Data Mining

Practical Machine Learning Tools and Techniques

Slides for Chapter 8 of *Data Mining* by I. H. Witten, E. Frank and M. A. Hall

Ensemble learning

- Combining multiple models
  - The basic idea
- Bagging
  - Bias-variance decomposition, bagging with costs
- Randomization
  - Rotation forests
- Boosting
  - AdaBoost, the power of boosting
- Additive regression
  - Numeric prediction, additive logistic regression
- Interpretable ensembles
  - Option trees, alternating decision trees, logistic model trees
- Stacking

Combining multiple models

- Basic idea:
  build different "experts", let them vote
- Advantage:
  - often improves predictive performance
- Disadvantage:
  - usually produces output that is very hard to analyze
  - but: there are approaches that aim to produce a single comprehensible structure

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
- Learning scheme is *unstable* ⇒ almost always improves performance
  - Small change in training data can make big change in model (e.g. decision trees)

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

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 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

Bagging classifiers

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
```

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: eg. initial weights in neural net
- Most algorithms can be randomized, eg. greedy algorithms:
  - Pick from the *N* best options at random instead of always picking the best options
  - Eg.: attribute selection in decision trees
- More generally applicable than bagging: e.g. random subsets in nearest-neighbor scheme
- Can be combined with bagging

Rotation forests

- Bagging creates ensembles of accurate classifiers with relatively low diversity
  - Bootstrap sampling creates training sets with a distribution that resembles the original data
- Randomness in the learning algorithm increases diversity but sacrifices accuracy of individual ensemble members
- Rotation forests have the goal of creating accurate **and** diverse ensemble members

Rotation forests

- Combine random attribute sets, bagging and principal components to generate an ensemble of decision trees
- An iteration involves
  - Randomly dividing the input attributes into *k* disjoint subsets
  - Applying PCA to each of the *k* subsets in turn
  - Learning a decision tree from the *k* sets of PCA directions
- Further increases in diversity can be achieved by creating a bootstrap sample in each iteration before applying PCA

Boosting

- Also uses voting/averaging
- Weights models according to performance
- Iterative: new models are influenced by 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

AdaBoost.M1

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
```

More on boosting I

- Boosting needs weights … but
- Can adapt learning algorithm ... or
- Can apply boosting *without* weights
  - resample with probability determined by weights
  - disadvantage: not all instances are used
  - advantage: if error > 0.5, can resample again
- Stems from *computational learning theory*
- Theoretical result:
  - training error decreases exponentially
- Also:
  - works if base classifiers are not too complex, and
  - their error doesn't become too large too quickly

More on boosting II

- Continue boosting after training error = 0?
- Puzzling fact:
  generalization error continues to decrease!
  - Seems to contradict Occam's Razor
- Explanation:
  consider *margin* (confidence), not error
  - Difference between estimated probability for true class and nearest other class (between –1 and 1)
- Boosting works with *weak* learners
  only condition: error doesn't exceed 0.5
- In practice, boosting sometimes overfits (in contrast to bagging)

Additive regression I

- Turns out that boosting is a greedy algorithm for fitting additive models
- More specifically, implements *forward stagewise additive modeling*
- Same kind of algorithm for numeric prediction:
  1. Build standard regression model (eg. tree)
  2. Gather residuals, learn model predicting residuals (eg. tree), and repeat
- To predict, simply sum up individual predictions from all models

Additive regression II

- Minimizes squared error of ensemble if base learner minimizes squared error
- Doesn't make sense to use it with standard multiple linear regression, why?
- Can use it with *simple* linear regression to build multiple linear regression model
- Use cross-validation to decide when to stop
- Another trick: shrink predictions of the base models by multiplying with pos. constant < 1
  - Caveat: need to start with model 0 that predicts the mean

Additive logistic regression

- Can use the logit transformation to get algorithm for classification
  - More precisely, class probability estimation
  - Probability estimation problem is transformed into regression problem
  - Regression scheme is used as base learner (eg. regression tree learner)
- Can use forward stagewise algorithm: at each stage, add model that maximizes probability of data
- If f_j is the jth regression model, the ensemble predicts probability for the first class

$$p(1 \mid \vec{a}) = \frac{1}{1+\exp(-\sum f_j(\vec{a}))}$$

LogitBoost

Model generation

```
For j = 1 to t iterations:
  For each instance a[i]:
    Set the target value for the regression to
      z[i] = (y[i] – p(1|a[i])) / [p(1|a[i]) × (1-p(1|a[i])]
    Set the weight of instance a[i] to p(1|a[i]) × (1-p(1|a[i])
  Fit a regression model f[j] to the data with class
    values z[i] and weights w[i]
```

