Machine Learning Techniques for Data Mining

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PART VII

Moving on: Engineering the input and output

Applying a learner is not all

- Already discussed: scheme/parameter selection
  - Important: selection process should be treated as part of the learning process
- Modifying the input: attribute selection, discretization, data cleansing, transformations
- Modifying the output: combining classification models to improve performance
  - Bagging, boosting, stacking, error-correcting output codes (and Bayesian model averaging)

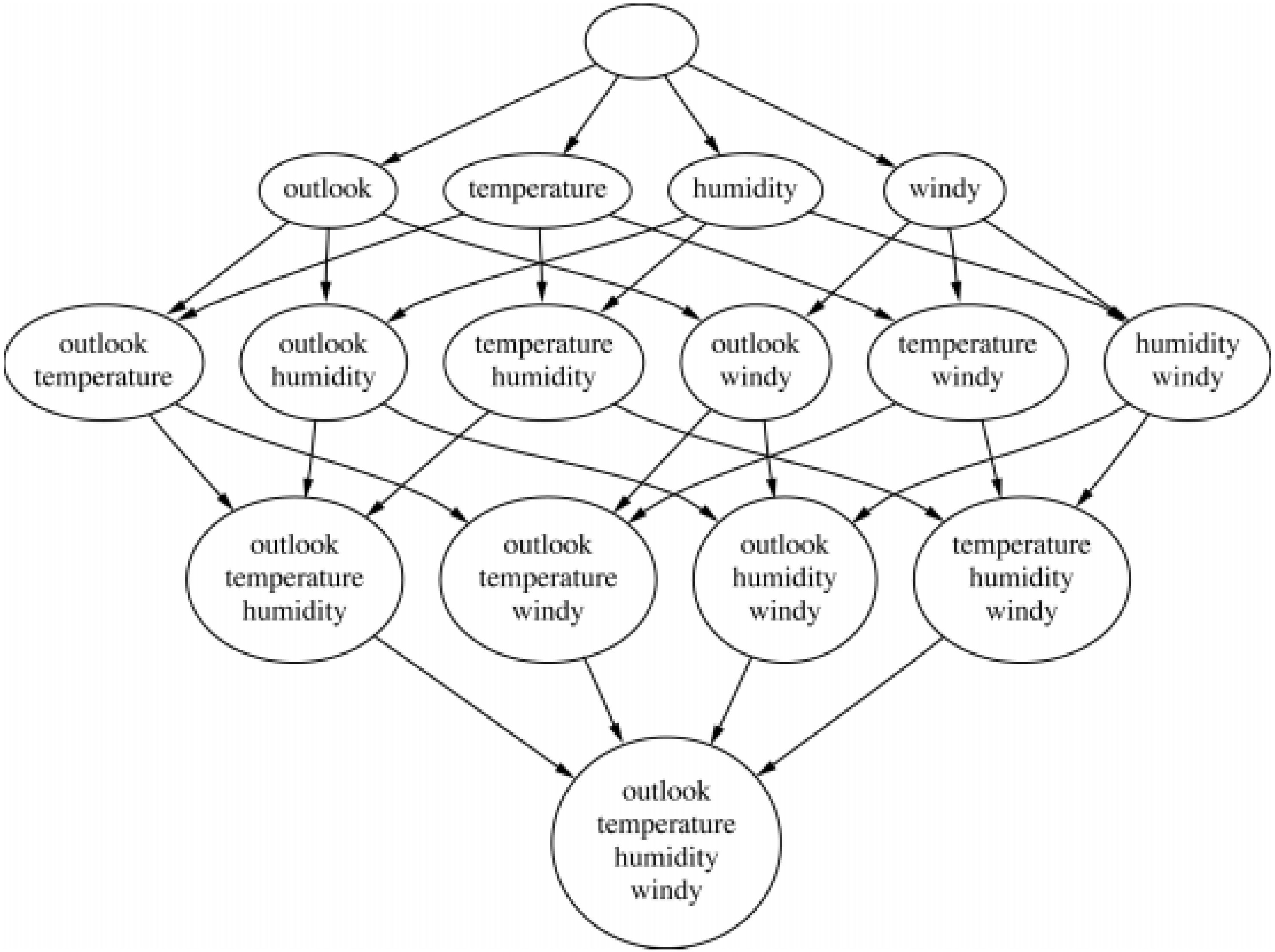
Attribute selection

- Adding a random (i.e. irrelevant) attribute can significantly degrade C4.5's performance
  - Problem: attribute selection based on smaller and smaller amounts of data
- IBL is also very susceptible to irrelevant attributes
  - Number of training instances required increases exponentially with number of irrelevant attributes
- Naïve Bayes doesn't have this problem
- *Relevant* attributes can also be harmful

