Decision Trees and Learning Ensembles for Classification/Ranking

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Outlines

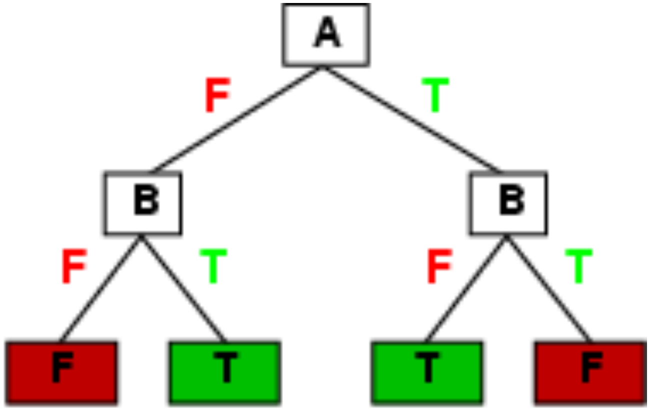
- **Example of classification algorithms**
  - Decision trees
- **Training data and cross-validation**
- **Learning Assembles**
- **Random Forest**
- **Adaboost**
- **Boosting regression trees**

Classification with Decision Trees

Decision Trees

- Decision trees can express any function of the input attributes.
- E.g., for Boolean functions, truth table row → path to leaf:

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



- Trivially, there is a consistent decision tree for any training set with one path to leaf for each example (unless *f* nondeterministic in *x*) but it probably won't generalize to new examples

- Prefer to find more compact decision trees: we don’t want to memorize the data, we want to find structure in the data!

Decision Trees: Application Example

Problem: decide whether to wait for a table at a restaurant, based on the following attributes, or called features

1. Alternative: is there an alternative restaurant nearby?
2. Bar: is there a comfortable bar area to wait in?
3. Fri/Sat: is today Friday or Saturday?
4. Hungry: are we hungry?
5. Patrons: number of people in the restaurant (None, Some, Full)
6. Price: price range ($, $$, $$$)
7. Raining: is it raining outside?
8. Reservation: have we made a reservation?
9. Type: kind of restaurant (French, Italian, Thai, Burger)
10. WaitEstimate: estimated waiting time (0-10, 10-30, 30-60, >60)

Training data: Restaurant waiting

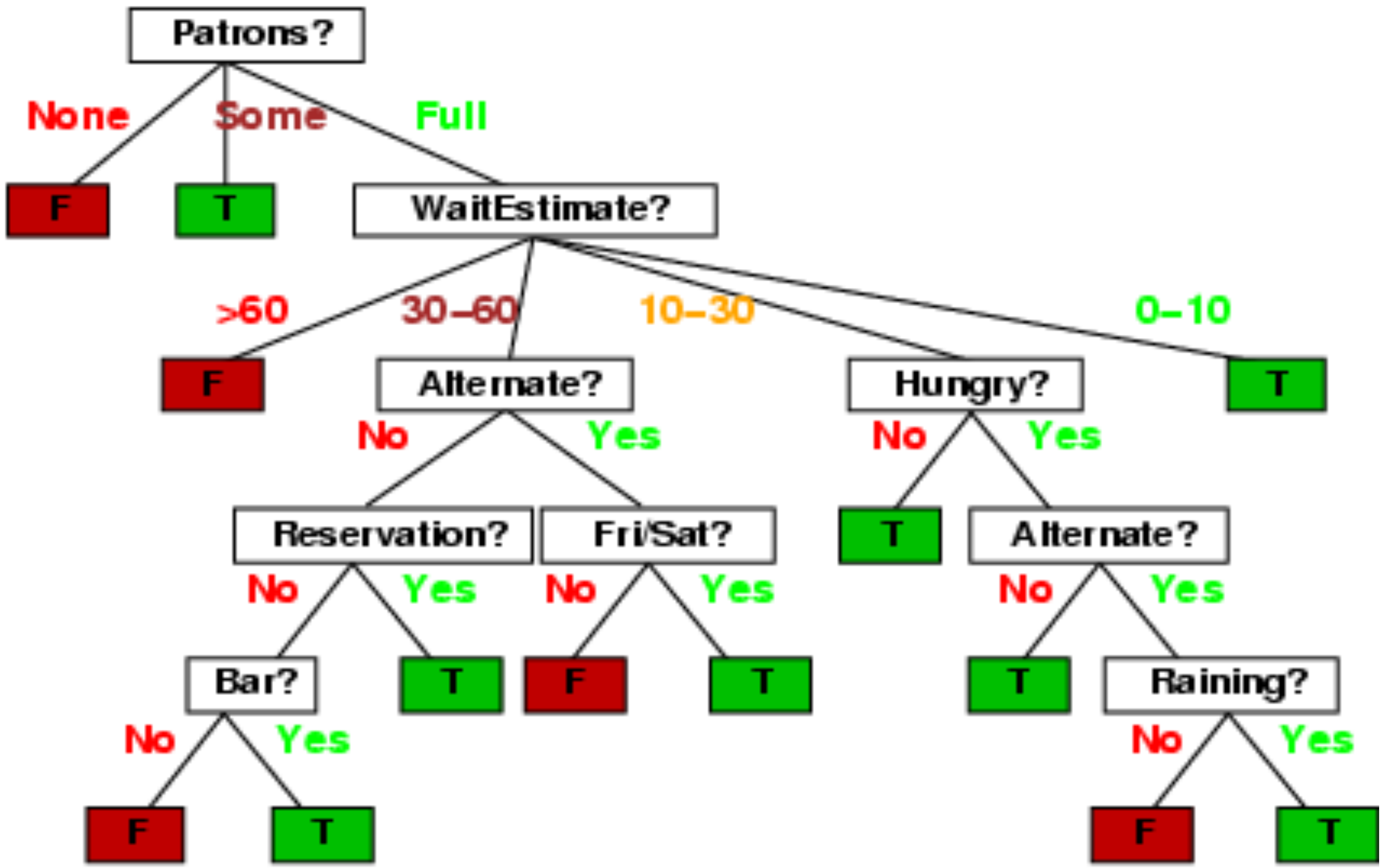
- Examples described by attribute values or feature value (Boolean, discrete, continuous)
- Decision: I will/won't wait for a table:

Example	Attributes										Target
	Alt	Bar	Fri	Hun	Pat	$Price$	$Rain$	Res	$Type$	Est	$Wait$
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

- Classification of examples is positive (T, wait) or negative (F, not wait)
- Each training instance is modeled as a feature vector

A decision tree to decide whether to wait

- imagine someone talking a sequence of decisions.



Decision tree learning

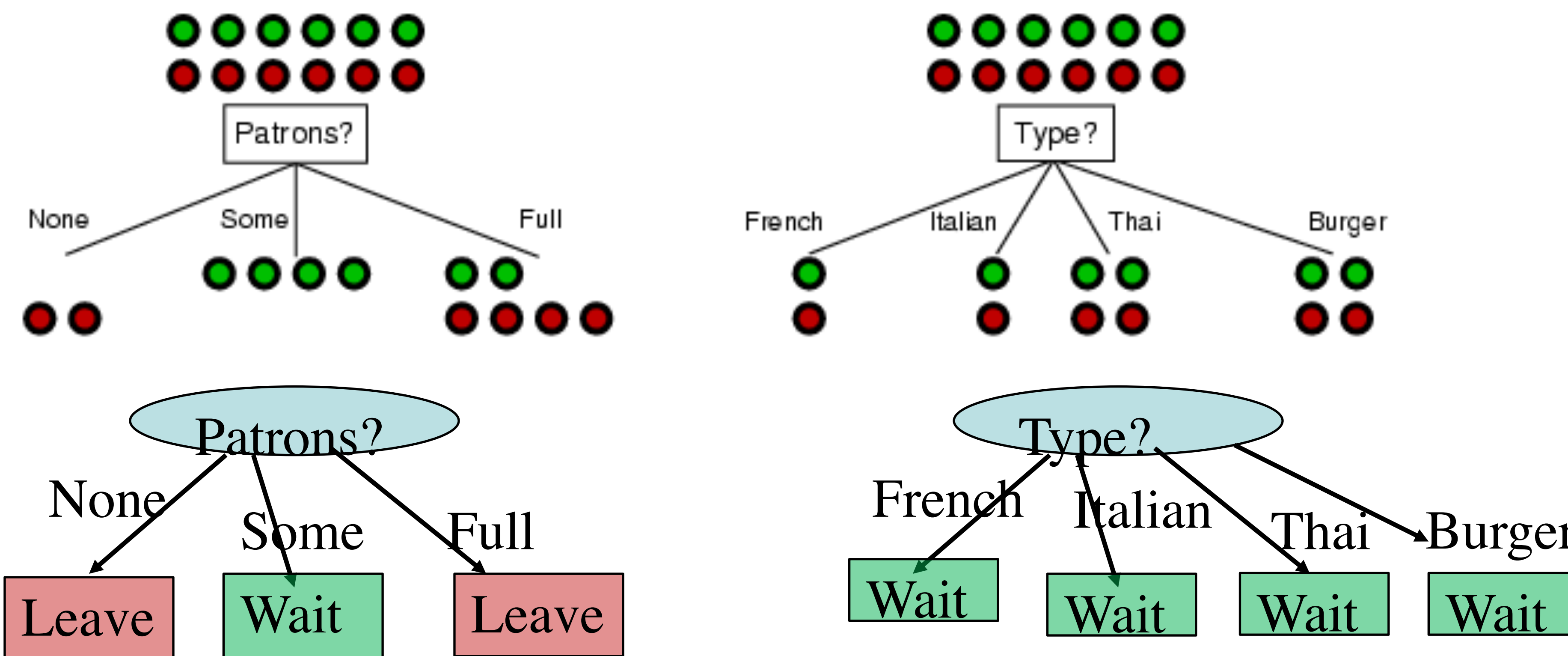
- The goal is to form a tree with the highest classification accuracy
- Test metric: Classification accuracy is the percentage of cases that the derived classifier prdicts correctly.

