POLITECNICO DI MILANO

Classifiers Ensembles

Data Mining and Text Mining (UIC 583 @ Politecnico di Milano)

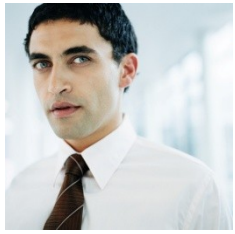
Prof. Pier Luca Lanzi

Lecture outline

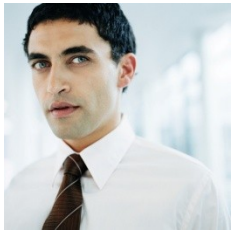
- Ensemble methods
- Bagging
- Boosting
- Random forests

Ensemble methods

What is the idea?



Final Diagnosis



Diagnosis

Diagnosis

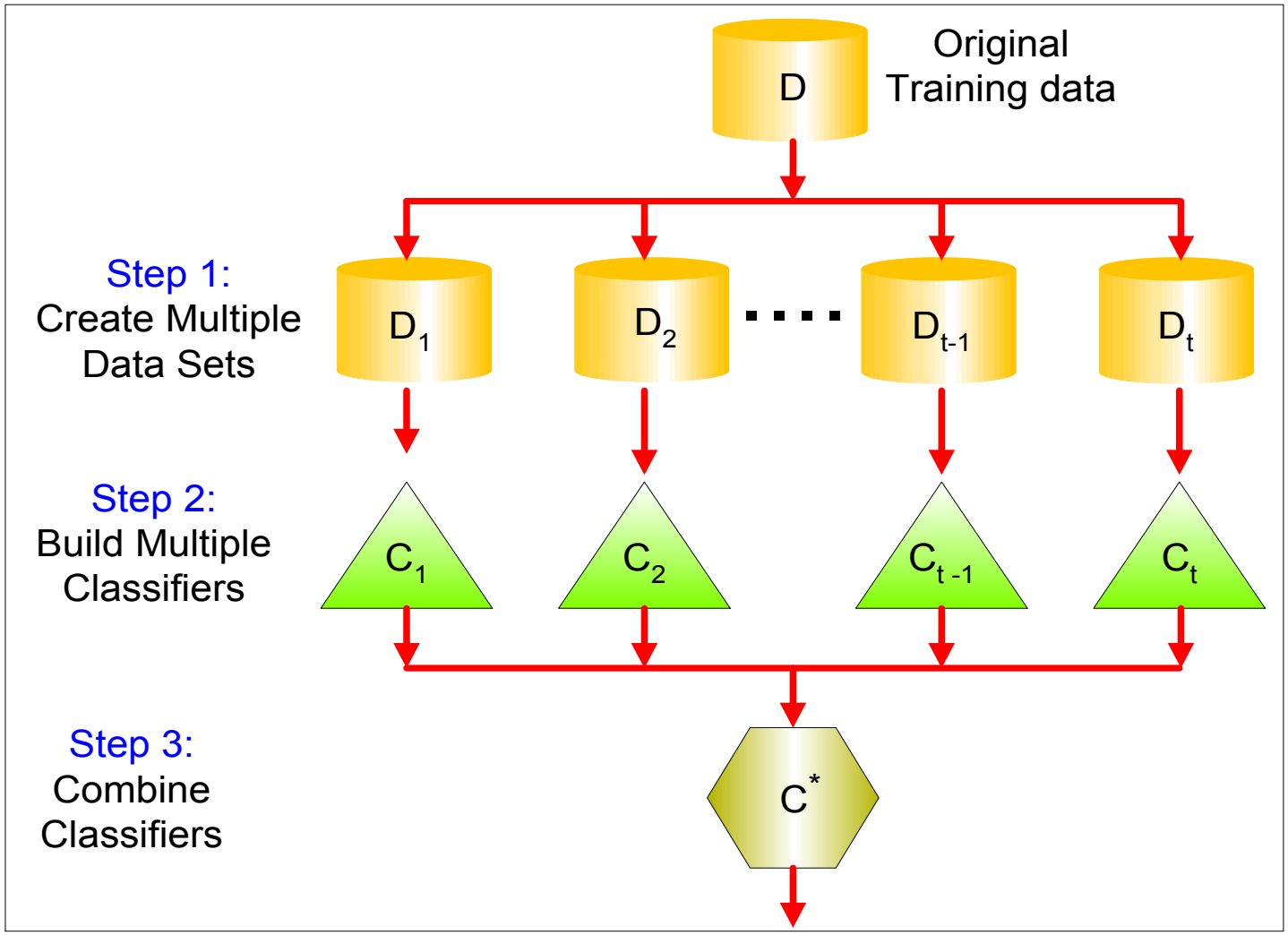
Diagnosis

Final Diagnosis

Ensemble Methods

- Construct a set of classifiers from the training data
- Predict class label of previously unseen records by aggregating predictions made by multiple classifiers

What is the General Idea?



Building models ensembles

- Basic idea
  - Build different “experts”, let them vote
- Advantage
  - Often improves predictive performance
- Disadvantage
  - Usually produces output that is very hard to analyze
- However, there are approaches that aim to produce a single comprehensible structure

Why does it work?

- Suppose there are 25 base classifiers
- Each classifier has error rate, $\varepsilon = 0.35$
- Assume classifiers are independent
- Probability that the ensemble classifier makes a wrong prediction:

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} = 0.06$$

How to generate an ensemble?

- Bootstrap Aggregating (Bagging)
- Boosting
- Random Forests

Bagging

What is Bagging? (Bootstrap Aggregation)

- Analogy: Diagnosis based on multiple doctors' majority vote
- Training
  - Given a set D of d tuples, at each iteration i, a training set D_i of d tuples is sampled with replacement from D (i.e., bootstrap)
  - A classifier model M_i is learned for each training set D_i
- Classification: classify an unknown sample X
  - Each classifier M_i returns its class prediction
  - The bagged classifier M* counts the votes and assigns the class with the most votes to X
- Prediction: can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple

What is Bagging?

- Combining predictions by voting/averaging
