Just apply a learner? NO!

- Scheme/parameter selection
  - ***treat selection process as part of the learning process***
- Modifying the input:
  - Data engineering to make learning possible or easier
- Modifying the output
  - Combining models to improve performance

Data transformations

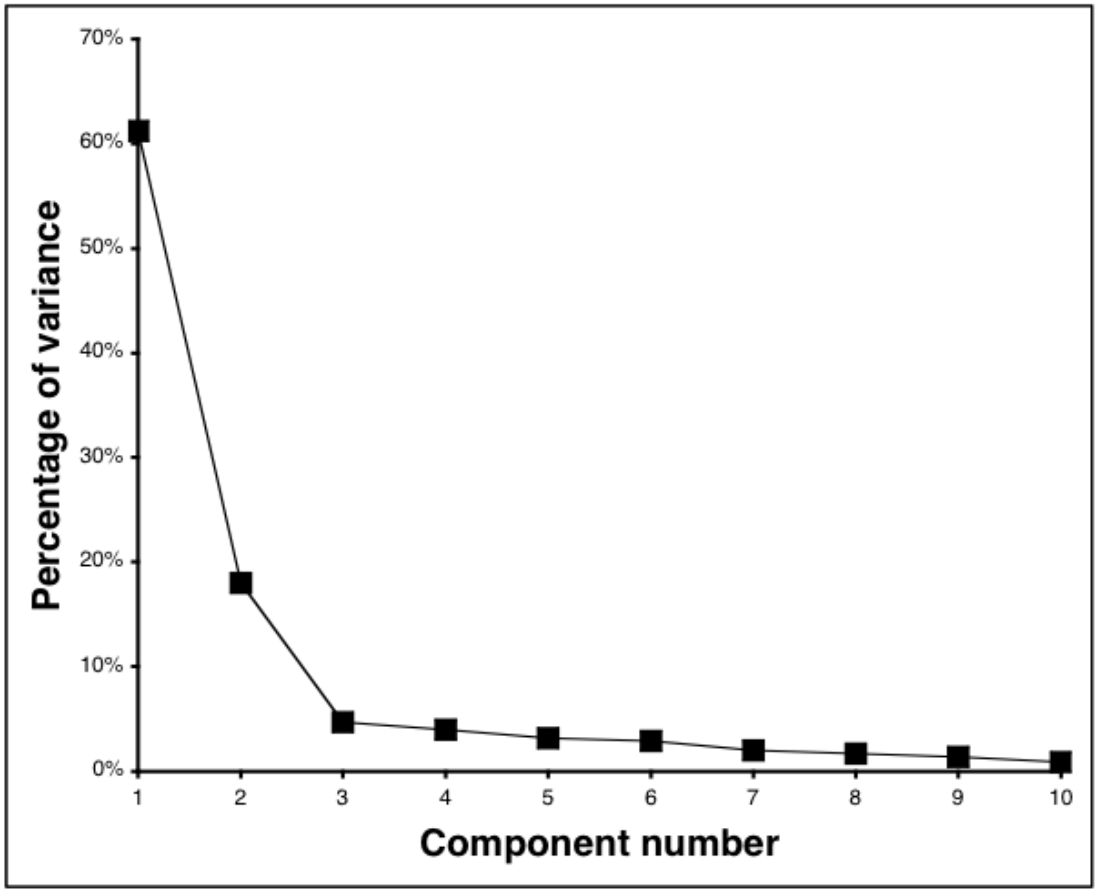
- Simple transformations can often make a large difference in performance
- Example transformations (not necessarily for performance improvement):
  - Difference of two date attributes
  - Ratio of two numeric (ratio-scale) attributes
  - Concatenating the values of nominal attributes
  - Encoding cluster membership
  - Adding noise to data
  - Removing data randomly or selectively
  - Obfuscating the data

Principal component analysis

- Method for identifying the important "directions" in the data
- Can rotate data into (reduced) coordinate system that is given by those directions
- Algorithm:
  1. Find direction (axis) of greatest variance
  2. Find direction of greatest variance that is perpendicular to previous direction and repeat
- Implementation: find eigenvectors of covariance matrix by diagonalization
  - Eigenvectors (sorted by eigenvalues) are the directions