If there are so many possible trees

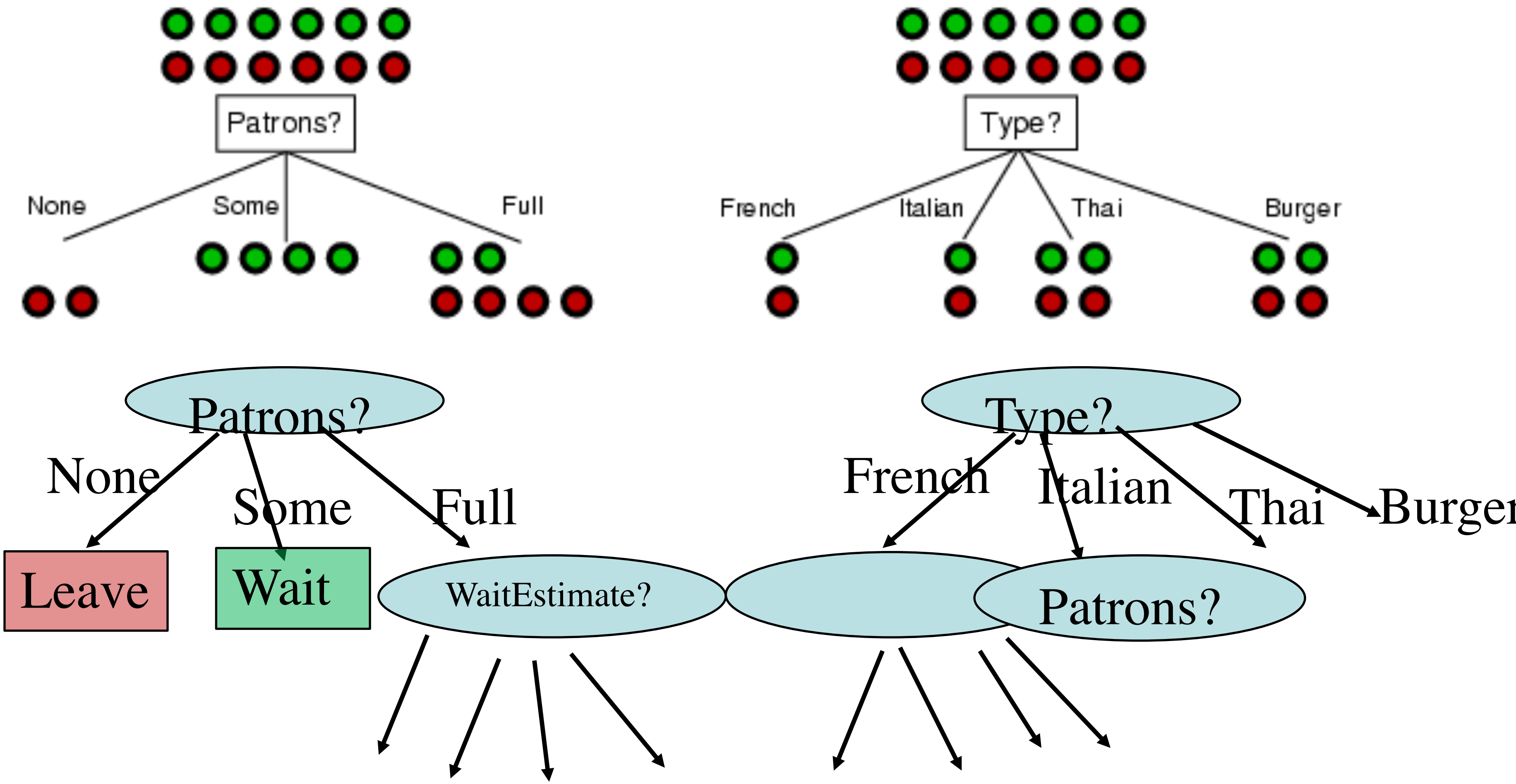
- Aim: find a small tree consistent with the training examples
- Idea: (recursively) choose "most significant" attribute as root of (sub)tree.

How to build a decision tree

- **Basic idea to form a decision node**
  - Pick up an attribute, and use the value range of this attribute as a branching condition
  - Expand each node by adding more children

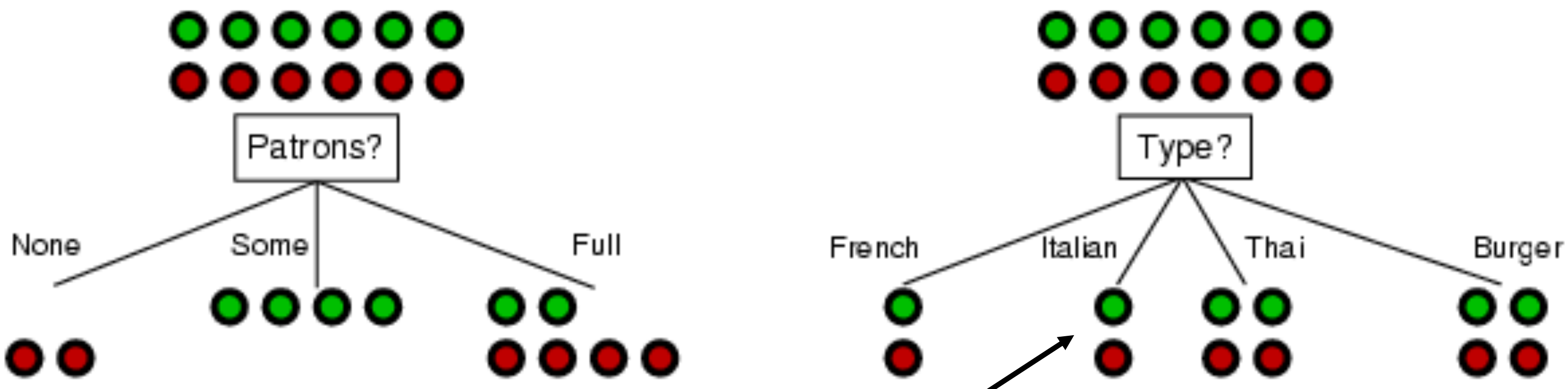


Grow a tree by adding children to some nodes



Choosing an attribute for a smaller tree

- **Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"**



- ***Patrons or type?***

To wait or not to wait is still at 50%.

- Probability of being positive is p.

P=0.5 is bad because it does not give any decidable information.

- Need to find a function f to measure uncertainty such that f(p)= bad when p=0.5 and f(p)=good when p=1 or 0.

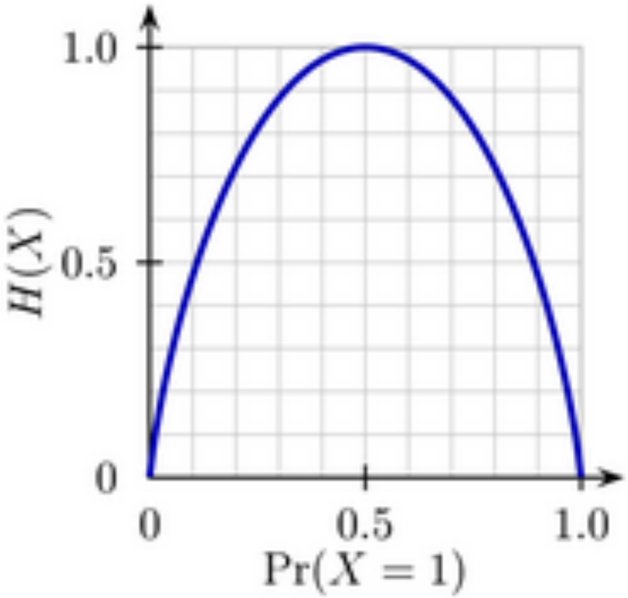
Information theory background: Entropy

- **Entropy measures uncertainty**

  H(p, 1-p)= -p log (p) - (1-p) log (1-p)

Consider tossing a biased coin.
If you toss the coin VERY often,
the frequency of heads is, say, p,
and hence the frequency of tails is
1-p.

Uncertainty (entropy) is zero if p=0 or 1
and maximal if we have p=0.5.



Using information theory for binary decisions

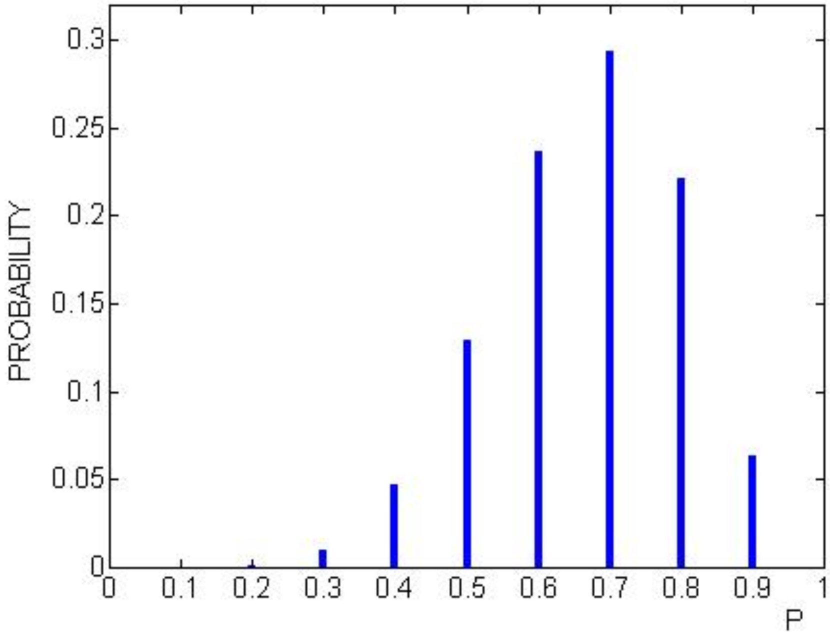
- **Imagine we have p examples which are true (positive) and n examples which are false (negative).**
- **Our best estimate of true or false is given by:**
  - Prob(true) = p/(p+n)
  - Prov(false)=n/(p+n)
- **Hence the entropy is given by:**

$$Entropy\left(\frac{p}{p+n},\frac{n}{p+n}\right) \approx -\frac{p}{p+n}\log\frac{p}{p+n}-\frac{n}{p+n}\log\frac{n}{p+n}$$

Using information theory for more than 2 classes

- **n classes**

$$\sum_{s=1}^{n} p(s) = 1$$

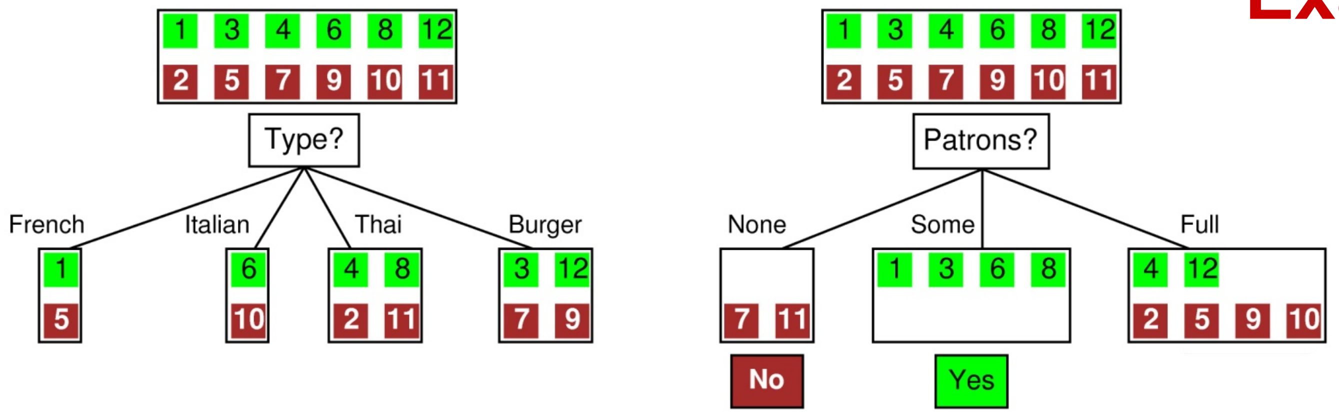


$$\begin{aligned} Entropy(p) = &-p(s=1)\log[p(s=1)] \\ &-p(s=2)\log[p(s=2)] \\ &\ldots \\ &-p(s=n)\log[p(s=n)] \end{aligned}$$

ID3 Algorithm: Using Information Theory to Choose an Attribute

- How much information do we gain if we disclose the value of some attribute?
- ID3 algorithm by Ross Quinlan uses information gained measured by maximum entropy reduction:
  - IG(A) = uncertainty before – uncertainty after
  - Choose an attribute with the maximum IA

Example



Before: Entropy = - ½ log(1/2) – ½ log(1/2)=log(2) = 1 bit:
There is "1 bit of information to be discovered".

After: for "Type:" If we go into branch "French" we have 1 bit, similarly for the others.

French: 1bit
Italian: 1 bit
Thai: 1 bit
Burger: 1bit

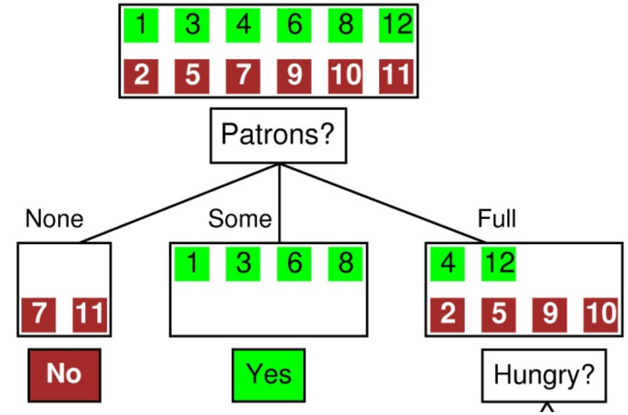
On average: 1 bit and gained nothing!