Classification

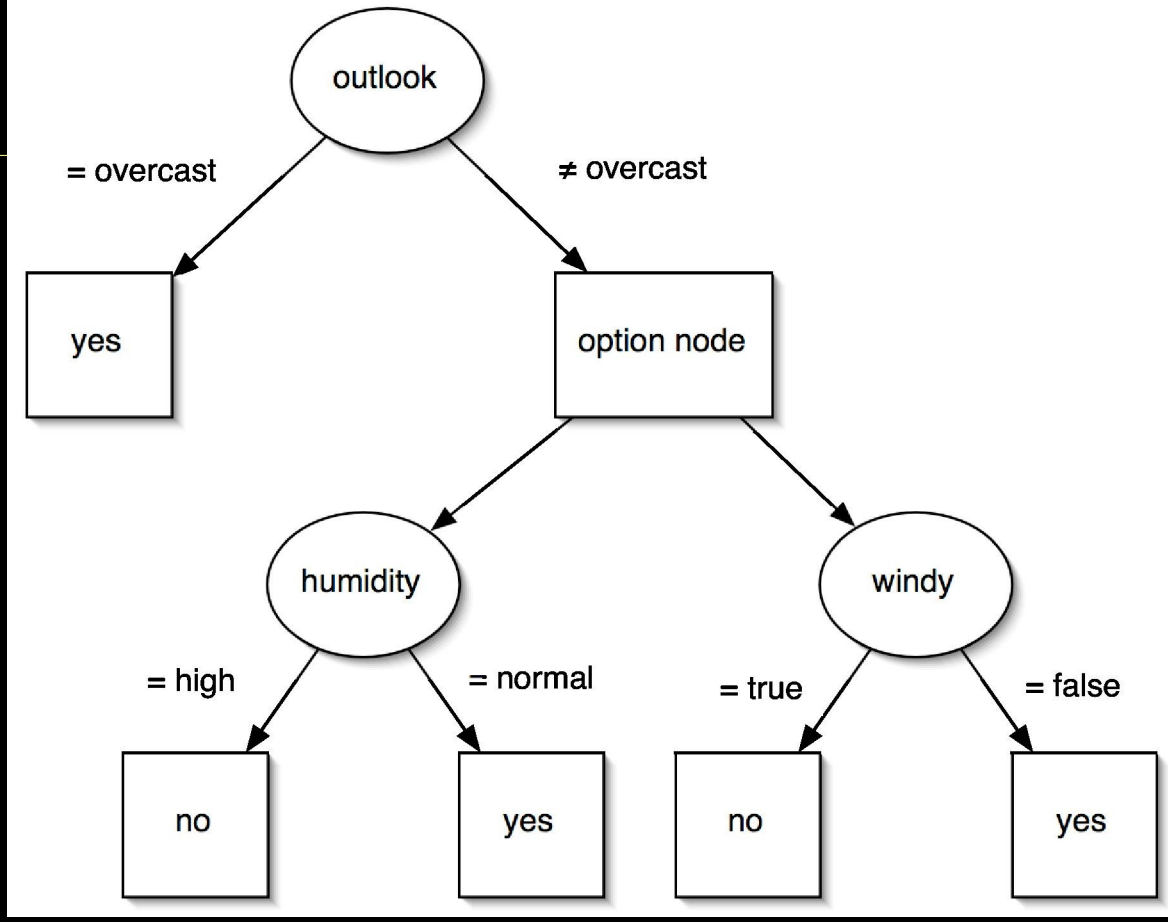
Predict 1st class if p(1 | a) > 0.5, otherwise predict 2nd class

- Maximizes probability if base learner minimizes squared error
- Difference to AdaBoost: optimizes probability/likelihood instead of exponential loss
- Can be adapted to multi-class problems
- Shrinking and cross-validation-based selection apply

Option trees

- Ensembles are not interpretable
- Can we generate a single model?
  - One possibility: "cloning" the ensemble by using lots of artificial data that is labeled by ensemble
  - Another possibility: generating a single structure that represents ensemble in compact fashion
- *Option tree*: decision tree with option nodes
  - Idea: follow all possible branches at option node
  - Predictions from different branches are merged using voting or by averaging probability estimates