Scheme-independent selection

- *Filter* approach: assessment based on general characteristics of the data
- One method: find subset of attributes that is enough to separate all the instances
- Another method: use different learning scheme (e.g. C4.5, 1R) to select attributes
- IBL-based attribute weighting techniques can also be used (but can’t find redundant attributes)
- CFS: uses correlation-based evaluation of subsets

Attribute subsets for weather data



Searching the attribute space

- Number of possible attribute subsets is exponential in the number of attributes
- Common greedy approaches: *forward selection* and *backward elimination*
- More sophisticated strategies:
  - *Bidirectional* search
  - *Best-first* search: can find the optimum solution
  - *Beam* search: approximation to best-first search
  - *Genetic algorithms*

Scheme-specific selection

- *Wrapper* approach: attribute selection implemented as wrapper around learning scheme
  - Evaluation criterion: cross-validation performance
- Time consuming: adds factor k^2 even for greedy approaches with k attributes
  - Linearity in k requires prior ranking of attributes
- Scheme-specific attribute selection essential for learning decision tables
- Can be done efficiently for DTs and Naïve Bayes

Discretizing numeric attributes

- Can be used to avoid making normality assumption in Naïve Bayes and Clustering
- Simple discretization scheme is used in 1R
- C4.5 performs *local* discretization
- *Global* discretization can be advantageous because it's based on more data
  - Learner can be applied to discretized attribute *or*
  - It can be applied to binary attributes coding the cut points in the discretized attribute

