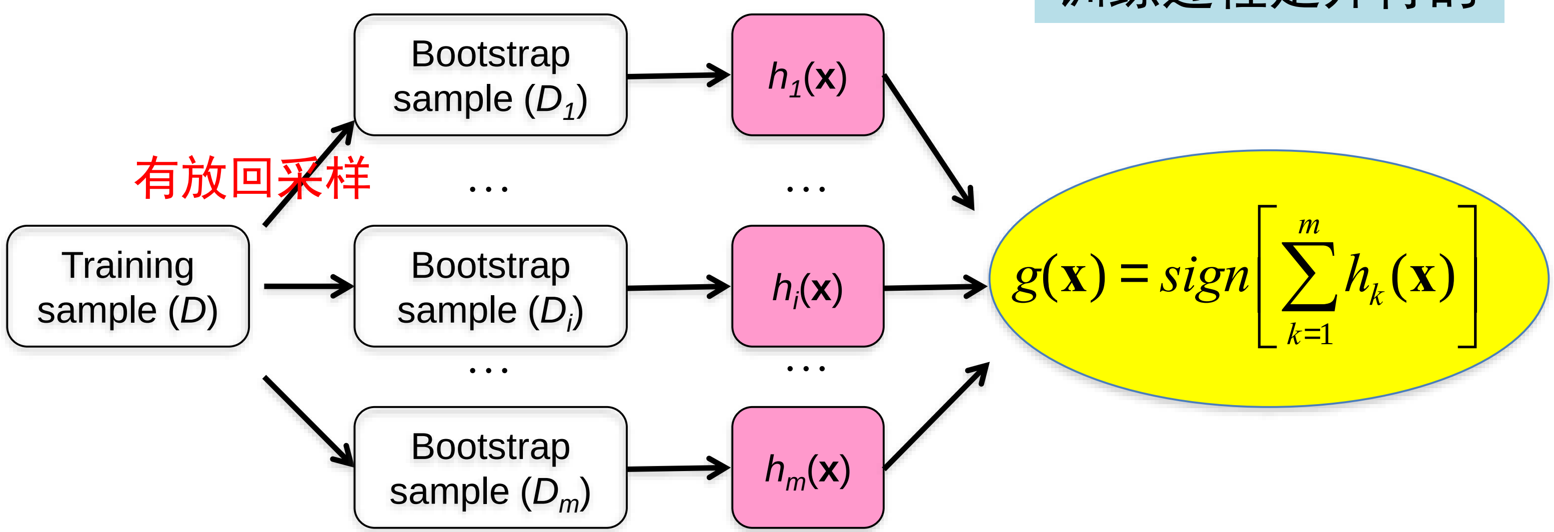
两种思路

- 个体学习器之间存在强依赖关系，串行生成学习器—Boosting
- 个体学习器之间不存在强依赖关系，可以并行生成学习器— Bagging, Random Forest
- 引入扰动：
  - 数据的扰动
  - 属性的扰动
  - 参数的扰动

Bagging (bootstrap aggregating)

- 对训练数据D有放回抽样生成m个数据集D_i, $(i=1,\ldots,m)$
- 在每一个数据集D_i上训练分类器h_i
- 对各个分类器的结果集成投票

训练过程是并行的



当D_i大小与D相同时，大约63.2% $(1-(1-1/n)^n)=1-1/e$的样本被抽到，有的样本出现两次或两次以上

防止过拟合，减小模型方差

- 随机森林 Random Forests

(Leo Breiman, *Machine Learning, 45: 5-32, 2001*)

(http://www.stat.berkeley.edu/users/breiman/RandomForests/cc_home.htm)