  - Simplest way
  - Each model receives equal weight
- "Idealized" version:
  - Sample several training sets of size n (instead of just having one training set of size n)
  - Build a classifier for each training set
  - Combine the classifiers' predictions

More on bagging

- Bagging works because it reduces variance by voting/averaging
  - Note: in some pathological hypothetical situations the overall error might increase
  - Usually, the more classifiers the better
- Problem: we only have one dataset!
- Solution: generate new ones of size n by Bootstrap, i.e., sampling from it with replacement
- Can help a lot if data is noisy
- Can also be applied to numeric prediction
  - Aside: bias-variance decomposition originally only known for numeric prediction

Model generation

```
Let n be the number of instances in the training data
For each of t iterations:
Sample n instances from training set
       (with replacement)
Apply learning algorithm to the sample
Store resulting model
```

Classification

```
For each of the t models:
Predict class of instance using model
Return class that is predicted most often
```

Bias-variance decomposition

- Used to analyze how much selection of any specific training set affects performance
- Assume infinitely many classifiers, built from different training sets of size n
- For any learning scheme,
  - Bias = expected error of the combined classifier on new data
  - Variance = expected error due to the particular training set used
- Total expected error ≈ bias + variance

When does Bagging work?

- Learning algorithm is unstable, if small changes to the training set cause large changes in the learned classifier
- If the learning algorithm is unstable, then Bagging almost always improves performance
- Bagging stable classifiers is not a good idea
- Which ones are unstable?
  - Neural nets, decision trees, regression trees, linear regression
- Which ones are stable?
  - K-nearest neighbors

Why Bagging works?