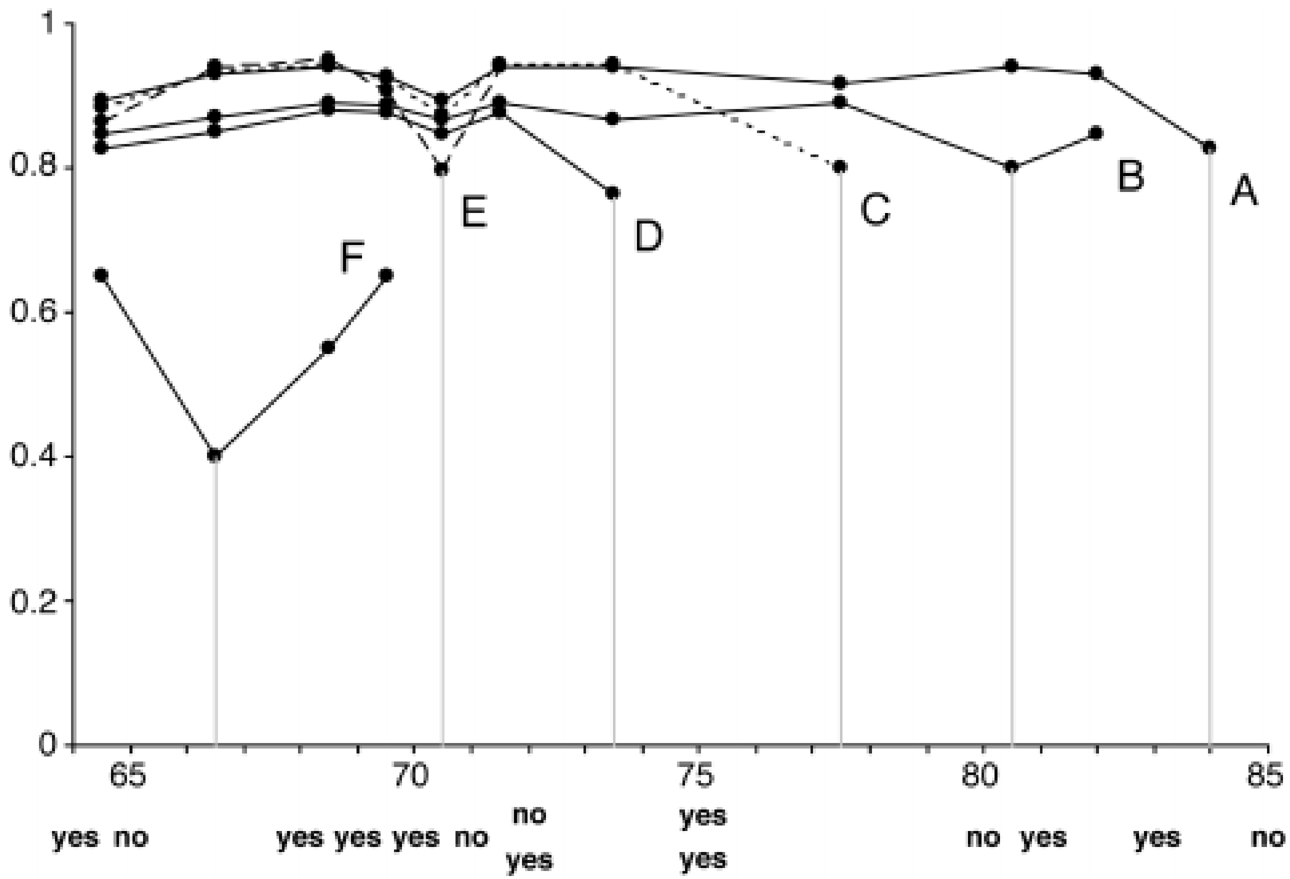
Unsupervised discretization

- *Unsupervised* discretization generates intervals without looking at class labels
  - Only possible way when clustering
- Two main strategies:
  - *Equal-interval binning*
  - *Equal-frequency binning* (also called *histogram equalization*)
- Inferior to supervised schemes in classification tasks

Entropy-based discretization

- *Supervised* method that builds a decision tree with pre-pruning on the attribute being discretized
  - Entropy used as splitting criterion
  - MDLP used as stopping criterion