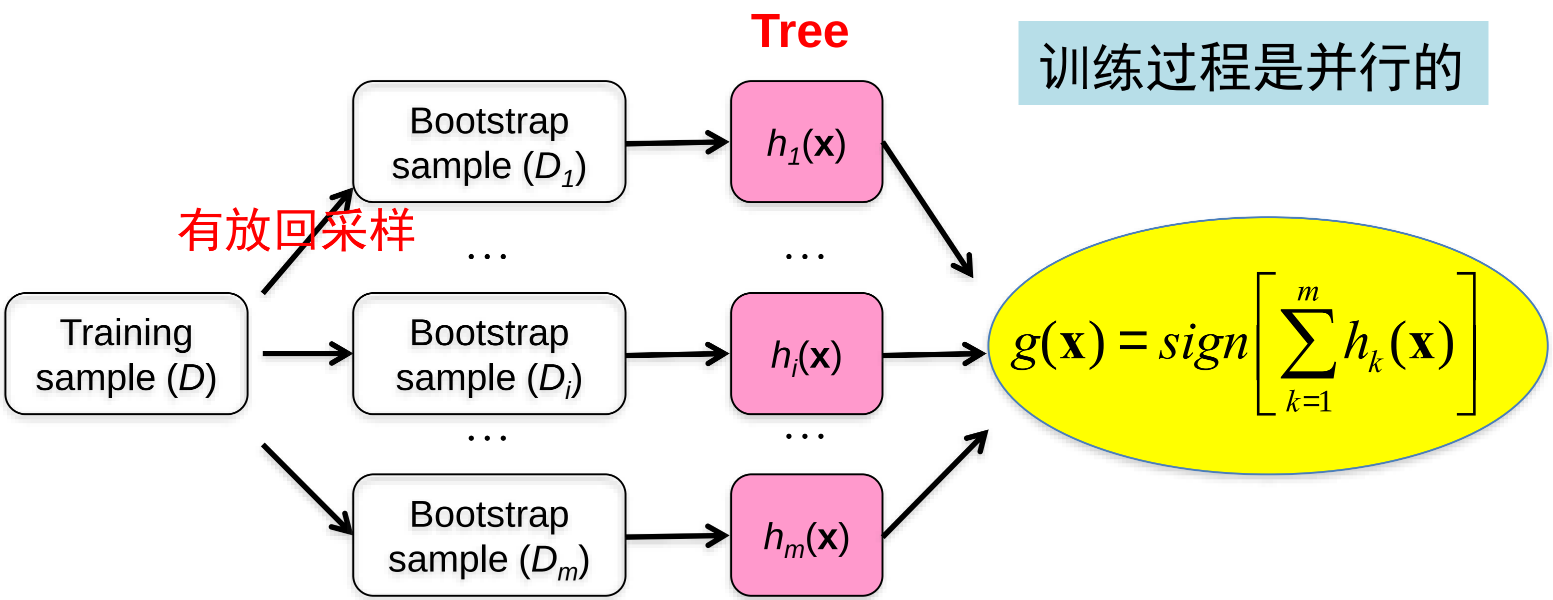
- Many decision trees

➔ Random Forest

Leo Breiman (1928-2005)

随机森林 Random Forests

- 利用bootstrapping的办法，训练多棵树(每次从*N*个训练样本中有放回地随机抽取*N*个样本作为当前训练集)
- 每次随机抽取*k*（*k*<*p*）个特征作为当前节点下决策的备选特征，从中选择特征进行划分（split）
- 最后对每一颗树的预测结果进行汇总投票，作为最终预测



Boosting

- 通过迭代对分类器的输入输出进行加权
  - 开始时所有训练样本同样权重
  - 每一轮学习一个“弱”分类器
  - 根据现有“弱”分类器的加权投票结果对训练样本分布进行调整，对分错的样本给予更多关注
  - 直到“弱”分类器数目达到预先制定的数目k_{max}，最终将k_{max}个分类器的结果加权组合

最终组合函数：
$$g(\mathbf{x}) = sign\left[\sum_{k=1}^{k\max} a_k h_k(\mathbf{x})\right]$$