- Let $T=\{<x_n, y_n>\}$ be the set of training data containing N examples
- Let $\{T_k\}$ be a sequence of training sets containing N examples independently sampled from T, for instance T_k can be generated using bootstrap
- Let P be the underlying distribution of T
- Bagging replaces the prediction of the model $\varphi(x,T)$ obtained by E, with the majority of the predictions given by the models $\{\varphi(x,T_k)\}$

$$\varphi_A(x,P) = E_T\,(\varphi(x,T_k))$$

- The algorithm is instable, if perturbing the learning set can cause significant changes in the predictor constructed
- Bagging can improve the accuracy of the predictor,

Why Bagging works?

- It is possible to prove that,

$$(y - E_T(\varphi(x,T)))^2 \leq E_T(y - \varphi(x,T))^2$$

- Thus, Bagging produces a smaller error

- How much is smaller the error is, depends on how much unequal are the two sides of,

$$[E_T(\varphi(x,T))\ ]^2 \leq E_T(\varphi^2(x,T))$$

- If the algorithm is stable, the two sides will be nearly equal
- If more highly variable the $\varphi(x,T)$ are the more improvement the aggregation produces

- However, φ_A always improves φ

Bagging with costs

- Bagging unpruned decision trees known to produce good probability estimates
  - Where, instead of voting, the individual classifiers' probability estimates are averaged
  - Note: this can also improve the success rate
- Can use this with minimum-expected cost approach for learning problems with costs
- Problem: not interpretable
  - MetaCost re-labels training data using bagging with costs and then builds single tree

Randomization

- Can randomize learning algorithm instead of input
- Some algorithms already have a random component:
  e.g. initial weights in neural net
- Most algorithms can be randomized, e.g. greedy algorithms:
  - Pick from the N best options at random instead of always picking the best options
  - E.g.: attribute selection in decision trees
- More generally applicable than bagging:
  e.g. random subsets in nearest-neighbor scheme
- Can be combined with bagging

Boosting

What is Boosting?

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - Weights are assigned to each training tuple
  - A series of k classifiers is iteratively learned
  - After a classifier Mi is learned, the weights are updated to allow the subsequent classifier, Mi+1, to pay more attention to the training tuples that were misclassified by Mi
  - The final M* combines the votes of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- The boosting algorithm can be extended for the prediction of continuous values
- Comparing with bagging: boosting tends to achieve greater accuracy, but it also risks overfitting the model to misclassified data

What is the Basic Idea?

- Suppose there are just 5 training examples {1,2,3,4,5}
- Initially each example has a 0.2 (1/5) probability of being sampled
- 1st round of boosting samples (with replacement) 5 examples: {2, 4, 4, 3, 2} and builds a classifier from them
- Suppose examples 2, 3, 5 are correctly predicted by this classifier, and examples 1, 4 are wrongly predicted:
  - Weight of examples 1 and 4 is increased,
  - Weight of examples 2, 3, 5 is decreased
- 2nd round of boosting samples again 5 examples, but now examples 1 and 4 are more likely to be sampled
- And so on … until some convergence is achieved

Boosting

- Also uses voting/averaging
- Weights models according to performance
- Iterative: new models are influenced by the performance of previously built ones
  - Encourage new model to become an "expert" for instances misclassified by earlier models
  - Intuitive justification: models should be experts that complement each other
- Several variants
  - Boosting by sampling, the weights are used to sample the data for training
  - Boosting by weighting, the weights are used by the learning algorithm

Model generation

```
Assign equal weight to each training instance
For t iterations:
  Apply learning algorithm to weighted dataset,
       store resulting model
  Compute model's error e on weighted dataset
  If e = 0 or e ≥ 0.5:
    Terminate model generation
  For each instance in dataset:
    If classified correctly by model:
       Multiply instance's weight by e/(1-e)
  Normalize weight of all instances
```

Classification

```
Assign weight = 0 to all classes
For each of the t (or less) models:
For the class this model predicts
       add -log e/(1-e) to this class's weight
Return class with highest weight
```