- State-of-the-art discretization method
- Application of MDLP:
  - "Theory" is the splitting point ($\log_2[N-1]$ bits) plus class distribution in each subset
  - DL before/after adding splitting point is compared

Example: temperature attribute



Formula for MDLP

- N instances and
  - k classes and entropy E in original set
  - k_1 classes and entropy E_1 in first subset
  - k_2 classes and entropy E_2 in first subset

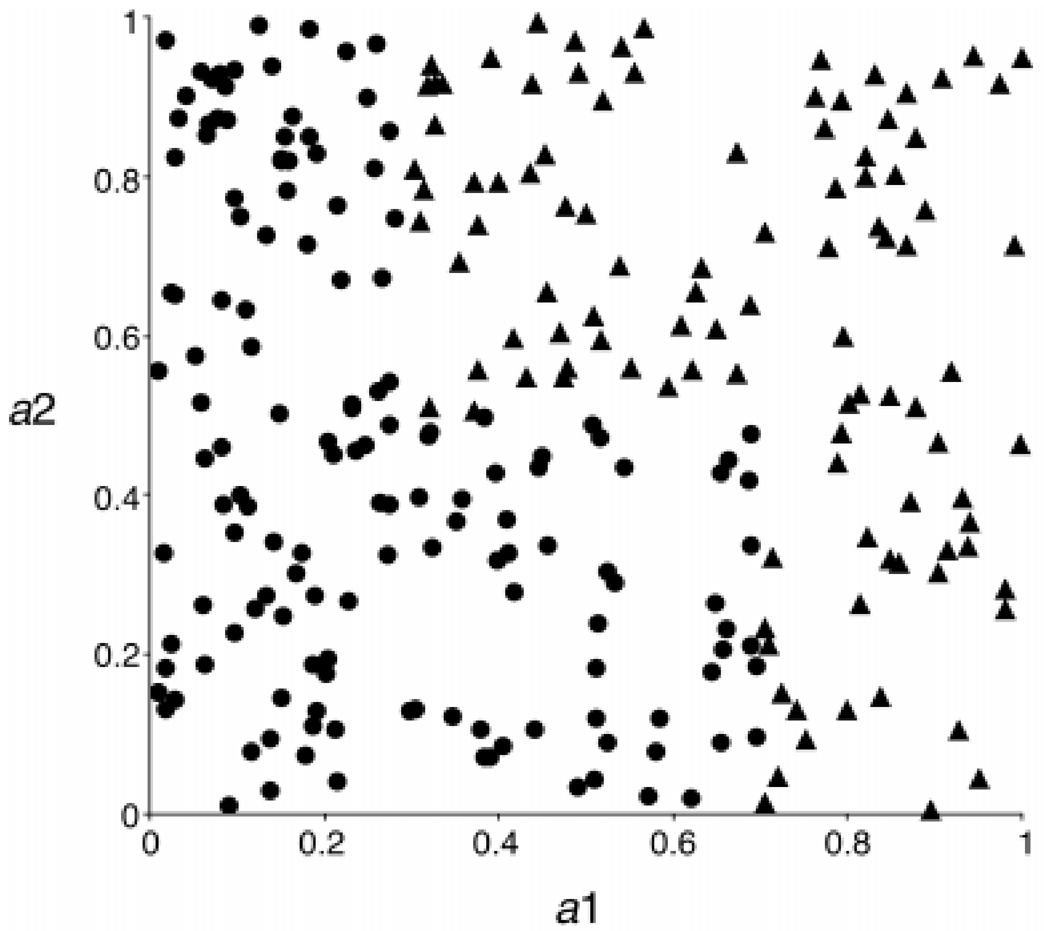
$$\text{gain} > \frac{\log_2(N-1)}{N} + \frac{\log_2(3^k-2) - kE + k_1E_1 + k_2E_2}{N}$$