After: for "Patrons:" In branch "None" and "Some" entropy = 0!,
In "Full" entropy = -1/3log(1/3)-2/3log(2/3)=0.92

So Patrons gains more information!

Information Gain: How to combine branches

- 1/6 of the time we enter "None", so we weight"None" with 1/6. Similarly: "Some" has weight: 1/3 and "Full" has weight ½.

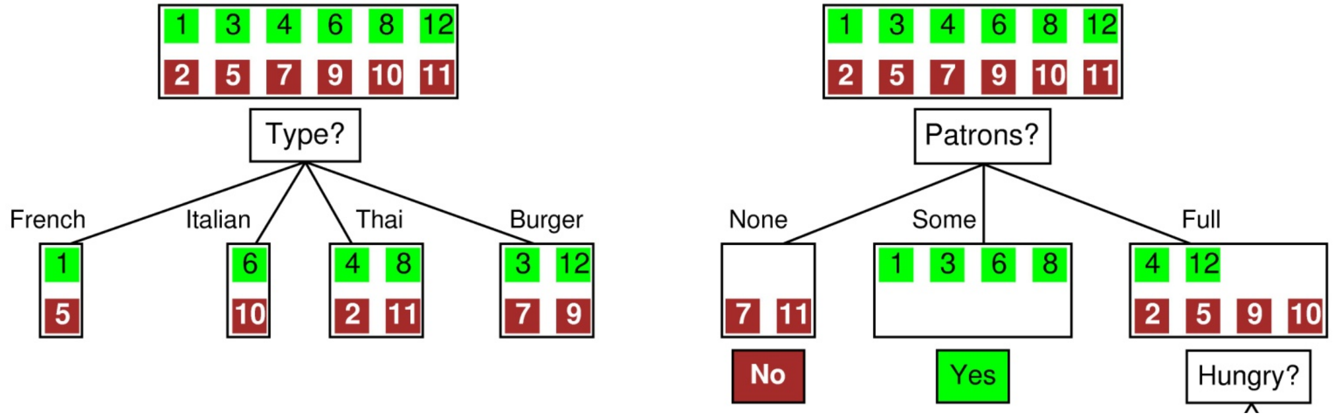


$$Entropy(A) = \sum_{i=1}^{n} \frac{p_i + n_i}{p + n} Entropy\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$$

entropy for each branch.

weight for each branch

Choose an attribute: Restaurant Example



For the training set, $p = n = 6$, *before split, I(6/12, 6/12) = 1* bit

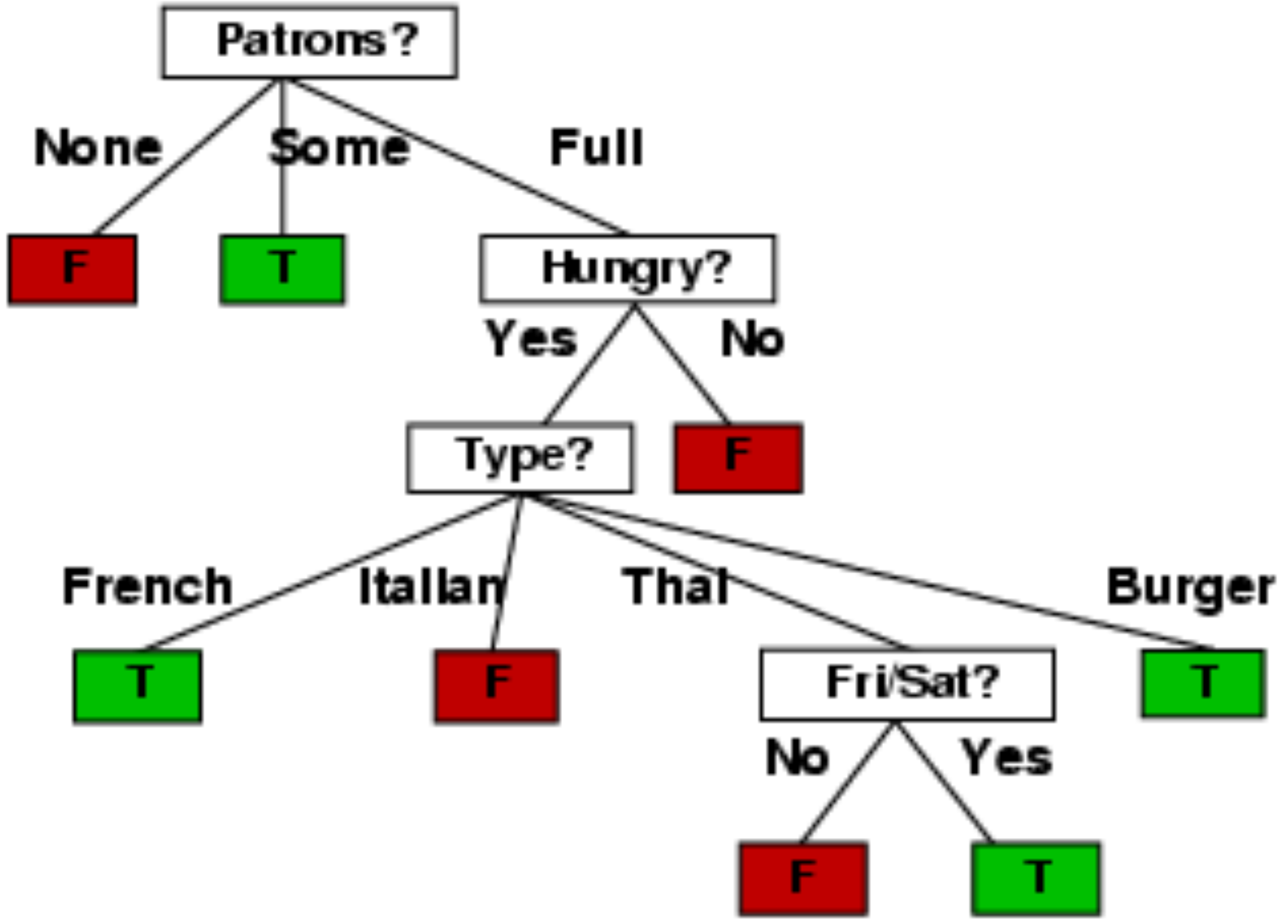
$$IG(Patrons) = 1 - [\frac{2}{12} I(0,1) + \frac{4}{12} I(1,0) + \frac{6}{12} I(\frac{2}{6}, \frac{4}{6})] = .0541 \text{ bits}$$

$$IG(Type) = 1 - [\frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4})] = 0 \text{ bits}$$

Patrons **has the highest IG of all attributes and so is chosen by the DTL algorithm as the root**

Example: Decision tree learned

- **Decision tree learned from the 12 examples:**



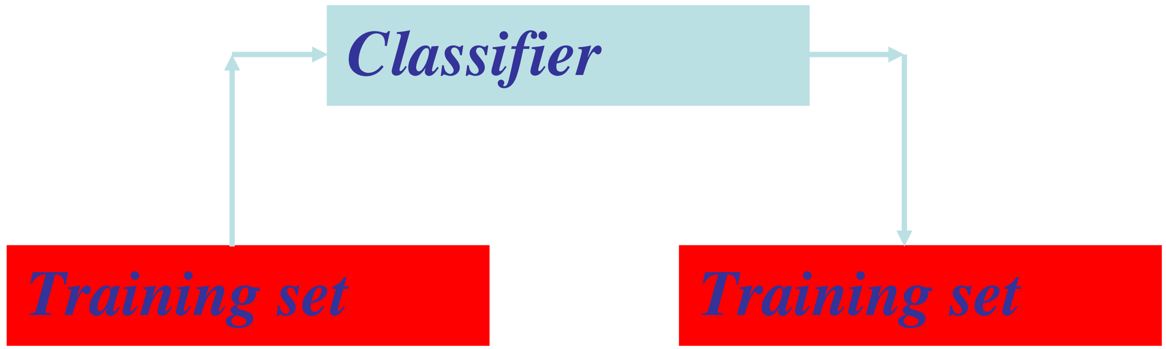
Issues and Discussion

- **When there are no attributes left:**
  - Stop growing and use majority vote.
- **Avoid over-fitting training data**
  - Control tree size with pruning
  - Stop growing a tree earlier
  - Grow first, and prune later.
- **Deal with continuous-valued attributes**
  - Dynamically select thresholds/intervals.
- **Handle missing attribute values**
  - Make up with common values
- **Other tree building methods: Regression with square error loss function**

Is it fair to use the training data to report final classification accuracy?

- **No fair. A labeled dataset is divided into two sets**
  - Training set is used to form a tree that fits data
  - Test set is used to report classification errors with no bias
  - Test metric:
    - Binary classification. Accuracy is the percentage of cases that the derived classifier prdicts correctly.
- **How to compute the error with more than 2 classes?**
  - For example, 3 Classes: class 1, class 2, class 3.
  - Sqared error sum
    - Sum (predicted class value – target value)^2
    - Normalized by dividing the number of cases
  - Another way: Measure # of cases classified correctly for Class 1, and # of cases classifed correctly for Case 2 etc. Then compute average, or weighted average.

How to Evaluate Accuracy with Training Data



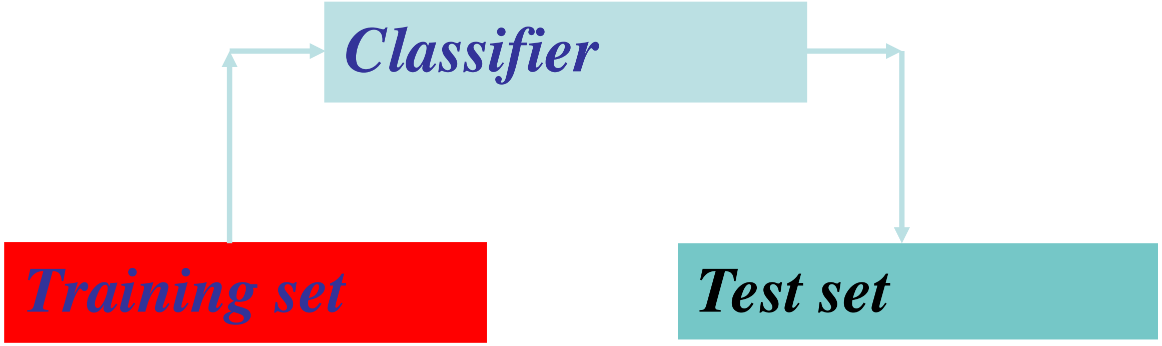
- The accuracy/error estimates on the training data are *not* good indicators of performance on future data
  - **Why?**
    - Because new data will probably not be **exactly** the same as the training data!
    - The algorithms do well on the training data may overfit

Divide a dataset into 3 sets: Training set, validation set, and test set

- **For more advanced setting, a labeled dataset is divided into 3 sets**
  - **Training set** is used to form a tree under some parameters (e.g. when to stop tree growing)
  - **Validation set** is used to assess the accuracy of the derived classifier, and then readjust training parameters, and reassess again for the best validation performance
  - **Test set** is used to report accuracy/error of the final classifier with no bias