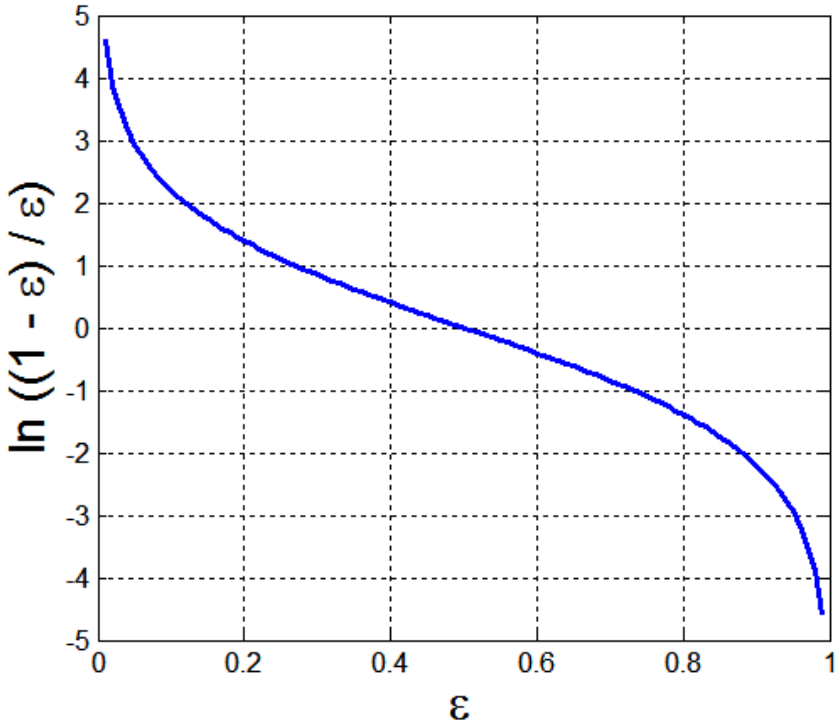
Example: AdaBoost

- Base classifiers: C_1, C_2, …, C_T
- Error rate:

$$\varepsilon_i = \frac{1}{N}\sum_{j=1}^{N} w_j \delta\left(C_i(x_j) \neq y_j\right)$$

- Importance of a classifier:

$$\alpha_i = \frac{1}{2}\ln\left(\frac{1-\varepsilon_i}{\varepsilon_i}\right)$$



Example: AdaBoost

- Weight update:

$$w_i^{(j+1)} = \frac{w_i^{(j)}}{Z_j} \begin{cases} \exp^{-\alpha_j} & \text{if } C_j(x_i) = y_i \\ \exp^{\alpha_j} & \text{if } C_j(x_i) \neq y_i \end{cases}$$