- Doesn't result in any discretization intervals for the temperature attribute

Other discretization methods

- Top-down procedure can be replaced by bottom-up method
- MDLP can be replaced by chi-squared test
- Dynamic programming can be used to find optimum *k*-way split for given additive criterion
  - Requires time quadratic in number of instances if entropy is used as criterion
  - Can be done in linear time if error rate is used as evaluation criterion

Error-based vs. entropy-based



The converse of discretization

- Scheme used by IB1: indicator attributes
- Doesn't make use of potential ordering information
- M5' generates ordering of nominal values and codes ordering using binary attributes
- This strategy can be used for any attribute for which values are ordered
  - Avoids problem of using integer attribute to code ordering: would imply a metric
- In general: subsets of attributes coded as binary attributes

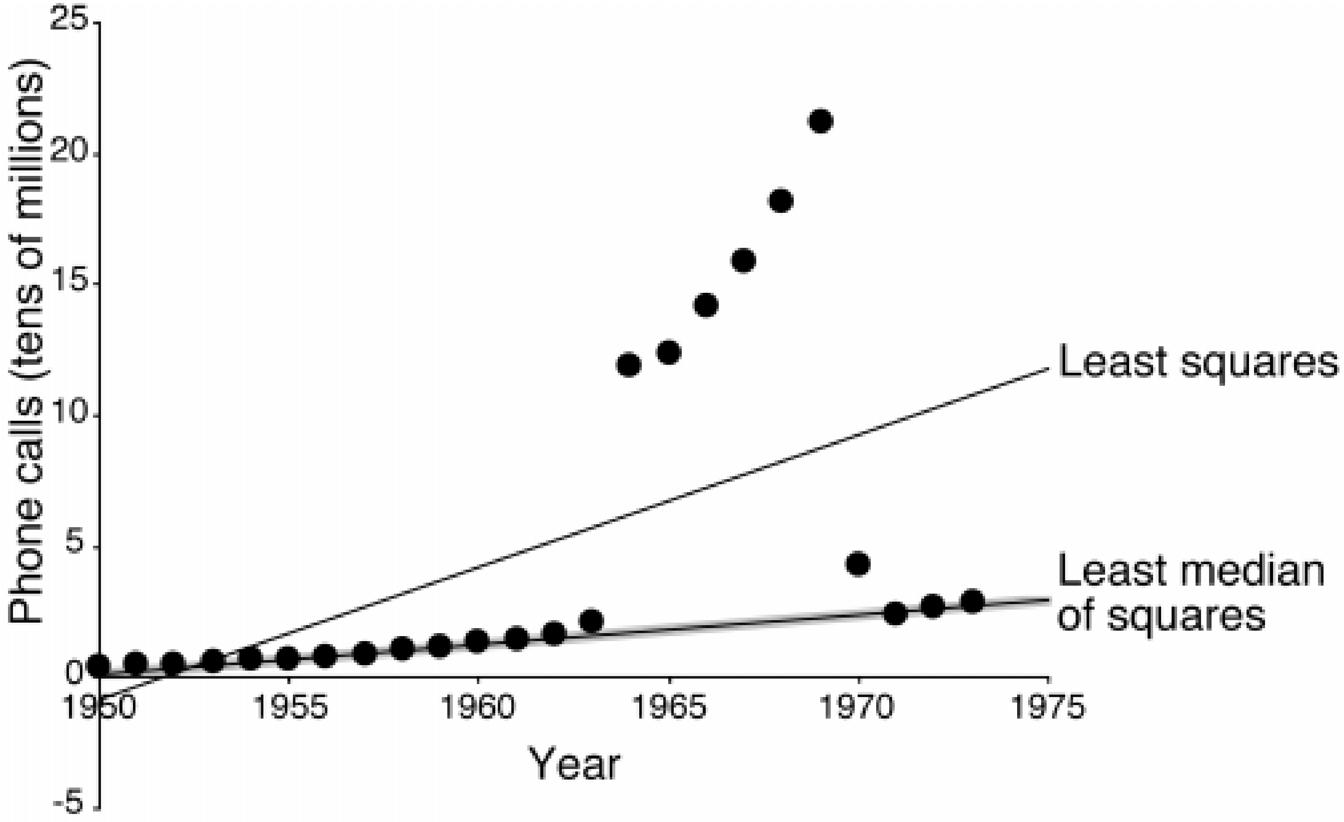
Automatic data cleansing

- Improving decision trees: relearn tree with misclassified instances removed
- Better strategy (of course): let human expert check misclassified instances
- When systematic noise is present it’s better not to modify the data
- Also: attribute noise should be left in training set
- (Unsystematic) class noise in training set should be eliminated if possible

Robust regression

- Statistical methods that address problem of *outliers* are called *robust*
- Possible way of making regression more robust:
  - Minimize absolute error instead of squared error
  - Remove outliers (i.e. 10% of points farthest from the regression plane)
  - Minimize *median* instead of *mean* of squares (copes with outliers in *x* and *y* direction)
    - Finds narrowest strip covering half the observations

Example: least median of squares



Detecting anomalies

- Visualization best way of detecting anomalies (but often can't be done)
- Automatic approach: committee of different learning schemes
  - E.g. decision tree, nearest-neighbor learner, and a linear discriminant function
  - Conservative approach: only delete instances which are incorrectly classified by all of them
  - Problem: might sacrifice instances of small classes

Combining multiple models

- Basic idea of “meta” learning schemes: build different “experts” and let them vote
- Advantage: often improves predictive performance
- Disadvantage: produces output that is very hard to analyze
- Schemes we will discuss: *bagging*, *boosting*, *stacking*, and *error-correcting output codes*
  - The first three can be applied to both classification and numeric prediction problems

Bagging

- Employs simplest way of combining predictions: voting/averaging
- Each model receives equal weight
- "Idealized" version of bagging:
  - 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 classifier's predictions
- This improves performance in almost all cases if learning scheme is *unstable* (i.e. decision trees)

Bias-variance decomposition

- Theoretical tool for analyzing how much *specific* training set affects performance of classifier
- Assume we have an infinite number of classifiers built from different training sets of size *n*
  - The *bias* of a learning scheme is the expected error of the combined classifier on new data
  - The *variance* of a learning scheme is the expected error due to the particular training set used
  - Total expected error: bias + variance

More on bagging

- Bagging reduces variance by voting/averaging, thus reducing the overall expected error
  - In the case of classification there are pathological situations where the overall error might increase
  - Usually, the more classifiers the better
- Problem: we only have one dataset!
- Solution: generate new datasets of size *n* by sampling with replacement from original dataset
- Can help a lot if data is noisy