Evaluation with Independent Test Data

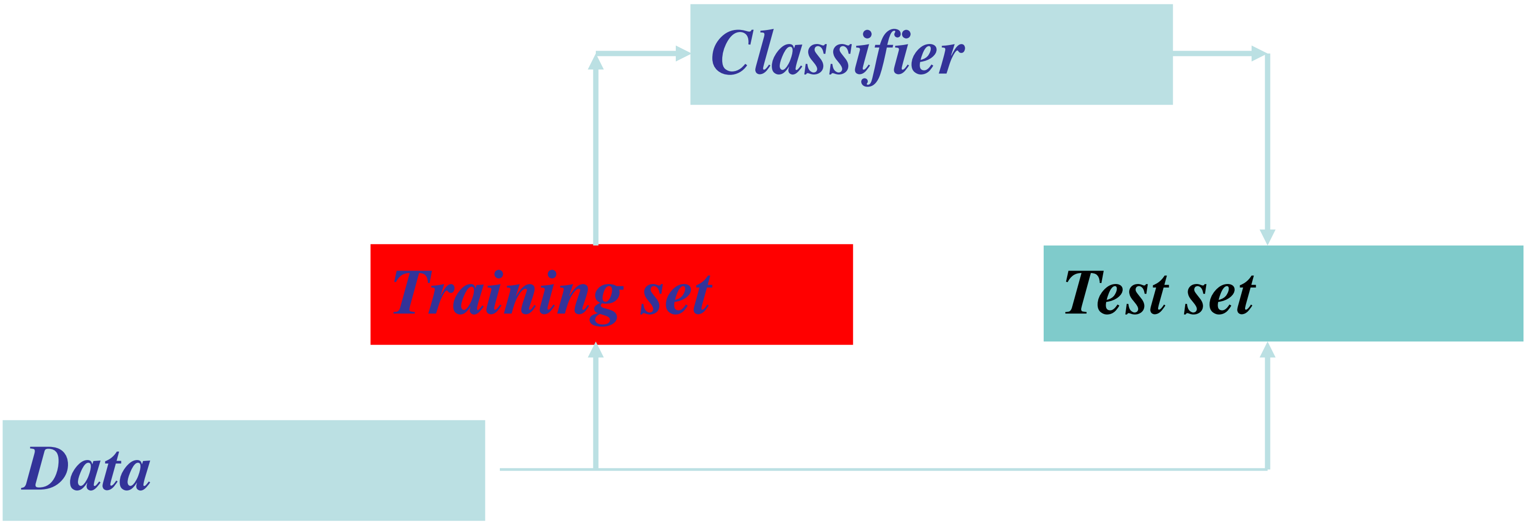
- Estimation with independent test data is used when we have plenty of data and there is a natural way to forming training and test data.



- *For example: reported experiments for which the classifiers were trained on data from 2017 and tested on data from 2018.*

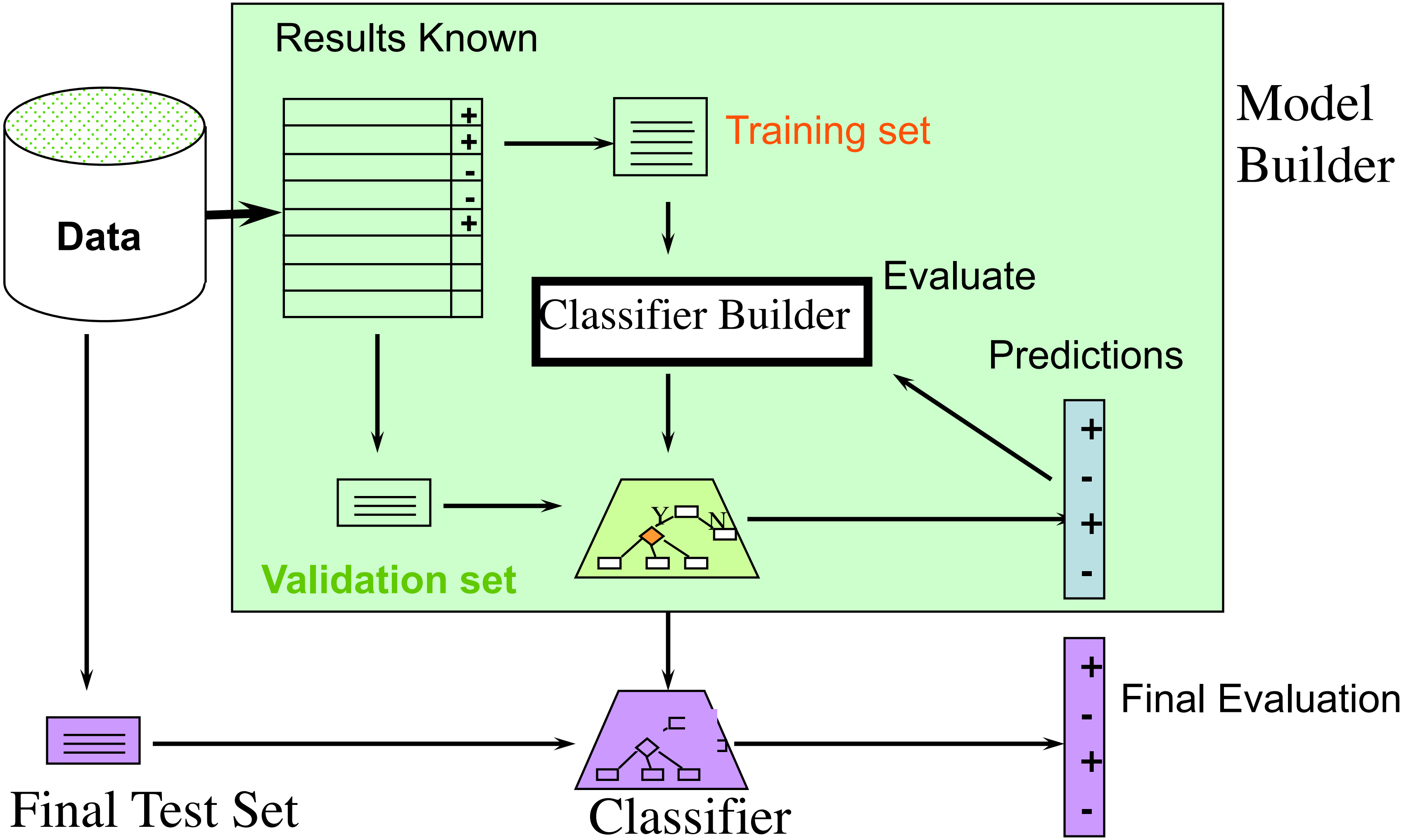
Hold-out Method

- The hold-out method splits the data into training data and test data (usually 2/3 for train, 1/3 for test). Then we build a classifier using the train data and test it using the test data.



- The hold-out method is usually used when we have a sufficient large dataset for training and testing separately

Classification: Train, Validation, Test Split



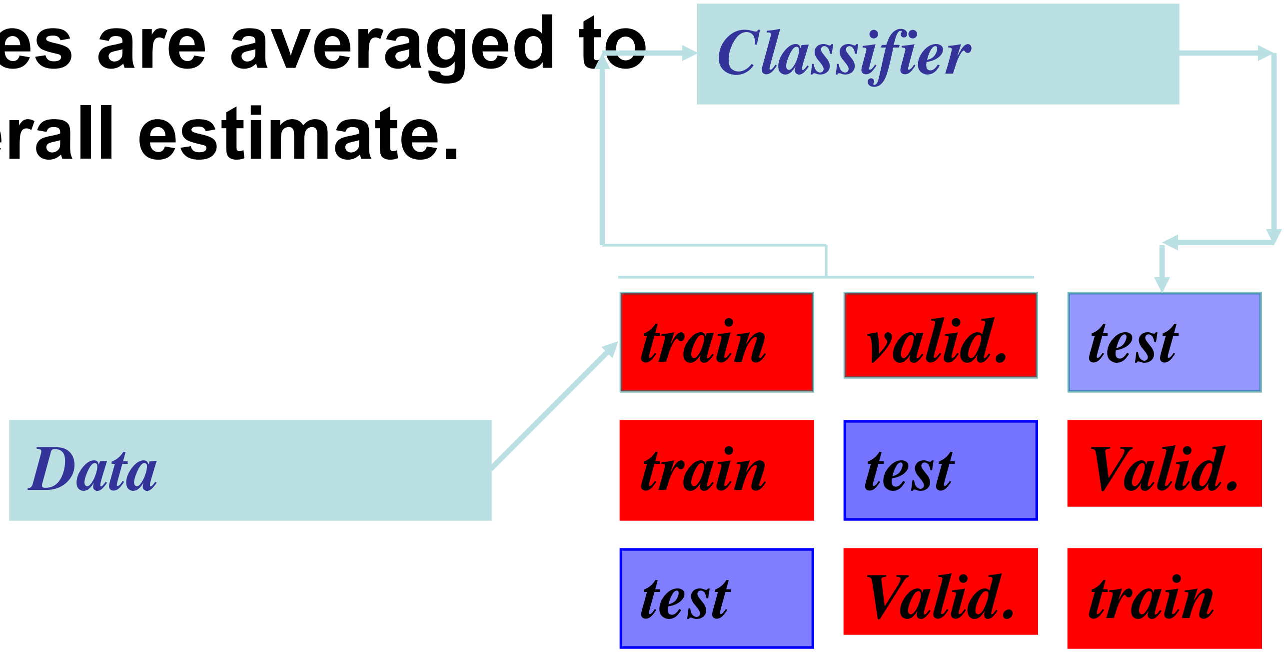
The test data can't be used for parameter tuning!

Making the Most of Available Data

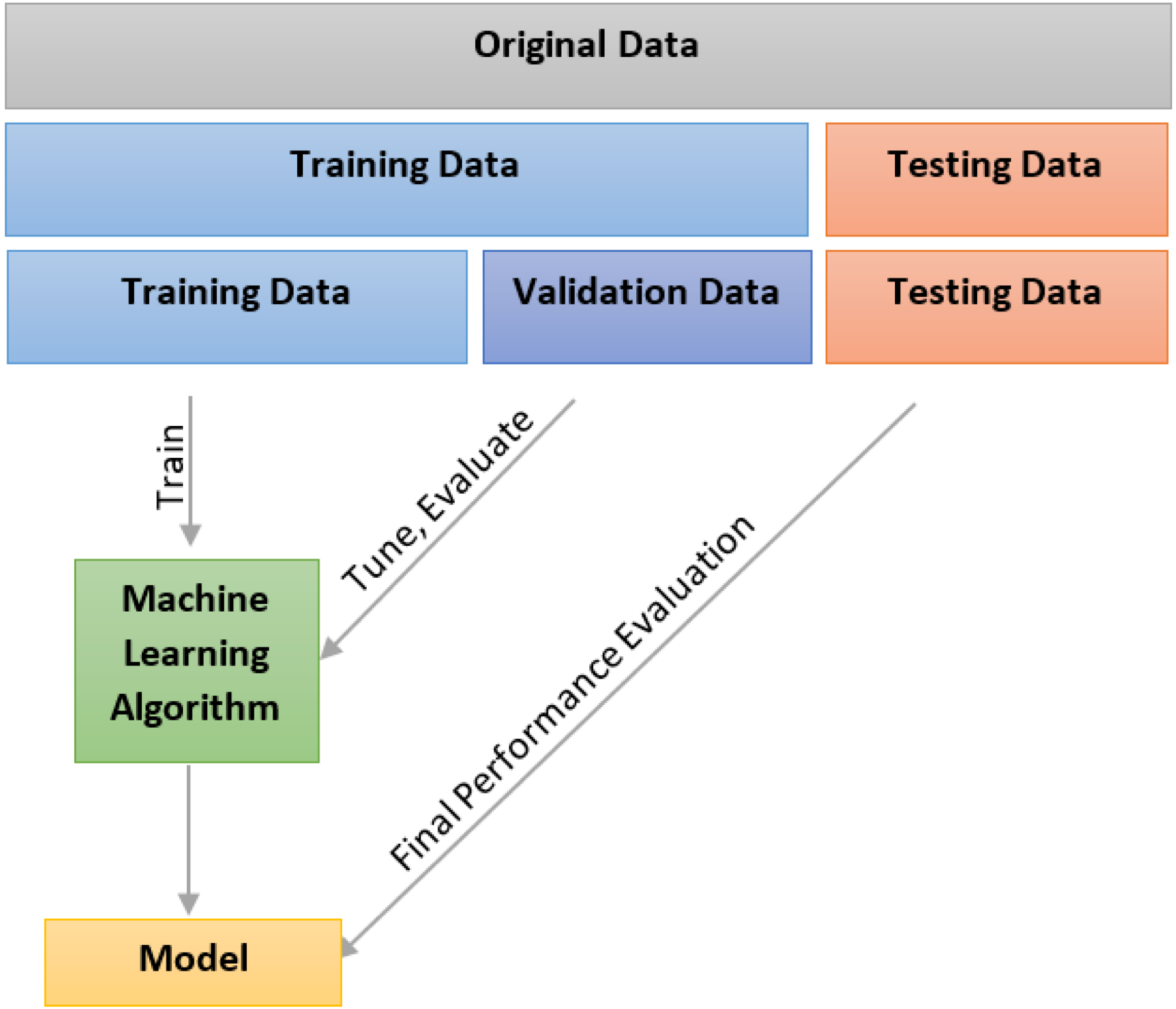
- **Difficult to obtain training/testing data**
- **Importance of more data**
  - Generally, the larger the training data the better the classifier (but returns diminish).
  - The larger the test data the more accurate the error estimate.
  - *Can we use all data* to build the final classifier.