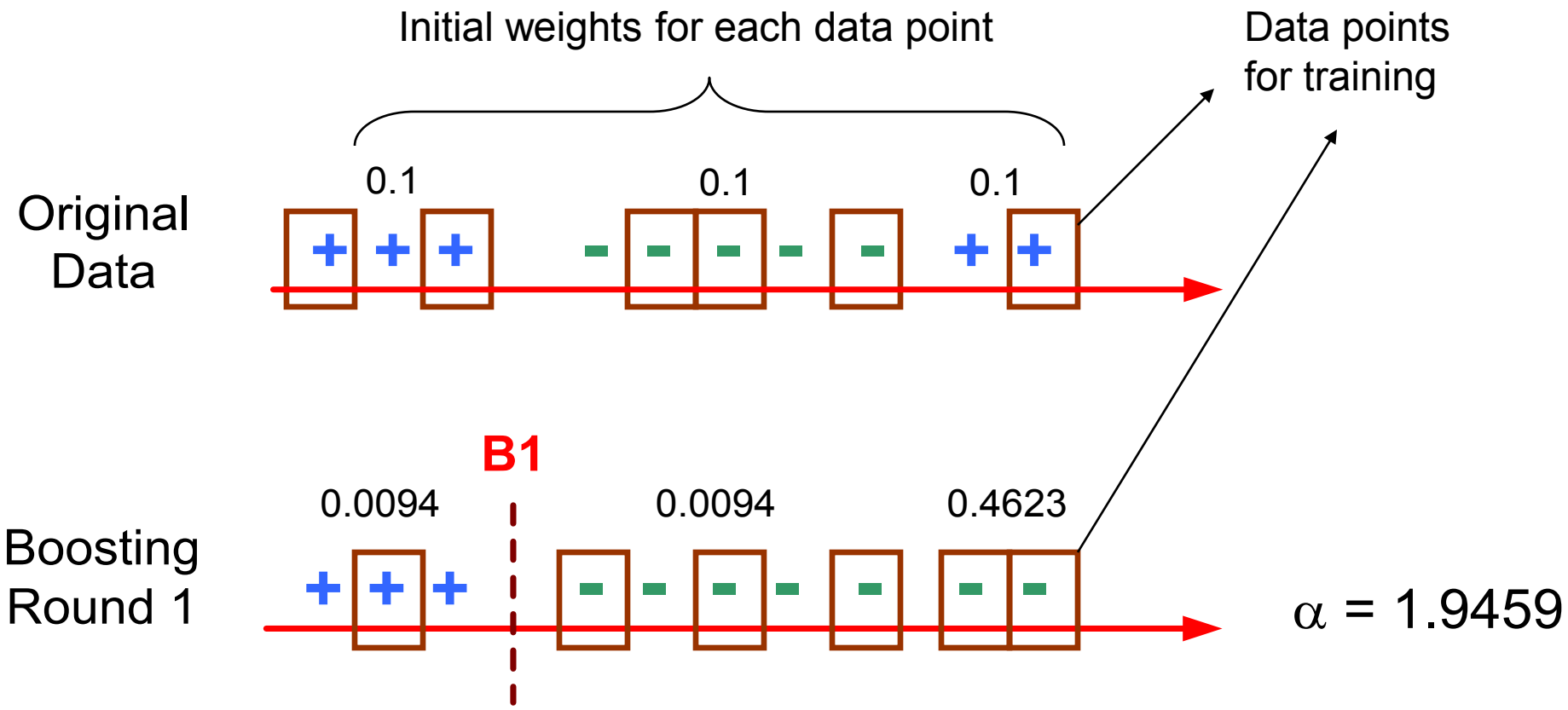
$$\text{where } Z_j \text{ is the normalization factor}$$

- If any intermediate rounds produce error rate higher than 50%, the weights are reverted back to 1/n and the resampling procedure is repeated