Bagging classifiers

model generation

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

classification

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

Boosting

- Also uses voting/averaging but models are weighted according to their performance
- Iterative procedure: new models are influenced by performance of previously built ones
  - New model is encouraged to become expert for instances classified incorrectly by earlier models
  - Intuitive justification: models should be experts that complement each other
- There are several variants of this algorithm

AdaBoost.M1

model generation

```
Assign equal weight to each training instance.
For each of t iterations:
  Apply learning algorithm to weighted dataset and store
     resulting model.
  Compute error e of model on weighted dataset and store error.
  If e equal to zero, or e greater or equal to 0.5:
    Terminate model generation.
  For each instance in dataset:
    If instance classified correctly by model:
       Multiply weight of instance by e / (1 - e).
  Normalize weight of all instances.
```

classification

```
Assign weight of zero to all classes.
For each of the t (or less) models:
  Add -log(e / (1 - e)) to weight of class predicted by model.
Return class with highest weight.
```

More on boosting

- Can be applied without weights using resampling with probability determined by weights
  - Disadvantage: not all instances are used
  - Advantage: resampling can be repeated if error exceeds 0.5
- Stems from *computational learning theory*
- Theoretical result: training error decreases exponentially
- Also: works if base classifiers not too complex and their error doesn’t become too large too quickly

A bit more on boosting

- Puzzling fact: generalization error can decrease long after training error has reached zero
  - Seems to contradict Occam's Razor!
  - However, problem disappears if *margin* (confidence) is considered instead of error
    - Margin: difference between estimated probability for true class and most likely other class (between –1, 1)
- Boosting works with *weak* learners: only condition is that error doesn't exceed 0.5
- LogitBoost: more sophisticated boosting scheme

Stacking

- Hard to analyze theoretically: "black magic"
- Uses *meta learner* instead of voting to combine predictions of base learners
  - Predictions of base learners (*level-0 models*) are used as input for meta learner (*level-1 model)*
- Base learners usually different learning schemes
- Predictions on training data can't be used to generate data for level-1 model!
  - Cross-validation-like scheme is employed

More on stacking

- If base learners can output probabilities it's better to use those as input to meta learner
- Which algorithm to use to generate meta learner?
  - In principle, any learning scheme can be applied
  - David Wolpert: "relatively global, smooth" model
    - Base learners do most of the work
    - Reduces risk of overfitting
- Stacking can also be applied to numeric prediction (and density estimation)

Error-correcting output codes

- Very elegant method of transforming multiclass problem into two-class problem
  - Simple scheme: as many binary class attributes as original classes using one-per-class coding

class	class vector
a	1000
b	0100
c	0010
d	0001

- Idea: use *error-correcting codes* instead

More on ECOCs

- Example:

class	class vector
a	1111111
b	0000111
c	0011001
d	0101010

  - What's the true class if base classifiers predict 1011111?
- We want code words for which minimum *hamming distance* between any pair of words *d* is large
  - Up to (*d*-1)/2 single-bit errors can be corrected

A bit more on ECOCs

- Two criteria for error-correcting output codes:
  - *Row-separation*: minimum distance between rows
  - *Column-separation*: minimum distance between columns (and columns' complements)
    - Why? Because if columns are identical, base classifiers will make the same errors
    - Error-correction is weakened if errors are correlated
- Only works for problems with more than 3 classes: for 3 classes there are only 2^3 possible columns

Exhaustive ECOCs

- With few classes *exhaustive* codes can be build (like the one on an earlier slide)
- Exhaustive code for *k* classes:
  - The columns comprise every possible *k*-string
  - Except for complements and all-zero/one strings
  - Each code word contains $2^{k-1}-1$ bits
- Code word for 1st class: all ones
- 2nd class: 2^{k-2} zeroes followed by $2^{k-2}-1$ ones
- i^{th} class: alternating runs of 2^{k-i} zeroes and ones, the last run being one short

One last slide on ECOCs

- With more classes, exhaustive codes are infeasible
  - Number of columns increases exponentially
- Random code words have good error-correcting properties on average!
- More sophisticated methods exist for generating ECOCs using a small number of columns
- ECOCs don't work with NN classifier
  - But: works if different attribute subsets are used to predict each output bit