k-Fold Cross-Validation

- ***Select a subset for training and another subset for testing without overlapping.***
  - data is split into *k* subsets of equal size; select one testing
- ***Repeat above process for k times***
  - each subset in turn is used for testing and the remainder for training or training/validation
- **The estimates are averaged to yield an overall estimate.**



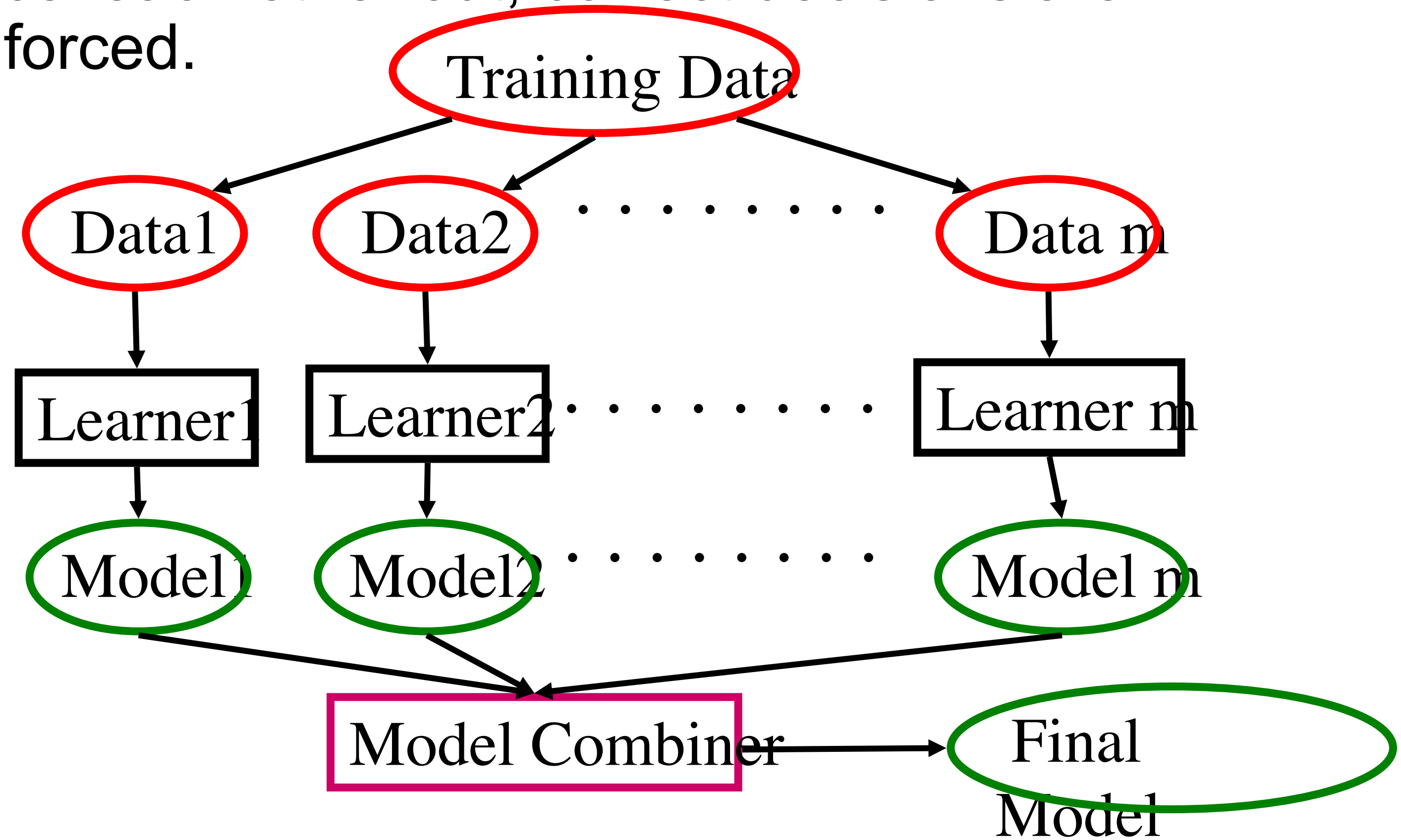
k-Fold Cross-Validation: Train, Validate and Test



Learning Ensembles

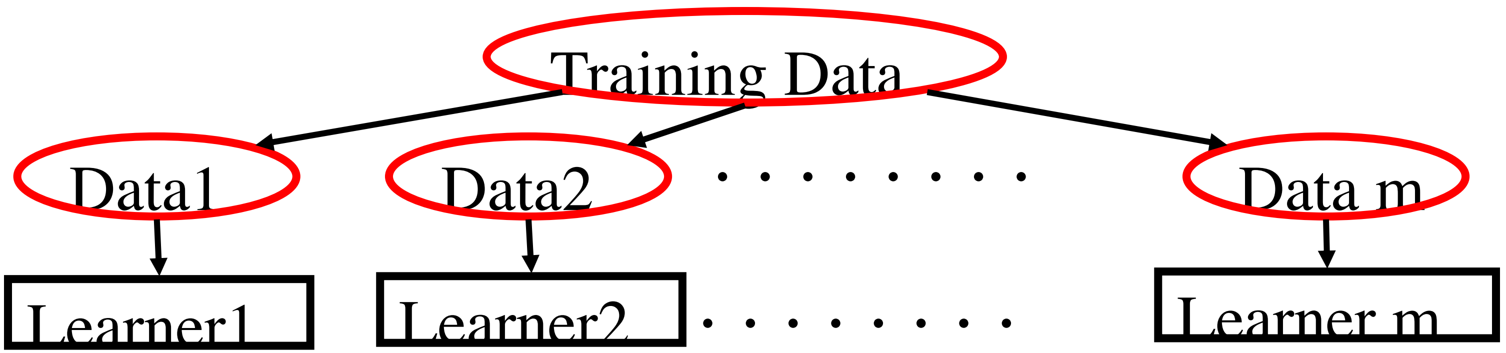
Learning Ensembles

- **Learn multiple classifiers separately**
- **Combine decisions (e.g. using weighted voting)**
- When combing multiple decisions, random errors cancel each other out, correct decisions are reinforced.



Homogenous Ensembles

- **Use a single, arbitrary learning algorithm but manipulate training data to make it learn multiple models.**
  - Data1 ≠ Data2 ≠ … ≠ Data m
  - Learner1 = Learner2 = … = Learner m
- **Methods for changing training data:**
  - **Bagging:** Resample training data
  - **Boosting:** Reweight training data
  - **DECORATE:** Add additional artificial training data



Bagging

- Create ensembles by repeatedly randomly resampling the training data (Brieman, 1996).
- Given a training set of size *n*, create *m* sample sets
  - Each *bootstrap sample set* will on average contain 63.2% of the unique training examples, the rest are replicates.
  - Combine the *m* resulting models using majority vote
- Advantages:
  - Decreases error by decreasing the variance in the results due to *unstable learners*, algorithms (like decision trees) whose output can change dramatically when the training data is slightly changed.
  - Avoid overfiting training data

Random Forests

- **Introduce two sources of randomness: “Bagging” and “Random input vectors”**
  - Each tree is grown using a bootstrap sample of training data
  - At each node, best split is chosen from random sample of *m* variables instead of all variables M (features).
  - Final result is aggregated through average or majority voting
- **Advantages:**
  - Good accuracy without over-fitting
  - Fast algorithm (can be faster than growing/pruning a single tree); easily parallelized
  - Handle high dimensional data without much problem

Random Forests

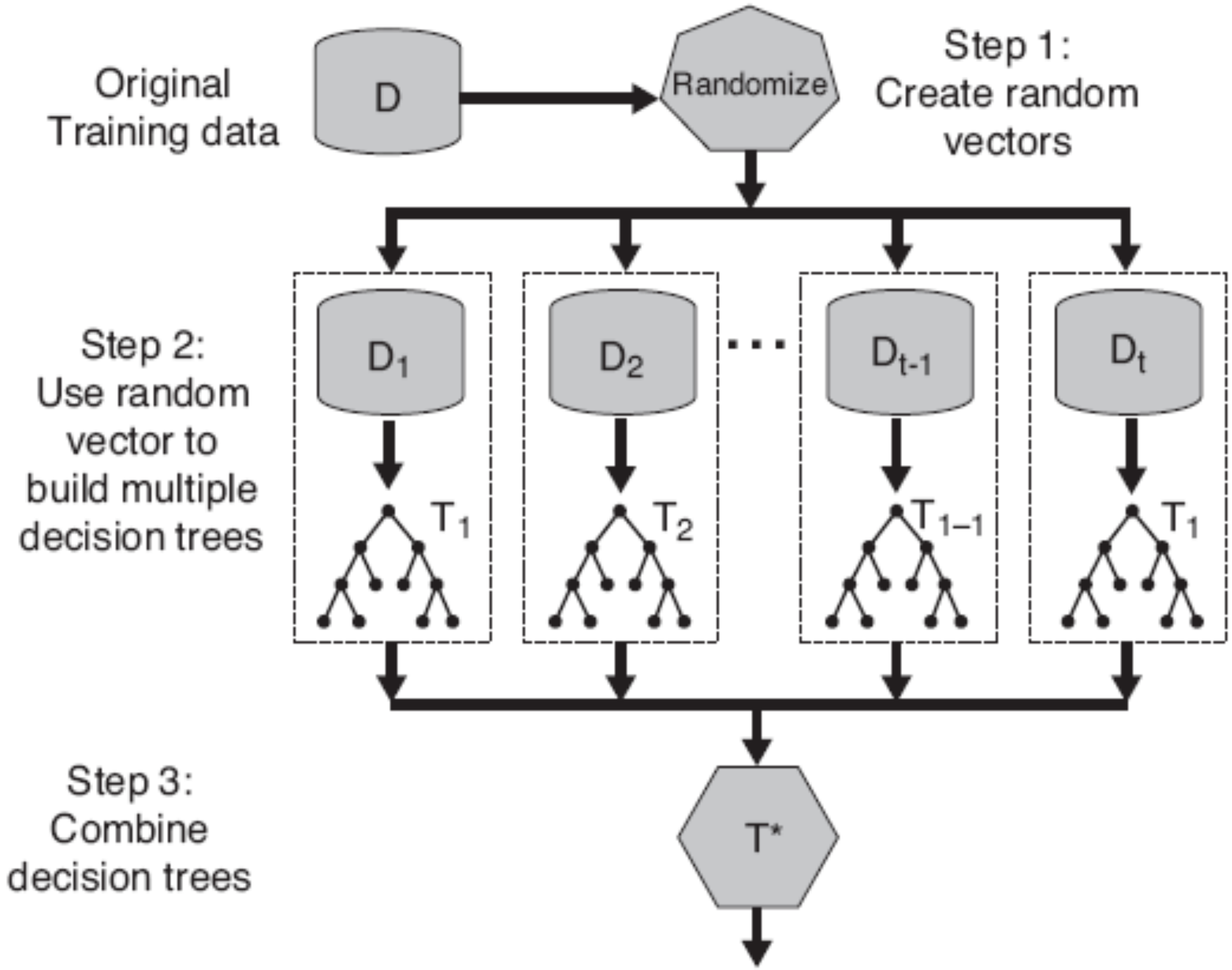


Figure 5.40. Random forests.