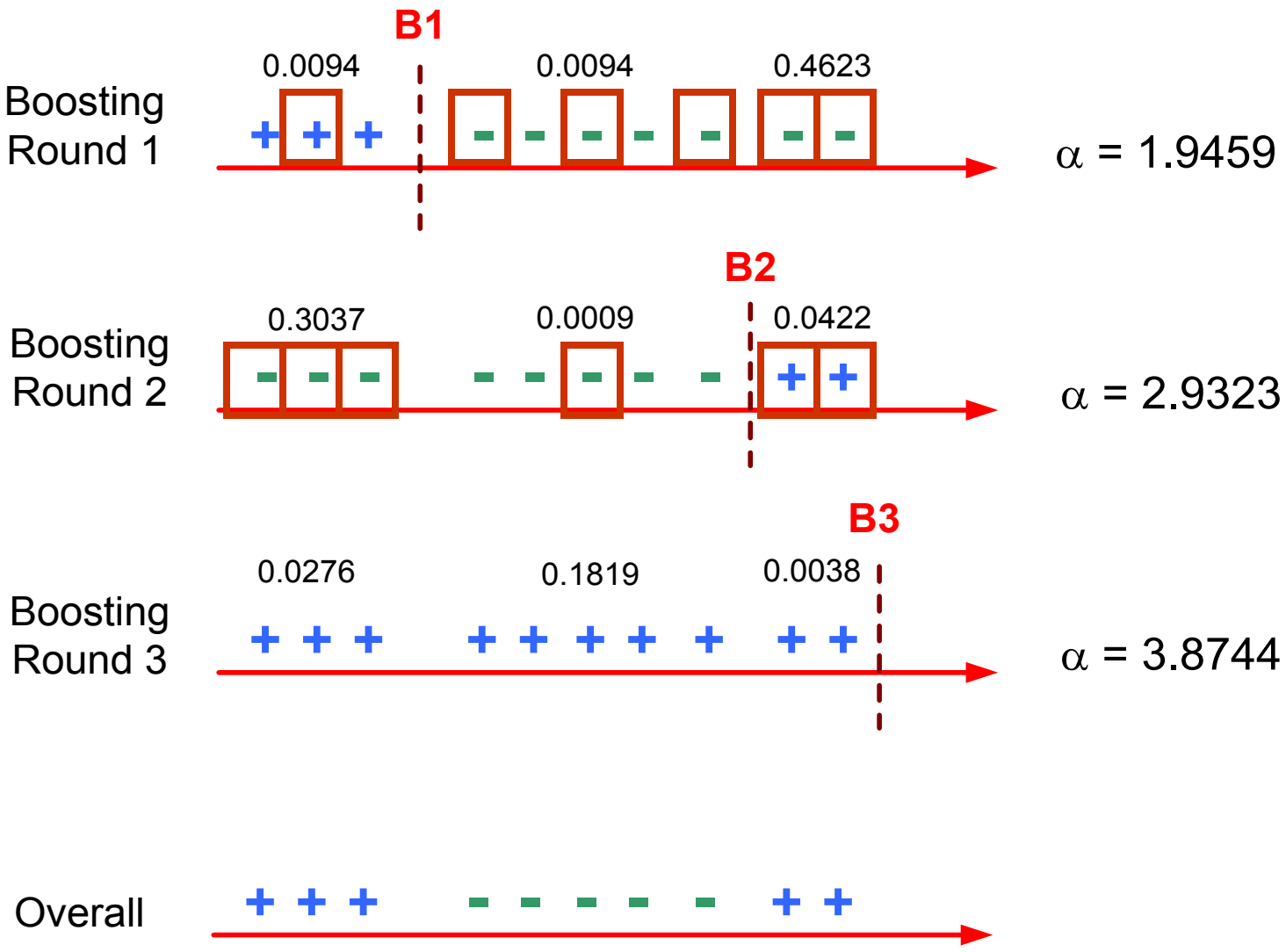
- Classification:

$$C^*(x) = \arg\max_y \sum_{j=1}^{T} \alpha_j \delta\left(C_j(x) = y\right)$$

Illustrating AdaBoost



Illustrating AdaBoost



Adaboost (Freund and Schapire, 1997)

- Given a set of *d* class-labeled tuples, $(\mathbf{X}_1, y_1), \ldots, (\mathbf{X}_d, y_d)$
- Initially, all the weights of tuples are set the same (1/d)
- Generate k classifiers in k rounds. At round i,
  - Tuples from D are sampled (with replacement) to form a training set D_i of the same size
  - Each tuple's chance of being selected is based on its weight
  - A classification model M_i is derived from D_i
  - Its error rate is calculated using D_i as a test set
  - If a tuple is misclassified, its weight is increased, o.w. it is decreased
- Error rate: $err(\mathbf{X}_j)$ is the misclassification error of tuple $\mathbf{X}_j$. Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_j^d w_j \times err(\mathbf{X_j})$$

- The weight of classifier M_i's vote is

$$\log \frac{1 - error(M_i)}{error(M_i)}$$

Random Forests

What is a Random Forest?