AdaBoost算法

核心思路：对错分样本进行加权

Algorithm 1. (AdaBoost)

begin **initialize** $\mathcal{D} = \{\mathbf{x}^1, y_1, \ldots, \mathbf{x}^n, y_n\}, k_{max}, W_1(i) = 1/n, i = 1, \ldots, n$

$k \leftarrow 0$

do $k \leftarrow k + 1$

train weak learner C_k using $\mathcal{D}$ sampled according to $W_k(i)$

$E_k \leftarrow$ training error of C_k measured on $\mathcal{D}$ using $W_k(i)$

$\alpha_k \leftarrow \frac{1}{2}\ln[(1 - E_k)/E_k]$

$W_{k+1}(i) \leftarrow \frac{W_k(i)}{Z_k} \times \begin{cases} e^{-\alpha_k} & \text{if } h_k(\mathbf{x}^i) = y_i \text{ (correctly classified)} \\ e^{\alpha_k} & \text{if } h_k(\mathbf{x}^i) \neq y_i \text{ (incorrectly classified)} \end{cases}$

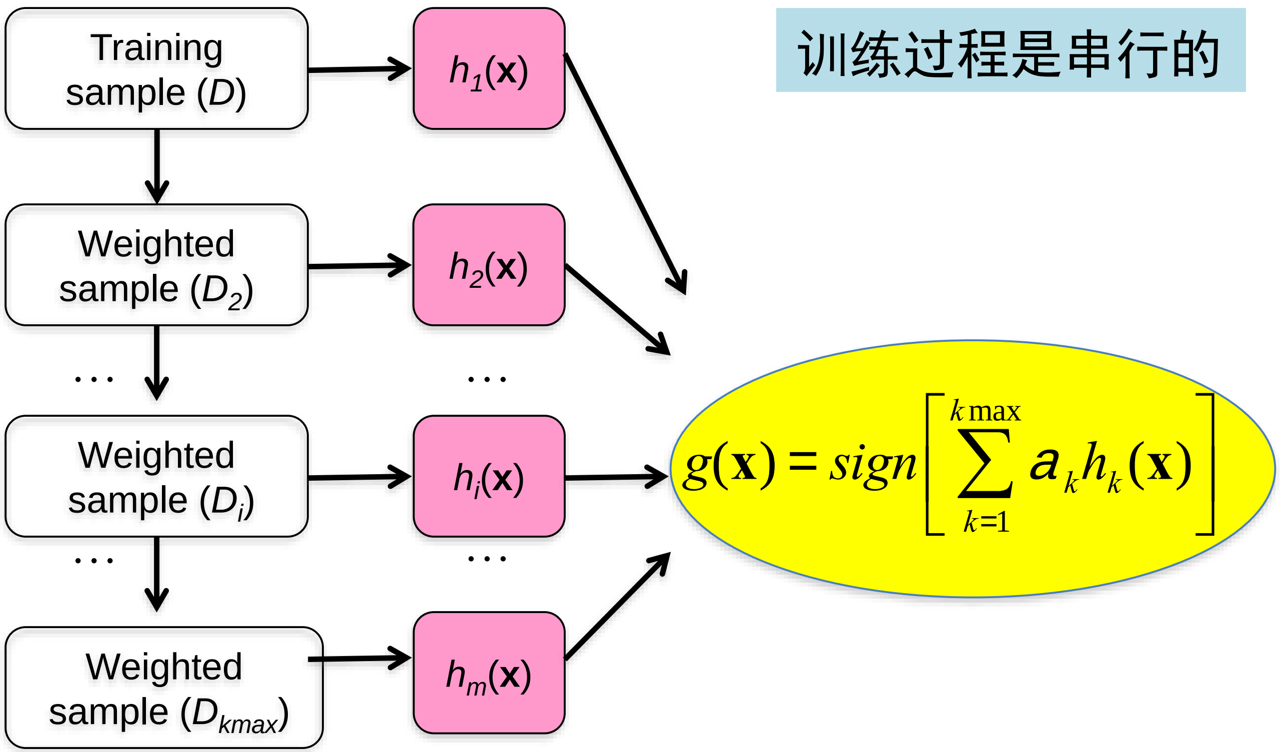
until $k = k_{max}$

return C_k and α_k for $k = 1$ to k_{max} (ensemble of classifiers with weights)

end

最终组合函数： $g(\mathbf{x}) = sign\left[\sum_{k=1}^{k\max} a_k h_k(\mathbf{x})\right]$