Boosting

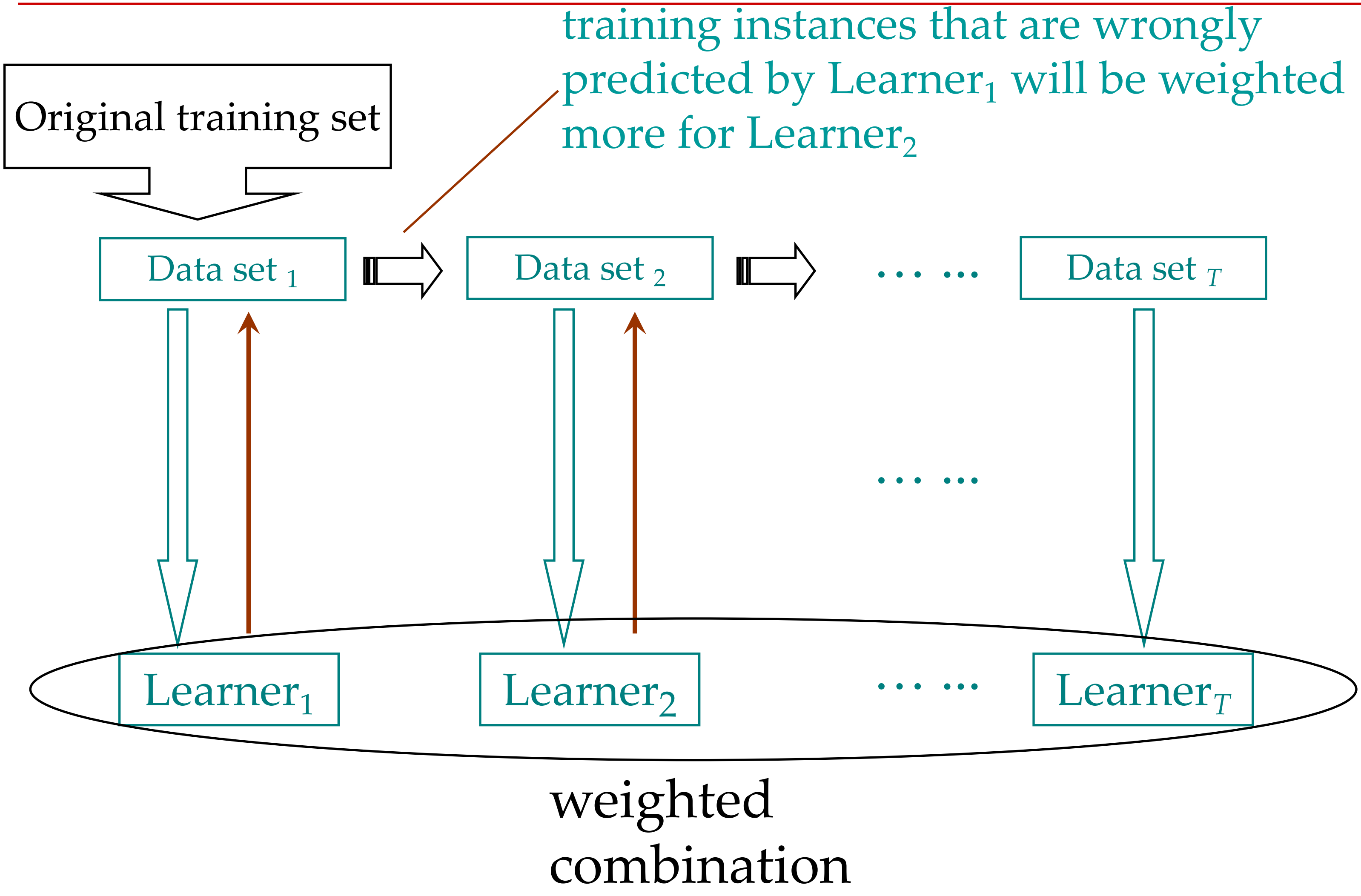
- Yoav Freund and Robert E. Schapire. A decision-theoretic generalization of on-line learning and an application to boosting. *Journal of Computer and System Sciences,* 55(1):119–139, August 1997.
  - Simple with theoretical foundation
- **Use training set re-weighting**
  - Each training sample uses a weight to determine the probability of being selected for a training set.

- **AdaBoost** is an algorithm for constructing a "strong" classifier as linear combination of a sequence of "simple" "weak" classifier

$$f(x) = \sum_{t=1}^{T} \alpha_t h_t(x)$$

- **A weak classifier** is built based on the previous weak classifiers

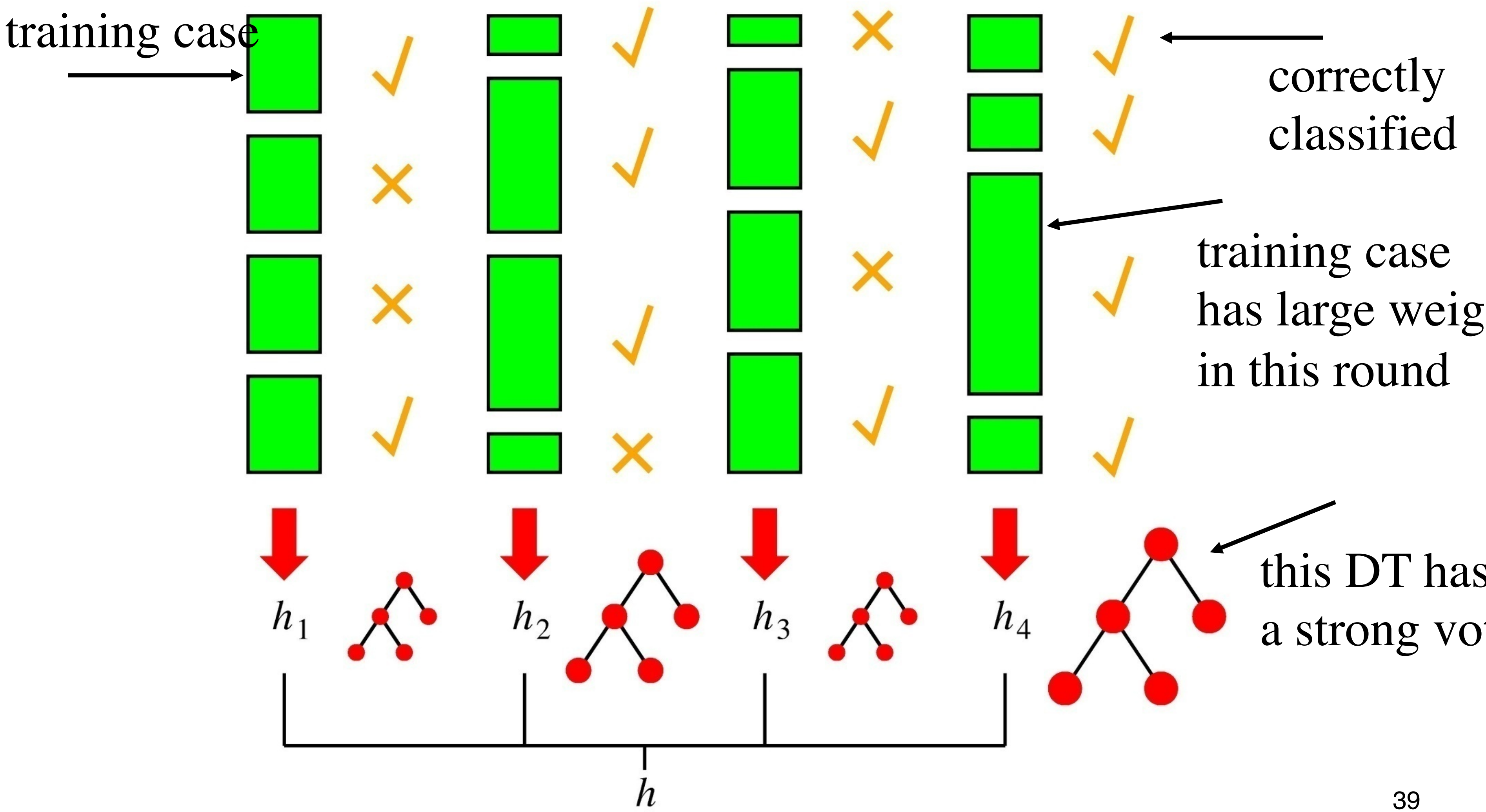
AdaBoost: An Easy Flow



Adaboost Terminology

- $h_t(x)$**… "weak" or basis classifier**
  - < 50% error over any distribution
- $H(x) = sign(f(x))$ **… "strong" or final classifier**
  - For binary classification: Positive vs negative
  - thresholded linear combination of weak classifier outputs

And in a Picture



Key idea of AdaBoost

- **Given training set $X=\{(x_1,y_1),\ldots,(x_m,y_m)\}$**
- **$y_i \in \{-1,+1\}$ correct label of instance $x_i \in X$**
- **Initialize distribution $D_1(i)=1/m$;** (weight of training cases)
- **for $t = 1,\ldots,T$:**
  - Find a weak classifier ("rule of thumb")

    $$h_t : X \to \{-1,+1\}$$

    with small error ε_t on D_t:
  - Update distribution D_t on $\{1,\ldots,m\}$ so that $D_{t+1}(i)$ becomes bigger for wrongly classified cases and smaller for correctly classified cases

    - how about by a factor of $1/\varepsilon_t$-1
    - how about by a factor of $\ln(1/\varepsilon_t$-1)
    - how about by a factor of sqrt($1/\varepsilon_t$-1))

- **Output final hypothesis**

$$H(x) = sign(\sum_{t=1}^{T} \alpha_t h_t(x))$$

AdaBoost.M1

- **Given training set $X=\{(x_1,y_1),\ldots,(x_m,y_m)\}$**
- **$y_i \in \{-1,+1\}$ correct label of instance $x_i \in X$**
- **Initialize distribution $D_1(i)=1/m$; (weight of training cases)**
- **for $t = 1,\ldots,T$:**
  - Find a weak classifier ("rule of thumb")

    $$h_t : X \rightarrow \{-1,+1\}$$

    with small error ε_t on D_t:
  - Update distribution D_t on $\{1,\ldots,m\}$. $\alpha_t = 0.5 \ln(1/\varepsilon_t - 1)$

$y_i * h_t(x_i) > 0$, if correct
$y_i * h_t(x_i) < 0$, if wrong

$$D_{t+1}(i) = \frac{D_t(i)\exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

where Z_t is a normalization factor (chosen so that D_{t+1} will be a distribution).