- Random forests (RF) are a combination of tree predictors
- Each tree depends on the values of a random vector sampled independently and with the same distribution for all trees in the forest
- The generalization error of a forest of tree classifiers depends on the strength of the individual trees in the forest and the correlation between them
- Using a random selection of features to split each node yields error rates that compare favorably to Adaboost, and are more robust with respect to noise

How do Random Forests Work?


```
D = training set                          F = set of tests
k = nb of trees in forest                 n = nb of tests

for i = 1 to k do:
   build data set Di by sampling with replacement from D
   learn tree Ti (Tilde) from Di:
      at each node:
         choose best split from random subset of F of size n
      allow aggregates and refinement of aggregates in tests

make predictions according to majority vote of the set of k trees.
```

Random Forests

- Ensemble method tailored for decision tree classifiers
- Creates k decision trees, where each tree is independently generated based on random decisions
- Bagging using decision trees can be seen as a special case of random forests where the random decisions are the random creations of the bootstrap samples

Two examples of Random Decisions in Decision Forests

- At each internal tree node, randomly select F attributes, and evaluate just those attributes to choose the partitioning attribute
  - Tends to produce trees larger than trees where all attributes are considered for selection at each node, but different classes will be eventually assigned to different leaf nodes, anyway
  - Saves processing time in the construction of each individual tree, since just a subset of attributes is considered at each internal node

- At each internal tree node, evaluate the quality of all possible partitioning attributes, but randomly select one of the F best attributes to label that node (based on InfoGain, etc.)
  - Unlike the previous approach, does not save processing time

Properties of Random Forests

- Easy to use ("off-the-shelve"), only 2 parameters (no. of trees, %variables for split)
- Very high accuracy
- No overfitting if selecting large number of trees (choose high)
- Insensitive to choice of split% (~20%)
- Returns an estimate of variable importance

Out of the Bag

- For every tree grown, about one-third of the cases are out-of-bag (out of the bootstrap sample). Abbreviated oob.
- Put these oob cases down the corresponding tree and get response estimates for them.
- For each case n, average or pluralize the response estimates over all time that n was oob to get a test set estimate y_n for y_n.
- Averaging the loss over all n give the test set estimate of prediction error.
- The only adjustable parameter in RF is m.
- The default value for m is M. But RF is not sensitive to the value of m over a wide range.

Variable Importance

- Because of the need to know which variables are important in the classification, RF has three different ways of looking at variable importance

- Measure
  - To estimate the importance of the mth variable, in the oob cases for the kth tree, randomly permute all values of the mth variable
  - Put these altered oob x-values down the tree and get classifications.
  - Proceed as though computing a new internal error rate.
  - The amount by which this new error exceeds the original test set error is defined as the importance of the mth variable.

The out-of-bag (oob) error estimate

- In random forests, there is no need for cross-validation or a separate test set to get an unbiased estimate of the test set error. It is estimated internally, during the run, as follows.

- Each tree is constructed using a different bootstrap sample from the original data. About one-third of the cases are left out of the bootstrap sample and not used in the construction of the kth tree.

- Put each case left out in the construction of the kth tree down the kth tree to get a classification. In this way, a test set classification is obtained for each case in about one-third of the trees. At the end of the run, take j to be the class that got most of the votes every time case n was oob. The proportion of times that j is not equal to the true class of n averaged over all cases is the oob error estimate. This has proven to be unbiased in many tests.

Summary of Random Forests

- Random forests are an effective tool in prediction.
- Forests give results competitive with boosting and adaptive bagging, yet do not progressively change the training set.
- Random inputs and random features produce good results in classification- less so in regression.
- For larger data sets, we can gain accuracy by combining random features with boosting.

Summary

Summary

- Ensembles in general improve predictive accuracy
  - Good results reported for most application domains, unlike algorithm variations whose success are more dependant on the application domain/dataset
- Improvement in accuracy, but interpretability decreases
  - Much more difficult for the user to interpret an ensemble of classification models than a single classification model
- Diversity of the base classifiers in the ensemble is important
  - Trade-off between each base classifier's error and diversity
  - Maximizing classifier diversity tends to increase the error of each individual base classifier