AdaBoost: Adaptive Boosting



训练过程是串行的

Ada Boost (Freund & Schapire, 1997)

Ada Boost for 2 Classes

Initialization step: for each example x, set

$$D(\mathbf{x}) = \frac{1}{N}, \text{ where } N \text{ is the number of examples}$$

Iteration step (for $t = 1 \ldots T$):

1. Find best weak classifier $h_t(x)$ using weights $D_t(x)$
2. Compute the error rate ε_t as

$$\varepsilon_t = \sum_{i=1}^{N} D(\mathbf{x}_i) \cdot \underbrace{\mathbf{I}[y_i \neq h_t(\mathbf{x}_i)]}_{= \begin{cases} 1 & \text{if } y_i \neq h_t(x_i) \\ 0 & \text{otherwise} \end{cases}}$$

3. assign weight α_t to classifier h_t in the final hypothesis

$$\alpha_t = \log((1 - \varepsilon_t)/\varepsilon_t)$$

4. For each x_i, $D(\mathbf{x}_i) = D(\mathbf{x}_i) \cdot \exp(\alpha_t \cdot \mathbf{I}[y_i \neq h_t(\mathbf{x}_i)])$
5. Normalize $D(x_i)$ so that $\sum_{i=1}^{N} D(\mathbf{x}_i) = 1$

$$\boxed{f_{final}(x) = \text{sign}\left[\sum \alpha_t h_t(x)\right]}$$

Ada Boost: step by step

1. Find best weak classifier $\boldsymbol{h_t(x)}$ using weights $\mathbf{D}(\boldsymbol{x})$

- Some classifiers accept weighted samples, but most don’t
- If the classifier does not take weighted samples, this step is done by sampling from the training samples according to the distribution $\boldsymbol{D}(\boldsymbol{x})$

1/16 1/4 1/16 1/16 1/4 1/16 1/4

- Draw **k** samples, each $\boldsymbol{x}$ with probability equal to $\boldsymbol{D}(\boldsymbol{x})$:

Ada Boost: step by step

1. Find best weak classifier $\boldsymbol{h}_t(\boldsymbol{x})$ using weights $\mathbf{D}(\boldsymbol{x})$

- Give to the classifier the following re-sampled examples:

- To find the best weak classifier, go through ALL weak classifiers, and find the one that works best (gives smallest error) on the collection above

	$\boldsymbol{h}_1(\boldsymbol{x})$	$\boldsymbol{h}_2(\boldsymbol{x})$	$\boldsymbol{h}_3(\boldsymbol{x})$	....	$\boldsymbol{h}_m(\boldsymbol{x})$
errors:	*0.46*	*0.36*	*0.16*		*0.43*

the best classifier $h_t(x)$ at iteration t

Ada Boost: step by step

2. Compute $\boldsymbol{\varepsilon_t}$ the error rate as

$$\varepsilon_t = \sum D(x_i) \cdot I[y_i \neq h_t(x_i)]$$

- where $I[y_i \neq h_t(x_i)] = \begin{cases} 1 & \text{if} \quad y_i \neq h_t(x_i) \\ 0 & \text{otherwise} \end{cases}$