Namely sum of $D_{t+1}=1$

- **Output final hypothesis**

$$H(x) = sign(\sum_{t=1}^{T} \alpha_t h_t(x))$$

Reweighting

Effect on the training set

Reweighting formula:

$$D_{t+1}(i) = \frac{D_t(i)exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

$$exp(-\alpha_t y_i h_t(x_i)) \begin{cases} < 1, & y_i = h_t(x_i) \\ > 1, & y_i \neq h_t(x_i) \end{cases}$$

y * h(x) = 1

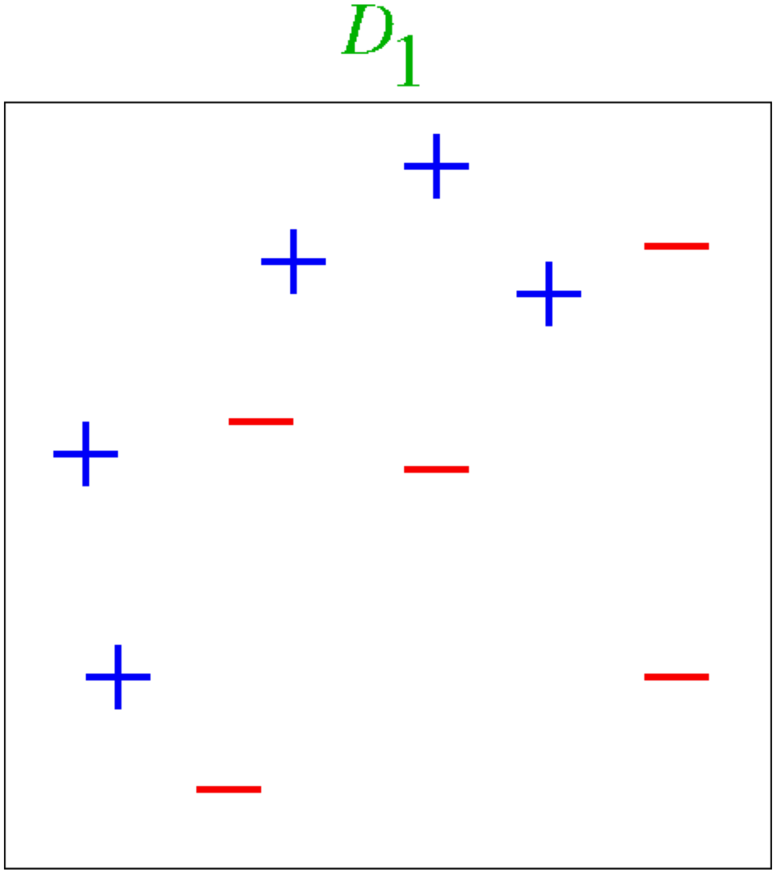
y * h(x) = -1

⇒ Increase (decrease) weight of wrongly (correctly) classified examples

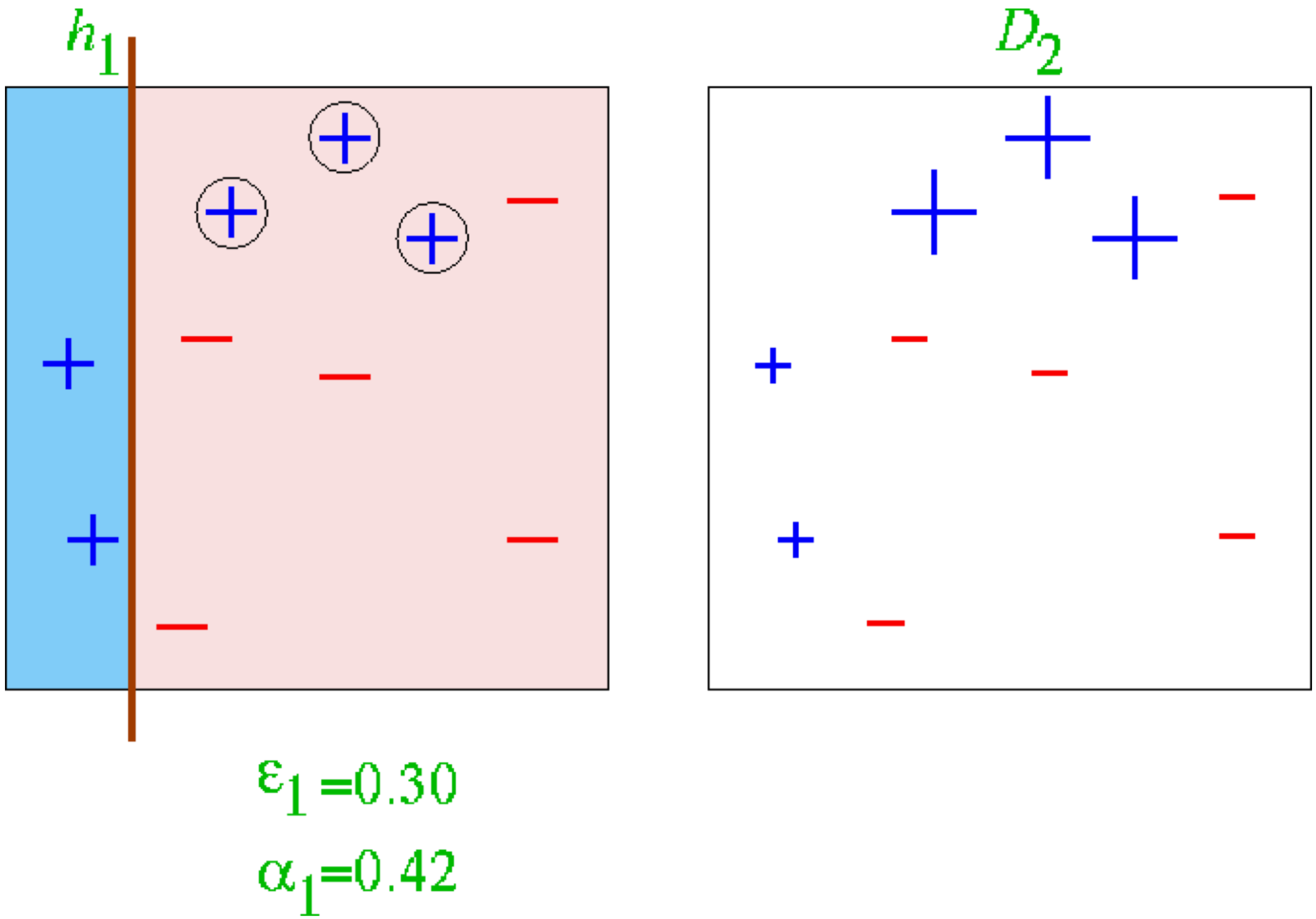
$Exp(0.5ln(1/\varepsilon_t-1)) = sqrt(1 /\varepsilon_t-1)$