Example

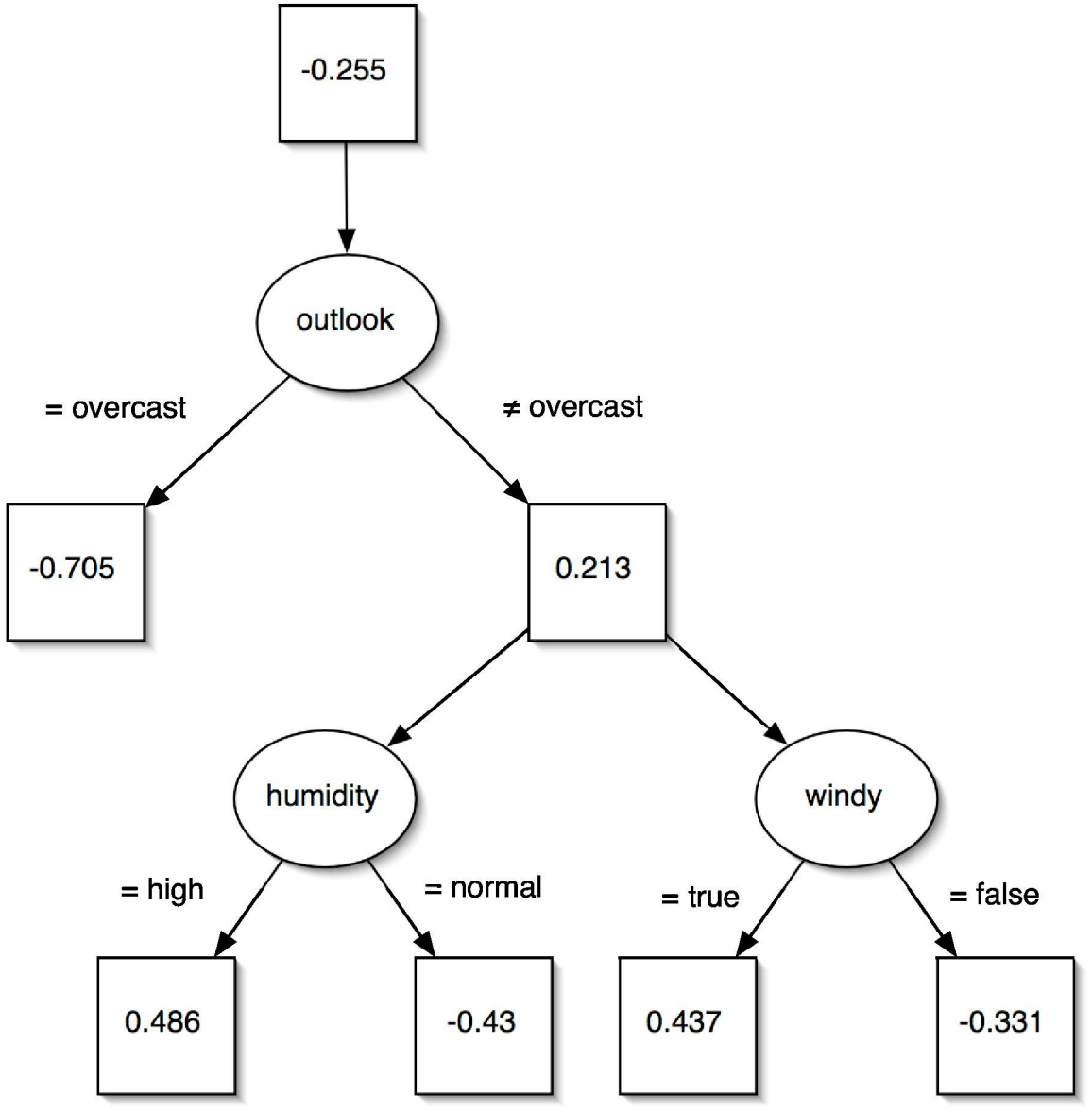


- Can be learned by modifying tree learner:
  - Create option node if there are several equally promising splits (within user-specified interval)
  - When pruning, error at option node is average error of options

Alternating decision trees

- Can also grow option tree by incrementally adding nodes to it
- Structure called *alternating decision tree*, with *splitter nodes* and *prediction* nodes
  - Prediction nodes are leaves if no splitter nodes have been added to them yet
  - Standard alternating tree applies to 2-class problems
  - To obtain prediction, filter instance down all applicable branches and sum predictions
    - Predict one class or the other depending on whether the sum is positive or negative

Example


-0.255
outlook
= overcast
≠ overcast
-0.705
0.213
humidity
windy
= high
= normal
= true
= false
0.486
-0.43
0.437
-0.331

Growing alternating trees

- Tree is grown using a boosting algorithm
  - Eg. LogitBoost described earlier
  - Assume that base learner produces single conjunctive rule in each boosting iteration (note: rule for regression)
  - Each rule could simply be added into the tree, including the numeric prediction obtained from the rule
  - Problem: tree would grow very large very quickly
  - Solution: base learner should only consider candidate rules that extend existing branches
    - Extension adds splitter node and two prediction nodes (assuming binary splits)
  - Standard algorithm chooses best extension among all possible extensions applicable to tree
  - More efficient heuristics can be employed instead

Logistic model trees

- Option trees may still be difficult to interpret
- Can also use boosting to build decision trees with linear models at the leaves (ie. trees without options)
- Algorithm for building logistic model trees:
  - Run LogitBoost with simple linear regression as base learner (choosing the best attribute in each iteration)
  - Interrupt boosting when cross-validated performance of additive model no longer increases
  - Split data (eg. as in C4.5) and resume boosting in subsets of data
  - Prune tree using cross-validation-based pruning strategy (from CART tree learner)

Stacking

- To combine predictions of base learners, don't vote, use *meta learner*
  - Base learners: *level-0 models*
  - Meta learner: *level-1 model*
  - Predictions of base learners are input to meta learner
- Base learners are usually different schemes
- Can't use predictions on training data to generate data for level-1 model!
  - Instead use cross-validation-like scheme
- Hard to analyze theoretically: "black magic"

More on stacking

- If base learners can output probabilities, use those as input to meta learner instead
- Which algorithm to use for meta learner?
  - In principle, any learning scheme
  - Prefer "relatively global, smooth" model
    - Base learners do most of the work
    - Reduces risk of overfitting
- Stacking can be applied to numeric prediction too