1/16	**1/4**	**1/16**	**1/16**	**1/4**	**1/16**	**1/4**
✓	✓	✓	✗	✗	✓	✓

$$\varepsilon_t = \frac{1}{4} + \frac{1}{16} = \frac{5}{16}$$

- $\boldsymbol{\varepsilon_t}$ is simply the weight of all misclassified examples added
  - notice that error rate is computed over original examples, not the re-sampled examples
- If a weak classifier is better than random, then $\boldsymbol{\varepsilon_t} < \frac{1}{2}$

Ada Boost: step by step

3. assign weight α_t to classifier h_t in the final hypothesis

$$\alpha_t = \log\left((1-\varepsilon_t)/\varepsilon_t\right)$$

Example from previous slide:

$$\varepsilon_t = \frac{5}{16} \quad \Rightarrow \quad \alpha_t = \log \frac{1-\frac{5}{16}}{\frac{5}{16}} = \log \frac{11}{5} \approx 0.8$$

- Recall that $\varepsilon_t < ½$
- Thus $(1-\varepsilon_t)/\varepsilon_t > 1 \Rightarrow \alpha_t > 0$
- The smaller is ε_t, the larger is α_t, and thus the more importance (weight) classifier $h_t(x)$ gets in the final classifier

$$f_{final}(x) = \text{sign}\left[\sum \alpha_t h_t(x)\right]$$

Ada Boost: step by step

4. For each $\boldsymbol{x}_i$, $\boldsymbol{D}(\boldsymbol{x}_i) = \boldsymbol{D}(\boldsymbol{x}_i) \cdot \exp[\boldsymbol{\alpha}_t \cdot \boldsymbol{I}(\boldsymbol{y}_i \neq \boldsymbol{h}_t(\boldsymbol{x}_i))]$

Example from previous slide: $\alpha_t = 0.8$

1/16	1/4	1/16	1/16	1/4	1/16	1/4
✓	✓	✓	✗	✗	✓	✓
$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$
1/16	1/4	1/16	(1/16) exp(0.8)	(1/4) exp(0.8)	1/16	1/4

- Weight of misclassified examples is increased and the new $\boldsymbol{D}(\boldsymbol{x}_i)$'s are normalized to be a distribution again

Ada Boost: step by step

5. Normalize $D(x_i)$ so that $\sum D(x_i) = 1$

Example from previous slide:

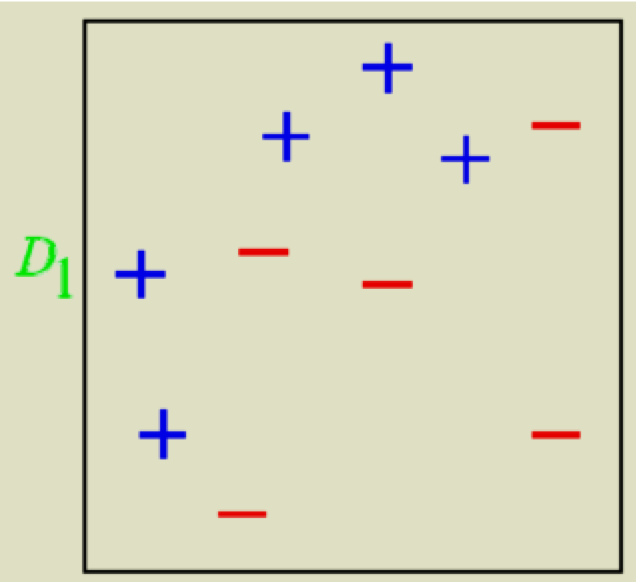
1/16 1/4 1/16 0.14 0.56 1/16 1/4

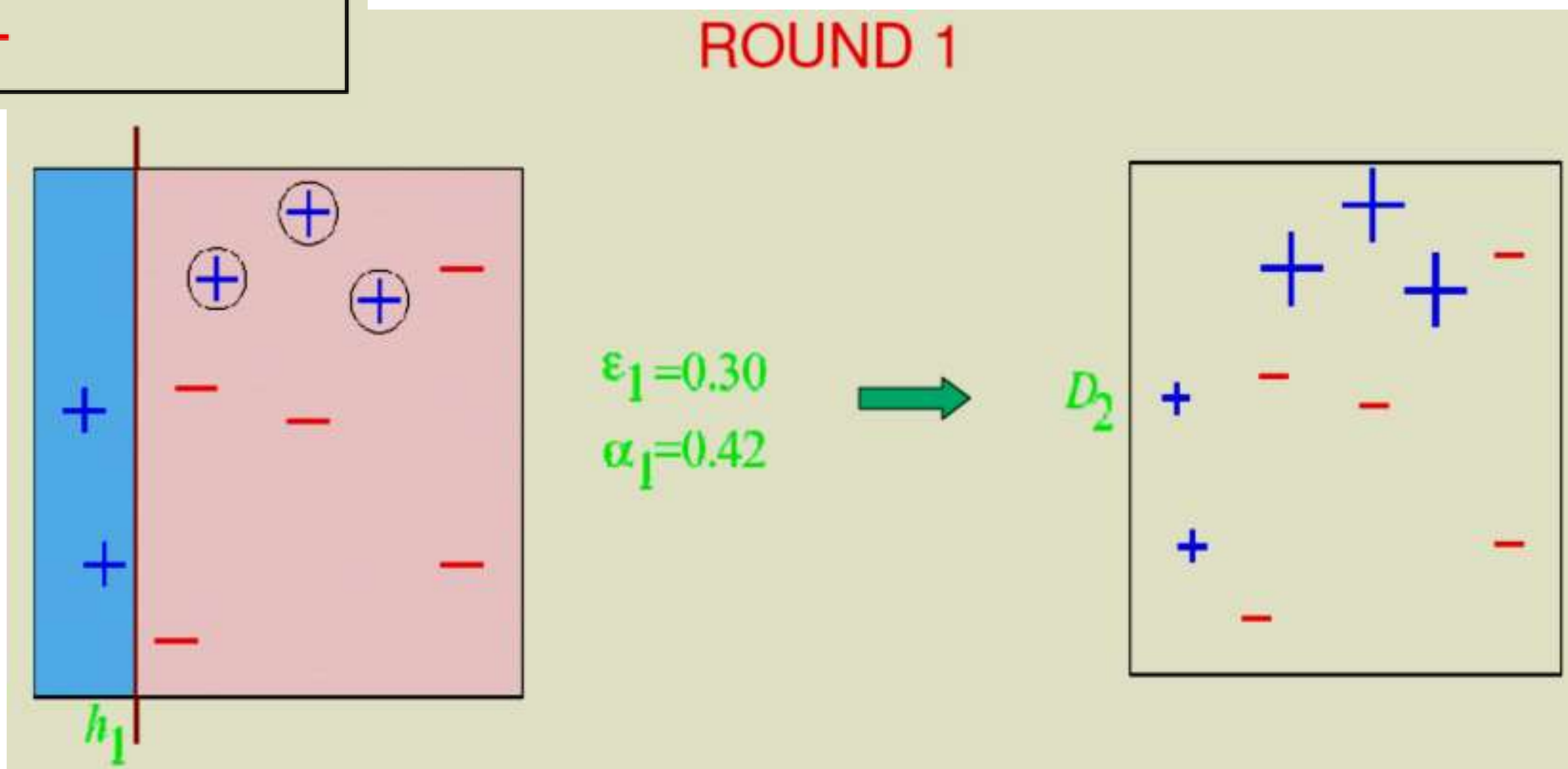
After normalization:

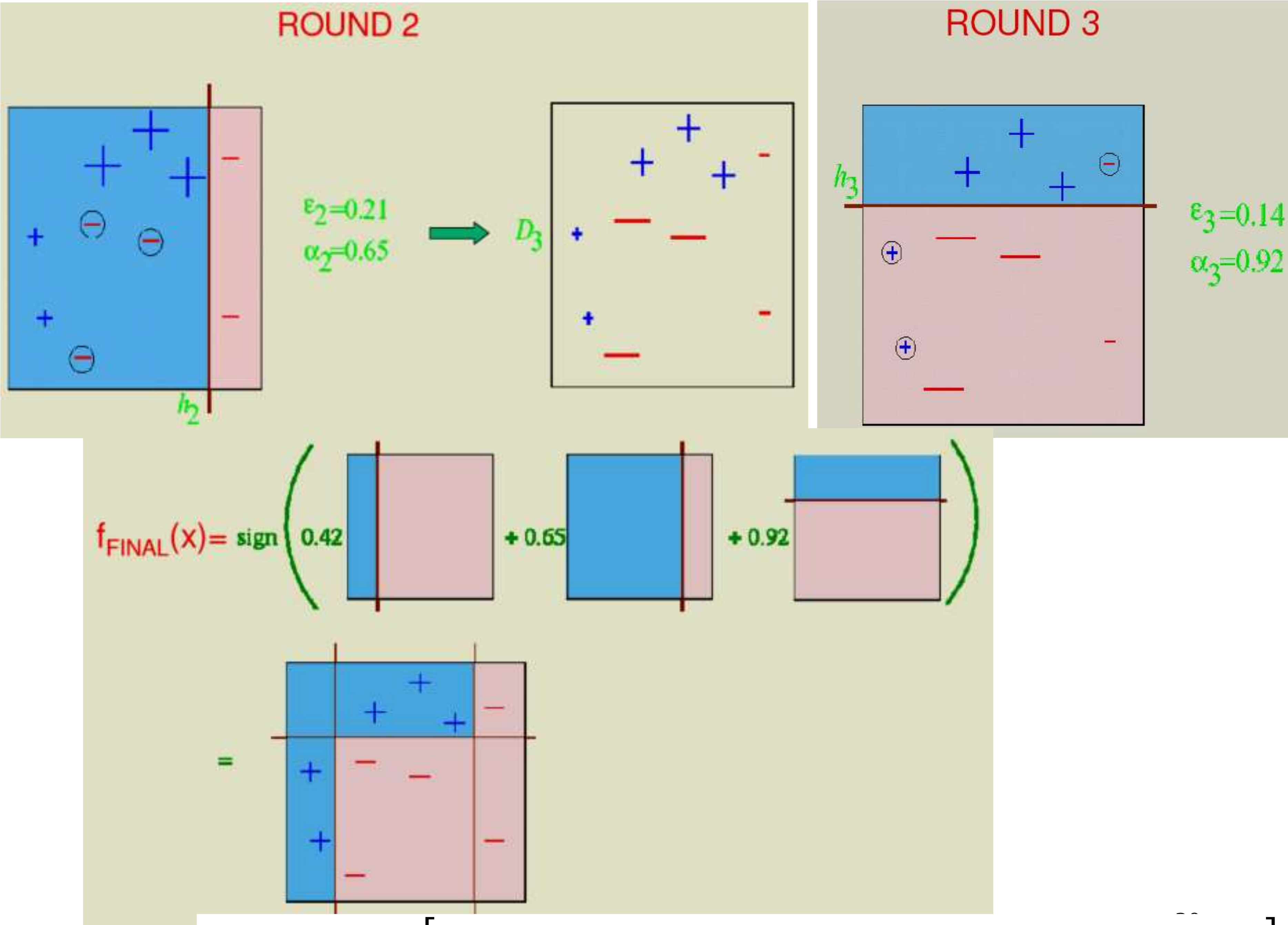
0.05 0.18 0.05 0.10 0.40 0.05 0.18

- In matlab, if D is a vector storing weights, D = D./sum(D)