$Exp(-0.5ln(1/\varepsilon_t-1)) = 1/sqrt(1 /\varepsilon_t-1)$

Toy Example



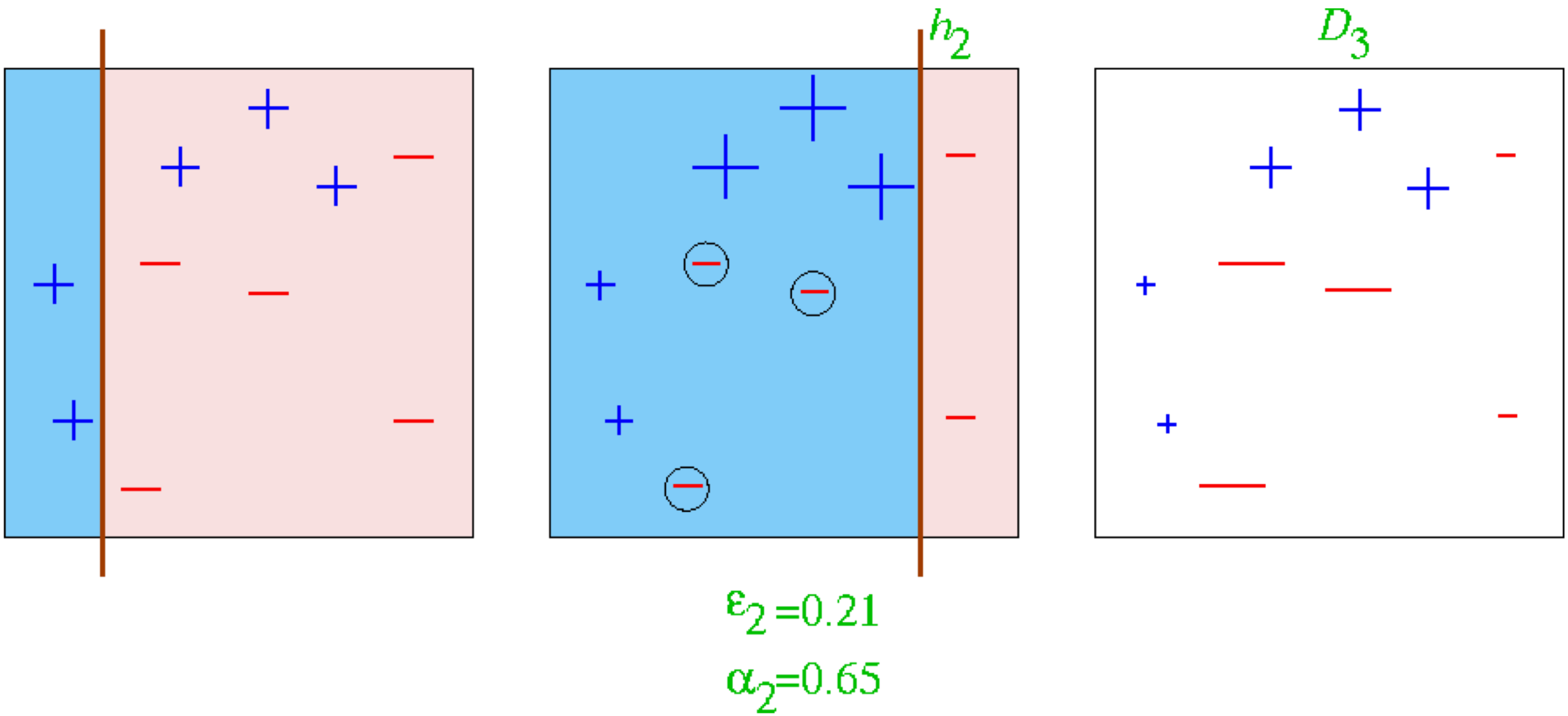
Round 1



Error rate is 30% $\alpha_1 = 0.5 \ln(1/\varepsilon_t - 1) = 0.4236$

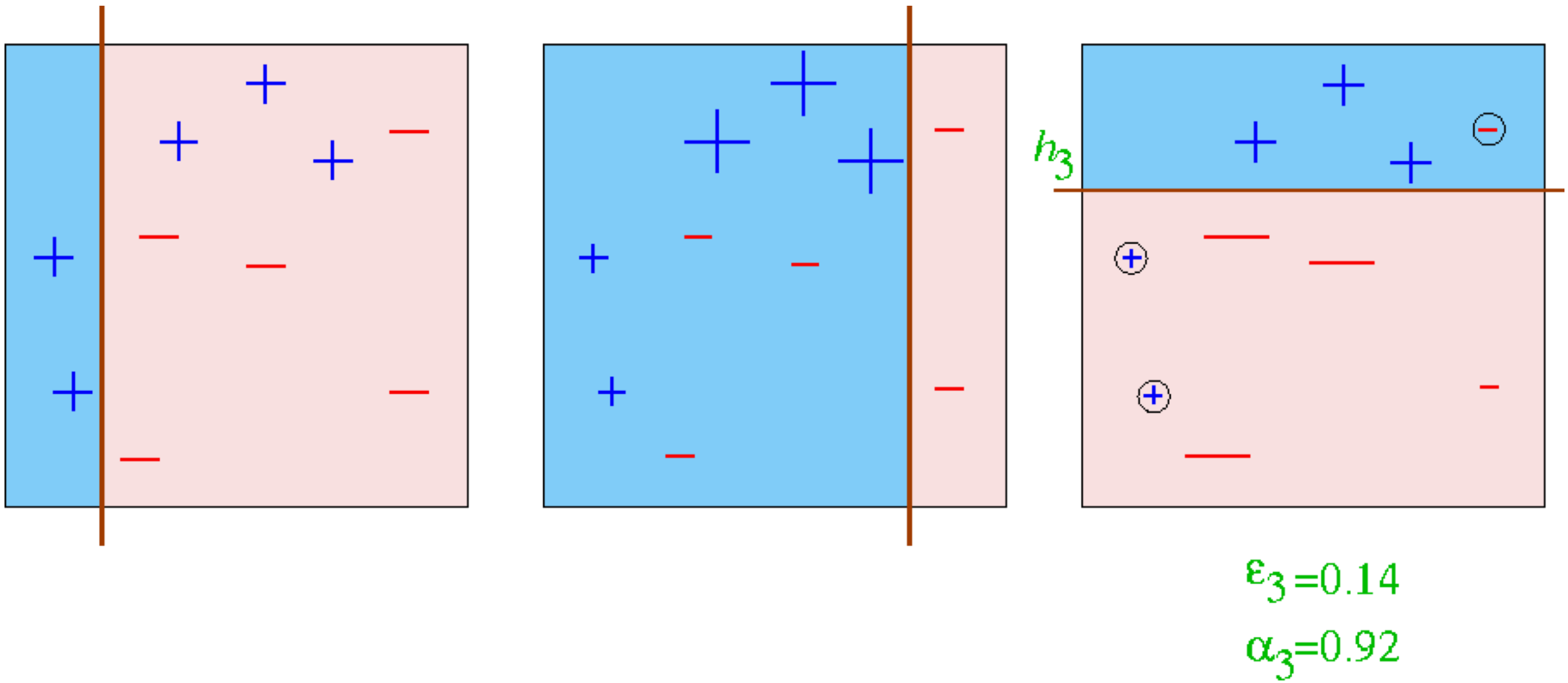
Weak classifier: if $h_1 < 0.2 \rightarrow 1$ else -1

Round 2



Weak classifier: if $h_2 < 0.8 \rightarrow 1$ else -1

Round 3

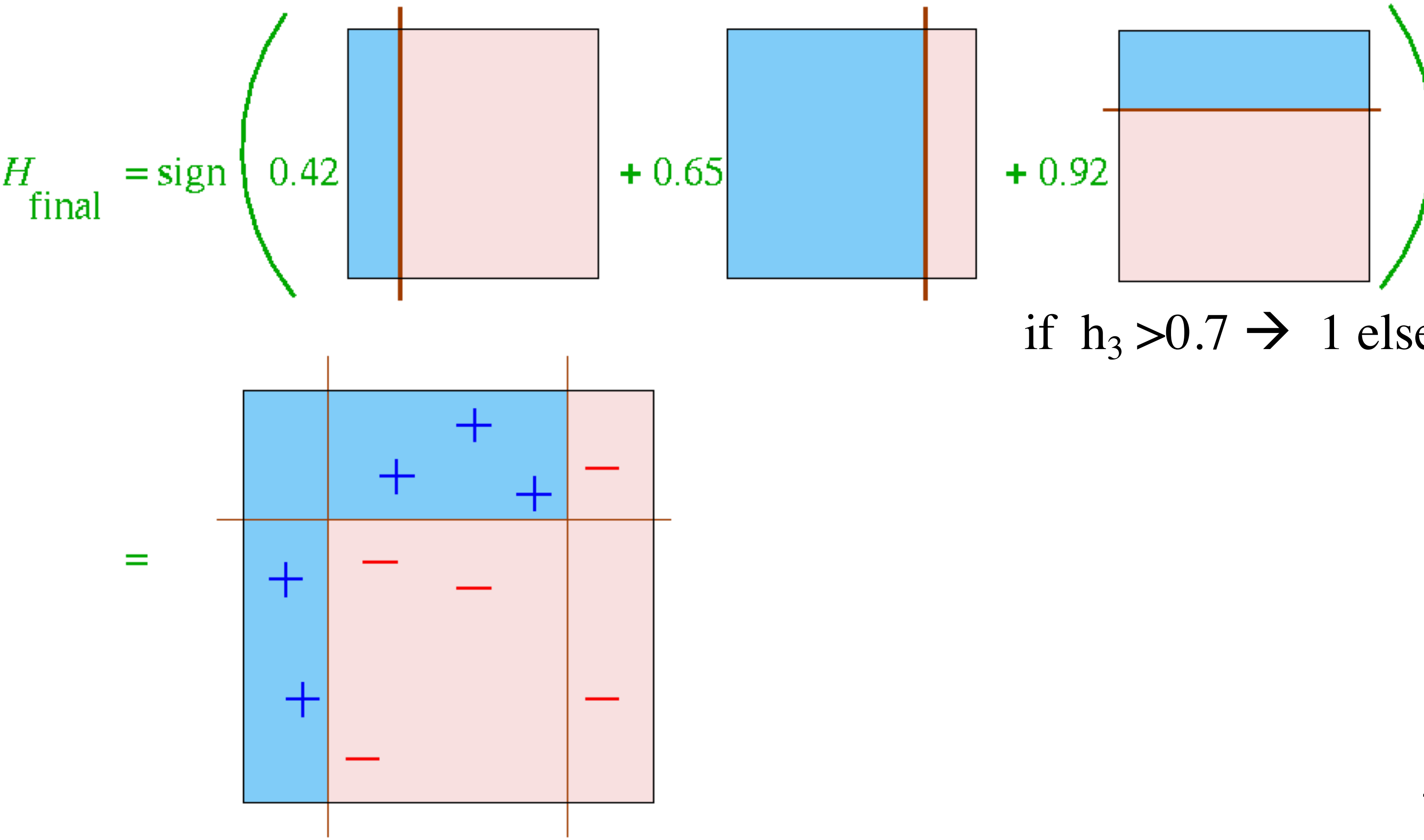


Weak classifier: if $h_3 > 0.7 \rightarrow$ 1 else -1

Final Combination

if $h_1 < 0.2 \rightarrow$ 1 else -1

if $h_2 < 0.8 \rightarrow$ 1 else -1



if $h_3 > 0.7 \rightarrow$ 1 else -1

Pros and Cons of AdaBoost and Extension

Advantages

- Very simple to implement
- Does feature selection resulting in relatively simple classifier
- Fairly good generalization

Disadvantages

- Suboptimal solution
- Sensitive to noisy data and outliers

- **RankBoost** extends AdaBoost for pairwise correctness of document ranking
  - +1: Correctly ordered for a pair of documents
  - -1: Incorrectly ordered

Rank Algorithms and Opensource Library

- **Linear**
  - RankSVM
    - SVM based weight computation
  - As an extension of AdaBoost/AdaRank, AdaRank is optimized for ranking based on NDCG cost metrics
- **Nonlinear Tree Ensembles**
  - GBRT (Gradient Boosting Regression Trees)
  - LambdaMART
    - Additive tree boosting
    - Optimzied based on NDCG
  - RandomForest
    - Bagging on top of GBRT or LambdaMART
- **Opensource Rank Library**
  - RankLib

Some References on Ranking & Boosting

- AdaRank,
  - Jun Xu and Hang Li. 2007. AdaRank: a boosting algorithm for information retrieval. In Proceedings of the 30th annual international ACM SIGIR conference on Research and development in information retrieval (SIGIR '07)
  - Generalization from Adaboost for NDCG optimization
- LambdaMart:
  - C.J.C. Burges, K.M. Svore, P.N. Bennett, A. Pastusiak and Q. Wu, *Learning to Rank Using an Ensemble of Lambda-Gradient Models*. Journal of Machine Learning Research: Workshop and Conference Proceedings, vol. 14, pp. 25-35, 2011
- RandomForest
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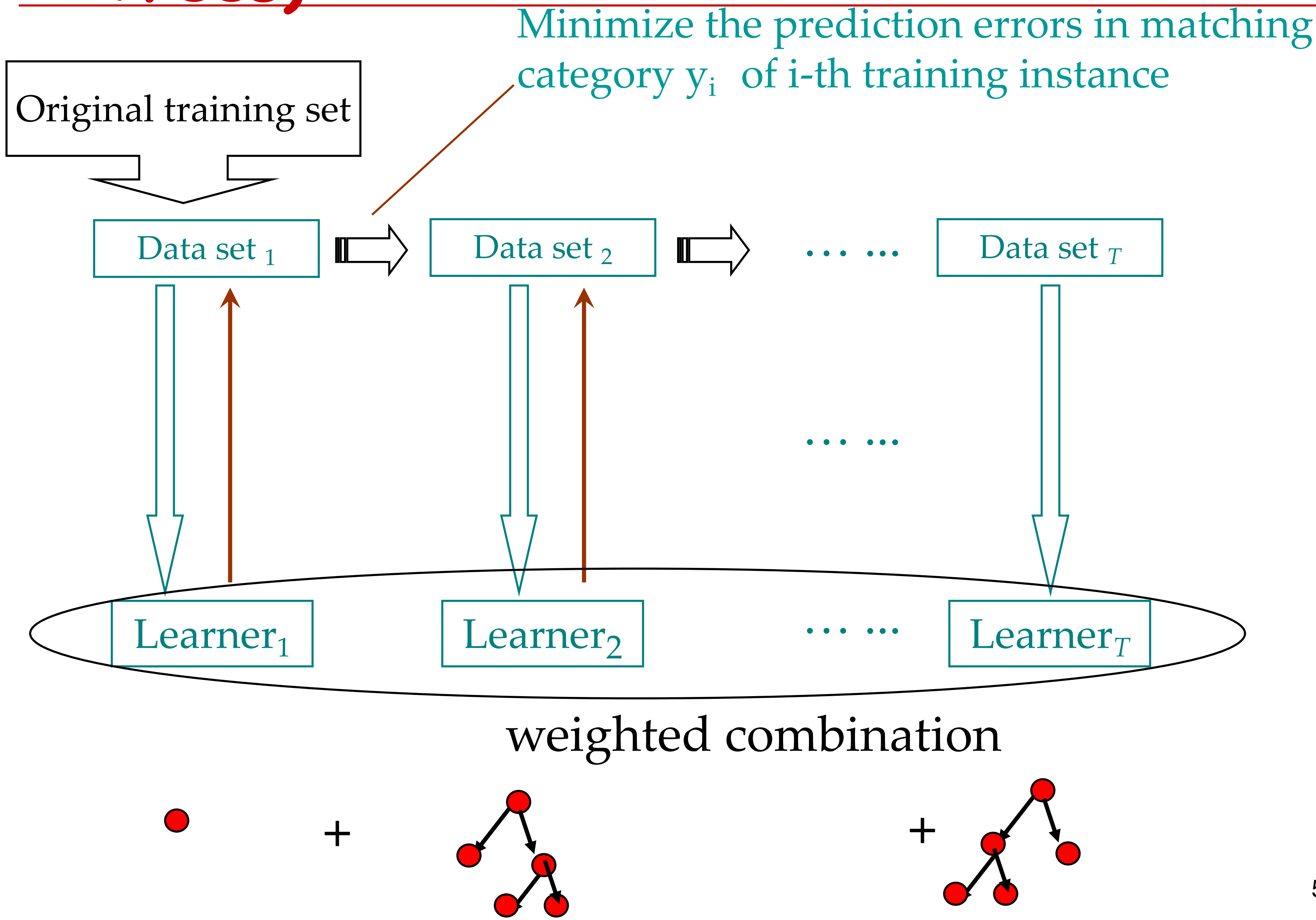
GBRT(Gradient Boosting Regression Trees)



GBRT example with 4 training instances