Example: 10-dimensional data

Axis	Variance	Cumulative
1	61.2%	61.2%
2	18.0%	79.2%
3	4.7%	83.9%
4	4.0%	87.9%
5	3.2%	91.1%
6	2.9%	94.0%
7	2.0%	96.0%
8	1.7%	97.7%
9	1.4%	99.1%
10	0.9%	100.0%



- Can transform data into space given by components
- Data is normally standardized for PCA
- Could also apply this recursively in tree learner

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
```

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

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
```

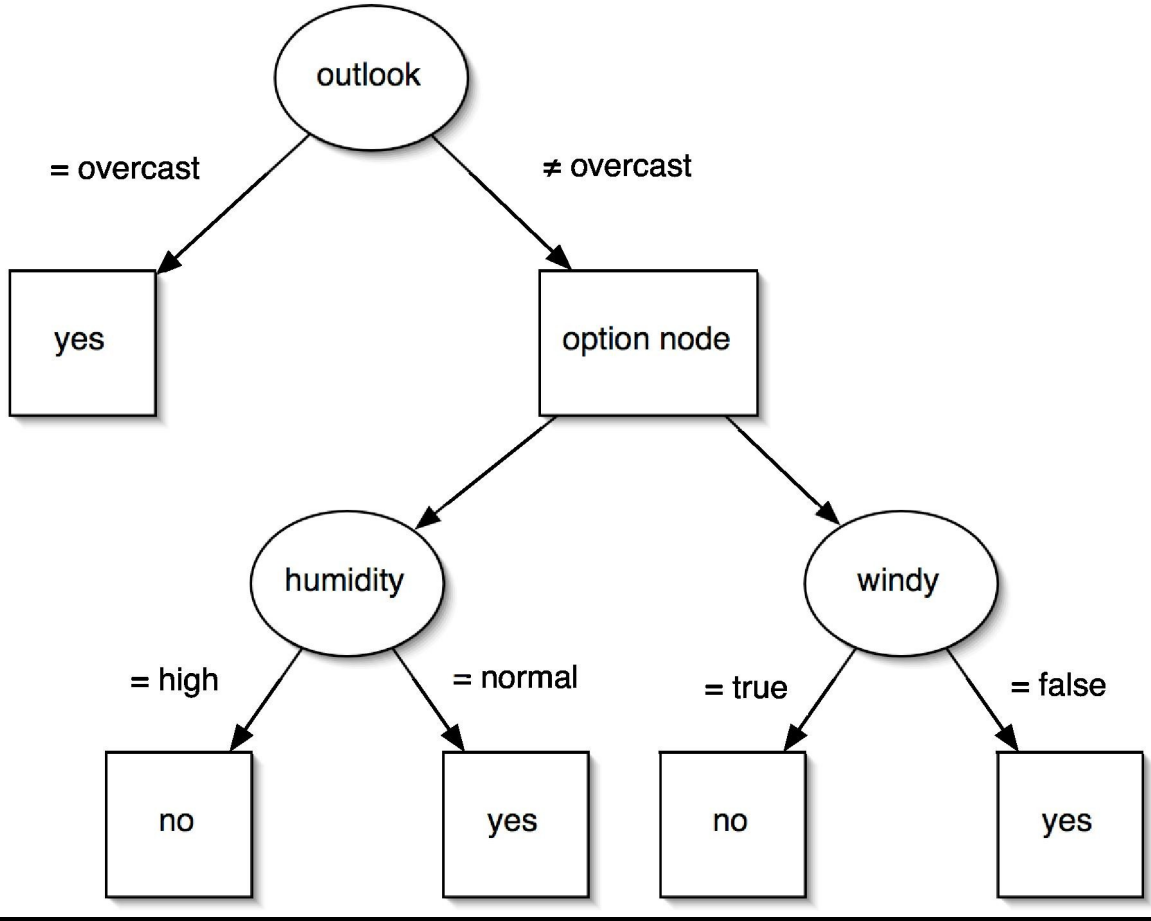
Classification

```
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

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

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