AdaBoost Example (Freund & Schapire)







$$f_{\text{final}}(\mathbf{x}) = \operatorname{sgn}\left[0.42\operatorname{sgn}(x_1 - 3) + 0.65\operatorname{sgn}(x_1 - 7) + 0.92\operatorname{sgn}(x_2 - 4)\right]$$

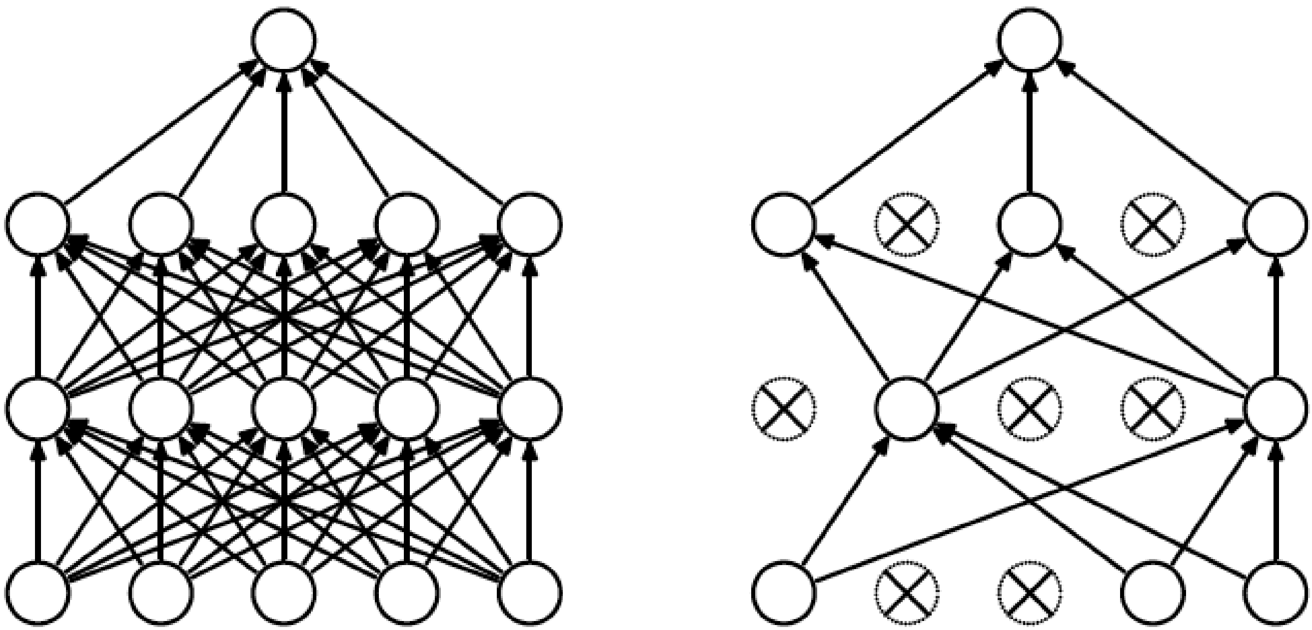
Boosting方法的特点

- 优点：
  - 快速
  - 简单
  - 只有一个参数k_{max}
  - 灵活：可以与任何分类器使用，只需要比随机好的“弱”分类器
- 缺点：
  - “弱”分类器不能太复杂（容易过拟合）
  - 对噪声敏感，例如会给标记错误的样本过大的权重

神经网络防止过拟合：Dropout

每次训练时随机把部分节点参数置零

相当于利用很多不同结构网络的结果的集合



(a) Standard Neural Net　　(b) After applying dropout.

Dropout: A Simple Way to Prevent Neural Networks from Overfitting

Journal of Machine Learning Research 15 (2014) 1929-1958

小结

- 将‘弱’分类器组合可以得到推广性更好的分类器
- 串行与并行（Boosting vs. Bagging, RF）
- 引入扰动 (样本，特征, …)
- 通常对不稳定的分类器（比如决策树）效果好，但不局限于树